



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:28 AM UTC

PDB ID : 3ZKB / pdb_00003zkb
Title : CRYSTAL STRUCTURE OF THE ATPASE REGION OF Mycobacterium tuberculosis GyrB WITH AMPPNP
Authors : Agrawal, A.; Roue, M.; Spitzfaden, C.; Petrella, S.; Aubry, A.; Volker, C.; Mossakowska, D.; Hann, M.; Bax, B.; Mayer, C.
Deposited on : 2013-01-22
Resolution : 2.90 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

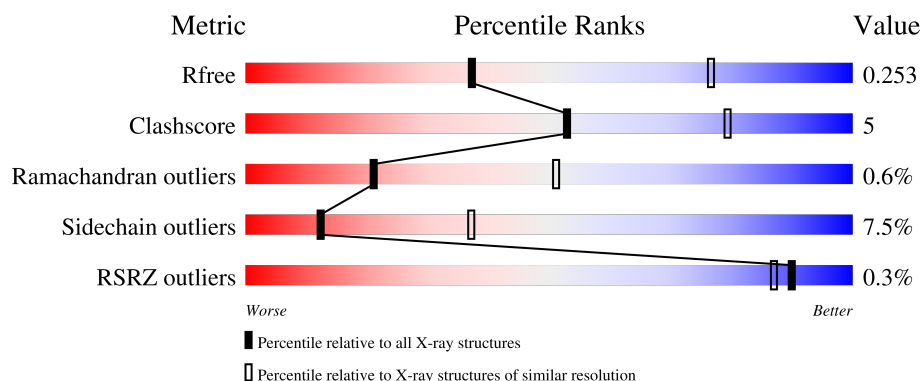
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	432	
1	B	432	
1	C	432	
1	D	432	

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Mol	Chain	Length	Quality of chain
1	E	432	
1	F	432	
1	G	432	
1	H	432	
1	I	432	
1	J	432	
1	K	432	
1	L	432	
1	M	432	
1	N	432	
1	O	432	
1	P	432	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 46952 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 DNA GYRASE SUBUNIT B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	380	Total	C	N	O	S	0	0	0
			2887	1809	509	563	6			
1	B	382	Total	C	N	O	S	0	0	0
			2874	1798	505	565	6			
1	C	387	Total	C	N	O	S	0	0	0
			2938	1842	516	574	6			
1	D	392	Total	C	N	O	S	0	0	0
			2954	1844	518	586	6			
1	E	386	Total	C	N	O	S	0	0	0
			2912	1821	511	574	6			
1	F	383	Total	C	N	O	S	0	0	0
			2888	1807	505	570	6			
1	G	381	Total	C	N	O	S	0	0	0
			2864	1796	502	560	6			
1	H	379	Total	C	N	O	S	0	0	0
			2866	1794	502	564	6			
1	I	375	Total	C	N	O	S	0	0	0
			2827	1768	494	559	6			
1	J	384	Total	C	N	O	S	0	0	0
			2884	1806	506	566	6			
1	K	376	Total	C	N	O	S	0	0	0
			2838	1778	497	557	6			
1	L	382	Total	C	N	O	S	0	0	0
			2862	1791	501	564	6			
1	M	383	Total	C	N	O	S	0	0	0
			2888	1808	509	565	6			
1	N	373	Total	C	N	O	S	0	0	0
			2816	1763	495	552	6			
1	O	379	Total	C	N	O	S	0	0	0
			2877	1803	506	562	6			
1	P	376	Total	C	N	O	S	0	0	0
			2822	1768	489	559	6			

There are 80 discrepancies between the modelled and reference sequences:

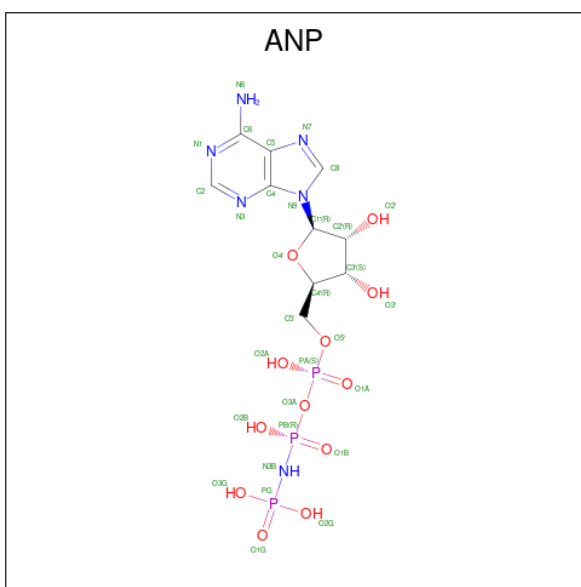
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A	-4	GLY	-	expression tag	UNP I6WX66
A	-3	PRO	-	expression tag	UNP I6WX66
A	-2	LEU	-	expression tag	UNP I6WX66
A	-1	GLY	-	expression tag	UNP I6WX66
A	0	SER	-	expression tag	UNP I6WX66
B	-4	GLY	-	expression tag	UNP I6WX66
B	-3	PRO	-	expression tag	UNP I6WX66
B	-2	LEU	-	expression tag	UNP I6WX66
B	-1	GLY	-	expression tag	UNP I6WX66
B	0	SER	-	expression tag	UNP I6WX66
C	-4	GLY	-	expression tag	UNP I6WX66
C	-3	PRO	-	expression tag	UNP I6WX66
C	-2	LEU	-	expression tag	UNP I6WX66
C	-1	GLY	-	expression tag	UNP I6WX66
C	0	SER	-	expression tag	UNP I6WX66
D	-4	GLY	-	expression tag	UNP I6WX66
D	-3	PRO	-	expression tag	UNP I6WX66
D	-2	LEU	-	expression tag	UNP I6WX66
D	-1	GLY	-	expression tag	UNP I6WX66
D	0	SER	-	expression tag	UNP I6WX66
E	-4	GLY	-	expression tag	UNP I6WX66
E	-3	PRO	-	expression tag	UNP I6WX66
E	-2	LEU	-	expression tag	UNP I6WX66
E	-1	GLY	-	expression tag	UNP I6WX66
E	0	SER	-	expression tag	UNP I6WX66
F	-4	GLY	-	expression tag	UNP I6WX66
F	-3	PRO	-	expression tag	UNP I6WX66
F	-2	LEU	-	expression tag	UNP I6WX66
F	-1	GLY	-	expression tag	UNP I6WX66
F	0	SER	-	expression tag	UNP I6WX66
G	-4	GLY	-	expression tag	UNP I6WX66
G	-3	PRO	-	expression tag	UNP I6WX66
G	-2	LEU	-	expression tag	UNP I6WX66
G	-1	GLY	-	expression tag	UNP I6WX66
G	0	SER	-	expression tag	UNP I6WX66
H	-4	GLY	-	expression tag	UNP I6WX66
H	-3	PRO	-	expression tag	UNP I6WX66
H	-2	LEU	-	expression tag	UNP I6WX66
H	-1	GLY	-	expression tag	UNP I6WX66
H	0	SER	-	expression tag	UNP I6WX66
I	-4	GLY	-	expression tag	UNP I6WX66
I	-3	PRO	-	expression tag	UNP I6WX66

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Chain	Residue	Modelled	Actual	Comment	Reference
I	-2	LEU	-	expression tag	UNP I6WX66
I	-1	GLY	-	expression tag	UNP I6WX66
I	0	SER	-	expression tag	UNP I6WX66
J	-4	GLY	-	expression tag	UNP I6WX66
J	-3	PRO	-	expression tag	UNP I6WX66
J	-2	LEU	-	expression tag	UNP I6WX66
J	-1	GLY	-	expression tag	UNP I6WX66
J	0	SER	-	expression tag	UNP I6WX66
K	-4	GLY	-	expression tag	UNP I6WX66
K	-3	PRO	-	expression tag	UNP I6WX66
K	-2	LEU	-	expression tag	UNP I6WX66
K	-1	GLY	-	expression tag	UNP I6WX66
K	0	SER	-	expression tag	UNP I6WX66
L	-4	GLY	-	expression tag	UNP I6WX66
L	-3	PRO	-	expression tag	UNP I6WX66
L	-2	LEU	-	expression tag	UNP I6WX66
L	-1	GLY	-	expression tag	UNP I6WX66
L	0	SER	-	expression tag	UNP I6WX66
M	-4	GLY	-	expression tag	UNP I6WX66
M	-3	PRO	-	expression tag	UNP I6WX66
M	-2	LEU	-	expression tag	UNP I6WX66
M	-1	GLY	-	expression tag	UNP I6WX66
M	0	SER	-	expression tag	UNP I6WX66
N	-4	GLY	-	expression tag	UNP I6WX66
N	-3	PRO	-	expression tag	UNP I6WX66
N	-2	LEU	-	expression tag	UNP I6WX66
N	-1	GLY	-	expression tag	UNP I6WX66
N	0	SER	-	expression tag	UNP I6WX66
O	-4	GLY	-	expression tag	UNP I6WX66
O	-3	PRO	-	expression tag	UNP I6WX66
O	-2	LEU	-	expression tag	UNP I6WX66
O	-1	GLY	-	expression tag	UNP I6WX66
O	0	SER	-	expression tag	UNP I6WX66
P	-4	GLY	-	expression tag	UNP I6WX66
P	-3	PRO	-	expression tag	UNP I6WX66
P	-2	LEU	-	expression tag	UNP I6WX66
P	-1	GLY	-	expression tag	UNP I6WX66
P	0	SER	-	expression tag	UNP I6WX66

- Molecule 2 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 31	C 10	N 6	O 12	P 3	0	0
2	B	1	Total 31	C 10	N 6	O 12	P 3	0	0
2	C	1	Total 31	C 10	N 6	O 12	P 3	0	0
2	D	1	Total 31	C 10	N 6	O 12	P 3	0	0
2	E	1	Total 31	C 10	N 6	O 12	P 3	0	0
2	F	1	Total 31	C 10	N 6	O 12	P 3	0	0
2	G	1	Total 31	C 10	N 6	O 12	P 3	0	0
2	H	1	Total 31	C 10	N 6	O 12	P 3	0	0
2	I	1	Total 31	C 10	N 6	O 12	P 3	0	0
2	J	1	Total 31	C 10	N 6	O 12	P 3	0	0
2	K	1	Total 31	C 10	N 6	O 12	P 3	0	0
2	L	1	Total 31	C 10	N 6	O 12	P 3	0	0
2	M	1	Total 31	C 10	N 6	O 12	P 3	0	0
2	N	1	Total 31	C 10	N 6	O 12	P 3	0	0

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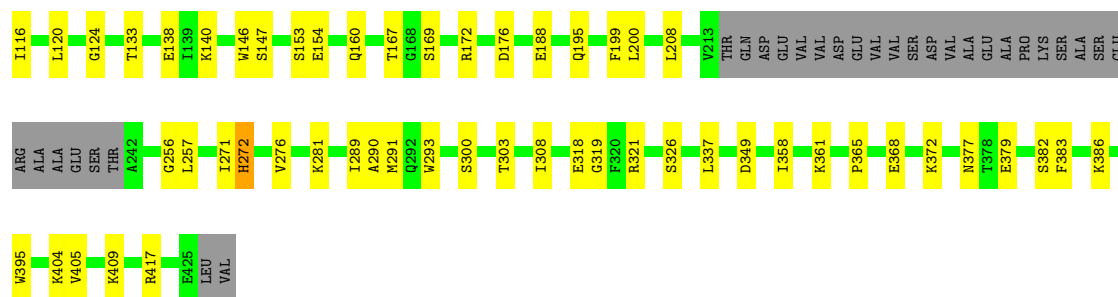
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	O	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
2	P	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	2	Total	Mg	0	0
			2	2		
3	C	2	Total	Mg	0	0
			2	2		
3	D	2	Total	Mg	0	0
			2	2		
3	E	1	Total	Mg	0	0
			1	1		
3	F	1	Total	Mg	0	0
			1	1		
3	G	2	Total	Mg	0	0
			2	2		
3	H	1	Total	Mg	0	0
			1	1		
3	I	1	Total	Mg	0	0
			1	1		
3	J	1	Total	Mg	0	0
			1	1		
3	K	1	Total	Mg	0	0
			1	1		
3	L	1	Total	Mg	0	0
			1	1		
3	M	1	Total	Mg	0	0
			1	1		
3	N	1	Total	Mg	0	0
			1	1		
3	O	1	Total	Mg	0	0
			1	1		
3	P	1	Total	Mg	0	0
			1	1		

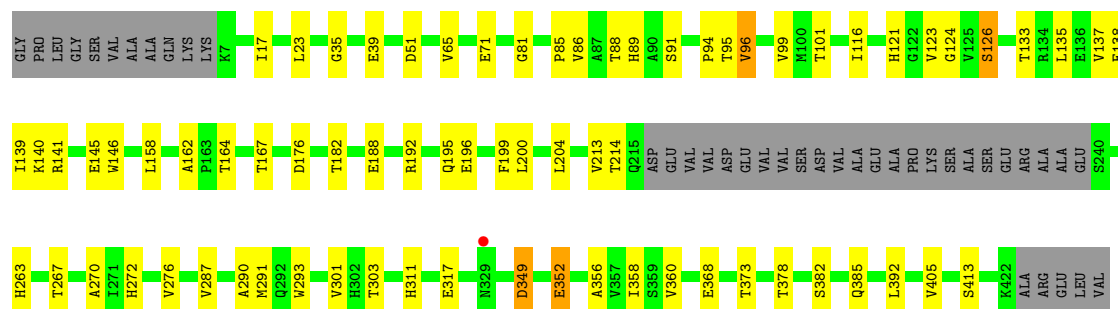
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	44	Total 44	O 44	0	0
4	B	31	Total 31	O 31	0	0
4	C	62	Total 62	O 62	0	0
4	D	40	Total 40	O 40	0	0
4	E	45	Total 45	O 45	0	0
4	F	26	Total 26	O 26	0	0
4	G	25	Total 25	O 25	0	0
4	H	29	Total 29	O 29	0	0
4	I	24	Total 24	O 24	0	0
4	J	33	Total 33	O 33	0	0
4	K	11	Total 11	O 11	0	0
4	L	13	Total 13	O 13	0	0
4	M	16	Total 16	O 16	0	0
4	N	14	Total 14	O 14	0	0
4	O	12	Total 12	O 12	0	0
4	P	14	Total 14	O 14	0	0



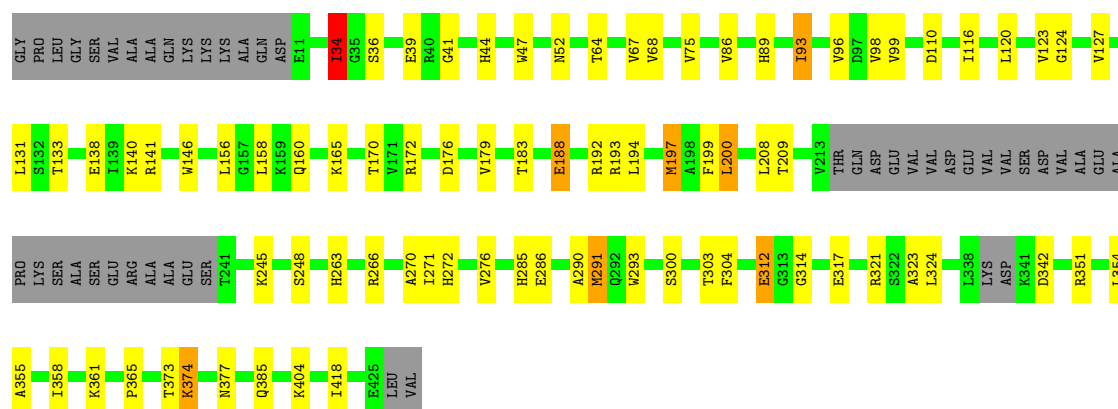
• Molecule 1: DNA GYRASE SUBUNIT B

Chain D: 74% 16% 9%



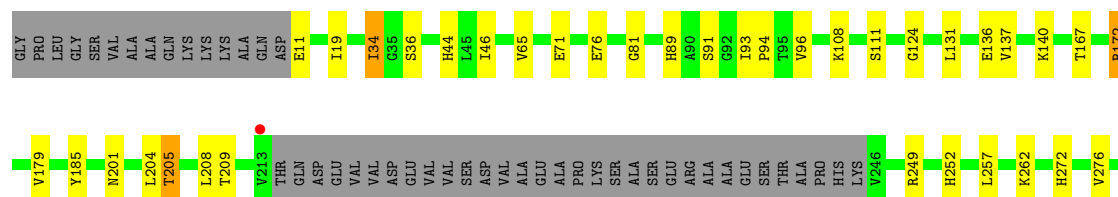
• Molecule 1: DNA GYRASE SUBUNIT B

Chain E: 70% 17% 11%

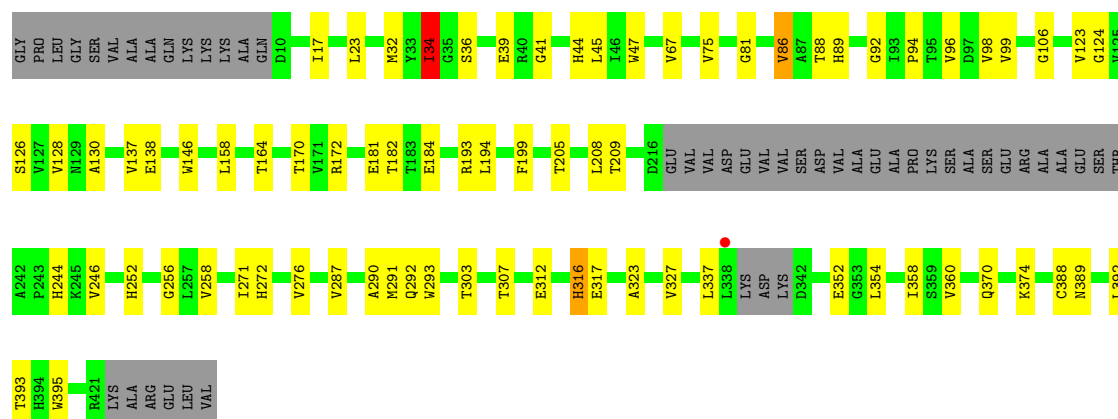


• Molecule 1: DNA GYRASE SUBUNIT B

Chain F: 75% 12% 11%

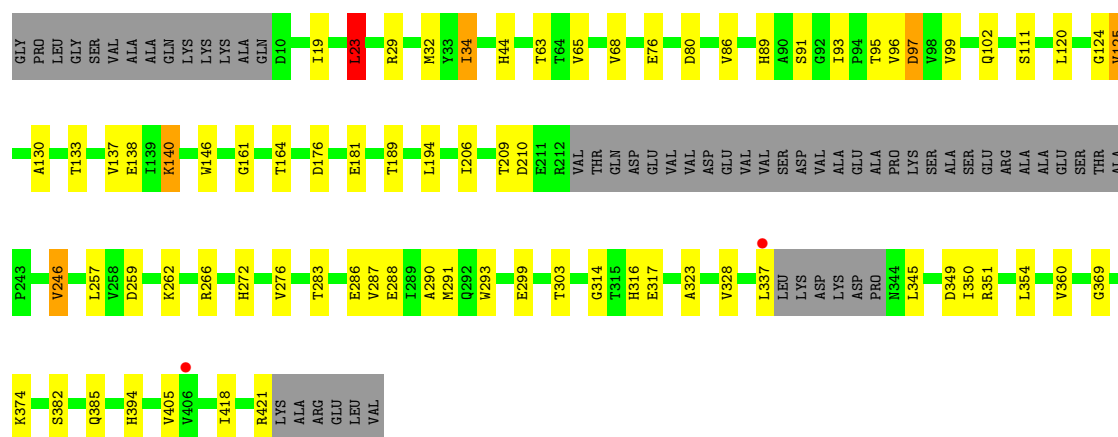


Chain J:  72% 17% 11%



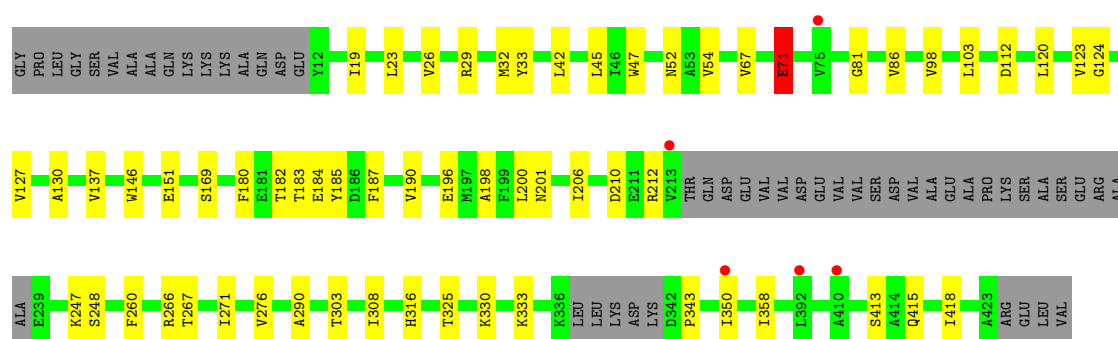
• Molecule 1: DNA GYRASE SUBUNIT B

Chain K:  70% 16% 13%



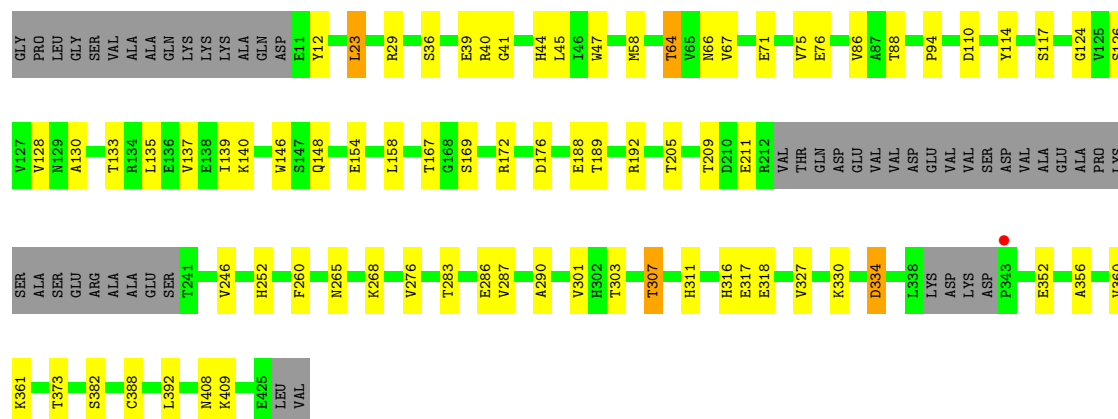
• Molecule 1: DNA GYRASE SUBUNIT B

Chain L:  74% 14% 12%

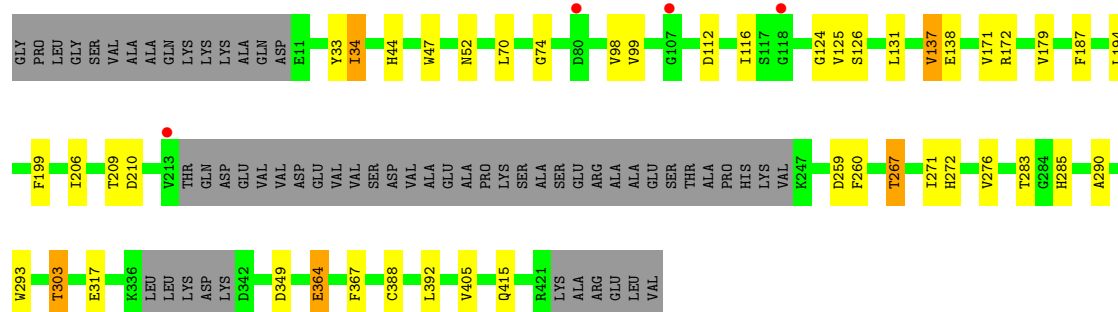
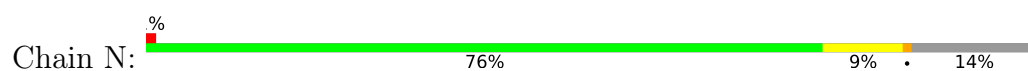


• Molecule 1: DNA GYRASE SUBUNIT B

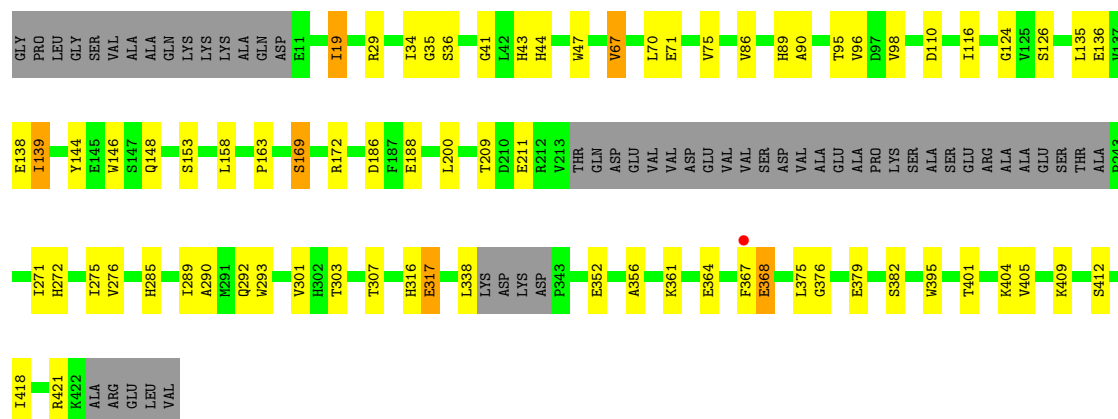
Chain M:  71% 17% 11%



- Molecule 1: DNA GYRASE SUBUNIT B

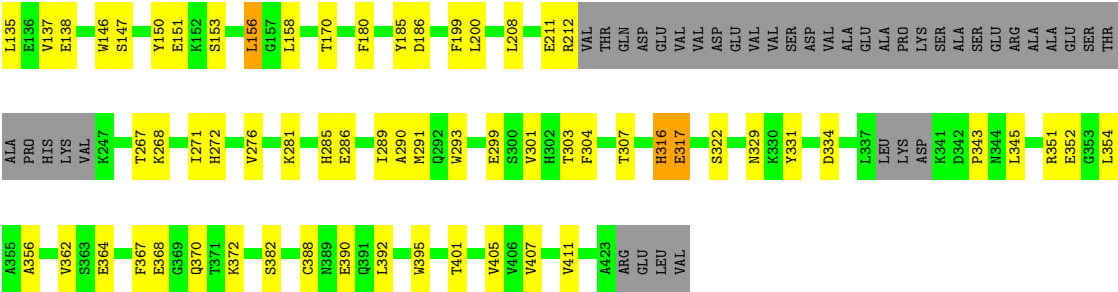


● Molecule 1: DNA GYRASE SUBUNIT B



• Molecule 1: DNA GYRASE SUBUNIT B





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	101.36Å 138.20Å 147.69Å 105.28° 92.31° 107.23°	Depositor
Resolution (Å)	24.94 – 2.90 24.94 – 2.90	Depositor EDS
% Data completeness (in resolution range)	98.2 (24.94-2.90) 98.0 (24.94-2.90)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.98 (at 2.89Å)	Xtriage
Refinement program	BUSTER 2.11.4	Depositor
R, R_{free}	0.182 , 0.240 0.195 , 0.253	Depositor DCC
R_{free} test set	7966 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	66.0	Xtriage
Anisotropy	0.668	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 58.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	46952	wwPDB-VP
Average B, all atoms (Å ²)	99.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.69% 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: ANP, MG

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	0.80	0/2942	1.40	26/3991 (0.7%)
1	B	0.79	0/2928	1.38	14/3978 (0.4%)
1	C	0.81	0/2994	1.40	26/4062 (0.6%)
1	D	0.79	0/3010	1.40	12/4091 (0.3%)
1	E	0.81	1/2967 (0.0%)	1.39	9/4030 (0.2%)
1	F	0.78	0/2942	1.36	4/3997 (0.1%)
1	G	0.77	0/2919	1.37	12/3967 (0.3%)
1	H	0.78	0/2920	1.40	13/3966 (0.3%)
1	I	0.76	0/2881	1.37	8/3913 (0.2%)
1	J	0.79	0/2938	1.39	7/3993 (0.2%)
1	K	0.80	0/2892	1.35	8/3927 (0.2%)
1	L	0.85	0/2916	1.41	9/3963 (0.2%)
1	M	0.79	0/2943	1.38	6/3995 (0.2%)
1	N	0.78	0/2869	1.38	10/3896 (0.3%)
1	O	0.77	0/2931	1.36	7/3975 (0.2%)
1	P	0.78	1/2875 (0.0%)	1.37	5/3907 (0.1%)
All	All	0.79	2/46867 (0.0%)	1.38	176/63651 (0.3%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	197	MET	SD-CE	-6.23	1.64	1.79
1	P	364	GLU	CA-C	5.55	1.58	1.52

