



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 27, 2026 – 11:32 AM UTC

PDB ID : 4PKN / pdb_00004pkn
Title : Crystal structure of the football-shaped GroEL-GroES2-(ADPBeFx)₁₄ complex containing substrate Rubisco
Authors : Fei, X.; Ye, X.; Laronde-Leblanc, N.; Lorimer, G.H.
Deposited on : 2014-05-15
Resolution : 3.66 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 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

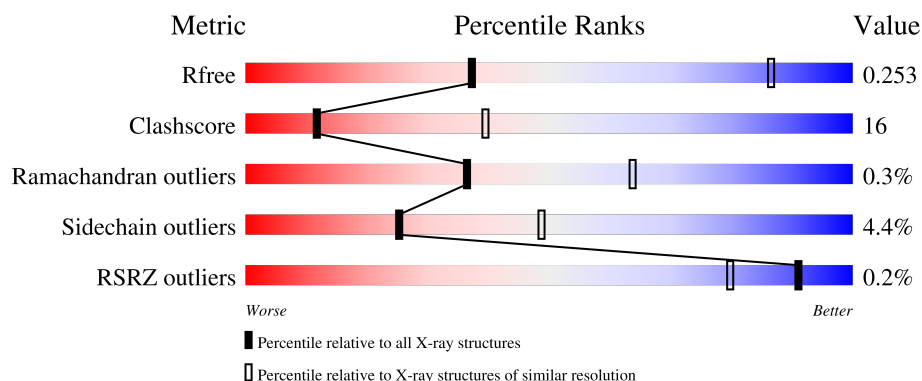
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.66 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.



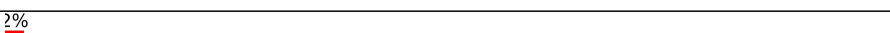
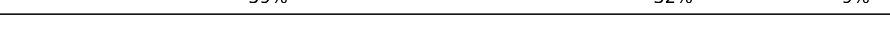
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1062 (3.78-3.54)
Clashscore	190562	1009 (3.76-3.56)
Ramachandran outliers	187476	1054 (3.78-3.54)
Sidechain outliers	187428	1052 (3.78-3.54)
RSRZ outliers	180081	1061 (3.78-3.54)

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

Mol	Chain	Length	Quality of chain
1	A	548	69% 25% • •
1	B	548	66% 28% • •
1	C	548	63% 30% • •
1	D	548	68% 26% • •
1	E	548	64% 30% • •

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Mol	Chain	Length	Quality of chain
1	F	548	
1	G	548	
1	H	548	
1	I	548	
1	J	548	
1	K	548	
1	L	548	
1	M	548	
1	N	548	
2	1	97	
2	2	97	
2	O	97	
2	P	97	
2	Q	97	
2	R	97	
2	S	97	
2	T	97	
2	U	97	
2	V	97	
2	W	97	
2	X	97	
2	Y	97	
2	Z	97	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	BEF	B	602	-	-	X	-
4	BEF	E	602	-	-	X	-
4	BEF	G	602	-	-	X	-
4	BEF	J	602	-	-	X	-
4	BEF	K	602	-	-	X	-
4	BEF	L	602	-	-	X	-
4	BEF	N	602	-	-	X	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 64579 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.