All (176) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	93	ILE	N-CA-CB	-9.66	105.16	111.83
1	N	34	ILE	N-CA-CB	-8.33	102.42	112.33
1	E	93	ILE	N-CA-CB	-8.24	104.67	111.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	34	ILE	N-CA-CB	-6.94	104.57	112.21
1	N	260	PHE	CA-CB-CG	6.87	120.67	113.80
1	E	199	PHE	CA-CB-CG	6.79	120.59	113.80
1	N	367	PHE	CA-C-N	6.77	129.65	120.38
1	N	367	PHE	C-N-CA	6.77	129.65	120.38
1	J	98	VAL	CA-C-N	6.34	129.14	120.46
1	J	98	VAL	C-N-CA	6.34	129.14	120.46
1	J	34	ILE	N-CA-CB	-6.31	100.82	111.23
1	H	112	ASP	CA-CB-CG	6.24	118.84	112.60
1	H	39	GLU	CA-C-N	6.24	128.92	120.38
1	H	39	GLU	C-N-CA	6.24	128.92	120.38
1	E	312	GLU	CB-CG-CD	6.21	123.16	112.60
1	F	201	ASN	CA-C-N	6.21	128.89	120.38
1	F	201	ASN	C-N-CA	6.21	128.89	120.38
1	L	201	ASN	CA-C-N	6.13	128.78	120.38
1	L	201	ASN	C-N-CA	6.13	128.78	120.38
1	I	90	ALA	CA-C-N	6.08	129.04	120.28
1	I	90	ALA	C-N-CA	6.08	129.04	120.28
1	K	97	ASP	CA-CB-CG	6.08	118.68	112.60
1	E	314	GLY	CA-C-N	6.05	128.67	120.38
1	E	314	GLY	C-N-CA	6.05	128.67	120.38
1	A	176	ASP	CA-CB-CG	6.04	118.64	112.60
1	P	199	PHE	CA-CB-CG	6.02	119.82	113.80
1	M	23	LEU	CA-C-N	6.01	128.82	120.29
1	M	23	LEU	C-N-CA	6.01	128.82	120.29
1	C	24	GLU	CA-C-N	5.98	128.88	120.28
1	C	24	GLU	C-N-CA	5.98	128.88	120.28
1	G	98	VAL	CA-C-N	5.90	128.54	120.46
1	G	98	VAL	C-N-CA	5.90	128.54	120.46
1	K	23	LEU	CA-C-N	5.89	128.18	120.28
1	K	23	LEU	C-N-CA	5.89	128.18	120.28
1	A	90	ALA	CA-C-N	5.86	128.94	120.38
1	A	90	ALA	C-N-CA	5.86	128.94	120.38
1	C	70	LEU	CA-C-N	5.86	129.61	120.82
1	C	70	LEU	C-N-CA	5.86	129.61	120.82
1	C	272	HIS	CA-C-N	5.82	128.00	120.44
1	C	272	HIS	C-N-CA	5.82	128.00	120.44
1	L	260	PHE	CA-CB-CG	5.81	119.61	113.80
1	E	34	ILE	N-CA-CB	-5.80	105.83	112.21
1	N	199	PHE	CA-CB-CG	5.79	119.59	113.80
1	P	51	ASP	CA-CB-CG	5.79	118.39	112.60
1	A	93	ILE	N-CA-CB	-5.76	103.15	111.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	270	ALA	CA-C-N	5.73	128.32	120.46
1	E	270	ALA	C-N-CA	5.73	128.32	120.46
1	D	126	SER	CA-C-N	5.73	127.78	120.56
1	D	126	SER	C-N-CA	5.73	127.78	120.56
1	D	199	PHE	CA-CB-CG	5.70	119.50	113.80
1	B	266	ARG	CA-C-N	5.69	128.37	120.29
1	B	266	ARG	C-N-CA	5.69	128.37	120.29
1	H	24	GLU	CA-C-N	5.68	128.22	120.54
1	H	24	GLU	C-N-CA	5.68	128.22	120.54
1	I	24	GLU	CA-C-N	5.64	127.84	120.28
1	I	24	GLU	C-N-CA	5.64	127.84	120.28
1	P	401	THR	CA-C-N	5.64	128.10	120.38
1	P	401	THR	C-N-CA	5.64	128.10	120.38
1	B	51	ASP	CA-CB-CG	5.64	118.24	112.60
1	C	98	VAL	CA-C-N	5.60	128.14	120.46
1	C	98	VAL	C-N-CA	5.60	128.14	120.46
1	D	349	ASP	CA-CB-CG	5.60	118.20	112.60
1	O	110	ASP	CA-CB-CG	5.60	118.20	112.60
1	A	259	ASP	CA-C-N	5.58	128.03	120.44
1	A	259	ASP	C-N-CA	5.58	128.03	120.44
1	H	403	ALA	CA-C-N	5.56	128.52	120.79
1	H	403	ALA	C-N-CA	5.56	128.52	120.79
1	A	260	PHE	CA-CB-CG	5.55	119.35	113.80
1	J	370	GLN	N-CA-C	-5.48	106.10	112.89
1	D	385	GLN	CA-C-N	5.47	127.56	120.44
1	D	385	GLN	C-N-CA	5.47	127.56	120.44
1	A	270	ALA	CA-C-N	5.46	127.94	120.46
1	A	270	ALA	C-N-CA	5.46	127.94	120.46
1	L	71	GLU	CA-C-N	5.43	128.31	120.38
1	L	71	GLU	C-N-CA	5.43	128.31	120.38
1	M	110	ASP	CA-CB-CG	5.38	117.97	112.60
1	F	342	ASP	CA-CB-CG	5.37	117.97	112.60
1	D	51	ASP	CA-C-N	5.35	127.45	120.28
1	D	51	ASP	C-N-CA	5.35	127.45	120.28
1	C	349	ASP	CA-CB-CG	5.34	117.94	112.60
1	G	96	VAL	CA-C-N	5.34	127.44	120.28
1	G	96	VAL	C-N-CA	5.34	127.44	120.28
1	B	97	ASP	CA-C-N	5.34	127.29	120.56
1	B	97	ASP	C-N-CA	5.34	127.29	120.56
1	N	267	THR	N-CA-C	-5.34	106.76	113.28
1	A	51	ASP	CA-CB-CG	5.32	117.92	112.60
1	B	270	ALA	CA-C-N	5.32	127.74	120.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	270	ALA	C-N-CA	5.32	127.74	120.46
1	G	404	LYS	CA-C-N	5.30	127.33	120.70
1	G	404	LYS	C-N-CA	5.30	127.33	120.70
1	J	199	PHE	CA-CB-CG	5.29	119.09	113.80
1	G	201	ASN	CA-C-N	5.28	127.62	120.38
1	G	201	ASN	C-N-CA	5.28	127.62	120.38
1	H	37	THR	CB-CA-C	5.28	118.83	109.65
1	E	165	LYS	N-CA-C	-5.25	106.92	113.38
1	B	34	ILE	N-CA-CB	-5.25	104.09	112.07
1	O	98	VAL	CA-C-N	5.25	127.93	120.53
1	O	98	VAL	C-N-CA	5.25	127.93	120.53
1	C	321	ARG	CA-C-N	5.25	127.57	120.65
1	C	321	ARG	C-N-CA	5.25	127.57	120.65
1	H	199	PHE	CA-CB-CG	5.23	119.03	113.80
1	O	70	LEU	CA-C-N	5.23	127.60	120.54
1	O	70	LEU	C-N-CA	5.23	127.60	120.54
1	C	86	VAL	N-CA-CB	-5.22	105.14	112.35
1	N	33	TYR	CA-C-N	5.22	127.93	122.14
1	N	33	TYR	C-N-CA	5.22	127.93	122.14
1	A	262	LYS	CA-C-N	5.21	127.26	120.28
1	A	262	LYS	C-N-CA	5.21	127.26	120.28
1	G	314	GLY	CA-C-N	5.19	127.49	120.38
1	G	314	GLY	C-N-CA	5.19	127.49	120.38
1	I	378	THR	CA-C-N	5.19	127.49	120.38
1	I	378	THR	C-N-CA	5.19	127.49	120.38
1	B	23	LEU	CA-C-N	5.18	127.23	120.28
1	B	23	LEU	C-N-CA	5.18	127.23	120.28
1	C	379	GLU	CB-CG-CD	5.18	121.41	112.60
1	H	34	ILE	N-CA-CB	-5.17	105.13	112.12
1	L	190	VAL	CA-C-N	5.17	127.46	120.38
1	L	190	VAL	C-N-CA	5.17	127.46	120.38
1	B	13	GLY	CA-C-N	5.17	127.20	120.28
1	B	13	GLY	C-N-CA	5.17	127.20	120.28
1	C	404	LYS	CA-C-N	5.16	127.06	120.56
1	C	404	LYS	C-N-CA	5.16	127.06	120.56
1	L	98	VAL	CA-C-N	5.16	127.53	120.46
1	L	98	VAL	C-N-CA	5.16	127.53	120.46
1	K	266	ARG	N-CA-C	-5.15	107.06	113.55
1	I	333	LYS	CA-C-N	5.15	127.18	120.28
1	I	333	LYS	C-N-CA	5.15	127.18	120.28
1	K	161	GLY	CA-C-N	5.15	127.54	120.39
1	K	161	GLY	C-N-CA	5.15	127.54	120.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	410	ALA	CA-C-N	5.14	127.03	120.56
1	G	410	ALA	C-N-CA	5.14	127.03	120.56
1	A	57	ALA	CA-C-N	5.12	128.10	120.31
1	A	57	ALA	C-N-CA	5.12	128.10	120.31
1	A	420	ALA	CA-C-N	5.12	127.66	120.28
1	A	420	ALA	C-N-CA	5.12	127.66	120.28
1	B	294	ASN	CA-C-N	5.12	127.86	120.38
1	B	294	ASN	C-N-CA	5.12	127.86	120.38
1	C	90	ALA	CA-C-N	5.12	131.31	121.54
1	C	90	ALA	C-N-CA	5.12	131.31	121.54
1	H	97	ASP	CA-CB-CG	5.12	117.72	112.60
1	O	367	PHE	CA-CB-CG	5.11	118.91	113.80
1	D	96	VAL	CA-C-N	5.11	127.63	120.28
1	D	96	VAL	C-N-CA	5.11	127.63	120.28
1	C	256	GLY	CA-C-N	5.10	127.11	120.28
1	C	256	GLY	C-N-CA	5.10	127.11	120.28
1	M	66	ASN	CA-CB-CG	5.07	117.67	112.60
1	A	126	SER	CA-C-N	5.07	126.95	120.56
1	A	126	SER	C-N-CA	5.07	126.95	120.56
1	M	334	ASP	CA-CB-CG	5.07	117.67	112.60
1	C	63	THR	N-CA-C	-5.07	107.76	114.04
1	N	98	VAL	CA-C-N	5.07	127.40	120.46
1	N	98	VAL	C-N-CA	5.07	127.40	120.46
1	C	51	ASP	CA-CB-CG	5.06	117.66	112.60
1	A	24	GLU	CA-C-N	5.06	127.47	120.29
1	A	24	GLU	C-N-CA	5.06	127.47	120.29
1	K	111	SER	CA-C-N	5.05	127.56	120.28
1	K	111	SER	C-N-CA	5.05	127.56	120.28
1	O	67	VAL	N-CA-CB	5.05	118.38	111.41
1	A	314	GLY	CA-C-N	5.05	127.30	120.38
1	A	314	GLY	C-N-CA	5.05	127.30	120.38
1	A	85	PRO	CA-C-N	5.05	127.54	121.84
1	A	85	PRO	C-N-CA	5.05	127.54	121.84
1	A	378	THR	CA-C-N	5.04	128.66	120.60
1	A	378	THR	C-N-CA	5.04	128.66	120.60
1	C	319	GLY	CA-C-N	5.03	126.98	120.44
1	C	319	GLY	C-N-CA	5.03	126.98	120.44
1	C	111	SER	CA-C-N	5.03	126.98	120.44
1	C	111	SER	C-N-CA	5.03	126.98	120.44
1	M	260	PHE	CA-CB-CG	5.03	118.83	113.80
1	J	393	THR	CA-C-N	5.02	127.01	120.28
1	J	393	THR	C-N-CA	5.02	127.01	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	378	THR	CA-C-N	5.01	127.49	120.28
1	H	378	THR	C-N-CA	5.01	127.49	120.28
1	D	270	ALA	CA-C-N	5.01	128.58	120.82
1	D	270	ALA	C-N-CA	5.01	128.58	120.82
1	P	401	THR	N-CA-C	-5.00	105.51	110.97

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2887	0	2803	35	0
1	B	2874	0	2760	27	0
1	C	2938	0	2857	33	0
1	D	2954	0	2823	30	0
1	E	2912	0	2795	40	0
1	F	2888	0	2772	21	0
1	G	2864	0	2755	30	0
1	H	2866	0	2764	34	0
1	I	2827	0	2701	27	0
1	J	2884	0	2769	34	0
1	K	2838	0	2730	34	0
1	L	2862	0	2749	21	0
1	M	2888	0	2784	30	0
1	N	2816	0	2714	15	0
1	O	2877	0	2791	32	0
1	P	2822	0	2700	39	0
2	A	31	0	13	1	0
2	B	31	0	13	0	0
2	C	31	0	13	0	0
2	D	31	0	13	0	0
2	E	31	0	13	1	0
2	F	31	0	13	1	0
2	G	31	0	13	1	0
2	H	31	0	13	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	I	31	0	13	2	0
2	J	31	0	13	1	0
2	K	31	0	13	1	0
2	L	31	0	13	1	0
2	M	31	0	13	0	0
2	N	31	0	13	0	0
2	O	31	0	13	2	0
2	P	31	0	13	0	0
3	A	1	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	1	0	0	0	0
3	F	1	0	0	0	0
3	G	2	0	0	0	0
3	H	1	0	0	0	0
3	I	1	0	0	0	0
3	J	1	0	0	0	0
3	K	1	0	0	0	0
3	L	1	0	0	0	0
3	M	1	0	0	0	0
3	N	1	0	0	0	0
3	O	1	0	0	0	0
3	P	1	0	0	0	0
4	A	44	0	0	0	0
4	B	31	0	0	0	0
4	C	62	0	0	0	0
4	D	40	0	0	1	0
4	E	45	0	0	0	0
4	F	26	0	0	0	0
4	G	25	0	0	1	0
4	H	29	0	0	0	0
4	I	24	0	0	0	0
4	J	33	0	0	0	0
4	K	11	0	0	0	0
4	L	13	0	0	0	0
4	M	16	0	0	0	0
4	N	14	0	0	0	0
4	O	12	0	0	1	0
4	P	14	0	0	0	0
All	All	46952	0	44475	458	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including

hydrogen atoms). The all-atom clashscore for this structure is 5.

All (458) 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:O:601:ANP:H8	2:O:601:ANP:H5'2	1.55	0.87
1:P:272:HIS:HE1	1:P:293:TRP:H	1.22	0.85
1:A:287:VAL:HG23	1:A:360:VAL:HG12	1.61	0.82
1:C:89:HIS:HD2	1:C:91:SER:HB2	1.44	0.81
1:H:272:HIS:HE1	1:H:293:TRP:H	1.28	0.80
1:E:193:ARG:HG3	1:E:197:MET:HE2	1.67	0.77
1:P:272:HIS:CE1	1:P:293:TRP:H	2.03	0.76
1:A:272:HIS:HE1	1:A:293:TRP:H	1.34	0.76
1:P:22:GLY:HA2	1:P:103:LEU:HD11	1.68	0.75
1:G:272:HIS:HE1	1:G:293:TRP:H	1.35	0.73
1:E:365:PRO:HA	1:E:377:ASN:HD21	1.56	0.71
1:B:348:ASP:O	1:B:352:GLU:HB2	1.91	0.71
1:L:123:VAL:HG12	1:L:127:VAL:HG23	1.74	0.70
1:P:329:ASN:HD21	1:P:345:LEU:H	1.39	0.70
1:G:272:HIS:CE1	1:G:293:TRP:H	2.09	0.69
1:K:272:HIS:CE1	1:K:293:TRP:H	2.11	0.69
1:E:272:HIS:HE1	1:E:293:TRP:H	1.40	0.68
1:A:299:GLU:HG3	1:A:351:ARG:HB3	1.76	0.68
1:K:272:HIS:HE1	1:K:293:TRP:H	1.40	0.68
1:E:291:MET:HB2	1:E:354:LEU:HD11	1.75	0.67
1:J:312:GLU:HB2	1:J:374:LYS:HG3	1.77	0.67
1:P:103:LEU:HB3	1:P:123:VAL:HG13	1.76	0.67
1:J:287:VAL:HG23	1:J:360:VAL:HG12	1.76	0.67
1:E:138:GLU:HB2	1:E:170:THR:HB	1.77	0.67
1:K:23:LEU:HG	1:K:130:ALA:HB2	1.77	0.67
1:O:272:HIS:HE1	1:O:293:TRP:H	1.41	0.66
1:M:86:VAL:HG11	1:M:146:TRP:CD2	2.30	0.66
1:K:29:ARG:HE	1:L:120:LEU:HB2	1.63	0.64
1:F:272:HIS:HE1	1:F:293:TRP:H	1.45	0.63
1:F:89:HIS:HD2	1:F:91:SER:H	1.45	0.63
1:K:287:VAL:HG23	1:K:360:VAL:HG12	1.81	0.62
1:B:303:THR:HG21	1:B:317:GLU:HB2	1.81	0.62
1:H:276:VAL:HB	1:H:291:MET:HG2	1.82	0.62
1:O:303:THR:HG21	1:O:317:GLU:HB2	1.81	0.62
1:E:276:VAL:HB	1:E:291:MET:HG2	1.80	0.61
1:O:301:VAL:HG22	1:O:356:ALA:HB3	1.82	0.61
1:E:36:SER:O	1:E:41:GLY:HA3	2.01	0.61
1:H:272:HIS:CE1	1:H:293:TRP:H	2.15	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:276:VAL:HB	1:I:291:MET:HG2	1.82	0.61
1:D:301:VAL:HG12	1:D:356:ALA:HB3	1.82	0.60
1:G:312:GLU:HG3	1:G:373:THR:HB	1.82	0.60
1:L:45:LEU:HD11	1:L:180:PHE:CZ	2.37	0.60
1:O:200:LEU:HD23	1:O:307:THR:HA	1.83	0.60
1:E:52:ASN:HB3	2:E:601:ANP:N7	2.15	0.60
1:G:257:LEU:HD22	1:G:288:GLU:HG3	1.83	0.60
1:K:418:ILE:HA	1:K:421:ARG:HE	1.67	0.59
1:M:330:LYS:O	1:M:334:ASP:HB2	2.02	0.59
1:D:276:VAL:O	1:D:290:ALA:HA	2.01	0.59
1:E:86:VAL:HG11	1:E:146:TRP:CD2	2.37	0.59
1:H:44:HIS:HA	1:H:47:TRP:CD1	2.37	0.59
1:E:323:ALA:HB2	1:E:385:GLN:HA	1.84	0.59
1:J:45:LEU:HD22	1:J:128:VAL:HA	1.84	0.59
1:C:89:HIS:HD2	1:C:91:SER:CB	2.14	0.59
1:O:316:HIS:CD2	1:O:375:LEU:HB3	2.38	0.59
1:D:188:GLU:HB3	1:D:192:ARG:HH21	1.68	0.58
1:K:68:VAL:HB	1:K:76:GLU:HB3	1.85	0.58
1:P:71:GLU:HA	1:P:212:ARG:HG2	1.86	0.58
1:N:276:VAL:O	1:N:290:ALA:HA	2.03	0.58
1:G:303:THR:HG22	1:G:358:ILE:HB	1.85	0.57
1:G:151:GLU:HB2	1:G:156:LEU:HD11	1.85	0.57
1:K:303:THR:HG21	1:K:317:GLU:HB2	1.85	0.57
1:B:291:MET:HB2	1:B:354:LEU:HD11	1.85	0.57
1:I:103:LEU:HD22	1:I:123:VAL:HG22	1.87	0.57
1:A:85:PRO:HB2	1:A:95:THR:HG21	1.86	0.57
1:E:86:VAL:HG13	1:E:158:LEU:HD21	1.86	0.57
1:A:82:ARG:HD2	1:B:12:TYR:HB3	1.87	0.57
1:M:303:THR:HB	1:M:316:HIS:CE1	2.40	0.57
1:A:272:HIS:CE1	1:A:293:TRP:H	2.19	0.56
1:N:272:HIS:HE1	1:N:293:TRP:H	1.51	0.56
1:A:411:VAL:O	1:A:415:GLN:HG2	2.05	0.56
1:J:316:HIS:H	1:J:316:HIS:CD2	2.23	0.56
1:A:86:VAL:HG11	1:A:146:TRP:CD2	2.40	0.56
1:G:303:THR:HG21	1:G:317:GLU:HB2	1.88	0.56
1:J:388:CYS:HB3	1:J:392:LEU:HD12	1.87	0.56
1:C:272:HIS:CE1	1:C:293:TRP:H	2.24	0.56
1:O:148:GLN:HB2	1:O:158:LEU:HD12	1.88	0.56
1:A:276:VAL:HB	1:A:291:MET:HG2	1.88	0.56
1:C:276:VAL:HB	1:C:291:MET:HG2	1.87	0.56
1:G:205:THR:HG23	1:G:252:HIS:HB2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:21:GLU:O	1:C:24:GLU:HB2	2.05	0.56
1:D:272:HIS:CE1	1:D:293:TRP:H	2.23	0.55
1:P:281:LYS:HG2	1:P:286:GLU:HG3	1.89	0.55
1:L:330:LYS:HA	1:L:333:LYS:HE2	1.88	0.55
1:I:276:VAL:O	1:I:290:ALA:HA	2.07	0.55
1:M:29:ARG:HH12	1:N:364:GLU:HG3	1.72	0.55
1:O:44:HIS:HA	1:O:47:TRP:CD1	2.42	0.55
1:G:303:THR:HB	1:G:316:HIS:CE1	2.42	0.55
1:H:303:THR:HG22	1:H:358:ILE:HB	1.89	0.55
1:A:388:CYS:O	1:A:392:LEU:HB2	2.07	0.55
1:C:272:HIS:HE1	1:C:293:TRP:H	1.54	0.55
1:N:272:HIS:CE1	1:N:293:TRP:H	2.25	0.55
1:A:136:GLU:HG2	1:A:149:VAL:HG22	1.89	0.54
1:B:276:VAL:HB	1:B:291:MET:HG2	1.90	0.54
1:I:272:HIS:HE1	1:I:293:TRP:H	1.56	0.54
1:O:271:ILE:HD12	1:O:405:VAL:HG12	1.88	0.54
1:D:89:HIS:HD2	1:D:91:SER:H	1.56	0.54
1:I:194:LEU:HD22	1:I:206:ILE:HG21	1.89	0.54
1:J:272:HIS:CE1	1:J:293:TRP:H	2.25	0.54
1:A:162:ALA:HB2	1:K:209:THR:HG21	1.90	0.54
1:D:86:VAL:HG13	1:D:158:LEU:HD21	1.90	0.54
1:E:34:ILE:HD13	1:E:127:VAL:HG11	1.88	0.54
1:P:316:HIS:CD2	1:P:316:HIS:H	2.26	0.54
1:B:205:THR:HG23	1:B:252:HIS:HB2	1.90	0.54
1:I:89:HIS:CD2	1:I:91:SER:H	2.25	0.54
1:L:86:VAL:HG11	1:L:146:TRP:CD2	2.43	0.54
1:H:45:LEU:HD22	1:H:128:VAL:HA	1.90	0.54
1:H:138:GLU:HB2	1:H:170:THR:HB	1.90	0.54
1:H:276:VAL:O	1:H:290:ALA:HA	2.07	0.54
1:D:301:VAL:HG21	4:D:2037:HOH:O	2.08	0.53
1:H:136:GLU:HG2	1:H:149:VAL:HG22	1.89	0.53
1:E:312:GLU:HG2	1:E:373:THR:HB	1.90	0.53
1:O:116:ILE:HD13	1:O:361:LYS:HB3	1.90	0.53
1:D:139:ILE:HG22	1:D:141:ARG:HG2	1.90	0.53
1:D:287:VAL:HG23	1:D:360:VAL:HG12	1.90	0.53
1:E:120:LEU:HD13	1:E:365:PRO:HG2	1.91	0.53
1:E:194:LEU:HA	1:E:197:MET:HE3	1.89	0.53
1:J:276:VAL:O	1:J:290:ALA:HA	2.07	0.53
1:J:276:VAL:HB	1:J:291:MET:HG2	1.91	0.53
1:B:312:GLU:HB2	1:B:374:LYS:HG3	1.90	0.53
1:C:308:ILE:HD13	1:C:372:LYS:HD3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:68:VAL:HG22	1:E:209:THR:HB	1.91	0.53
1:H:327:VAL:HG11	1:H:392:LEU:HB3	1.91	0.53
1:C:86:VAL:HA	1:C:96:VAL:HG22	1.90	0.53
1:J:34:ILE:HD13	1:J:44:HIS:HB3	1.90	0.52
1:A:120:LEU:HD13	1:A:365:PRO:HG2	1.92	0.52
1:E:188:GLU:O	1:E:192:ARG:HG2	2.10	0.52
1:G:95:THR:CG2	1:H:17:ILE:HG13	2.40	0.52
1:N:131:LEU:HG	1:N:179:VAL:HG11	1.92	0.52
1:B:140:LYS:O	1:B:167:THR:HA	2.09	0.52
1:C:383:PHE:HA	1:C:386:LYS:HE3	1.90	0.52
1:D:133:THR:HG23	1:D:176:ASP:HA	1.90	0.52
1:M:36:SER:O	1:M:41:GLY:HA3	2.10	0.52
1:M:148:GLN:HB2	1:M:158:LEU:HA	1.90	0.52
1:N:388:CYS:O	1:N:392:LEU:HB2	2.09	0.52
1:E:34:ILE:HG13	1:E:44:HIS:HB3	1.91	0.51
1:M:205:THR:HG23	1:M:252:HIS:HB2	1.92	0.51
1:P:44:HIS:HA	1:P:47:TRP:CD1	2.46	0.51
1:B:34:ILE:HD13	1:B:127:VAL:HG11	1.92	0.51
1:B:276:VAL:O	1:B:290:ALA:HA	2.10	0.51
1:C:96:VAL:O	1:C:100:MET:HB2	2.10	0.51
1:J:86:VAL:HG11	1:J:146:TRP:CD2	2.46	0.51
1:K:63:THR:HG22	1:K:80:ASP:OD2	2.11	0.51
1:D:272:HIS:HE1	1:D:293:TRP:H	1.57	0.51
1:F:281:LYS:HD2	1:F:286:GLU:HG3	1.93	0.51
1:A:369:GLY:HA2	1:B:32:MET:HA	1.92	0.50
1:C:89:HIS:HE1	1:D:17:ILE:O	1.94	0.50
1:H:311:HIS:CE1	1:H:373:THR:HG22	2.46	0.50
1:H:325:THR:HA	1:H:350:ILE:HD13	1.93	0.50
1:M:86:VAL:HG11	1:M:146:TRP:CE3	2.46	0.50
1:B:44:HIS:HA	1:B:47:TRP:CD1	2.46	0.50
1:H:289:ILE:HD12	1:H:358:ILE:HG13	1.93	0.50
1:P:43:HIS:CE1	1:P:186:ASP:H	2.30	0.50
1:C:138:GLU:CD	1:C:172:ARG:HH22	2.19	0.50
1:E:200:LEU:HD21	1:E:304:PHE:CD1	2.47	0.50
1:J:88:THR:HA	1:J:94:PRO:HA	1.94	0.50
1:O:36:SER:O	1:O:41:GLY:HA3	2.11	0.50
1:A:343:PRO:O	1:A:344:ASN:HB2	2.12	0.50
2:O:601:ANP:H5'2	2:O:601:ANP:C8	2.37	0.50
1:P:271:ILE:HD12	1:P:293:TRP:HB3	1.92	0.50
1:A:65:VAL:HG23	1:A:204:LEU:HD11	1.94	0.50
1:D:276:VAL:HB	1:D:291:MET:HG2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:415:GLN:HA	1:L:418:ILE:HD12	1.93	0.49
1:F:140:LYS:O	1:F:167:THR:HA	2.12	0.49
1:F:34:ILE:HG22	1:F:36:SER:O	2.12	0.49
1:B:276:VAL:HG22	1:B:395:TRP:CE2	2.47	0.49
1:G:287:VAL:HG23	1:G:360:VAL:HG12	1.94	0.49
1:L:276:VAL:O	1:L:290:ALA:HA	2.13	0.49
1:M:301:VAL:HG22	1:M:356:ALA:HB3	1.95	0.49
1:A:103:LEU:HD22	1:A:123:VAL:HG22	1.94	0.49
1:A:286:GLU:HB3	1:A:361:LYS:HB2	1.95	0.49
1:J:272:HIS:HE1	1:J:293:TRP:H	1.59	0.49
1:P:303:THR:HG21	1:P:317:GLU:HB2	1.94	0.49
1:E:303:THR:HG21	1:E:317:GLU:HB2	1.95	0.49
1:A:311:HIS:CE1	1:A:373:THR:HG22	2.47	0.49
1:D:85:PRO:HB2	1:D:95:THR:HG21	1.95	0.49
1:F:89:HIS:CD2	1:F:91:SER:H	2.29	0.49
1:H:37:THR:HG23	1:H:180:PHE:HA	1.95	0.49
1:I:385:GLN:O	1:I:389:ASN:HB2	2.13	0.49
1:K:34:ILE:HG13	1:K:44:HIS:HB3	1.95	0.49
1:K:93:ILE:HG22	1:K:97:ASP:HB2	1.95	0.48
1:K:133:THR:HG23	1:K:176:ASP:HA	1.95	0.48
1:M:265:ASN:HA	1:M:268:LYS:HB2	1.95	0.48
1:A:303:THR:HG21	1:A:317:GLU:HB2	1.94	0.48
1:L:23:LEU:HD22	1:L:130:ALA:HB2	1.96	0.48
1:B:140:LYS:HG2	1:B:145:GLU:HG2	1.94	0.48
1:L:26:VAL:HG13	1:L:33:TYR:CD2	2.48	0.48
1:M:286:GLU:HB2	1:M:361:LYS:HB2	1.95	0.48
1:A:18:THR:O	1:B:105:ALA:HA	2.13	0.48
1:J:23:LEU:HD22	1:J:130:ALA:HB2	1.95	0.48
1:C:368:GLU:HG3	1:D:35:GLY:HA2	1.96	0.48
1:D:89:HIS:CD2	1:D:91:SER:H	2.32	0.48
1:O:368:GLU:HG2	1:P:35:GLY:HA2	1.96	0.48
1:P:301:VAL:HG22	1:P:356:ALA:HB3	1.95	0.48
1:E:300:SER:HB2	1:E:355:ALA:HA	1.95	0.48
1:I:68:VAL:HG22	1:I:209:THR:HG23	1.94	0.48
1:M:276:VAL:O	1:M:290:ALA:HA	2.14	0.48
1:N:194:LEU:HD22	1:N:206:ILE:HG21	1.96	0.48
1:N:303:THR:HG21	1:N:317:GLU:HB2	1.96	0.48
1:O:409:LYS:HD2	4:O:2007:HOH:O	2.14	0.48
1:H:32:MET:HG2	1:H:33:TYR:CE2	2.49	0.48
1:J:303:THR:HG22	1:J:358:ILE:HB	1.95	0.48
1:I:34:ILE:HG13	1:I:44:HIS:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:299:GLU:HG3	1:K:351:ARG:HB3	1.95	0.48
1:B:116:ILE:HD13	1:B:361:LYS:HB3	1.96	0.48
1:G:190:VAL:HG12	1:G:194:LEU:HD11	1.96	0.48
1:H:257:LEU:HD22	1:H:357:VAL:HG11	1.95	0.48
1:K:120:LEU:HB2	1:L:29:ARG:HE	1.79	0.48
1:A:291:MET:HB2	1:A:354:LEU:HD11	1.95	0.47
1:F:205:THR:HG23	1:F:252:HIS:HB2	1.96	0.47
1:K:86:VAL:HG11	1:K:146:TRP:CD2	2.49	0.47
1:B:271:ILE:HD12	1:B:293:TRP:HB3	1.96	0.47
1:D:65:VAL:HG23	1:D:204:LEU:HD11	1.96	0.47
1:O:19:ILE:HG23	1:P:105:ALA:HB2	1.97	0.47
1:G:310:THR:OG1	1:G:316:HIS:CE1	2.67	0.47
1:J:316:HIS:H	1:J:316:HIS:HD2	1.62	0.47
1:P:135:LEU:HB3	1:P:150:TYR:HB2	1.96	0.47
1:C:276:VAL:HG22	1:C:395:TRP:CE2	2.49	0.47
1:K:257:LEU:HD11	1:K:288:GLU:HB3	1.97	0.47
1:M:287:VAL:HG23	1:M:360:VAL:HG12	1.96	0.47
1:O:89:HIS:CG	1:O:90:ALA:H	2.32	0.47
1:K:276:VAL:HB	1:K:291:MET:HG2	1.96	0.47
1:O:138:GLU:HA	1:O:146:TRP:O	2.14	0.47
1:A:63:THR:HG22	1:A:80:ASP:OD2	2.15	0.47
1:I:106:GLY:HA2	2:I:601:ANP:H4'	1.96	0.47
1:M:45:LEU:HD22	1:M:128:VAL:HA	1.96	0.47
1:N:44:HIS:HA	1:N:47:TRP:CD1	2.50	0.47
1:G:75:VAL:O	1:G:172:ARG:HA	2.15	0.47
1:H:388:CYS:O	1:H:392:LEU:HB2	2.15	0.47
1:K:259:ASP:HA	1:K:262:LYS:HD2	1.97	0.47
1:K:314:GLY:HA2	1:K:374:LYS:HE3	1.97	0.47
1:P:151:GLU:HB2	1:P:156:LEU:HD11	1.96	0.47
1:A:289:ILE:HD12	1:A:358:ILE:HG13	1.97	0.47
1:F:276:VAL:O	1:F:290:ALA:HA	2.15	0.47
1:C:93:ILE:HG23	1:C:94:PRO:HD2	1.97	0.47
1:G:286:GLU:HB3	1:G:361:LYS:HB2	1.96	0.47
1:I:36:SER:O	1:I:41:GLY:HA3	2.15	0.47
1:K:316:HIS:CD2	1:K:316:HIS:H	2.33	0.47
1:L:42:LEU:HG	1:L:185:TYR:CE1	2.49	0.47
1:P:276:VAL:O	1:P:290:ALA:HA	2.14	0.47
1:J:138:GLU:HB2	1:J:170:THR:HB	1.95	0.46
1:H:34:ILE:HG22	1:H:36:SER:O	2.15	0.46
1:I:366:GLN:H	1:I:377:ASN:HD21	1.64	0.46
1:J:34:ILE:HD13	1:J:44:HIS:CD2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:189:THR:HG22	1:M:192:ARG:HH22	1.79	0.46
1:H:89:HIS:CD2	1:H:91:SER:H	2.34	0.46
1:L:303:THR:HG22	1:L:358:ILE:HB	1.97	0.46
1:P:45:LEU:HD11	1:P:180:PHE:CZ	2.50	0.46
1:H:368:GLU:HB2	1:H:374:LYS:HB2	1.98	0.46
1:H:116:ILE:HD13	1:H:361:LYS:HB3	1.97	0.46
1:L:187:PHE:CD1	1:L:210:ASP:HB2	2.50	0.46
1:F:289:ILE:HG22	1:F:291:MET:HE2	1.98	0.46
1:O:71:GLU:HG3	1:O:211:GLU:O	2.15	0.46
1:A:367:PHE:CD1	1:A:372:LYS:HB3	2.51	0.46
1:C:89:HIS:CD2	1:C:91:SER:HB2	2.36	0.46
1:I:386:LYS:O	1:I:390:GLU:HB2	2.16	0.46
1:B:135:LEU:HB3	1:B:150:TYR:HB2	1.96	0.46
1:M:44:HIS:HA	1:M:47:TRP:CD1	2.51	0.46
1:G:388:CYS:O	1:G:392:LEU:HB2	2.16	0.45
1:H:271:ILE:HD12	1:H:295:ALA:HA	1.97	0.45
1:M:36:SER:HB2	1:M:40:ARG:HH21	1.80	0.45
1:O:136:GLU:HB2	1:O:172:ARG:HB2	1.98	0.45
1:E:312:GLU:HB2	1:E:374:LYS:HG3	1.97	0.45
1:O:29:ARG:HD2	1:P:120:LEU:HD12	1.98	0.45
1:P:388:CYS:HB3	1:P:392:LEU:HD12	1.97	0.45
1:A:276:VAL:O	1:A:290:ALA:HA	2.16	0.45
1:A:327:VAL:HG11	1:A:392:LEU:HB3	1.99	0.45
1:D:86:VAL:HG11	1:D:146:TRP:CD2	2.52	0.45
1:M:140:LYS:O	1:M:167:THR:HA	2.15	0.45
1:O:139:ILE:HG23	1:O:169:SER:HB3	1.98	0.45
1:E:303:THR:HG22	1:E:358:ILE:HB	1.99	0.45
1:G:45:LEU:HD22	1:G:128:VAL:HA	1.98	0.45
1:I:89:HIS:HD2	1:I:91:SER:H	1.64	0.45
1:K:328:VAL:HG11	1:K:350:ILE:HG12	1.98	0.45
1:M:88:THR:HA	1:M:94:PRO:HA	1.97	0.45
1:O:276:VAL:HG22	1:O:395:TRP:CE2	2.51	0.45
1:P:299:GLU:HG3	1:P:351:ARG:HB3	1.98	0.45
1:F:303:THR:HG22	1:F:358:ILE:HB	1.99	0.45
1:G:276:VAL:HB	1:G:291:MET:HG3	1.97	0.45
1:I:89:HIS:HE1	1:J:17:ILE:O	2.00	0.45
1:C:44:HIS:HA	1:C:47:TRP:CD1	2.52	0.45
1:F:65:VAL:HG23	1:F:204:LEU:HD11	1.99	0.45
1:F:276:VAL:HG22	1:F:395:TRP:CE2	2.52	0.45
1:G:58:MET:HE3	1:G:361:LYS:HE2	1.98	0.45
1:H:194:LEU:HD22	1:H:206:ILE:HG21	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:366:GLN:N	1:I:377:ASN:HD21	2.15	0.45
1:M:388:CYS:O	1:M:392:LEU:HB2	2.17	0.45
1:F:367:PHE:CD1	1:F:372:LYS:HB3	2.52	0.45
1:C:86:VAL:HG11	1:C:146:TRP:CE2	2.52	0.44
1:C:116:ILE:HG21	1:C:361:LYS:HB3	1.99	0.44
1:D:303:THR:HG21	1:D:317:GLU:HB2	1.99	0.44
1:H:308:ILE:HD12	1:H:372:LYS:HD3	1.99	0.44
1:I:120:LEU:HD13	1:I:365:PRO:HG2	1.99	0.44
1:K:369:GLY:HA2	1:L:32:MET:HA	1.98	0.44
1:M:311:HIS:CE1	1:M:373:THR:HG22	2.52	0.44
1:O:75:VAL:O	1:O:172:ARG:HA	2.17	0.44
1:A:129:ASN:OD1	1:A:153:SER:HA	2.18	0.44
1:B:86:VAL:HG12	1:B:158:LEU:HD21	1.99	0.44
1:C:32:MET:HG3	1:D:121:HIS:CE1	2.52	0.44
1:F:108:LYS:HD2	2:F:601:ANP:O1B	2.18	0.44
1:K:89:HIS:CD2	1:K:91:SER:H	2.35	0.44
1:P:138:GLU:HB2	1:P:170:THR:HB	2.00	0.44
1:E:140:LYS:O	1:E:141:ARG:HB3	2.17	0.44
1:E:351:ARG:HG2	1:E:354:LEU:HD23	2.00	0.44
1:I:303:THR:HG21	1:I:317:GLU:HB2	2.00	0.44
1:J:327:VAL:HG11	1:J:392:LEU:HB3	1.99	0.44
1:P:407:VAL:O	1:P:411:VAL:HG23	2.17	0.44
1:C:195:GLN:HG2	1:C:199:PHE:CE2	2.53	0.44
1:E:276:VAL:O	1:E:290:ALA:HA	2.18	0.44
1:E:272:HIS:CE1	1:E:293:TRP:H	2.28	0.44
1:O:418:ILE:HG23	1:O:421:ARG:HH21	1.82	0.44
1:P:200:LEU:HD21	1:P:304:PHE:CD2	2.52	0.44
1:L:303:THR:HB	1:L:316:HIS:CE1	2.53	0.44
1:I:377:ASN:HB3	1:I:379:GLU:OE1	2.18	0.44
1:J:205:THR:HG23	1:J:252:HIS:HB2	2.00	0.44
1:O:272:HIS:CE1	1:O:293:TRP:H	2.29	0.44
1:P:331:TYR:HD2	1:P:407:VAL:HG21	1.82	0.44
1:F:131:LEU:HD22	1:F:179:VAL:HG11	2.00	0.43
1:G:140:LYS:O	1:G:167:THR:HA	2.18	0.43
1:I:301:VAL:HG22	1:I:356:ALA:HB3	2.00	0.43
1:N:70:LEU:HD12	1:N:74:GLY:HA3	1.99	0.43
1:O:316:HIS:CD2	1:O:316:HIS:H	2.35	0.43
1:C:85:PRO:HB2	1:C:95:THR:HG21	2.00	0.43
1:I:123:VAL:HG13	1:I:127:VAL:HG23	2.00	0.43
1:M:23:LEU:HD22	1:M:130:ALA:HB2	2.00	0.43
1:O:89:HIS:CG	1:O:90:ALA:N	2.86	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:291:MET:HB2	1:P:354:LEU:HD11	2.00	0.43
1:A:140:LYS:O	1:A:167:THR:HA	2.19	0.43
1:B:272:HIS:CE1	1:B:293:TRP:H	2.37	0.43
1:H:43:HIS:HB3	1:H:47:TRP:CZ2	2.53	0.43
1:J:44:HIS:HA	1:J:47:TRP:CD1	2.54	0.43
1:O:275:ILE:HG12	1:O:292:GLN:HB2	1.99	0.43
1:O:276:VAL:O	1:O:290:ALA:HA	2.18	0.43
1:G:368:GLU:HG2	1:H:35:GLY:HA2	2.00	0.43
1:K:323:ALA:HB2	1:K:385:GLN:HG3	2.00	0.43
1:P:276:VAL:HG22	1:P:395:TRP:CE2	2.54	0.43
1:C:35:GLY:HA2	1:D:368:GLU:HG3	2.00	0.43
1:E:34:ILE:HD13	1:E:127:VAL:CG1	2.47	0.43
1:E:317:GLU:HG2	1:E:321:ARG:HD2	1.99	0.43
1:H:138:GLU:CD	1:H:172:ARG:HH22	2.26	0.43
1:K:276:VAL:O	1:K:290:ALA:HA	2.19	0.43
1:M:303:THR:HG21	1:M:317:GLU:HB2	2.01	0.43
1:O:376:GLY:HA3	1:P:36:SER:HB3	2.01	0.43
1:F:93:ILE:HB	1:F:94:PRO:HD2	1.98	0.43
1:H:86:VAL:HG11	1:H:146:TRP:CD2	2.54	0.43
1:L:103:LEU:HD22	1:L:123:VAL:HG13	2.01	0.43
1:E:44:HIS:HA	1:E:47:TRP:CD1	2.54	0.43
1:L:325:THR:HA	1:L:350:ILE:HD13	2.00	0.43
1:G:291:MET:HE1	1:G:324:LEU:HD13	1.99	0.43
1:J:86:VAL:HG11	1:J:146:TRP:CE2	2.54	0.43
1:K:194:LEU:HD22	1:K:206:ILE:HG21	2.01	0.43
1:O:35:GLY:HA2	1:P:368:GLU:HG3	2.01	0.43
1:J:323:ALA:CB	1:J:388:CYS:HB2	2.49	0.43
1:K:181:GLU:HA	1:N:283:THR:HB	2.00	0.43
1:I:17:ILE:O	1:J:89:HIS:HE1	2.02	0.42
1:K:65:VAL:HB	1:K:206:ILE:HG12	2.00	0.42
1:K:140:LYS:HG2	1:K:164:THR:HG21	2.00	0.42
1:P:67:VAL:HG23	1:P:77:VAL:HG22	2.01	0.42
1:B:309:ASN:HD21	1:B:311:HIS:HB3	1.84	0.42
1:K:291:MET:HB2	1:K:354:LEU:HD11	2.01	0.42
1:E:89:HIS:HD2	1:E:98:VAL:HG21	1.84	0.42
1:E:133:THR:HG23	1:E:176:ASP:HA	1.99	0.42
1:G:327:VAL:HG11	1:G:392:LEU:HB3	2.01	0.42
1:J:86:VAL:HG13	1:J:158:LEU:HD21	2.00	0.42
1:O:144:TYR:HA	1:O:163:PRO:HA	2.00	0.42
1:C:120:LEU:HD13	1:C:365:PRO:HG2	2.00	0.42
1:L:71:GLU:HG2	1:L:212:ARG:HA	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:137:VAL:HG12	1:N:171:VAL:HG22	2.00	0.42
1:B:259:ASP:O	1:B:263:HIS:HD2	2.02	0.42
1:K:125:VAL:HG12	2:K:601:ANP:O1A	2.19	0.42
1:M:58:MET:SD	1:M:307:THR:HB	2.59	0.42
1:N:52:ASN:HD21	1:N:125:VAL:HB	1.85	0.42
1:O:86:VAL:HG22	1:O:158:LEU:HD21	2.01	0.42
1:B:196:GLU:O	1:B:200:LEU:HD22	2.19	0.42
1:D:352:GLU:OE1	1:D:413:SER:HB2	2.19	0.42
1:H:86:VAL:HG11	1:H:146:TRP:CE2	2.54	0.42
1:M:133:THR:HG23	1:M:176:ASP:HA	2.01	0.42
1:P:54:VAL:HG11	1:P:307:THR:HG21	2.00	0.42
1:G:67:VAL:HA	1:G:76:GLU:O	2.19	0.42
1:J:75:VAL:O	1:J:172:ARG:HA	2.20	0.42
1:P:316:HIS:H	1:P:316:HIS:HD2	1.65	0.42
1:B:272:HIS:HE1	1:B:293:TRP:H	1.67	0.42
1:C:67:VAL:HG22	1:C:208:LEU:HD13	2.01	0.42
1:J:194:LEU:HD12	1:J:208:LEU:HB2	2.01	0.42
1:D:23:LEU:HD11	1:D:101:THR:HA	2.02	0.42
1:D:311:HIS:CE1	1:D:373:THR:HG22	2.54	0.42
1:E:208:LEU:O	1:E:248:SER:HA	2.20	0.42
1:H:316:HIS:H	1:H:316:HIS:CD2	2.38	0.42
1:J:36:SER:O	1:J:41:GLY:HA3	2.20	0.42
1:J:272:HIS:NE2	1:J:292:GLN:HG3	2.34	0.42
1:K:210:ASP:O	1:K:246:VAL:HG13	2.19	0.42
1:N:34:ILE:HD12	1:N:44:HIS:HB3	2.02	0.42
1:A:44:HIS:HA	1:A:47:TRP:CD1	2.54	0.42
1:B:83:GLY:HA2	1:B:169:SER:HB2	2.01	0.42
1:I:257:LEU:HD13	1:I:357:VAL:HG12	2.02	0.42
1:P:86:VAL:HG13	1:P:158:LEU:HD21	2.01	0.41
1:P:367:PHE:CD1	1:P:372:LYS:HB3	2.55	0.41
1:D:88:THR:HA	1:D:94:PRO:HA	2.01	0.41
1:A:283:THR:HB	1:A:284:GLY:H	1.70	0.41
1:D:140:LYS:O	1:D:167:THR:HA	2.20	0.41
1:J:291:MET:HB2	1:J:354:LEU:HD11	2.02	0.41
1:O:43:HIS:CE1	1:O:186:ASP:H	2.38	0.41
1:A:36:SER:O	1:A:41:GLY:HA3	2.20	0.41
1:E:131:LEU:HD22	1:E:179:VAL:HG11	2.02	0.41
1:E:146:TRP:CZ3	1:E:160:GLN:HB2	2.55	0.41
1:L:52:ASN:HB3	2:L:601:ANP:N7	2.36	0.41
1:A:35:GLY:HA2	1:B:368:GLU:HA	2.02	0.41
1:C:276:VAL:O	1:C:290:ALA:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:276:VAL:HB	1:F:291:MET:HG2	2.02	0.41
1:G:137:VAL:HG23	1:G:148:GLN:HB3	2.03	0.41
1:C:160:GLN:HB3	1:E:245:LYS:HA	2.03	0.41
1:D:303:THR:HG22	1:D:358:ILE:HB	2.03	0.41
1:M:114:TYR:HB3	1:M:117:SER:HB3	2.02	0.41
1:I:45:LEU:HD22	1:I:128:VAL:HA	2.02	0.41
1:M:64:THR:HG23	1:M:205:THR:HB	2.02	0.41
1:P:123:VAL:HG12	1:P:127:VAL:HG23	2.02	0.41
1:C:133:THR:HG23	1:C:176:ASP:HA	2.02	0.41
1:F:46:ILE:HD11	1:F:185:TYR:CD1	2.55	0.41
1:G:52:ASN:HB3	2:G:601:ANP:N7	2.35	0.41
1:H:200:LEU:HD13	1:H:307:THR:HA	2.03	0.41
1:M:327:VAL:HG11	1:M:392:LEU:HB3	2.02	0.41
1:P:146:TRP:HB3	1:P:158:LEU:HD11	2.03	0.41
1:A:276:VAL:HG22	1:A:395:TRP:CE2	2.55	0.41
1:B:299:GLU:CD	1:B:351:ARG:HE	2.29	0.41
1:C:200:LEU:HD23	1:C:257:LEU:HD21	2.02	0.41
1:I:52:ASN:HB3	2:I:601:ANP:N7	2.35	0.41
1:L:198:ALA:HB2	1:L:206:ILE:HD12	2.02	0.41
1:M:75:VAL:O	1:M:172:ARG:HA	2.20	0.41
1:N:187:PHE:CD2	1:N:210:ASP:HB2	2.56	0.41
1:P:46:ILE:HD11	1:P:185:TYR:CD1	2.56	0.41
1:C:140:LYS:O	1:C:167:THR:HA	2.21	0.41
1:F:257:LEU:HD11	1:F:359:SER:HB3	2.03	0.41
1:C:303:THR:HG22	1:C:358:ILE:HB	2.03	0.40
1:G:312:GLU:HB2	1:G:374:LYS:HG3	2.03	0.40
1:I:72:ASP:CG	1:I:174:TRP:HE1	2.29	0.40
1:J:106:GLY:HA2	2:J:601:ANP:H4'	2.03	0.40
1:A:106:GLY:HA2	2:A:601:ANP:H4'	2.04	0.40
1:C:17:ILE:O	1:D:89:HIS:HE1	2.03	0.40
1:D:145:GLU:HG2	1:D:162:ALA:O	2.21	0.40
1:E:286:GLU:HB3	1:E:361:LYS:HB2	2.03	0.40
1:H:182:THR:HG22	1:H:184:GLU:H	1.86	0.40
1:J:303:THR:HG21	1:J:317:GLU:HB2	2.03	0.40
1:C:89:HIS:CD2	1:C:91:SER:H	2.39	0.40
1:F:44:HIS:CE1	1:F:371:THR:HA	2.57	0.40
1:G:188:GLU:HB2	4:G:2018:HOH:O	2.20	0.40
1:I:370:GLN:HB2	1:J:32:MET:HE3	2.03	0.40
1:J:276:VAL:HG22	1:J:395:TRP:CE2	2.56	0.40
1:K:93:ILE:HD13	1:K:102:GLN:HE22	1.86	0.40
1:P:71:GLU:HB2	1:P:211:GLU:O	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:195:GLN:HE22	1:D:263:HIS:CE1	2.40	0.40
1:F:76:GLU:HG3	1:F:172:ARG:HG3	2.04	0.40
1:G:276:VAL:HB	1:G:291:MET:CG	2.52	0.40
1:M:76:GLU:HG3	1:M:172:ARG:HH11	1.86	0.40
1:E:75:VAL:O	1:E:172:ARG:HA	2.20	0.40
1:E:200:LEU:HD21	1:E:304:PHE:CG	2.56	0.40
1:E:263:HIS:O	1:E:266:ARG:HG2	2.22	0.40
1:G:63:THR:HG22	1:G:80:ASP:OD2	2.22	0.40
1:H:299:GLU:HG3	1:H:351:ARG:HB3	2.04	0.40
1:L:86:VAL:HG11	1:L:146:TRP:CE2	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	374/432 (87%)	354 (95%)	17 (4%)	3 (1%)	16	44
1	B	378/432 (88%)	362 (96%)	13 (3%)	3 (1%)	16	44
1	C	383/432 (89%)	368 (96%)	13 (3%)	2 (0%)	24	54
1	D	388/432 (90%)	375 (97%)	11 (3%)	2 (0%)	24	54
1	E	380/432 (88%)	365 (96%)	14 (4%)	1 (0%)	36	65
1	F	379/432 (88%)	366 (97%)	11 (3%)	2 (0%)	24	54
1	G	375/432 (87%)	361 (96%)	13 (4%)	1 (0%)	36	65
1	H	375/432 (87%)	360 (96%)	13 (4%)	2 (0%)	24	54
1	I	369/432 (85%)	355 (96%)	12 (3%)	2 (0%)	24	54
1	J	378/432 (88%)	360 (95%)	13 (3%)	5 (1%)	9	32
1	K	370/432 (86%)	351 (95%)	17 (5%)	2 (0%)	24	54
1	L	376/432 (87%)	356 (95%)	17 (4%)	3 (1%)	16	44

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	M	377/432 (87%)	358 (95%)	18 (5%)	1 (0%)	36	65
1	N	367/432 (85%)	350 (95%)	16 (4%)	1 (0%)	36	65
1	O	373/432 (86%)	358 (96%)	14 (4%)	1 (0%)	36	65
1	P	370/432 (86%)	353 (95%)	14 (4%)	3 (1%)	16	44
All	All	6012/6912 (87%)	5752 (96%)	226 (4%)	34 (1%)	21	51

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	344	ASN
1	L	343	PRO
1	B	124	GLY
1	D	124	GLY
1	E	124	GLY
1	F	124	GLY
1	G	124	GLY
1	H	124	GLY
1	I	124	GLY
1	J	81	GLY
1	J	124	GLY
1	J	256	GLY
1	L	81	GLY
1	P	124	GLY
1	A	124	GLY
1	B	120	LEU
1	H	112	ASP
1	J	244	HIS
1	K	124	GLY
1	P	343	PRO
1	C	124	GLY
1	K	95	THR
1	O	124	GLY
1	C	377	ASN
1	I	120	LEU
1	J	92	GLY
1	M	124	GLY
1	A	343	PRO
1	B	343	PRO
1	L	124	GLY
1	P	120	LEU
1	F	81	GLY

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Mol	Chain	Res	Type
1	N	124	GLY
1	D	81	GLY

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	302/350 (86%)	279 (92%)	23 (8%)	12	36
1	B	297/350 (85%)	281 (95%)	16 (5%)	20	51
1	C	307/350 (88%)	282 (92%)	25 (8%)	11	33
1	D	306/350 (87%)	283 (92%)	23 (8%)	12	37
1	E	302/350 (86%)	280 (93%)	22 (7%)	13	38
1	F	299/350 (85%)	278 (93%)	21 (7%)	14	40
1	G	296/350 (85%)	275 (93%)	21 (7%)	13	40
1	H	299/350 (85%)	271 (91%)	28 (9%)	8	26
1	I	293/350 (84%)	270 (92%)	23 (8%)	11	35
1	J	298/350 (85%)	275 (92%)	23 (8%)	12	35
1	K	295/350 (84%)	275 (93%)	20 (7%)	14	42
1	L	297/350 (85%)	276 (93%)	21 (7%)	13	40
1	M	299/350 (85%)	277 (93%)	22 (7%)	13	38
1	N	293/350 (84%)	276 (94%)	17 (6%)	18	49
1	O	301/350 (86%)	277 (92%)	24 (8%)	11	34
1	P	292/350 (83%)	265 (91%)	27 (9%)	8	27
All	All	4776/5600 (85%)	4420 (92%)	356 (8%)	12	37

All (356) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	MET
1	A	34	ILE

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Mol	Chain	Res	Type
1	A	39	GLU
1	A	47	TRP
1	A	86	VAL
1	A	96	VAL
1	A	99	VAL
1	A	100	MET
1	A	123	VAL
1	A	131	LEU
1	A	133	THR
1	A	184	GLU
1	A	197	MET
1	A	246	VAL
1	A	283	THR
1	A	285	HIS
1	A	300	SER
1	A	316	HIS
1	A	337	LEU
1	A	392	LEU
1	A	405	VAL
1	A	411	VAL
1	A	417	ARG
1	B	10	ASP
1	B	34	ILE
1	B	86	VAL
1	B	96	VAL
1	B	99	VAL
1	B	116	ILE
1	B	123	VAL
1	B	181	GLU
1	B	200	LEU
1	B	289	ILE
1	B	298	SER
1	B	337	LEU
1	B	378	THR
1	B	382	SER
1	B	389	ASN
1	B	405	VAL
1	C	21	GLU
1	C	32	MET
1	C	39	GLU
1	C	40	ARG
1	C	63	THR

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Mol	Chain	Res	Type
1	C	67	VAL
1	C	86	VAL
1	C	96	VAL
1	C	99	VAL
1	C	147	SER
1	C	153	SER
1	C	154	GLU
1	C	169	SER
1	C	188	GLU
1	C	271	ILE
1	C	281	LYS
1	C	289	ILE
1	C	300	SER
1	C	318	GLU
1	C	326	SER
1	C	337	LEU
1	C	382	SER
1	C	405	VAL
1	C	409	LYS
1	C	417	ARG
1	D	39	GLU
1	D	71	GLU
1	D	96	VAL
1	D	99	VAL
1	D	116	ILE
1	D	123	VAL
1	D	126	SER
1	D	135	LEU
1	D	137	VAL
1	D	138	GLU
1	D	164	THR
1	D	182	THR
1	D	196	GLU
1	D	200	LEU
1	D	213	VAL
1	D	214	THR
1	D	267	THR
1	D	349	ASP
1	D	352	GLU
1	D	378	THR
1	D	382	SER
1	D	392	LEU

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Mol	Chain	Res	Type
1	D	405	VAL
1	E	34	ILE
1	E	39	GLU
1	E	64	THR
1	E	67	VAL
1	E	93	ILE
1	E	96	VAL
1	E	99	VAL
1	E	110	ASP
1	E	116	ILE
1	E	123	VAL
1	E	156	LEU
1	E	183	THR
1	E	188	GLU
1	E	200	LEU
1	E	271	ILE
1	E	285	HIS
1	E	291	MET
1	E	324	LEU
1	E	342	ASP
1	E	374	LYS
1	E	404	LYS
1	E	418	ILE
1	F	11	GLU
1	F	19	ILE
1	F	71	GLU
1	F	96	VAL
1	F	111	SER
1	F	136	GLU
1	F	137	VAL
1	F	172	ARG
1	F	205	THR
1	F	208	LEU
1	F	209	THR
1	F	249	ARG
1	F	262	LYS
1	F	281	LYS
1	F	289	ILE
1	F	338	LEU
1	F	349	ASP
1	F	381	LYS
1	F	382	SER

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Mol	Chain	Res	Type
1	F	388	CYS
1	F	389	ASN
1	G	16	SER
1	G	34	ILE
1	G	64	THR
1	G	96	VAL
1	G	104	HIS
1	G	137	VAL
1	G	153	SER
1	G	167	THR
1	G	169	SER
1	G	188	GLU
1	G	209	THR
1	G	246	VAL
1	G	257	LEU
1	G	271	ILE
1	G	277	ASP
1	G	285	HIS
1	G	289	ILE
1	G	308	ILE
1	G	346	THR
1	G	368	GLU
1	G	389	ASN
1	H	18	THR
1	H	32	MET
1	H	37	THR
1	H	39	GLU
1	H	64	THR
1	H	68	VAL
1	H	71	GLU
1	H	86	VAL
1	H	96	VAL
1	H	99	VAL
1	H	123	VAL
1	H	134	ARG
1	H	137	VAL
1	H	153	SER
1	H	183	THR
1	H	189	THR
1	H	196	GLU
1	H	267	THR
1	H	271	ILE

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Mol	Chain	Res	Type
1	H	281	LYS
1	H	300	SER
1	H	308	ILE
1	H	316	HIS
1	H	326	SER
1	H	330	LYS
1	H	346	THR
1	H	352	GLU
1	H	389	ASN
1	I	16	SER
1	I	34	ILE
1	I	39	GLU
1	I	70	LEU
1	I	86	VAL
1	I	93	ILE
1	I	96	VAL
1	I	99	VAL
1	I	123	VAL
1	I	138	GLU
1	I	169	SER
1	I	184	GLU
1	I	188	GLU
1	I	192	ARG
1	I	208	LEU
1	I	209	THR
1	I	291	MET
1	I	316	HIS
1	I	330	LYS
1	I	366	GLN
1	I	379	GLU
1	I	389	ASN
1	I	405	VAL
1	J	34	ILE
1	J	39	GLU
1	J	67	VAL
1	J	86	VAL
1	J	96	VAL
1	J	99	VAL
1	J	123	VAL
1	J	126	SER
1	J	137	VAL
1	J	164	THR

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Mol	Chain	Res	Type
1	J	181	GLU
1	J	182	THR
1	J	184	GLU
1	J	193	ARG
1	J	209	THR
1	J	246	VAL
1	J	258	VAL
1	J	271	ILE
1	J	307	THR
1	J	316	HIS
1	J	337	LEU
1	J	352	GLU
1	J	389	ASN
1	K	19	ILE
1	K	23	LEU
1	K	32	MET
1	K	34	ILE
1	K	96	VAL
1	K	99	VAL
1	K	125	VAL
1	K	137	VAL
1	K	138	GLU
1	K	140	LYS
1	K	189	THR
1	K	246	VAL
1	K	283	THR
1	K	286	GLU
1	K	337	LEU
1	K	345	LEU
1	K	349	ASP
1	K	382	SER
1	K	394	HIS
1	K	405	VAL
1	L	19	ILE
1	L	47	TRP
1	L	54	VAL
1	L	67	VAL
1	L	71	GLU
1	L	112	ASP
1	L	137	VAL
1	L	151	GLU
1	L	169	SER

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Mol	Chain	Res	Type
1	L	182	THR
1	L	183	THR
1	L	184	GLU
1	L	196	GLU
1	L	200	LEU
1	L	247	LYS
1	L	248	SER
1	L	266	ARG
1	L	267	THR
1	L	271	ILE
1	L	308	ILE
1	L	413	SER
1	M	12	TYR
1	M	39	GLU
1	M	64	THR
1	M	67	VAL
1	M	71	GLU
1	M	126	SER
1	M	135	LEU
1	M	137	VAL
1	M	139	ILE
1	M	154	GLU
1	M	169	SER
1	M	188	GLU
1	M	209	THR
1	M	211	GLU
1	M	246	VAL
1	M	283	THR
1	M	307	THR
1	M	318	GLU
1	M	352	GLU
1	M	382	SER
1	M	408	ASN
1	M	409	LYS
1	N	99	VAL
1	N	112	ASP
1	N	116	ILE
1	N	126	SER
1	N	137	VAL
1	N	138	GLU
1	N	172	ARG
1	N	209	THR

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Mol	Chain	Res	Type
1	N	259	ASP
1	N	267	THR
1	N	271	ILE
1	N	285	HIS
1	N	303	THR
1	N	349	ASP
1	N	364	GLU
1	N	405	VAL
1	N	415	GLN
1	O	19	ILE
1	O	34	ILE
1	O	67	VAL
1	O	95	THR
1	O	96	VAL
1	O	126	SER
1	O	135	LEU
1	O	139	ILE
1	O	153	SER
1	O	169	SER
1	O	188	GLU
1	O	209	THR
1	O	285	HIS
1	O	289	ILE
1	O	317	GLU
1	O	338	LEU
1	O	352	GLU
1	O	364	GLU
1	O	368	GLU
1	O	379	GLU
1	O	382	SER
1	O	401	THR
1	O	404	LYS
1	O	412	SER
1	P	67	VAL
1	P	71	GLU
1	P	86	VAL
1	P	99	VAL
1	P	103	LEU
1	P	110	ASP
1	P	123	VAL
1	P	126	SER
1	P	137	VAL

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Mol	Chain	Res	Type
1	P	147	SER
1	P	153	SER
1	P	156	LEU
1	P	208	LEU
1	P	267	THR
1	P	268	LYS
1	P	285	HIS
1	P	289	ILE
1	P	316	HIS
1	P	317	GLU
1	P	322	SER
1	P	334	ASP
1	P	352	GLU
1	P	362	VAL
1	P	370	GLN
1	P	382	SER
1	P	390	GLU
1	P	405	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (120) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	104	HIS
1	A	272	HIS
1	A	311	HIS
1	A	366	GLN
1	A	408	ASN
1	B	104	HIS
1	B	252	HIS
1	B	263	HIS
1	B	265	ASN
1	B	272	HIS
1	B	294	ASN
1	B	309	ASN
1	B	389	ASN
1	B	399	ASN
1	C	44	HIS
1	C	89	HIS
1	C	102	GLN
1	C	104	HIS
1	C	272	HIS
1	C	285	HIS

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Mol	Chain	Res	Type
1	C	309	ASN
1	C	316	HIS
1	C	389	ASN
1	C	408	ASN
1	D	44	HIS
1	D	66	ASN
1	D	89	HIS
1	D	244	HIS
1	D	263	HIS
1	D	272	HIS
1	D	294	ASN
1	D	389	ASN
1	E	207	ASN
1	E	252	HIS
1	E	272	HIS
1	E	309	ASN
1	E	377	ASN
1	E	385	GLN
1	E	389	ASN
1	E	408	ASN
1	F	89	HIS
1	F	104	HIS
1	F	195	GLN
1	F	272	HIS
1	F	285	HIS
1	F	309	ASN
1	F	311	HIS
1	F	399	ASN
1	G	44	HIS
1	G	160	GLN
1	G	272	HIS
1	G	316	HIS
1	G	408	ASN
1	H	44	HIS
1	H	89	HIS
1	H	129	ASN
1	H	272	HIS
1	H	316	HIS
1	H	415	GLN
1	I	89	HIS
1	I	207	ASN
1	I	311	HIS

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Mol	Chain	Res	Type
1	I	385	GLN
1	I	408	ASN
1	J	44	HIS
1	J	89	HIS
1	J	285	HIS
1	J	311	HIS
1	J	316	HIS
1	J	385	GLN
1	J	394	HIS
1	J	399	ASN
1	K	89	HIS
1	K	102	GLN
1	K	263	HIS
1	K	272	HIS
1	K	309	ASN
1	K	311	HIS
1	K	329	ASN
1	K	389	ASN
1	K	391	GLN
1	K	408	ASN
1	L	89	HIS
1	L	102	GLN
1	L	104	HIS
1	L	129	ASN
1	L	201	ASN
1	L	272	HIS
1	L	294	ASN
1	L	316	HIS
1	L	344	ASN
1	L	389	ASN
1	L	399	ASN
1	M	89	HIS
1	M	160	GLN
1	M	263	HIS
1	M	309	ASN
1	M	311	HIS
1	M	316	HIS
1	M	399	ASN
1	N	89	HIS
1	N	272	HIS
1	N	309	ASN
1	N	366	GLN

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Mol	Chain	Res	Type
1	N	389	ASN
1	O	44	HIS
1	O	160	GLN
1	O	207	ASN
1	O	272	HIS
1	O	311	HIS
1	O	316	HIS
1	O	385	GLN
1	P	66	ASN
1	P	195	GLN
1	P	272	HIS
1	P	309	ASN
1	P	316	HIS
1	P	329	ASN
1	P	389	ASN
1	P	399	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 36 ligands modelled in this entry, 20 are monoatomic - leaving 16 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	E	601	3	33,33,33	3.54	15 (45%)	45,52,52	2.08	10 (22%)
2	ANP	N	601	3	33,33,33	3.56	14 (42%)	45,52,52	2.02	9 (20%)
2	ANP	D	601	3	33,33,33	3.40	14 (42%)	45,52,52	2.00	9 (20%)
2	ANP	A	601	3	33,33,33	3.51	15 (45%)	45,52,52	1.95	9 (20%)
2	ANP	C	601	3	33,33,33	3.51	14 (42%)	45,52,52	1.94	10 (22%)
2	ANP	H	601	3	33,33,33	3.57	13 (39%)	45,52,52	2.00	10 (22%)
2	ANP	B	601	3	33,33,33	3.63	15 (45%)	45,52,52	2.04	12 (26%)
2	ANP	K	601	3	33,33,33	3.52	14 (42%)	45,52,52	1.99	11 (24%)
2	ANP	O	601	3	33,33,33	3.53	15 (45%)	45,52,52	2.02	11 (24%)
2	ANP	I	601	3	33,33,33	3.54	15 (45%)	45,52,52	2.12	11 (24%)
2	ANP	P	601	3	33,33,33	3.56	14 (42%)	45,52,52	2.10	11 (24%)
2	ANP	L	601	3	33,33,33	3.48	13 (39%)	45,52,52	2.02	11 (24%)
2	ANP	F	601	3	33,33,33	3.54	14 (42%)	45,52,52	1.93	10 (22%)
2	ANP	M	601	3	33,33,33	3.57	15 (45%)	45,52,52	2.03	11 (24%)
2	ANP	J	601	3	33,33,33	3.51	13 (39%)	45,52,52	1.90	9 (20%)
2	ANP	G	601	3	33,33,33	3.55	14 (42%)	45,52,52	2.01	11 (24%)

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	E	601	3	-	2/18/38/38	0/3/3/3
2	ANP	N	601	3	-	3/18/38/38	0/3/3/3
2	ANP	D	601	3	-	4/18/38/38	0/3/3/3
2	ANP	A	601	3	-	5/18/38/38	0/3/3/3
2	ANP	C	601	3	-	4/18/38/38	0/3/3/3
2	ANP	H	601	3	-	4/18/38/38	0/3/3/3
2	ANP	B	601	3	-	3/18/38/38	0/3/3/3
2	ANP	K	601	3	-	1/18/38/38	0/3/3/3
2	ANP	O	601	3	-	4/18/38/38	0/3/3/3
2	ANP	I	601	3	-	3/18/38/38	0/3/3/3
2	ANP	P	601	3	-	3/18/38/38	0/3/3/3
2	ANP	L	601	3	-	3/18/38/38	0/3/3/3
2	ANP	F	601	3	-	2/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ANP	M	601	3	-	2/18/38/38	0/3/3/3
2	ANP	J	601	3	-	5/18/38/38	0/3/3/3
2	ANP	G	601	3	-	3/18/38/38	0/3/3/3

All (227) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	ANP	PB-O1B	11.32	1.63	1.46
2	C	601	ANP	PB-O1B	11.31	1.63	1.46
2	M	601	ANP	PB-O1B	11.24	1.63	1.46
2	P	601	ANP	PB-O1B	11.22	1.63	1.46
2	H	601	ANP	PB-O1B	11.19	1.63	1.46
2	L	601	ANP	PB-O1B	11.16	1.63	1.46
2	E	601	ANP	PB-O1B	11.16	1.63	1.46
2	G	601	ANP	PB-O1B	10.87	1.62	1.46
2	J	601	ANP	PB-O1B	10.82	1.62	1.46
2	N	601	ANP	PB-O1B	10.77	1.62	1.46
2	I	601	ANP	PB-O1B	10.71	1.62	1.46
2	K	601	ANP	PB-O1B	10.64	1.62	1.46
2	F	601	ANP	PB-O1B	10.63	1.62	1.46
2	D	601	ANP	PB-O1B	10.56	1.62	1.46
2	O	601	ANP	PB-O1B	10.55	1.62	1.46
2	A	601	ANP	PB-O1B	10.55	1.62	1.46
2	N	601	ANP	PG-O1G	8.09	1.58	1.46
2	A	601	ANP	PG-O1G	7.89	1.58	1.46
2	O	601	ANP	PG-O1G	7.83	1.58	1.46
2	F	601	ANP	PG-O1G	7.74	1.57	1.46
2	B	601	ANP	PG-O1G	7.73	1.57	1.46
2	I	601	ANP	PG-O1G	7.72	1.57	1.46
2	M	601	ANP	PG-O1G	7.68	1.57	1.46
2	H	601	ANP	PG-O1G	7.65	1.57	1.46
2	E	601	ANP	PG-O1G	7.59	1.57	1.46
2	K	601	ANP	PG-O1G	7.57	1.57	1.46
2	G	601	ANP	PG-O1G	7.46	1.57	1.46
2	P	601	ANP	PG-O1G	7.36	1.57	1.46
2	J	601	ANP	PG-O1G	7.27	1.57	1.46
2	C	601	ANP	PG-O1G	7.12	1.57	1.46
2	J	601	ANP	C6-N6	7.04	1.52	1.34
2	L	601	ANP	C6-N6	7.04	1.52	1.34
2	D	601	ANP	PG-O1G	7.00	1.56	1.46
2	A	601	ANP	C6-N6	6.99	1.52	1.34
2	P	601	ANP	C6-N6	6.94	1.51	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	ANP	C6-N6	6.94	1.51	1.34
2	H	601	ANP	C6-N6	6.91	1.51	1.34
2	K	601	ANP	C6-N6	6.90	1.51	1.34
2	I	601	ANP	C6-N6	6.88	1.51	1.34
2	E	601	ANP	C6-N6	6.85	1.51	1.34
2	G	601	ANP	C6-N6	6.84	1.51	1.34
2	F	601	ANP	C6-N6	6.83	1.51	1.34
2	L	601	ANP	PG-O1G	6.83	1.56	1.46
2	M	601	ANP	C6-N6	6.78	1.51	1.34
2	C	601	ANP	C6-N6	6.75	1.51	1.34
2	N	601	ANP	C6-N6	6.75	1.51	1.34
2	O	601	ANP	C6-N6	6.74	1.51	1.34
2	D	601	ANP	C6-N6	6.72	1.51	1.34
2	J	601	ANP	C8-N7	6.27	1.43	1.31
2	G	601	ANP	C8-N7	6.10	1.43	1.31
2	F	601	ANP	C8-N7	6.08	1.43	1.31
2	B	601	ANP	C4-N3	6.07	1.45	1.34
2	E	601	ANP	C8-N7	6.06	1.43	1.31
2	P	601	ANP	C8-N7	6.03	1.43	1.31
2	M	601	ANP	C8-N7	6.00	1.43	1.31
2	B	601	ANP	C8-N7	5.97	1.43	1.31
2	N	601	ANP	C8-N7	5.93	1.43	1.31
2	N	601	ANP	C4-N3	5.90	1.45	1.34
2	H	601	ANP	C8-N7	5.90	1.43	1.31
2	O	601	ANP	C4-N3	5.89	1.45	1.34
2	O	601	ANP	C8-N7	5.89	1.43	1.31
2	K	601	ANP	C8-N7	5.85	1.42	1.31
2	C	601	ANP	C8-N7	5.80	1.42	1.31
2	A	601	ANP	C8-N7	5.78	1.42	1.31
2	I	601	ANP	C8-N7	5.74	1.42	1.31
2	D	601	ANP	C8-N7	5.72	1.42	1.31
2	H	601	ANP	C4-N3	5.71	1.45	1.34
2	L	601	ANP	C4-N3	5.69	1.45	1.34
2	D	601	ANP	C4-N3	5.67	1.45	1.34
2	M	601	ANP	C4-N3	5.64	1.45	1.34
2	L	601	ANP	C8-N7	5.62	1.42	1.31
2	G	601	ANP	C4-N3	5.61	1.44	1.34
2	E	601	ANP	C4-N3	5.57	1.44	1.34
2	I	601	ANP	C4-N3	5.52	1.44	1.34
2	P	601	ANP	C4-N3	5.48	1.44	1.34
2	J	601	ANP	C4-N3	5.39	1.44	1.34
2	K	601	ANP	C4-N3	5.39	1.44	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	601	ANP	C4-N3	5.39	1.44	1.34
2	C	601	ANP	C4-N3	5.36	1.44	1.34
2	A	601	ANP	C4-N3	5.34	1.44	1.34
2	K	601	ANP	PA-O3A	-5.22	1.53	1.59
2	G	601	ANP	PA-O3A	-5.01	1.54	1.59
2	F	601	ANP	PA-O3A	-4.95	1.54	1.59
2	B	601	ANP	PA-O3A	-4.70	1.54	1.59
2	J	601	ANP	PA-O3A	-4.55	1.54	1.59
2	D	601	ANP	C2-N1	4.46	1.41	1.33
2	O	601	ANP	C2-N1	4.42	1.41	1.33
2	I	601	ANP	PA-O3A	-4.39	1.54	1.59
2	L	601	ANP	C2-N1	4.36	1.41	1.33
2	J	601	ANP	C2-N1	4.30	1.41	1.33
2	P	601	ANP	C2-N1	4.29	1.41	1.33
2	N	601	ANP	C2-N1	4.29	1.41	1.33
2	P	601	ANP	PG-N3B	-4.28	1.52	1.63
2	M	601	ANP	PG-N3B	-4.23	1.52	1.63
2	A	601	ANP	PG-N3B	-4.23	1.52	1.63
2	A	601	ANP	PA-O3A	-4.19	1.55	1.59
2	P	601	ANP	PA-O3A	-4.18	1.55	1.59
2	C	601	ANP	PG-N3B	-4.18	1.52	1.63
2	F	601	ANP	C2-N1	4.16	1.41	1.33
2	N	601	ANP	PG-N3B	-4.15	1.52	1.63
2	H	601	ANP	C2-N1	4.15	1.41	1.33
2	O	601	ANP	PA-O3A	-4.11	1.55	1.59
2	G	601	ANP	PG-N3B	-4.10	1.52	1.63
2	C	601	ANP	C2-N1	4.10	1.41	1.33
2	D	601	ANP	PG-N3B	-4.07	1.52	1.63
2	E	601	ANP	C2-N1	4.05	1.41	1.33
2	K	601	ANP	C2-N1	4.04	1.41	1.33
2	G	601	ANP	C2-N1	4.02	1.41	1.33
2	I	601	ANP	PG-N3B	-4.01	1.52	1.63
2	K	601	ANP	PG-N3B	-4.01	1.52	1.63
2	H	601	ANP	PA-O3A	-4.01	1.55	1.59
2	I	601	ANP	C2-N1	4.01	1.41	1.33
2	B	601	ANP	PG-N3B	-4.00	1.52	1.63
2	M	601	ANP	C2-N1	3.98	1.41	1.33
2	A	601	ANP	C2-N1	3.93	1.40	1.33
2	L	601	ANP	PG-N3B	-3.85	1.53	1.63
2	B	601	ANP	C2-N1	3.85	1.40	1.33
2	O	601	ANP	PG-N3B	-3.84	1.53	1.63
2	O	601	ANP	C3'-C4'	-3.84	1.43	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	601	ANP	PA-O3A	-3.83	1.55	1.59
2	B	601	ANP	C3'-C4'	-3.83	1.43	1.53
2	I	601	ANP	C3'-C4'	-3.83	1.43	1.53
2	E	601	ANP	PG-N3B	-3.83	1.53	1.63
2	F	601	ANP	PG-N3B	-3.73	1.53	1.63
2	A	601	ANP	C3'-C4'	-3.73	1.43	1.53
2	L	601	ANP	PA-O3A	-3.73	1.55	1.59
2	N	601	ANP	PA-O3A	-3.72	1.55	1.59
2	M	601	ANP	PA-O3A	-3.70	1.55	1.59
2	F	601	ANP	C3'-C4'	-3.66	1.43	1.53
2	H	601	ANP	PG-N3B	-3.62	1.53	1.63
2	N	601	ANP	C3'-C4'	-3.59	1.43	1.53
2	K	601	ANP	C3'-C4'	-3.58	1.43	1.53
2	H	601	ANP	C3'-C4'	-3.57	1.43	1.53
2	L	601	ANP	C3'-C4'	-3.54	1.44	1.53
2	D	601	ANP	C3'-C4'	-3.50	1.44	1.53
2	M	601	ANP	C2-N3	-3.48	1.27	1.33
2	J	601	ANP	C3'-C4'	-3.46	1.44	1.53
2	J	601	ANP	PG-N3B	-3.44	1.54	1.63
2	P	601	ANP	C3'-C4'	-3.42	1.44	1.53
2	G	601	ANP	C3'-C4'	-3.40	1.44	1.53
2	B	601	ANP	C2-N3	-3.39	1.27	1.33
2	G	601	ANP	C4-N9	3.37	1.44	1.37
2	E	601	ANP	PA-O3A	-3.36	1.55	1.59
2	N	601	ANP	C4-N9	3.35	1.44	1.37
2	E	601	ANP	C3'-C4'	-3.35	1.44	1.53
2	H	601	ANP	C4-N9	3.33	1.44	1.37
2	C	601	ANP	C3'-C4'	-3.33	1.44	1.53
2	M	601	ANP	C3'-C4'	-3.33	1.44	1.53
2	I	601	ANP	C2-N3	-3.31	1.28	1.33
2	I	601	ANP	C4-N9	3.28	1.44	1.37
2	O	601	ANP	C4-N9	3.27	1.44	1.37
2	C	601	ANP	C2-N3	-3.25	1.28	1.33
2	B	601	ANP	C4-N9	3.19	1.44	1.37
2	E	601	ANP	C2-N3	-3.19	1.28	1.33
2	F	601	ANP	C2-N3	-3.18	1.28	1.33
2	H	601	ANP	C2-N3	-3.17	1.28	1.33
2	K	601	ANP	C2-N3	-3.16	1.28	1.33
2	L	601	ANP	C4-N9	3.14	1.44	1.37
2	M	601	ANP	C4-N9	3.14	1.44	1.37
2	P	601	ANP	C4-N9	3.13	1.44	1.37
2	K	601	ANP	C4-N9	3.11	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	ANP	C2-N3	-3.09	1.28	1.33
2	G	601	ANP	C2-N3	-3.09	1.28	1.33
2	J	601	ANP	C2-N3	-3.06	1.28	1.33
2	O	601	ANP	C2-N3	-3.06	1.28	1.33
2	F	601	ANP	C4-N9	3.03	1.44	1.37
2	J	601	ANP	C4-N9	3.03	1.44	1.37
2	E	601	ANP	C4-N9	3.00	1.43	1.37
2	D	601	ANP	C2-N3	-3.00	1.28	1.33
2	A	601	ANP	C4-N9	2.97	1.43	1.37
2	P	601	ANP	C2-N3	-2.91	1.28	1.33
2	C	601	ANP	C2'-C3'	-2.90	1.45	1.53
2	D	601	ANP	C4-N9	2.86	1.43	1.37
2	L	601	ANP	C2-N3	-2.82	1.28	1.33
2	C	601	ANP	C4-N9	2.81	1.43	1.37
2	P	601	ANP	C2'-C3'	-2.79	1.45	1.53
2	N	601	ANP	C2-N3	-2.78	1.29	1.33
2	M	601	ANP	C2'-C1'	-2.77	1.44	1.53
2	F	601	ANP	C2'-C3'	-2.75	1.45	1.53
2	I	601	ANP	C2'-C3'	-2.75	1.45	1.53
2	C	601	ANP	C2'-C1'	-2.74	1.44	1.53
2	K	601	ANP	C2'-C3'	-2.73	1.46	1.53
2	H	601	ANP	C2'-C3'	-2.71	1.46	1.53
2	E	601	ANP	C2'-C3'	-2.71	1.46	1.53
2	J	601	ANP	C2'-C1'	-2.69	1.45	1.53
2	H	601	ANP	C2'-C1'	-2.69	1.45	1.53
2	O	601	ANP	C2'-C3'	-2.66	1.46	1.53
2	D	601	ANP	C2'-C1'	-2.65	1.45	1.53
2	D	601	ANP	PA-O3A	-2.63	1.56	1.59
2	N	601	ANP	C2'-C3'	-2.62	1.46	1.53
2	I	601	ANP	C2'-C1'	-2.61	1.45	1.53
2	A	601	ANP	C2'-C3'	-2.59	1.46	1.53
2	D	601	ANP	C2'-C3'	-2.59	1.46	1.53
2	G	601	ANP	C2'-C1'	-2.57	1.45	1.53
2	O	601	ANP	C2'-C1'	-2.55	1.45	1.53
2	L	601	ANP	C2'-C3'	-2.54	1.46	1.53
2	P	601	ANP	PB-N3B	-2.52	1.56	1.63
2	E	601	ANP	C2'-C1'	-2.51	1.45	1.53
2	M	601	ANP	C2'-C3'	-2.50	1.46	1.53
2	F	601	ANP	C2'-C1'	-2.50	1.45	1.53
2	K	601	ANP	C2'-C1'	-2.50	1.45	1.53
2	G	601	ANP	C2'-C3'	-2.49	1.46	1.53
2	N	601	ANP	C2'-C1'	-2.48	1.45	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	601	ANP	PB-N3B	-2.47	1.56	1.63
2	J	601	ANP	C2'-C3'	-2.44	1.46	1.53
2	B	601	ANP	C2'-C3'	-2.44	1.46	1.53
2	A	601	ANP	C2'-C1'	-2.43	1.45	1.53
2	L	601	ANP	C2'-C1'	-2.42	1.45	1.53
2	A	601	ANP	PB-N3B	-2.40	1.57	1.63
2	B	601	ANP	C2'-C1'	-2.40	1.45	1.53
2	P	601	ANP	C2'-C1'	-2.40	1.45	1.53
2	E	601	ANP	PB-O3A	2.39	1.62	1.59
2	O	601	ANP	PB-N3B	-2.30	1.57	1.63
2	G	601	ANP	PB-N3B	-2.27	1.57	1.63
2	M	601	ANP	PB-N3B	-2.25	1.57	1.63
2	B	601	ANP	PB-N3B	-2.25	1.57	1.63
2	N	601	ANP	PB-N3B	-2.23	1.57	1.63
2	K	601	ANP	PB-N3B	-2.19	1.57	1.63
2	F	601	ANP	PB-N3B	-2.17	1.57	1.63
2	C	601	ANP	PB-N3B	-2.13	1.57	1.63
2	I	601	ANP	C5'-C4'	-2.13	1.45	1.51
2	M	601	ANP	PB-O3A	2.13	1.61	1.59
2	D	601	ANP	PB-N3B	-2.12	1.57	1.63
2	O	601	ANP	C5'-C4'	-2.08	1.45	1.51
2	A	601	ANP	C5'-C4'	-2.05	1.45	1.51
2	E	601	ANP	PB-N3B	-2.01	1.58	1.63
2	B	601	ANP	C5'-C4'	-2.01	1.45	1.51

All (165) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	601	ANP	C5-C4-N3	-6.51	117.75	126.72
2	B	601	ANP	N3-C2-N1	-6.42	118.86	128.58
2	I	601	ANP	C5-C4-N3	-6.40	117.91	126.72
2	L	601	ANP	C5-C4-N3	-6.38	117.93	126.72
2	H	601	ANP	C5-C4-N3	-6.32	118.01	126.72
2	G	601	ANP	C5-C4-N3	-6.25	118.11	126.72
2	E	601	ANP	N3-C2-N1	-6.15	119.27	128.58
2	O	601	ANP	C5-C4-N3	-6.11	118.30	126.72
2	A	601	ANP	C5-C4-N3	-6.08	118.34	126.72
2	F	601	ANP	C5-C4-N3	-6.04	118.40	126.72
2	K	601	ANP	C5-C4-N3	-5.96	118.52	126.72
2	P	601	ANP	C5-C4-N3	-5.95	118.53	126.72
2	E	601	ANP	C5-C4-N3	-5.89	118.61	126.72
2	B	601	ANP	C5-C4-N3	-5.86	118.65	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	601	ANP	C5-C4-N3	-5.78	118.76	126.72
2	M	601	ANP	C5-C4-N3	-5.75	118.81	126.72
2	J	601	ANP	N3-C2-N1	-5.70	119.95	128.58
2	J	601	ANP	C5-C4-N3	-5.68	118.90	126.72
2	H	601	ANP	N3-C2-N1	-5.61	120.09	128.58
2	I	601	ANP	N3-C2-N1	-5.55	120.17	128.58
2	C	601	ANP	N3-C2-N1	-5.54	120.20	128.58
2	M	601	ANP	N3-C2-N1	-5.53	120.21	128.58
2	A	601	ANP	N3-C2-N1	-5.48	120.28	128.58
2	C	601	ANP	C5-C4-N3	-5.47	119.18	126.72
2	N	601	ANP	N3-C2-N1	-5.47	120.30	128.58
2	P	601	ANP	N3-C2-N1	-5.45	120.33	128.58
2	O	601	ANP	N3-C2-N1	-5.38	120.44	128.58
2	D	601	ANP	N3-C2-N1	-5.25	120.64	128.58
2	G	601	ANP	N3-C2-N1	-5.23	120.66	128.58
2	F	601	ANP	N3-C2-N1	-5.21	120.70	128.58
2	L	601	ANP	N3-C2-N1	-5.19	120.72	128.58
2	K	601	ANP	N3-C2-N1	-5.05	120.94	128.58
2	L	601	ANP	N3-C4-N9	5.01	135.68	127.17
2	H	601	ANP	N3-C4-N9	5.00	135.66	127.17
2	N	601	ANP	N3-C4-N9	4.97	135.61	127.17
2	B	601	ANP	N3-C4-N9	4.73	135.21	127.17
2	I	601	ANP	N3-C4-N9	4.72	135.20	127.17
2	A	601	ANP	N3-C4-N9	4.65	135.08	127.17
2	G	601	ANP	N3-C4-N9	4.63	135.05	127.17
2	M	601	ANP	N3-C4-N9	4.61	135.01	127.17
2	P	601	ANP	N3-C4-N9	4.53	134.87	127.17
2	O	601	ANP	N3-C4-N9	4.52	134.85	127.17
2	N	601	ANP	C2-N3-C4	4.49	122.80	111.83
2	I	601	ANP	C2-N3-C4	4.47	122.74	111.83
2	B	601	ANP	C2-N3-C4	4.46	122.73	111.83
2	E	601	ANP	C2-N3-C4	4.46	122.73	111.83
2	K	601	ANP	N3-C4-N9	4.43	134.71	127.17
2	D	601	ANP	O1B-PB-N3B	-4.42	105.26	111.77
2	E	601	ANP	N3-C4-N9	4.41	134.66	127.17
2	F	601	ANP	N3-C4-N9	4.39	134.64	127.17
2	L	601	ANP	C2-N3-C4	4.32	122.39	111.83
2	G	601	ANP	C2-N3-C4	4.31	122.36	111.83
2	O	601	ANP	C2-N3-C4	4.30	122.34	111.83
2	H	601	ANP	C2-N3-C4	4.30	122.33	111.83
2	D	601	ANP	N3-C4-N9	4.28	134.45	127.17
2	P	601	ANP	C2-N3-C4	4.28	122.28	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	601	ANP	C2-N3-C4	4.24	122.18	111.83
2	A	601	ANP	C2-N3-C4	4.23	122.16	111.83
2	M	601	ANP	C2-N3-C4	4.20	122.09	111.83
2	E	601	ANP	N9-C8-N7	-4.19	107.98	113.94
2	F	601	ANP	C2-N3-C4	4.19	122.05	111.83
2	D	601	ANP	C2-N3-C4	4.16	121.98	111.83
2	C	601	ANP	C2-N3-C4	4.14	121.95	111.83
2	P	601	ANP	N9-C8-N7	-4.14	108.07	113.94
2	J	601	ANP	N3-C4-N9	4.06	134.06	127.17
2	K	601	ANP	C2-N3-C4	4.02	121.66	111.83
2	C	601	ANP	N3-C4-N9	3.99	133.95	127.17
2	C	601	ANP	N9-C8-N7	-3.97	108.30	113.94
2	M	601	ANP	N9-C8-N7	-3.84	108.48	113.94
2	I	601	ANP	N9-C8-N7	-3.76	108.61	113.94
2	N	601	ANP	N9-C8-N7	-3.68	108.71	113.94
2	K	601	ANP	N9-C8-N7	-3.66	108.74	113.94
2	G	601	ANP	N9-C8-N7	-3.65	108.75	113.94
2	A	601	ANP	N9-C8-N7	-3.61	108.82	113.94
2	L	601	ANP	N9-C8-N7	-3.59	108.84	113.94
2	F	601	ANP	N9-C8-N7	-3.58	108.85	113.94
2	D	601	ANP	N9-C8-N7	-3.58	108.86	113.94
2	H	601	ANP	N9-C8-N7	-3.42	109.09	113.94
2	J	601	ANP	N9-C8-N7	-3.39	109.12	113.94
2	I	601	ANP	O1B-PB-N3B	-3.38	106.79	111.77
2	E	601	ANP	C5-N7-C8	3.29	108.62	103.45
2	P	601	ANP	C5-N7-C8	3.26	108.57	103.45
2	I	601	ANP	C5-N7-C8	3.23	108.53	103.45
2	C	601	ANP	C5-N7-C8	3.20	108.49	103.45
2	N	601	ANP	C5-N7-C8	3.17	108.43	103.45
2	M	601	ANP	O1B-PB-N3B	-3.11	107.19	111.77
2	B	601	ANP	N9-C8-N7	-3.10	109.54	113.94
2	K	601	ANP	C5-N7-C8	3.09	108.31	103.45
2	G	601	ANP	C5-N7-C8	3.08	108.29	103.45
2	P	601	ANP	O3G-PG-O1G	-3.05	105.81	113.45
2	P	601	ANP	O5'-C5'-C4'	3.04	119.35	108.99
2	D	601	ANP	C5-N7-C8	3.03	108.22	103.45
2	L	601	ANP	C5-N7-C8	3.02	108.20	103.45
2	B	601	ANP	O1B-PB-N3B	-3.00	107.35	111.77
2	J	601	ANP	O3G-PG-O1G	-2.96	106.02	113.45
2	F	601	ANP	C5-N7-C8	2.96	108.10	103.45
2	M	601	ANP	C4-N9-C8	2.96	108.84	105.74
2	H	601	ANP	C5-N7-C8	2.93	108.06	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	601	ANP	C4-N9-C8	2.93	108.81	105.74
2	I	601	ANP	O1G-PG-N3B	-2.91	107.48	111.77
2	K	601	ANP	O5'-C5'-C4'	2.88	118.79	108.99
2	A	601	ANP	C5-N7-C8	2.87	107.97	103.45
2	C	601	ANP	C4-N9-C8	2.87	108.75	105.74
2	O	601	ANP	N9-C8-N7	-2.87	109.87	113.94
2	O	601	ANP	O5'-C5'-C4'	2.86	118.73	108.99
2	M	601	ANP	C5-N7-C8	2.84	107.92	103.45
2	E	601	ANP	C4-N9-C8	2.82	108.70	105.74
2	G	601	ANP	O1G-PG-N3B	-2.78	107.68	111.77
2	J	601	ANP	C5-N7-C8	2.77	107.81	103.45
2	B	601	ANP	O3G-PG-O1G	-2.75	106.54	113.45
2	P	601	ANP	O1B-PB-N3B	-2.71	107.79	111.77
2	C	601	ANP	O3G-PG-O1G	-2.68	106.73	113.45
2	K	601	ANP	C3'-C2'-C1'	2.67	106.51	101.46
2	O	601	ANP	O4'-C1'-N9	2.66	113.19	108.09
2	O	601	ANP	C5-N7-C8	2.61	107.55	103.45
2	C	601	ANP	C4-C5-N7	-2.58	107.63	110.58
2	L	601	ANP	O2G-PG-O1G	-2.54	107.08	113.45
2	B	601	ANP	C3'-C2'-C1'	2.53	106.26	101.46
2	L	601	ANP	C3'-C2'-C1'	2.53	106.24	101.46
2	A	601	ANP	O3G-PG-O1G	-2.52	107.13	113.45
2	G	601	ANP	O5'-C5'-C4'	2.51	117.54	108.99
2	O	601	ANP	O3G-PG-O1G	-2.49	107.20	113.45
2	C	601	ANP	O5'-C5'-C4'	2.49	117.46	108.99
2	F	601	ANP	O3G-PG-O1G	-2.47	107.25	113.45
2	D	601	ANP	C4-N9-C8	2.46	108.32	105.74
2	E	601	ANP	C3'-C2'-C1'	2.45	106.11	101.46
2	H	601	ANP	O3G-PG-O1G	-2.45	107.30	113.45
2	A	601	ANP	C4-N9-C8	2.44	108.30	105.74
2	D	601	ANP	C4-C5-N7	-2.43	107.80	110.58
2	B	601	ANP	C5-N7-C8	2.39	107.21	103.45
2	H	601	ANP	O5'-C5'-C4'	2.38	117.09	108.99
2	N	601	ANP	C4-N9-C8	2.37	108.23	105.74
2	J	601	ANP	O5'-C5'-C4'	2.37	117.06	108.99
2	O	601	ANP	C5'-C4'-C3'	-2.35	106.76	115.21
2	P	601	ANP	C4-C5-N7	-2.34	107.91	110.58
2	E	601	ANP	C4-C5-N7	-2.33	107.92	110.58
2	M	601	ANP	O3G-PG-O1G	-2.33	107.61	113.45
2	I	601	ANP	C4-C5-N7	-2.29	107.97	110.58
2	K	601	ANP	C2'-C1'-N9	-2.28	107.64	113.30
2	B	601	ANP	O5'-C5'-C4'	2.28	116.75	108.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	601	ANP	C4-C5-N7	-2.28	107.98	110.58
2	G	601	ANP	O2B-PB-O3A	2.27	112.22	104.64
2	G	601	ANP	C4-C5-N7	-2.27	107.99	110.58
2	A	601	ANP	O5'-C5'-C4'	2.26	116.70	108.99
2	K	601	ANP	C4-N9-C8	2.26	108.11	105.74
2	G	601	ANP	C4-N9-C8	2.26	108.11	105.74
2	K	601	ANP	C4-C5-N7	-2.26	108.00	110.58
2	L	601	ANP	O5'-C5'-C4'	2.25	116.66	108.99
2	L	601	ANP	C4-N9-C8	2.22	108.07	105.74
2	F	601	ANP	C4-C5-N7	-2.22	108.05	110.58
2	N	601	ANP	O5'-C5'-C4'	2.21	116.53	108.99
2	H	601	ANP	C4-N9-C8	2.19	108.04	105.74
2	B	601	ANP	C4-N9-C8	2.18	108.03	105.74
2	F	601	ANP	C4-N9-C8	2.17	108.02	105.74
2	M	601	ANP	O2B-PB-O3A	2.17	111.88	104.64
2	F	601	ANP	O2B-PB-O3A	2.16	111.84	104.64
2	B	601	ANP	C2-N1-C6	2.11	122.20	118.73
2	I	601	ANP	C4-N9-C8	2.11	107.95	105.74
2	L	601	ANP	O3G-PG-O1G	-2.11	108.16	113.45
2	J	601	ANP	C4-C5-N7	-2.09	108.19	110.58
2	M	601	ANP	O5'-C5'-C4'	2.08	116.08	108.99
2	H	601	ANP	C3'-C2'-C1'	2.04	105.32	101.46
2	I	601	ANP	O4'-C1'-N9	2.04	112.00	108.09
2	O	601	ANP	C3'-C2'-C1'	2.03	105.30	101.46
2	E	601	ANP	C2'-C1'-N9	-2.02	108.30	113.30

There are no chirality outliers.

All (51) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
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	B	601	ANP	PG-N3B-PB-O1B
2	B	601	ANP	PA-O3A-PB-O1B
2	C	601	ANP	PB-N3B-PG-O1G
2	C	601	ANP	PG-N3B-PB-O1B
2	C	601	ANP	PA-O3A-PB-O1B
2	D	601	ANP	PA-O3A-PB-O2B
2	D	601	ANP	C5'-O5'-PA-O1A
2	E	601	ANP	PG-N3B-PB-O1B
2	E	601	ANP	PB-O3A-PA-O5'

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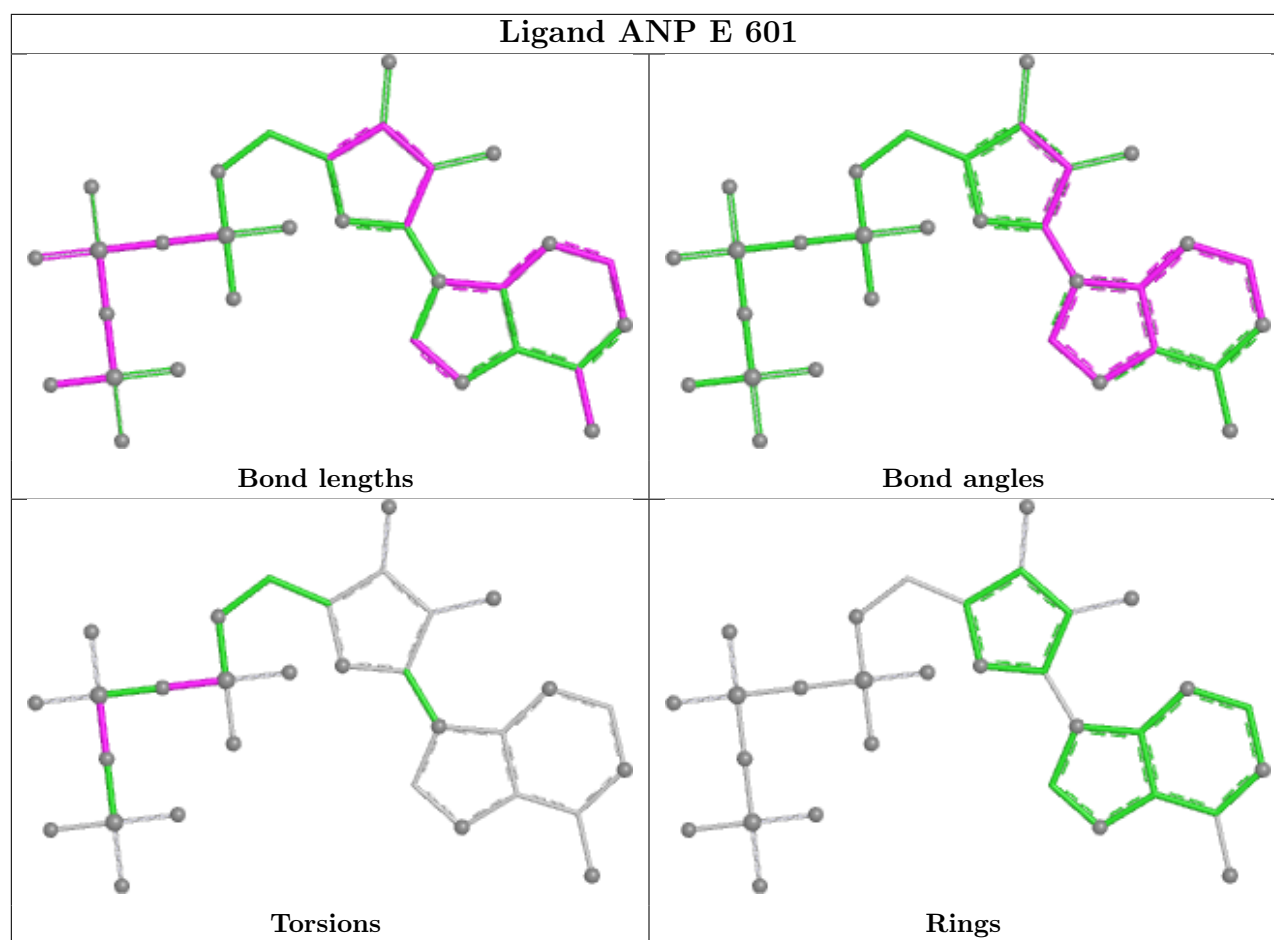
Mol	Chain	Res	Type	Atoms
2	F	601	ANP	PB-N3B-PG-O1G
2	G	601	ANP	PB-N3B-PG-O1G
2	G	601	ANP	PA-O3A-PB-O2B
2	H	601	ANP	PB-N3B-PG-O1G
2	H	601	ANP	PG-N3B-PB-O1B
2	H	601	ANP	PA-O3A-PB-O2B
2	I	601	ANP	PG-N3B-PB-O1B
2	J	601	ANP	PB-N3B-PG-O1G
2	J	601	ANP	PG-N3B-PB-O1B
2	J	601	ANP	PA-O3A-PB-O2B
2	J	601	ANP	C5'-O5'-PA-O1A
2	K	601	ANP	PB-O3A-PA-O5'
2	L	601	ANP	PB-N3B-PG-O1G
2	L	601	ANP	PG-N3B-PB-O1B
2	M	601	ANP	PB-N3B-PG-O1G
2	M	601	ANP	PB-O3A-PA-O5'
2	N	601	ANP	PG-N3B-PB-O1B
2	O	601	ANP	PB-N3B-PG-O1G
2	O	601	ANP	PG-N3B-PB-O1B
2	P	601	ANP	PG-N3B-PB-O1B
2	P	601	ANP	PA-O3A-PB-O2B
2	O	601	ANP	C3'-C4'-C5'-O5'
2	O	601	ANP	O4'-C4'-C5'-O5'
2	C	601	ANP	PB-O3A-PA-O5'
2	L	601	ANP	PB-O3A-PA-O5'
2	N	601	ANP	PB-O3A-PA-O5'
2	A	601	ANP	C5'-O5'-PA-O1A
2	G	601	ANP	C5'-O5'-PA-O1A
2	B	601	ANP	PA-O3A-PB-O2B
2	F	601	ANP	PA-O3A-PB-O2B
2	A	601	ANP	PA-O3A-PB-O1B
2	D	601	ANP	PA-O3A-PB-O1B
2	H	601	ANP	PA-O3A-PB-O1B
2	I	601	ANP	PA-O3A-PB-O1B
2	J	601	ANP	PA-O3A-PB-O1B
2	N	601	ANP	PA-O3A-PB-O1B
2	P	601	ANP	PA-O3A-PB-O1B
2	D	601	ANP	PB-N3B-PG-O1G
2	I	601	ANP	PB-N3B-PG-O1G

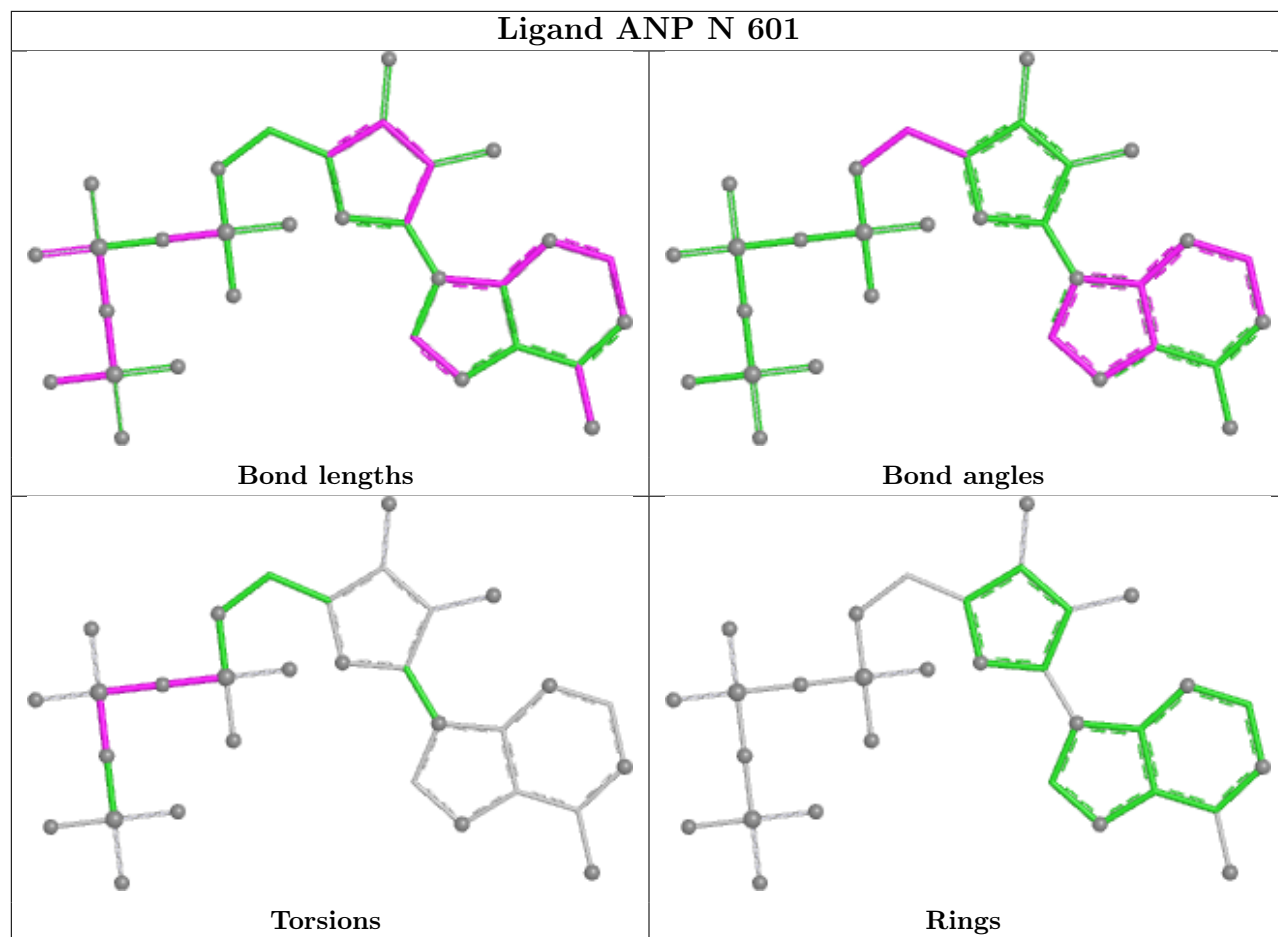
There are no ring outliers.

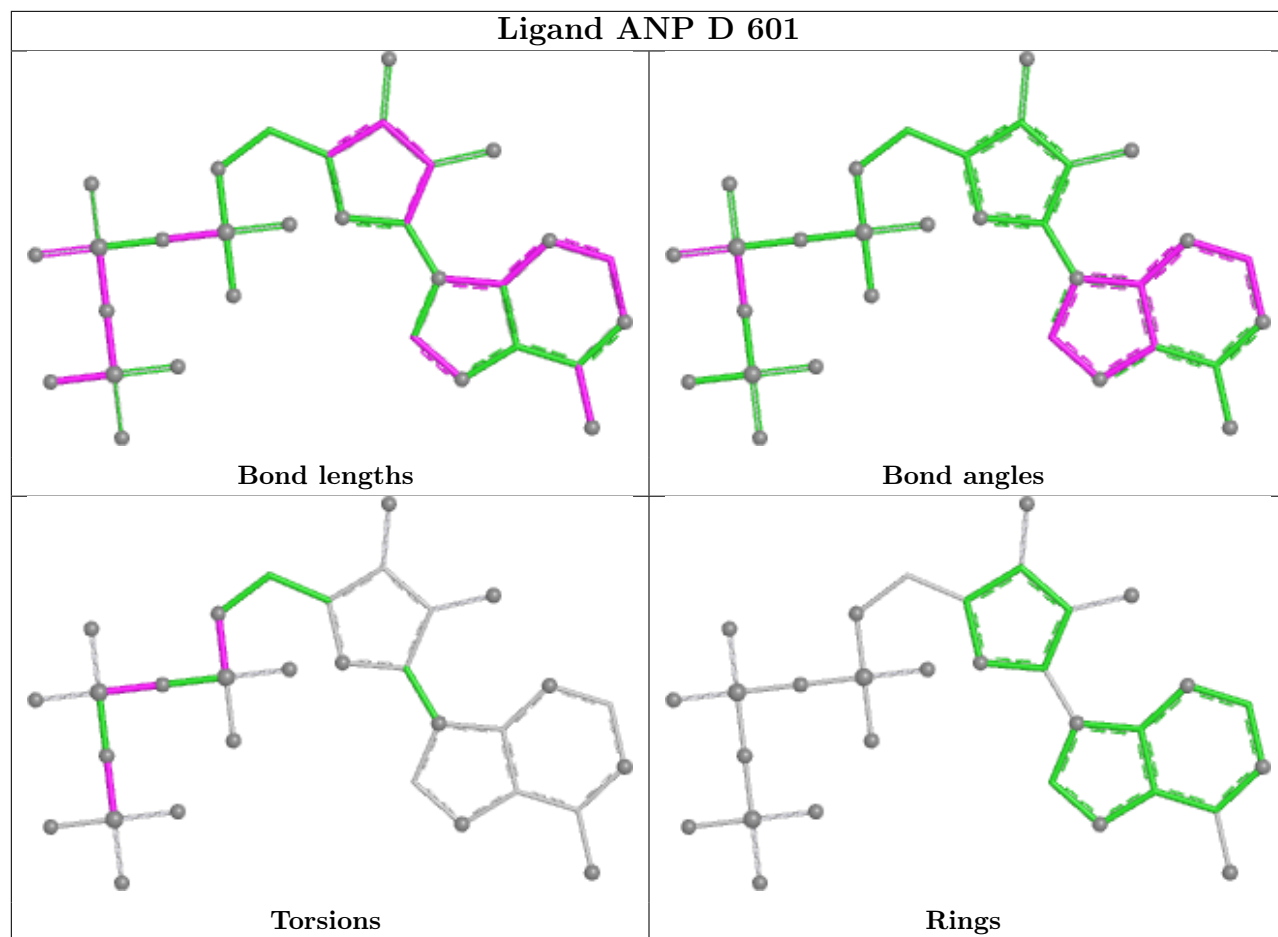
9 monomers are involved in 11 short contacts:

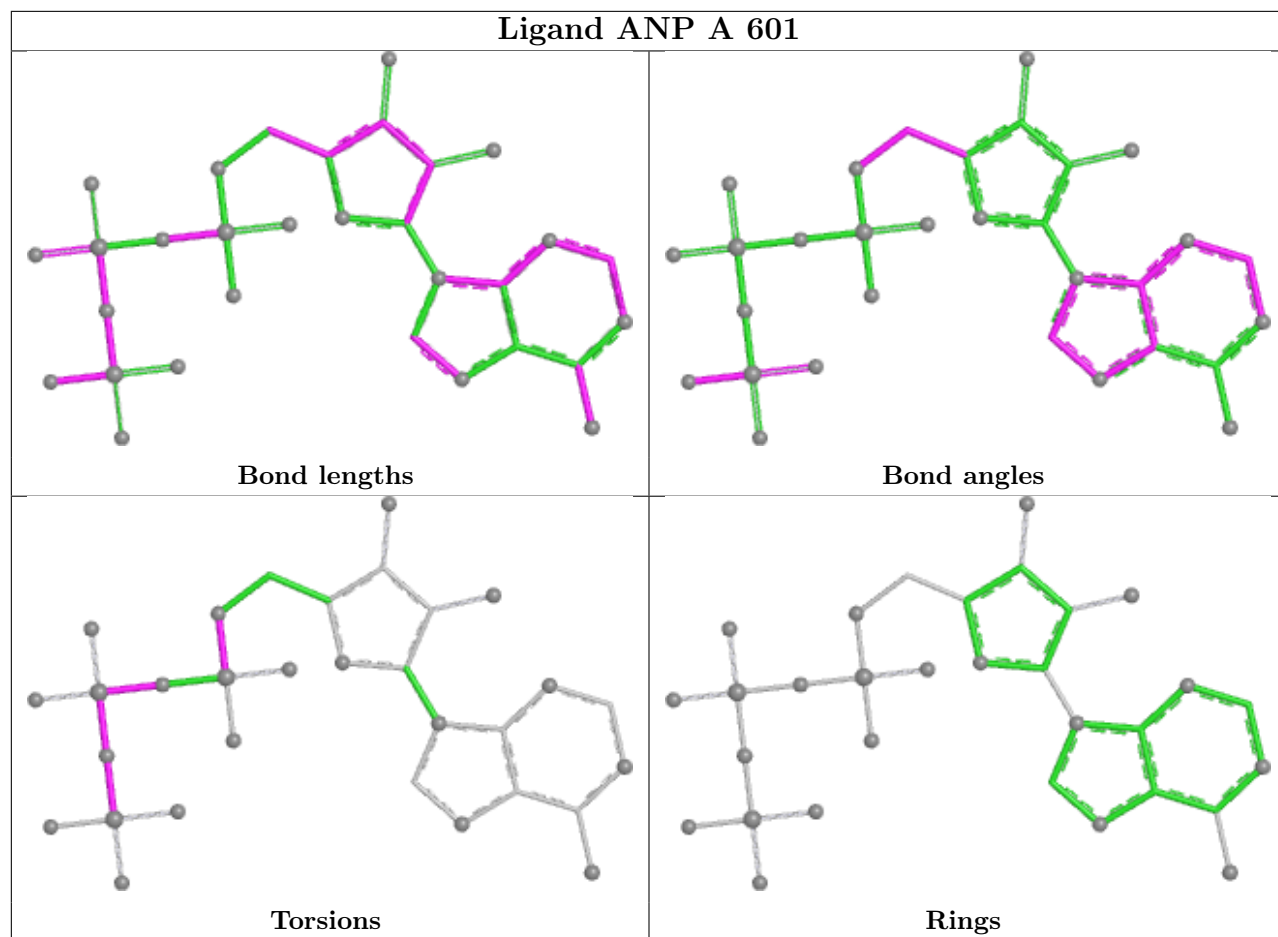
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	601	ANP	1	0
2	A	601	ANP	1	0
2	K	601	ANP	1	0
2	O	601	ANP	2	0
2	I	601	ANP	2	0
2	L	601	ANP	1	0
2	F	601	ANP	1	0
2	J	601	ANP	1	0
2	G	601	ANP	1	0

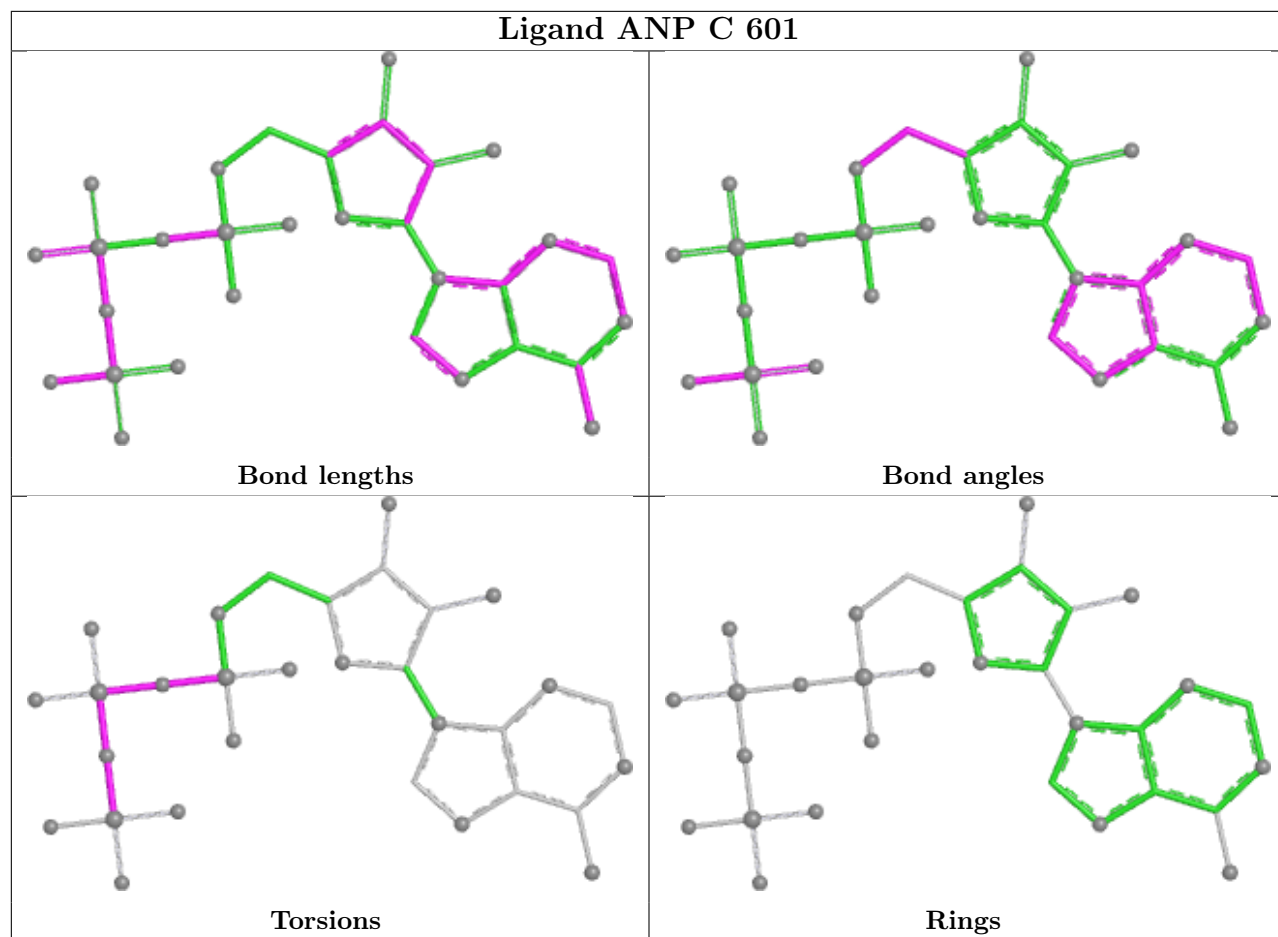
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

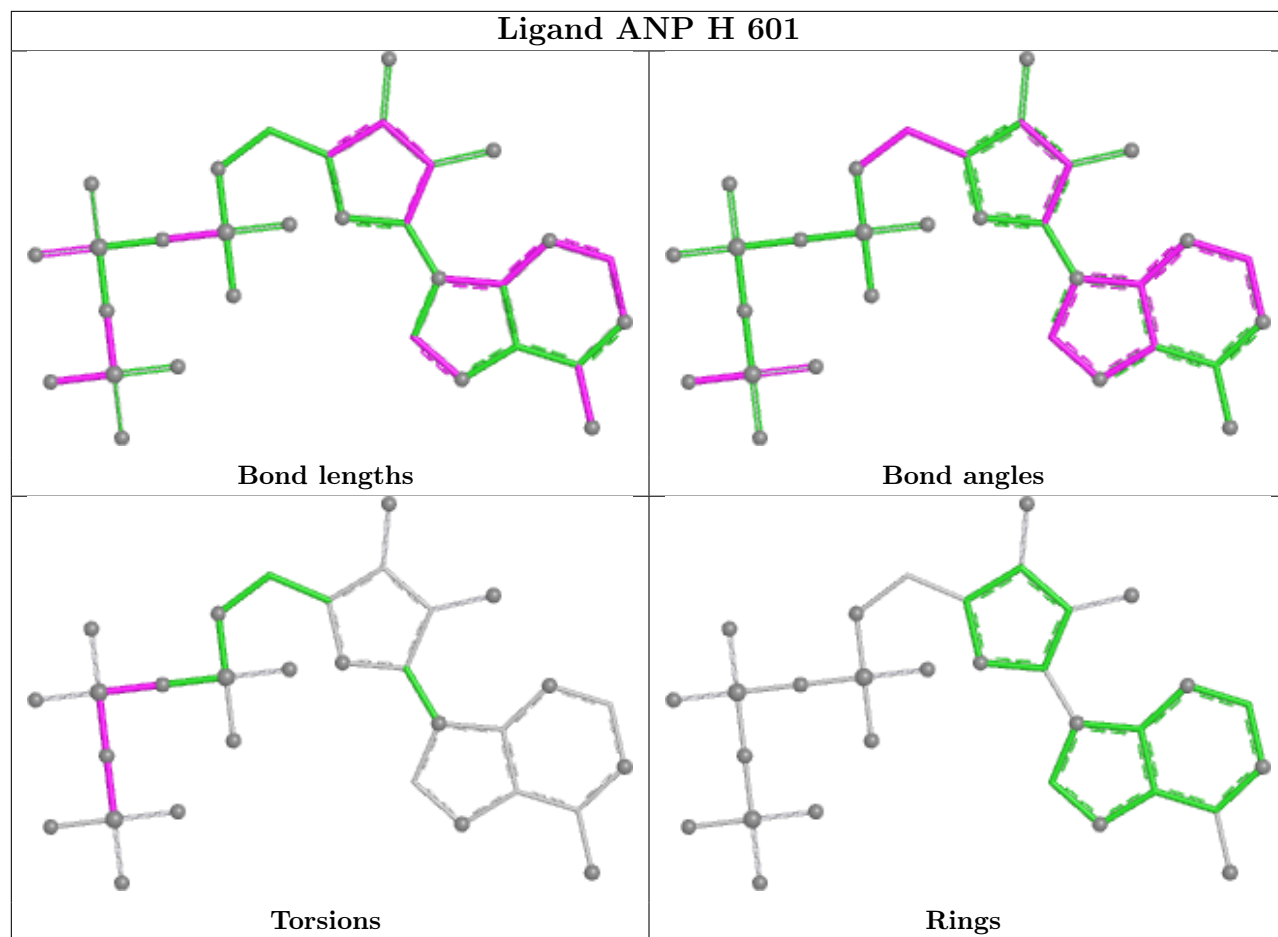


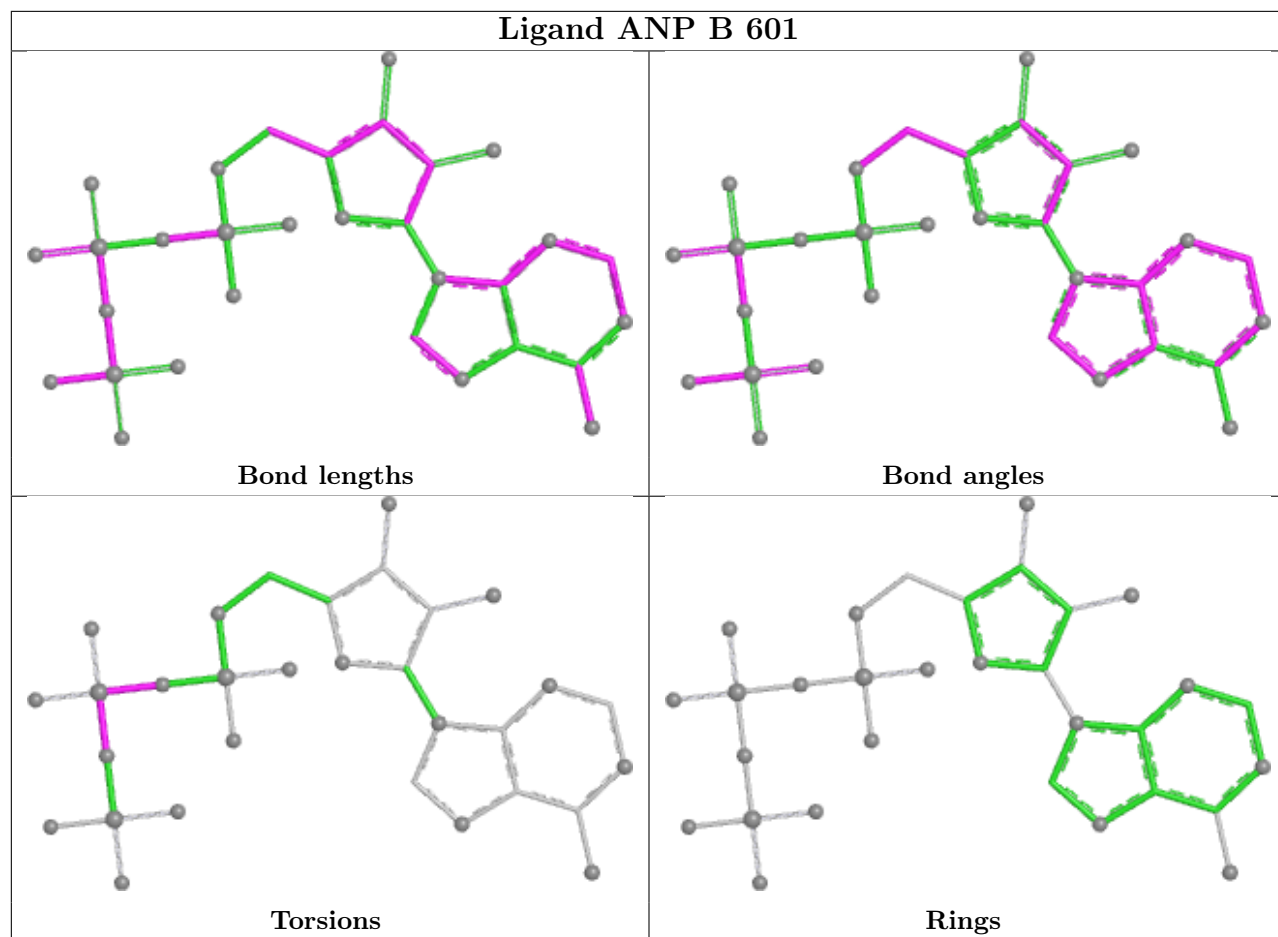


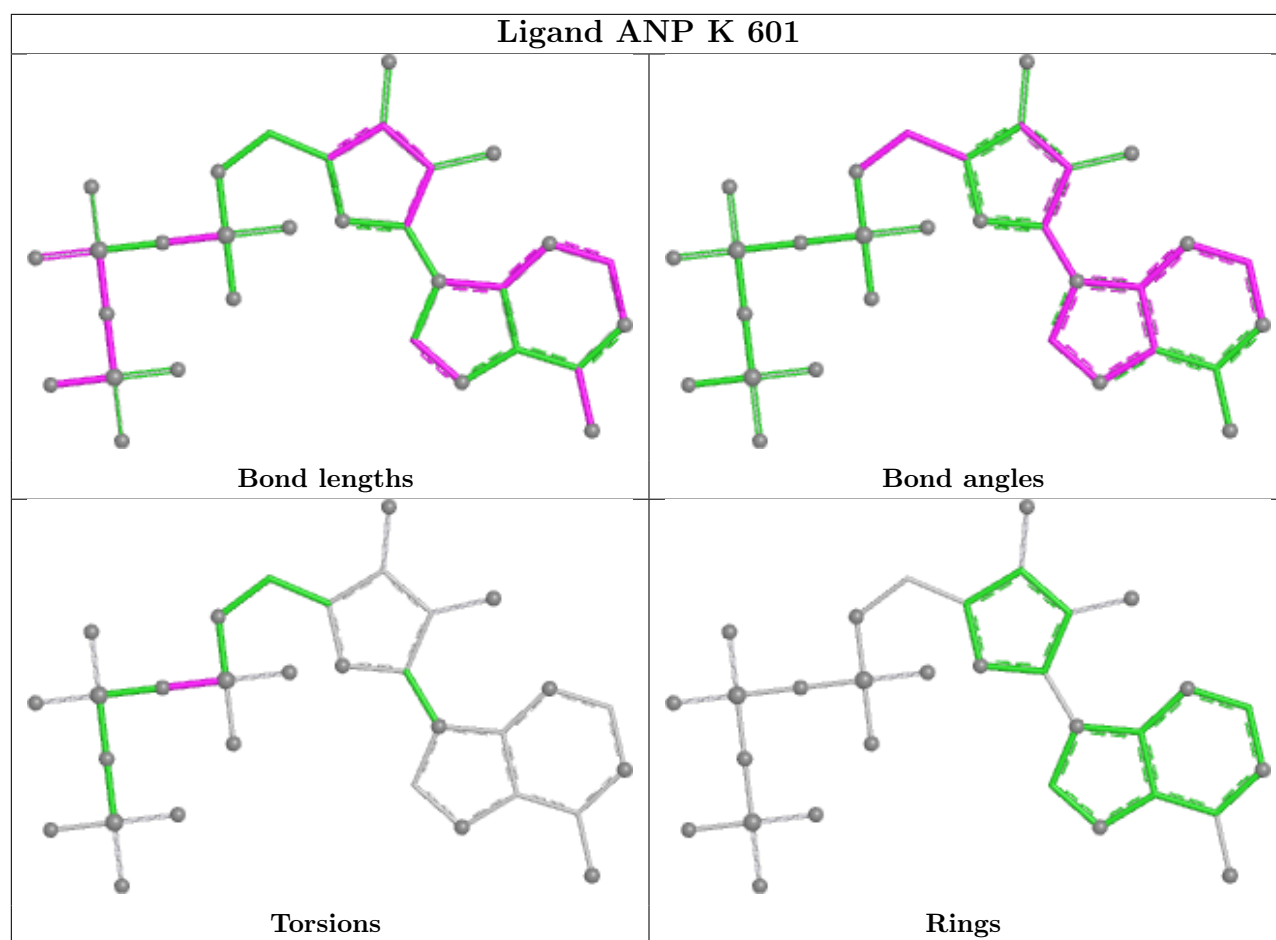


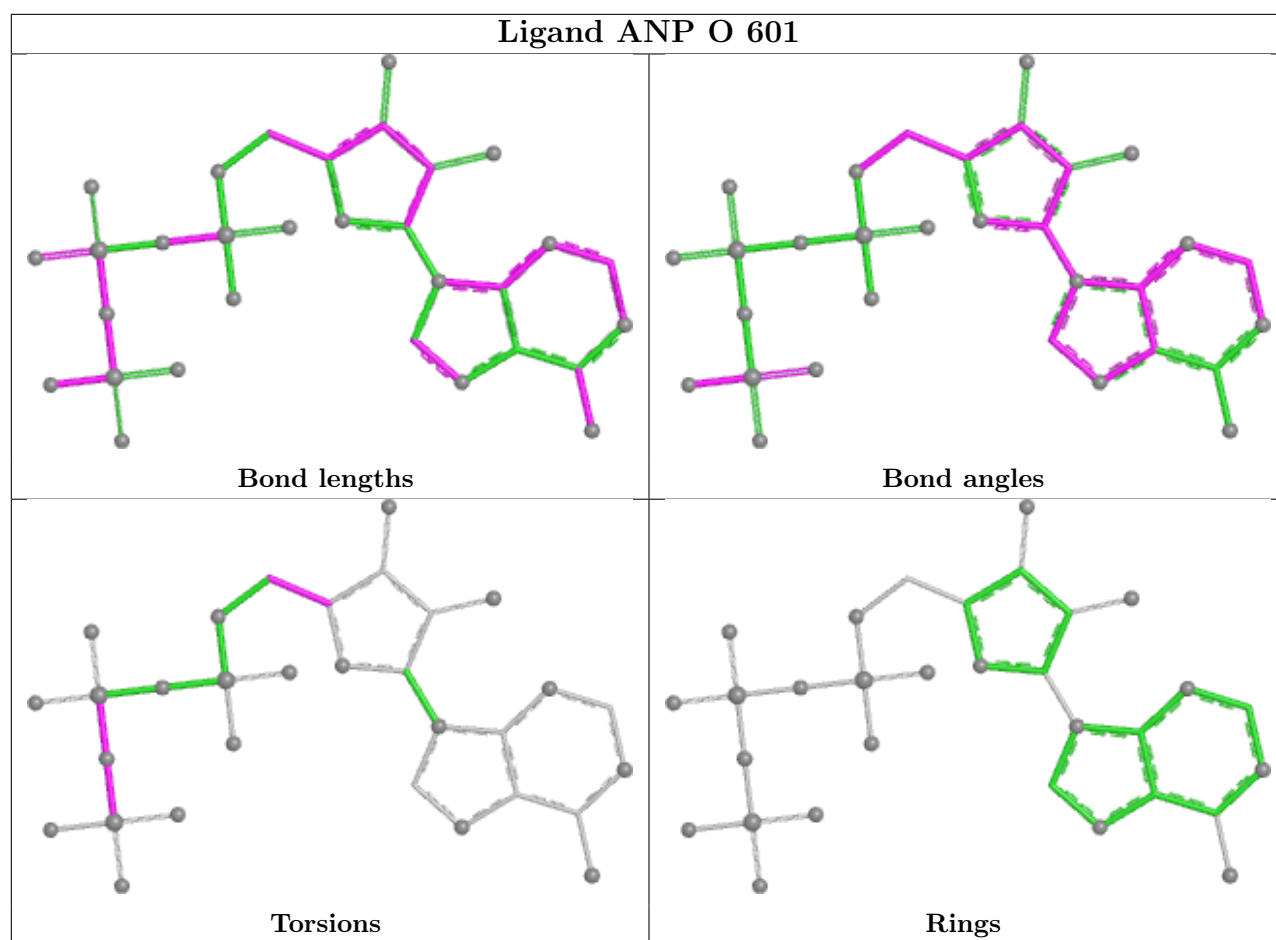


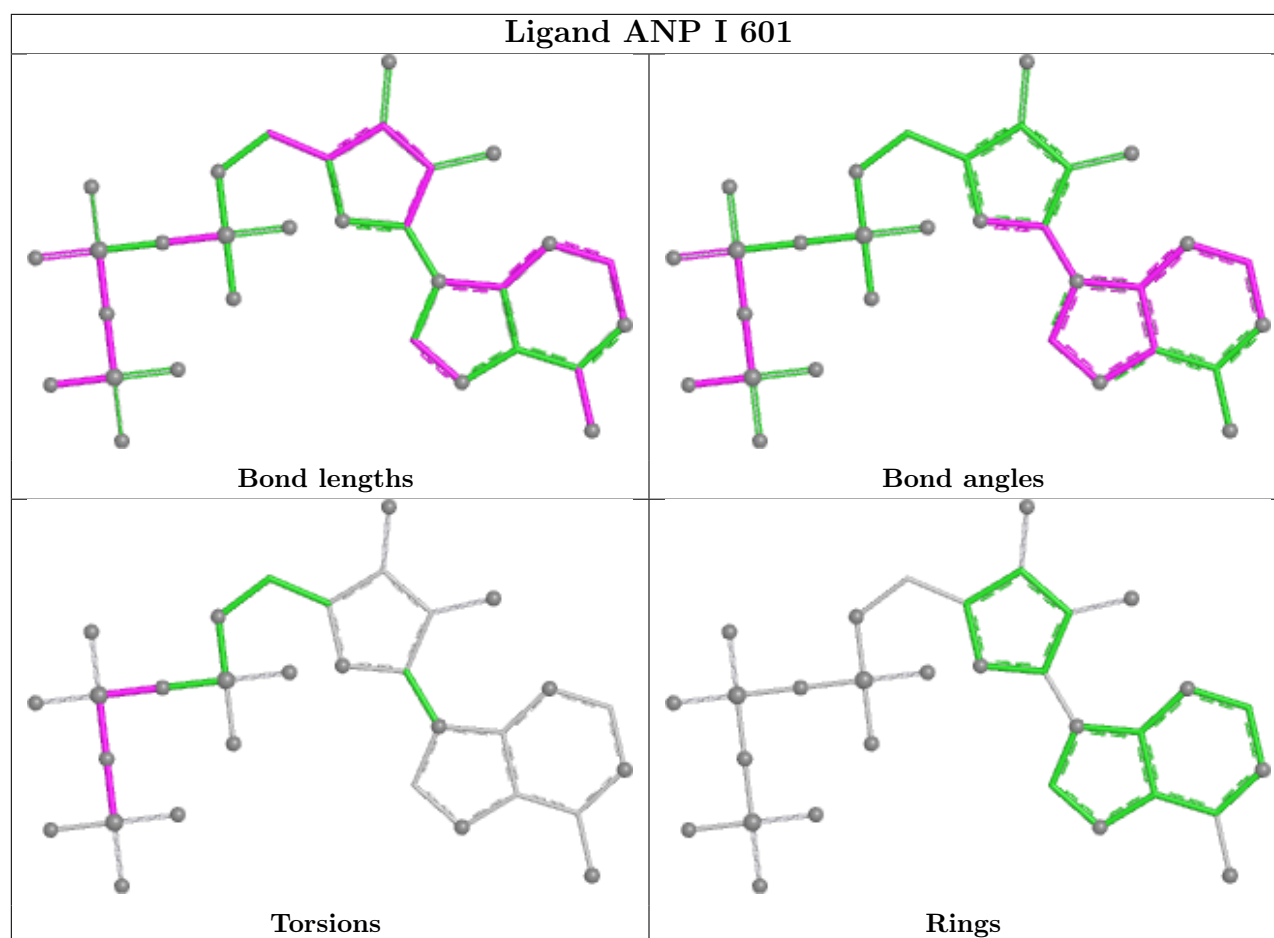


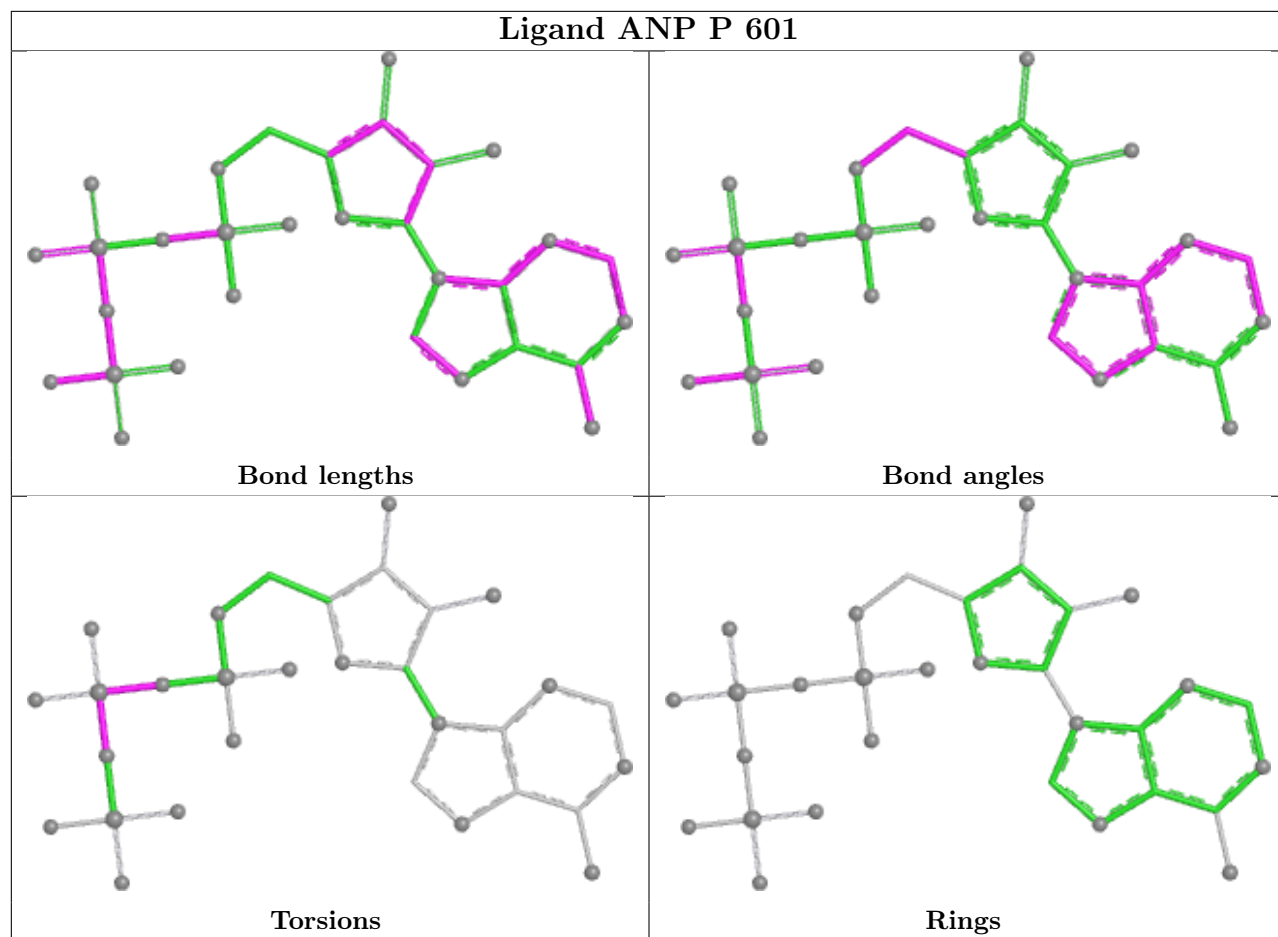


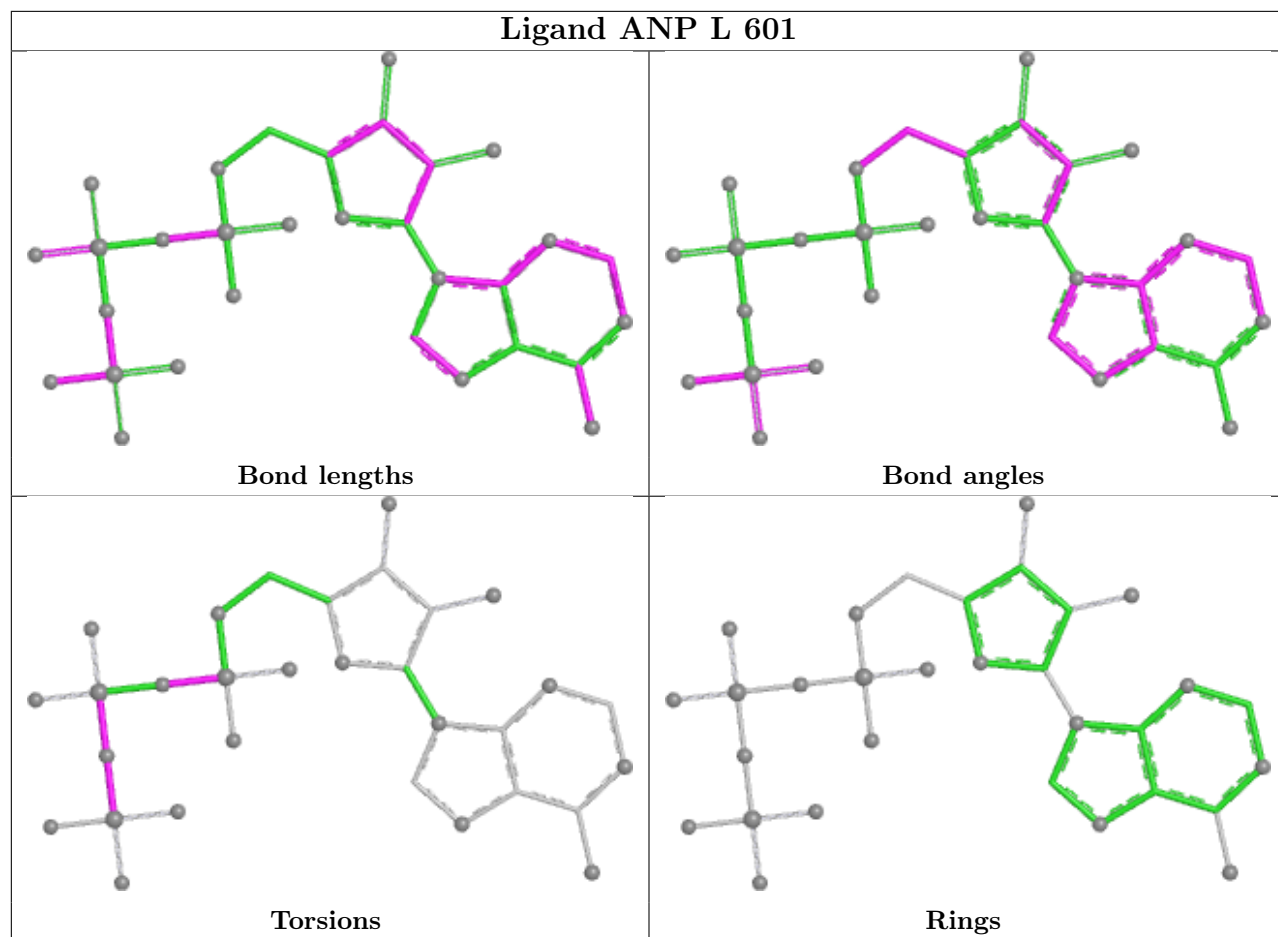


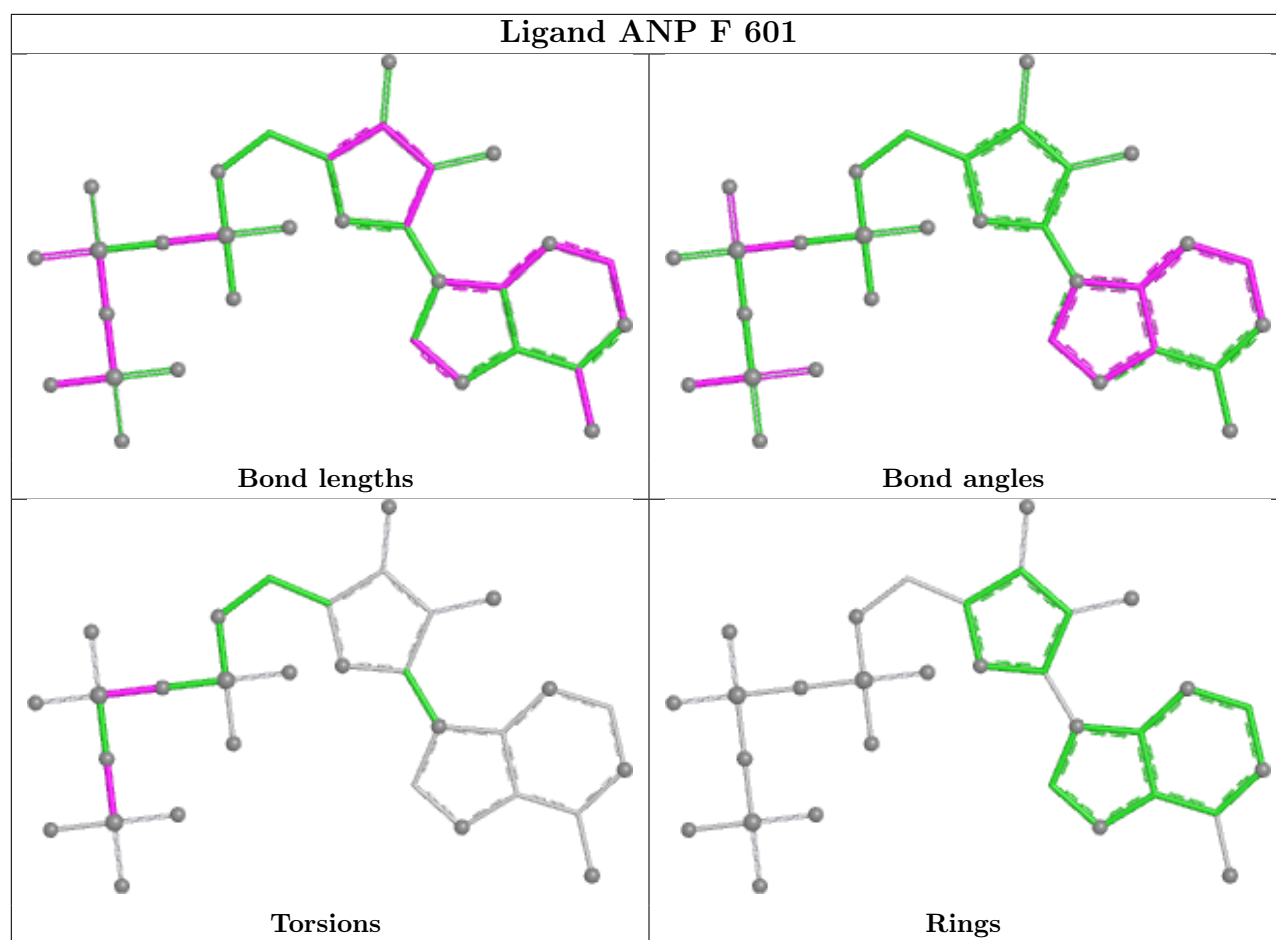


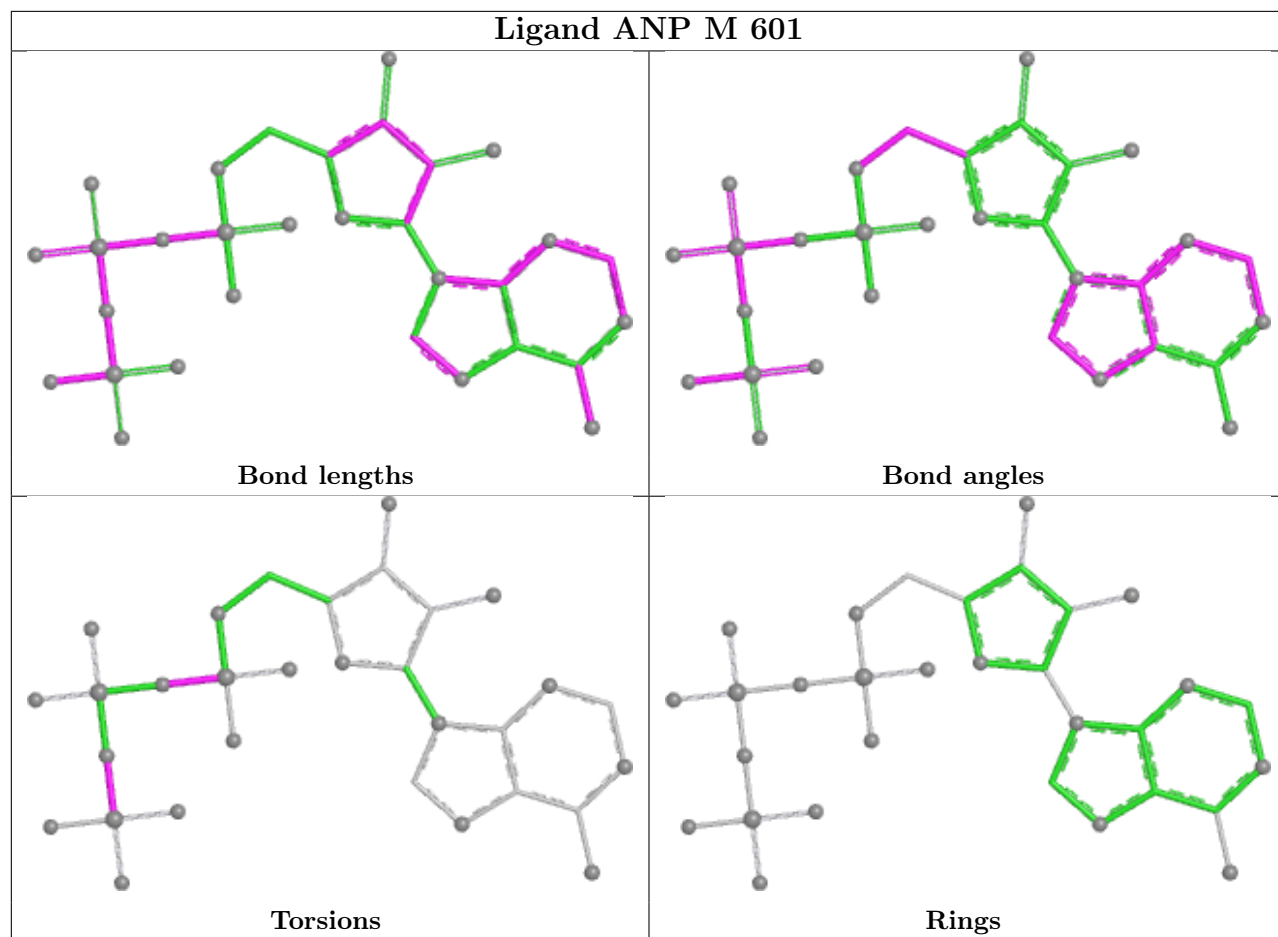




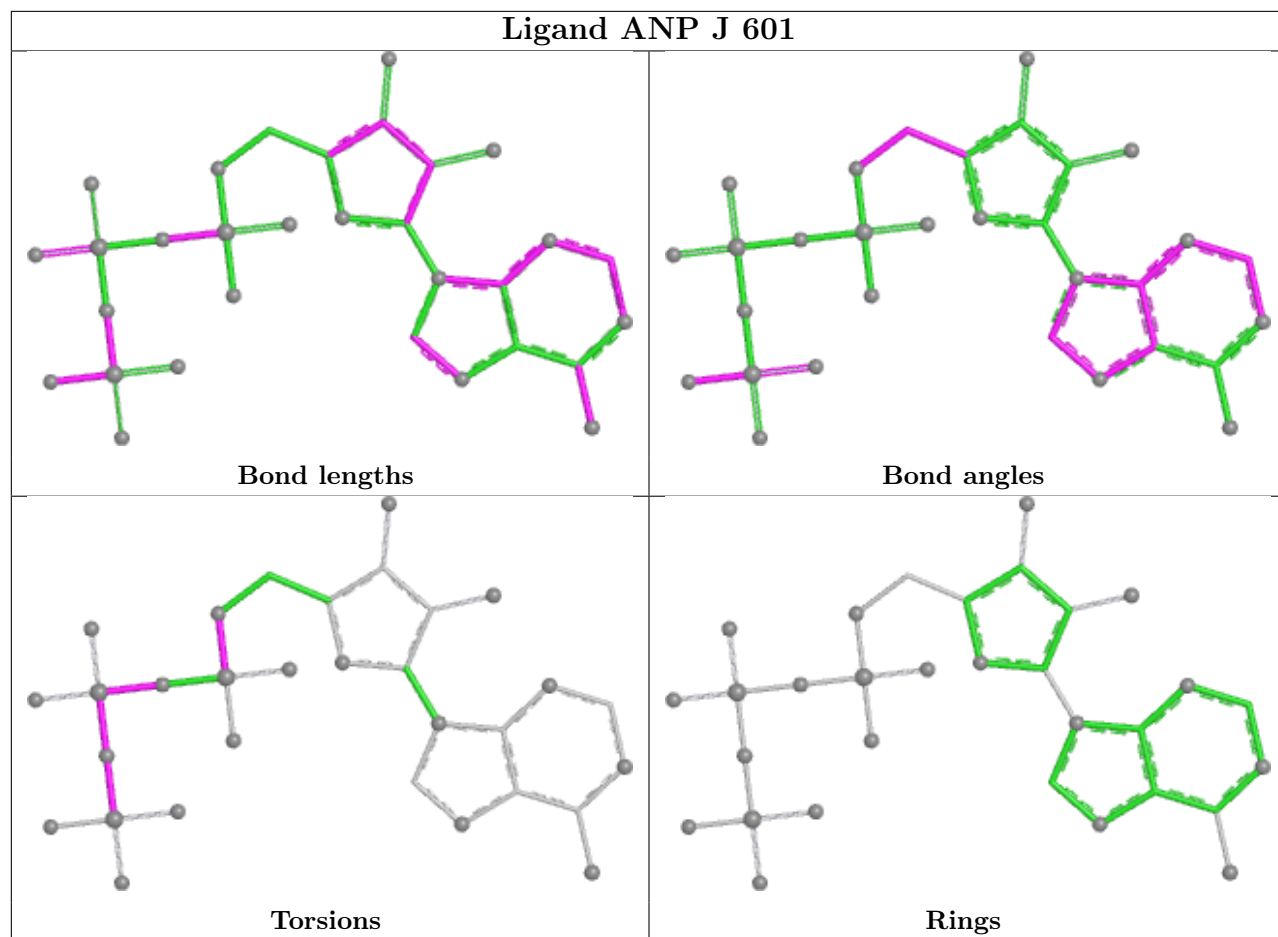


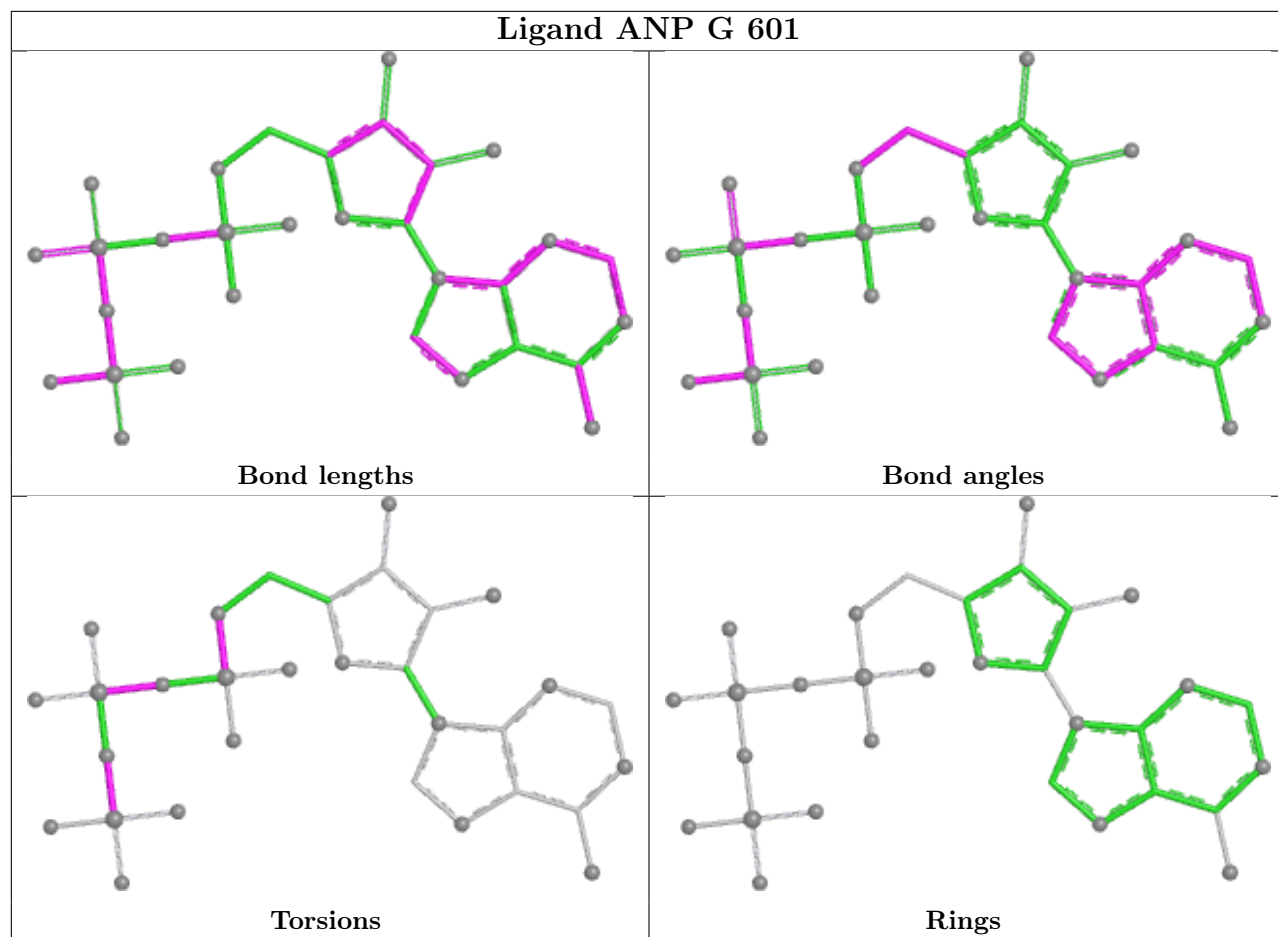






Ligand ANP J 601





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	380/432 (87%)	-0.46	2 (0%) 87 83	53, 85, 146, 167	0
1	B	382/432 (88%)	-0.46	0 100 100	49, 93, 147, 176	0
1	C	387/432 (89%)	-0.61	0 100 100	50, 72, 122, 151	0
1	D	392/432 (90%)	-0.53	1 (0%) 90 87	51, 79, 132, 170	0
1	E	386/432 (89%)	-0.58	0 100 100	50, 78, 132, 161	0
1	F	383/432 (88%)	-0.46	1 (0%) 90 87	65, 96, 138, 156	0
1	G	381/432 (88%)	-0.48	0 100 100	67, 93, 122, 156	0
1	H	379/432 (87%)	-0.43	0 100 100	64, 91, 122, 137	0
1	I	375/432 (86%)	-0.39	1 (0%) 90 87	66, 101, 176, 192	0
1	J	384/432 (88%)	-0.50	1 (0%) 90 87	56, 83, 144, 172	0
1	K	376/432 (87%)	-0.29	2 (0%) 87 83	71, 104, 176, 190	0
1	L	382/432 (88%)	-0.11	5 (1%) 75 67	74, 112, 180, 195	0
1	M	383/432 (88%)	-0.35	1 (0%) 90 87	78, 108, 145, 166	0
1	N	373/432 (86%)	-0.27	4 (1%) 78 71	74, 109, 152, 173	0
1	O	379/432 (87%)	-0.38	1 (0%) 90 87	78, 100, 131, 161	0
1	P	376/432 (87%)	-0.30	2 (0%) 87 83	76, 108, 139, 151	0
All	All	6098/6912 (88%)	-0.41	21 (0%) 90 87	49, 96, 149, 195	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	75	VAL	3.6
1	K	406	VAL	3.0
1	N	107	GLY	3.0
1	F	213	VAL	2.9
1	A	342	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	J	338	LEU	2.6
1	L	410	ALA	2.4
1	N	118	GLY	2.4
1	I	421	ARG	2.4
1	N	80	ASP	2.2
1	P	118	GLY	2.2
1	A	423	ALA	2.2
1	M	343	PRO	2.2
1	K	337	LEU	2.2
1	D	329	ASN	2.1
1	P	75	VAL	2.1
1	L	350	ILE	2.1
1	L	392	LEU	2.0
1	O	367	PHE	2.0
1	N	213	VAL	2.0
1	L	213	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	MG	C	1001	1/1	0.81	0.23	85,85,85,85	0
3	MG	B	1001	1/1	0.83	0.06	83,83,83,83	0
3	MG	G	1001	1/1	0.92	0.04	76,76,76,76	0
3	MG	B	602	1/1	0.93	0.06	57,57,57,57	0
2	ANP	O	601	31/31	0.93	0.08	98,102,105,106	0
3	MG	D	1001	1/1	0.95	0.06	78,78,78,78	0
2	ANP	K	601	31/31	0.95	0.07	90,96,104,106	0

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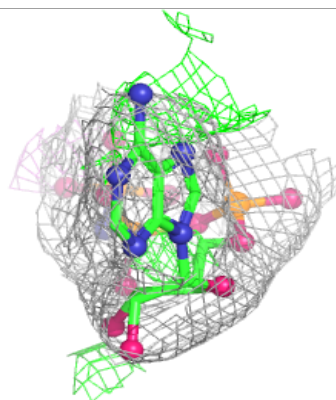
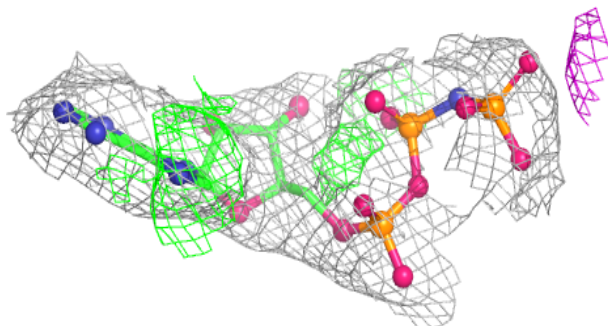
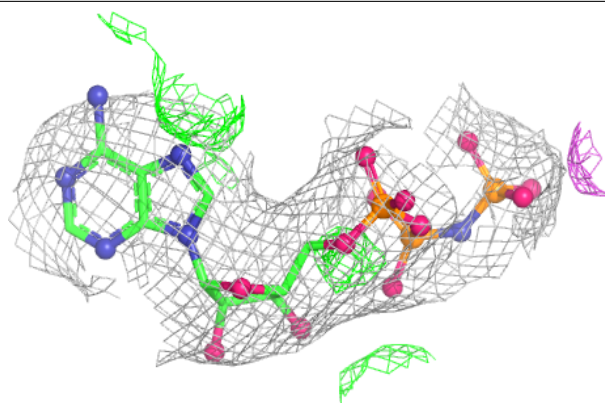
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	MG	I	602	1/1	0.95	0.18	82,82,82,82	0
3	MG	J	602	1/1	0.95	0.12	60,60,60,60	0
3	MG	O	602	1/1	0.95	0.09	76,76,76,76	0
2	ANP	P	601	31/31	0.96	0.07	94,98,108,111	0
2	ANP	F	601	31/31	0.96	0.07	72,90,100,102	0
3	MG	L	602	1/1	0.96	0.05	74,74,74,74	0
2	ANP	H	601	31/31	0.96	0.06	69,77,80,83	0
2	ANP	D	601	31/31	0.97	0.06	58,64,68,74	0
2	ANP	I	601	31/31	0.97	0.07	70,75,80,83	0
2	ANP	J	601	31/31	0.97	0.06	49,63,68,69	0
2	ANP	E	601	31/31	0.97	0.06	62,69,73,76	0
2	ANP	L	601	31/31	0.97	0.06	74,92,98,99	0
2	ANP	M	601	31/31	0.97	0.05	76,87,92,93	0
2	ANP	N	601	31/31	0.97	0.06	81,89,95,97	0
2	ANP	B	601	31/31	0.97	0.06	56,81,90,93	0
2	ANP	G	601	31/31	0.97	0.05	63,78,82,83	0
3	MG	P	602	1/1	0.97	0.05	97,97,97,97	0
2	ANP	C	601	31/31	0.98	0.05	43,56,63,65	0
3	MG	K	602	1/1	0.98	0.04	54,54,54,54	0
2	ANP	A	601	31/31	0.98	0.06	56,65,76,81	0
3	MG	H	602	1/1	0.98	0.09	58,58,58,58	0
3	MG	A	602	1/1	0.98	0.09	50,50,50,50	0
3	MG	F	602	1/1	0.99	0.07	53,53,53,53	0
3	MG	G	602	1/1	0.99	0.04	63,63,63,63	0
3	MG	D	602	1/1	0.99	0.04	58,58,58,58	0
3	MG	N	602	1/1	0.99	0.05	75,75,75,75	0
3	MG	C	602	1/1	0.99	0.07	51,51,51,51	0
3	MG	E	602	1/1	0.99	0.03	56,56,56,56	0
3	MG	M	602	1/1	1.00	0.04	51,51,51,51	0

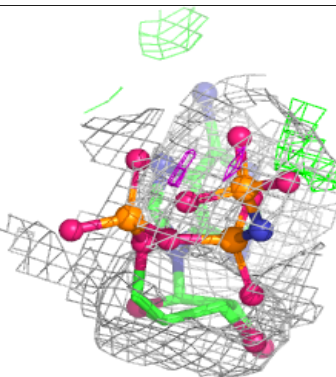
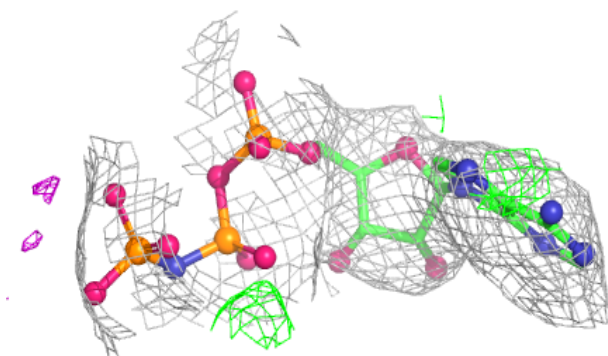
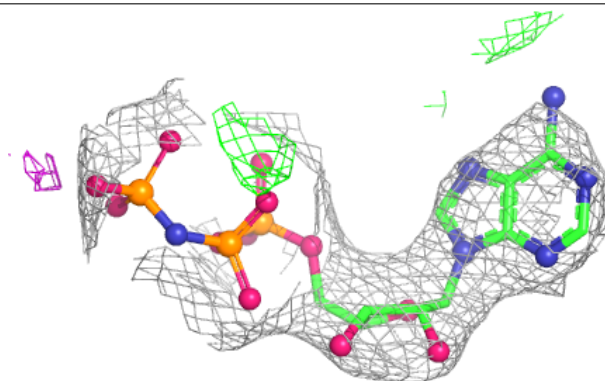
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ANP O 601:

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

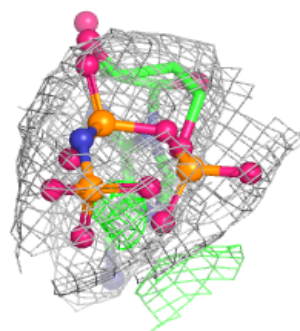
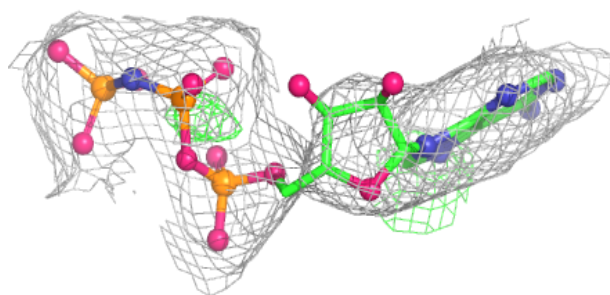
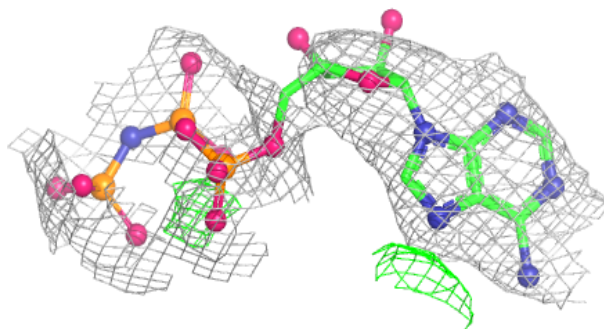
**Electron density around ANP K 601:**

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

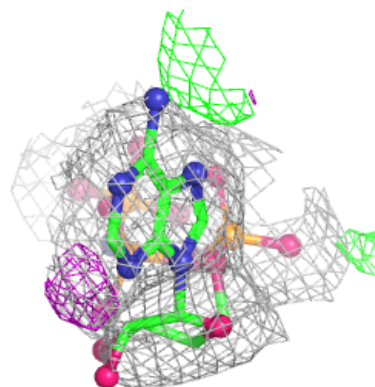
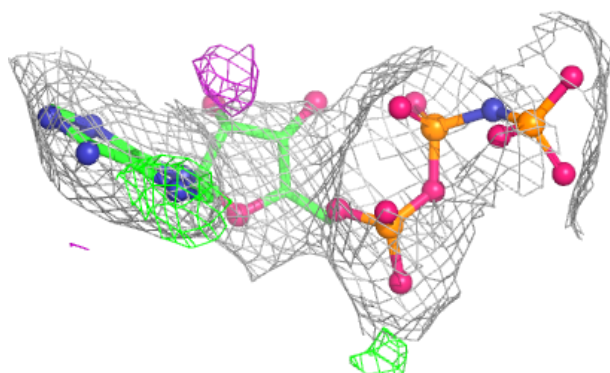
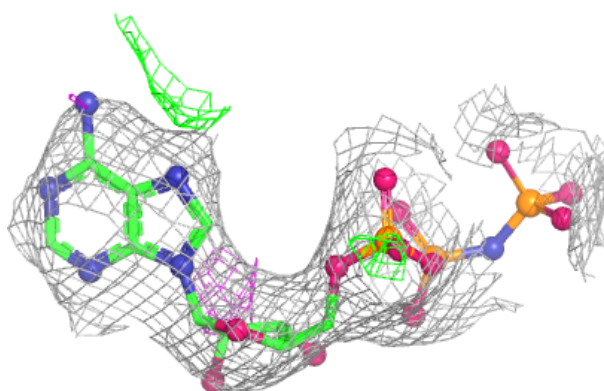


Electron density around ANP P 601:

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

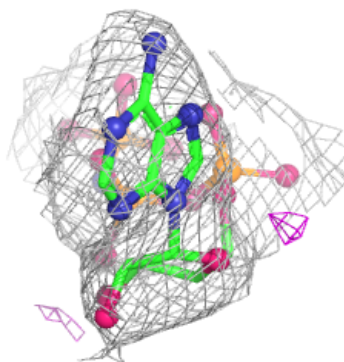
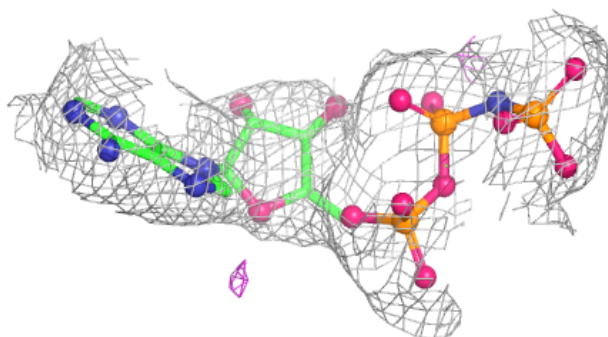
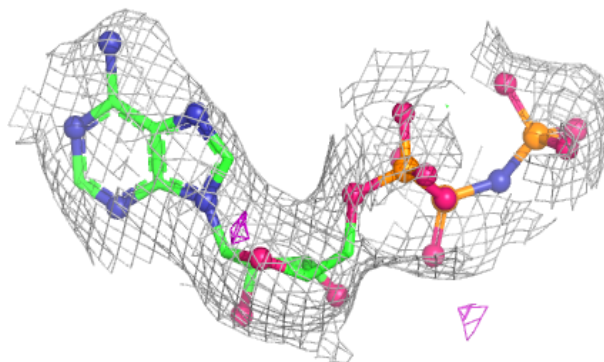
**Electron density around ANP F 601:**

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and green (positive)

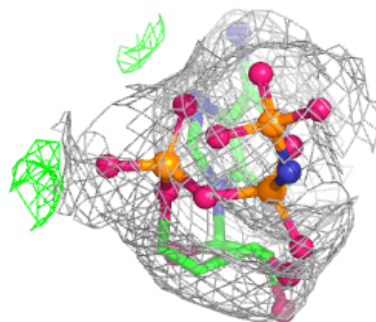
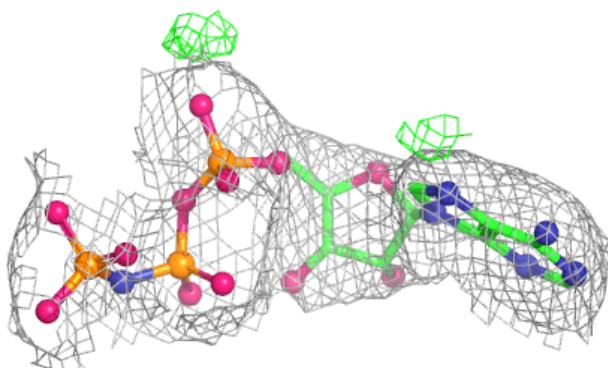
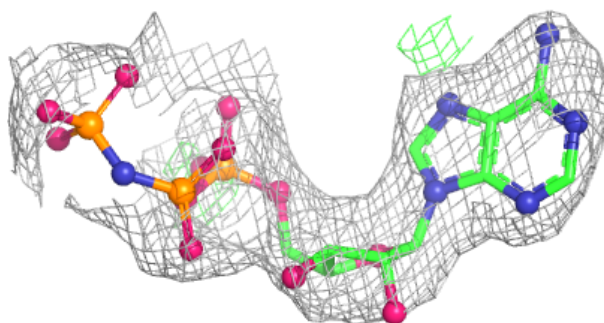


Electron density around ANP H 601:

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

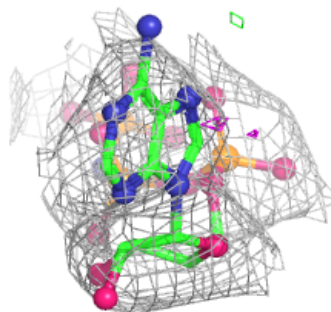
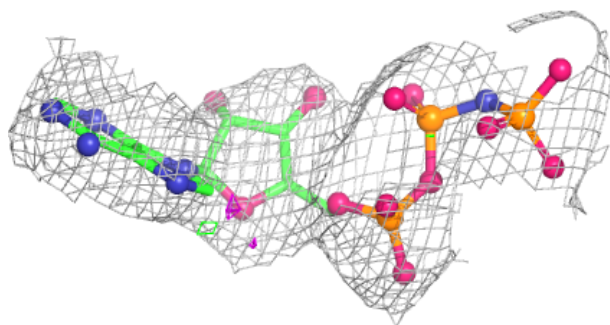
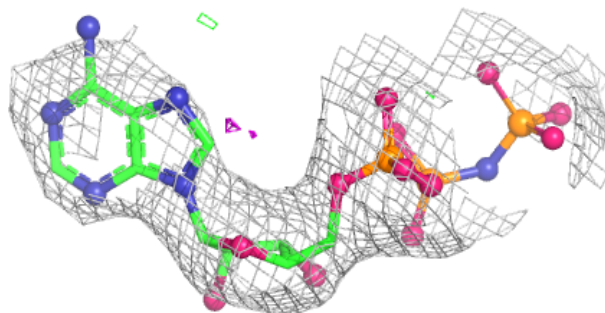
**Electron density around ANP D 601:**

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

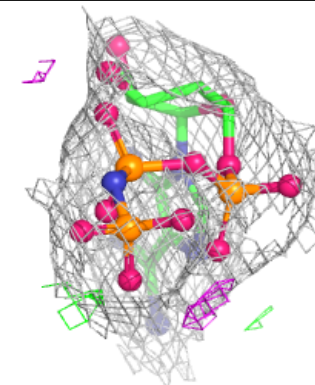
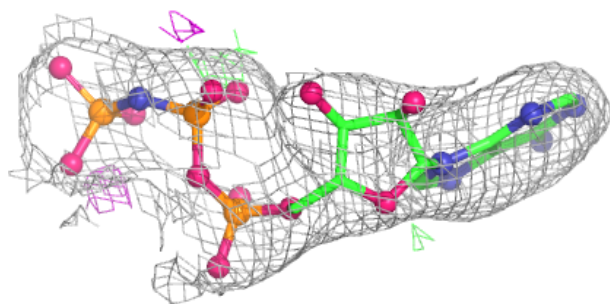
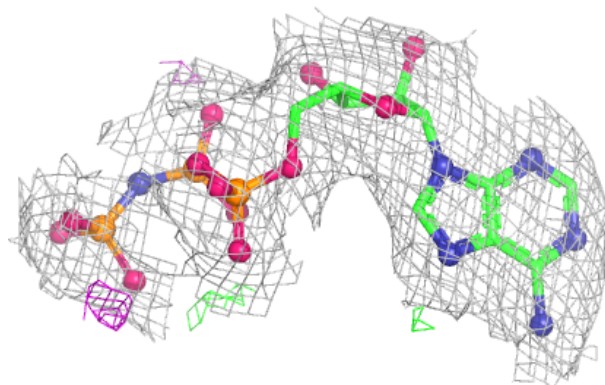


Electron density around ANP I 601:

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

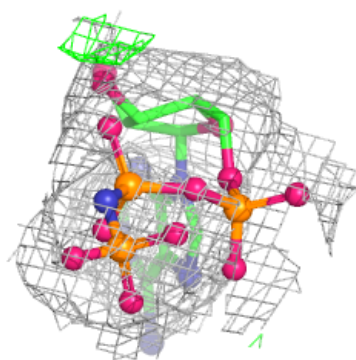
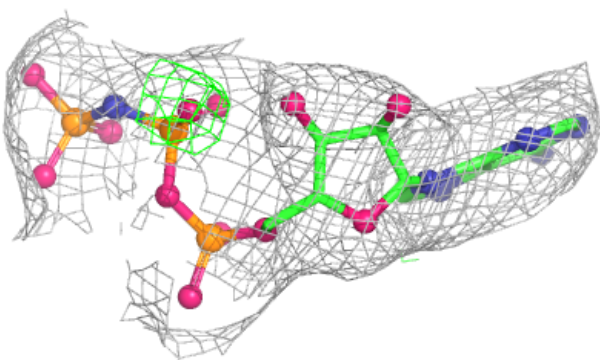
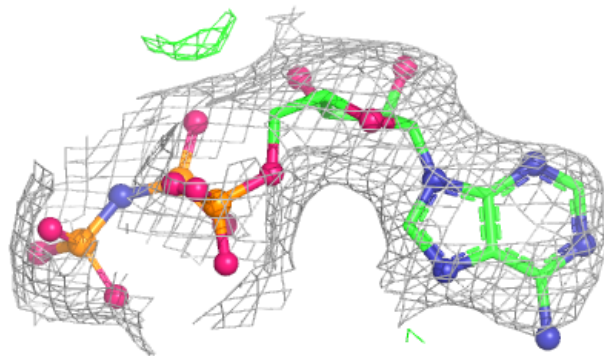
**Electron density around ANP J 601:**

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



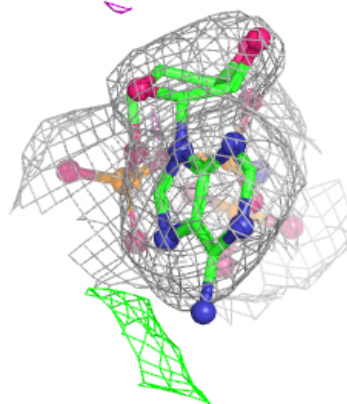
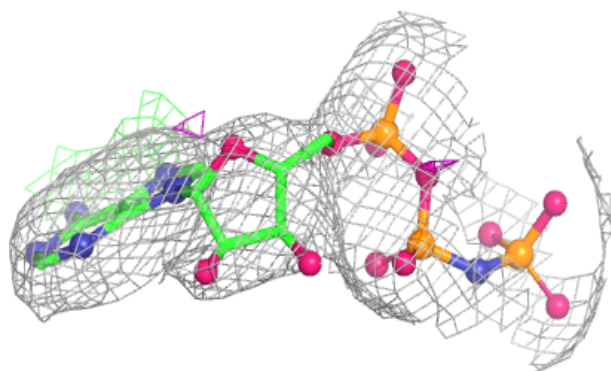
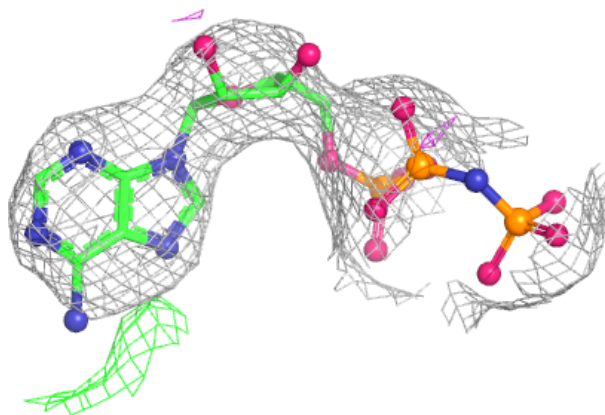
Electron density around ANP E 601:

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

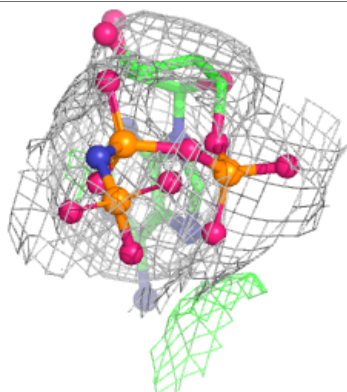
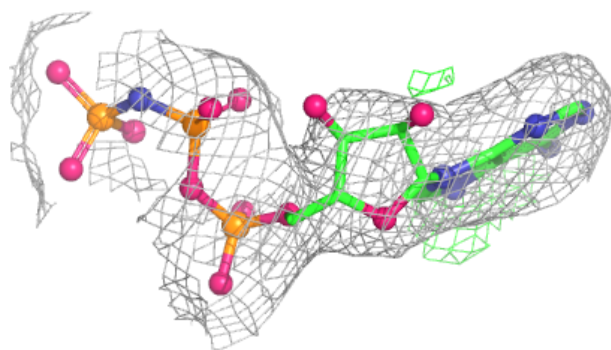
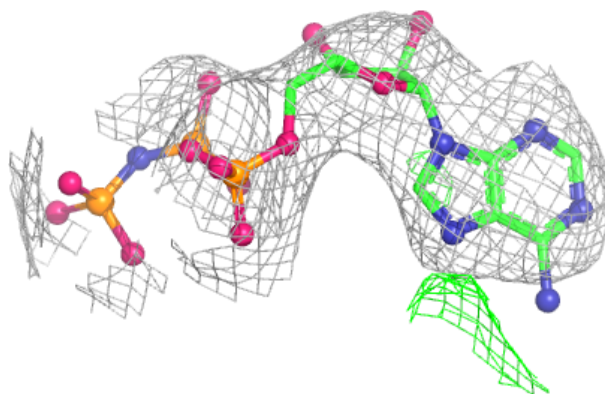


Electron density around ANP L 601:

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

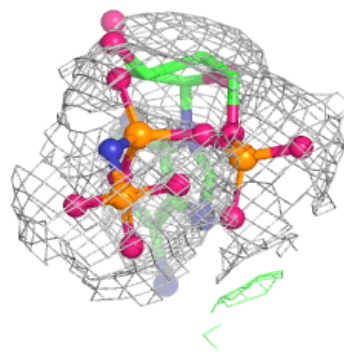
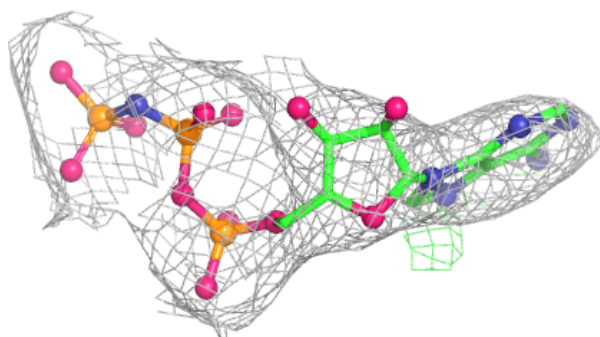
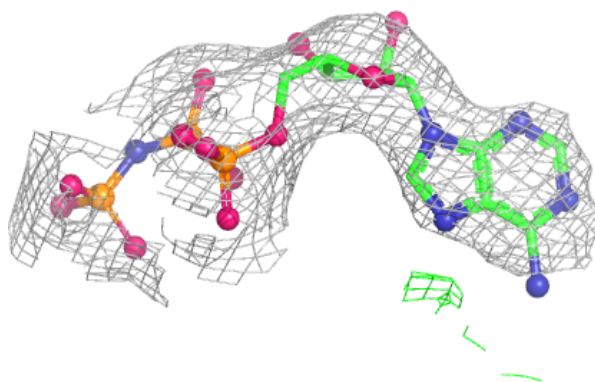
**Electron density around ANP M 601:**

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

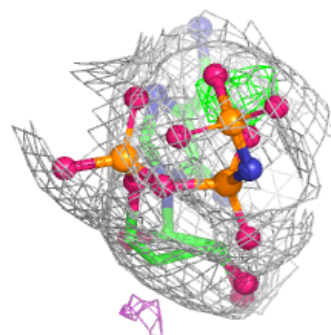
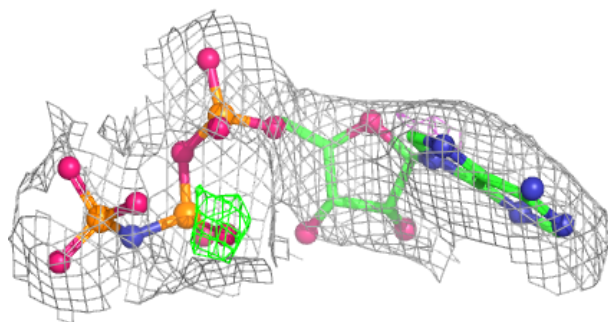
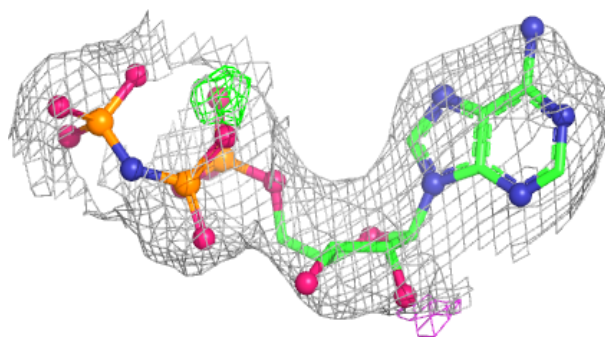


Electron density around ANP N 601:

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

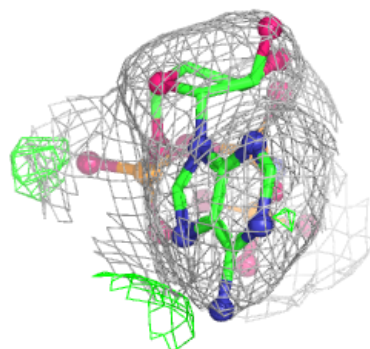
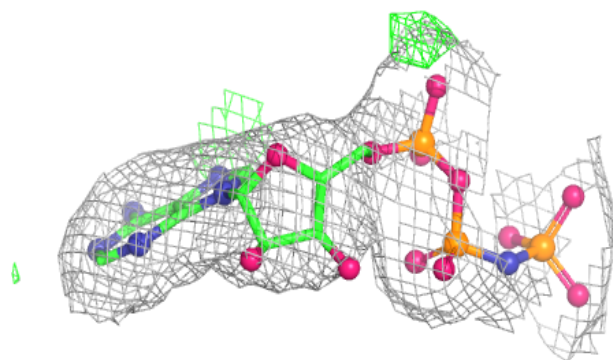
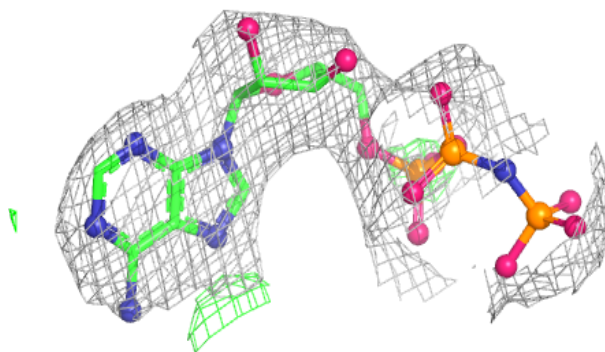
**Electron density around ANP B 601:**

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

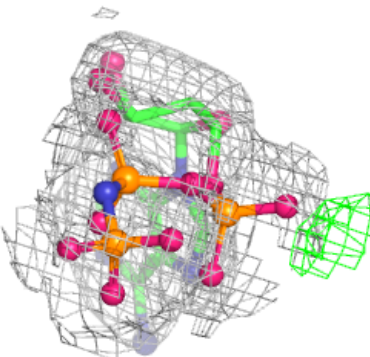
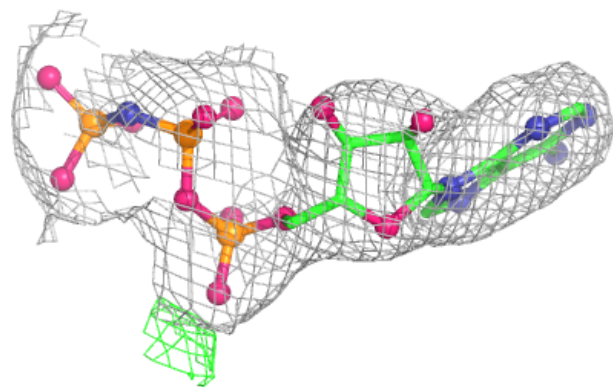
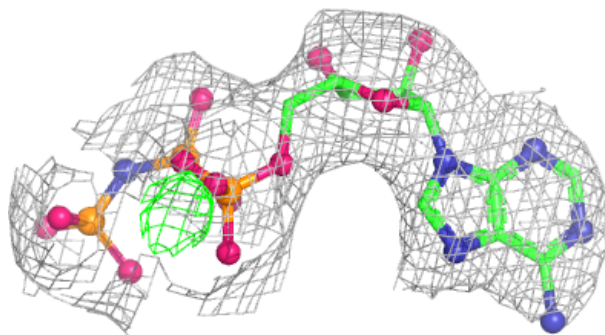


Electron density around ANP G 601:

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

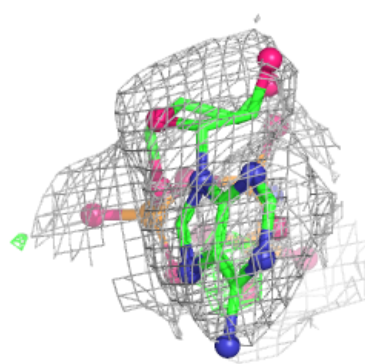
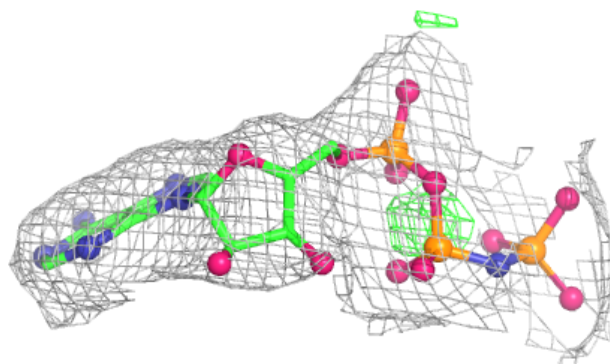
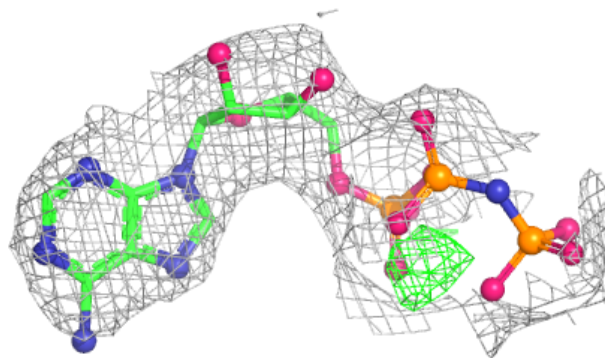
**Electron density around ANP C 601:**

$2mF_o-DF_c$ (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)



6.5 Other polymers [i](#)

There are no such residues in this entry.