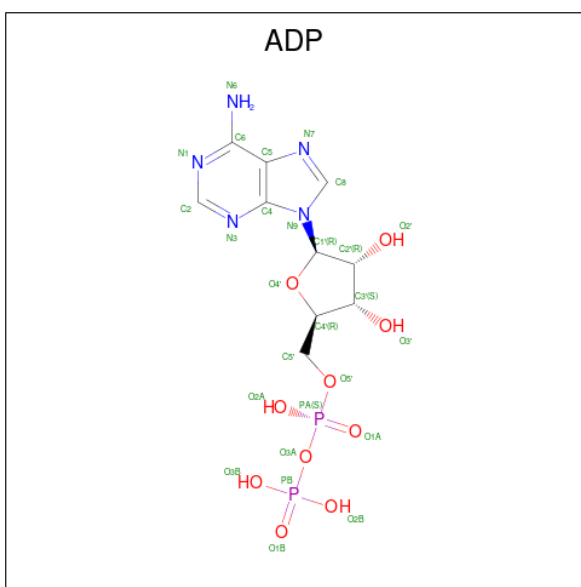
- Molecule 1 is a protein called 60 kDa chaperonin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	G	524	Total	C	N	O	S	0	0	0
			3855	2397	665	773	20			
1	A	524	Total	C	N	O	S	0	0	0
			3855	2397	665	773	20			
1	B	524	Total	C	N	O	S	0	0	0
			3855	2397	665	773	20			
1	F	524	Total	C	N	O	S	0	0	0
			3855	2397	665	773	20			
1	E	524	Total	C	N	O	S	0	0	0
			3855	2397	665	773	20			
1	C	524	Total	C	N	O	S	0	0	0
			3855	2397	665	773	20			
1	D	524	Total	C	N	O	S	0	0	0
			3855	2397	665	773	20			
1	K	524	Total	C	N	O	S	0	0	0
			3855	2397	665	773	20			
1	J	524	Total	C	N	O	S	0	0	0
			3855	2397	665	773	20			
1	I	524	Total	C	N	O	S	0	0	0
			3855	2397	665	773	20			
1	L	524	Total	C	N	O	S	0	0	0
			3855	2397	665	773	20			
1	M	524	Total	C	N	O	S	0	0	0
			3855	2397	665	773	20			
1	H	524	Total	C	N	O	S	0	0	0
			3855	2397	665	773	20			
1	N	524	Total	C	N	O	S	0	0	0
			3855	2397	665	773	20			

- Molecule 2 is a protein called 10 kDa chaperonin.

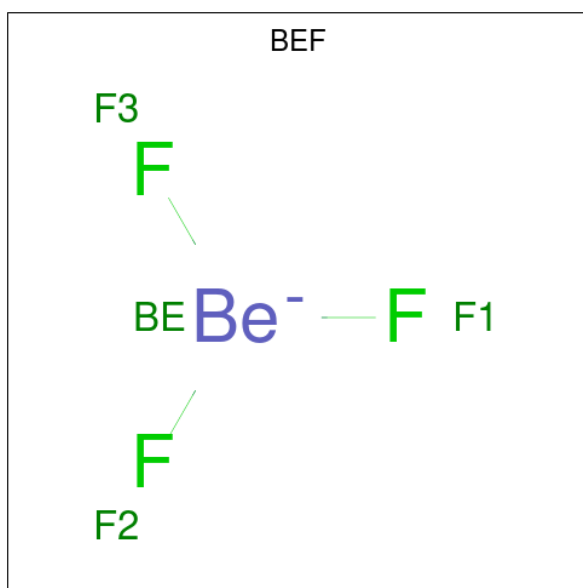
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	O	97	Total	C	N	O	S	0	0	0
			727	454	127	144	2			
2	P	97	Total	C	N	O	S	0	0	0
			727	454	127	144	2			
2	Q	97	Total	C	N	O	S	0	0	0
			727	454	127	144	2			
2	U	97	Total	C	N	O	S	0	0	0
			727	454	127	144	2			
2	T	97	Total	C	N	O	S	0	0	0
			727	454	127	144	2			
2	R	97	Total	C	N	O	S	0	0	0
			727	454	127	144	2			
2	S	97	Total	C	N	O	S	0	0	0
			727	454	127	144	2			
2	X	95	Total	C	N	O	S	0	0	0
			714	446	125	142	1			
2	W	96	Total	C	N	O	S	0	0	0
			719	449	126	143	1			
2	V	96	Total	C	N	O	S	0	0	0
			722	451	126	143	2			
2	Y	96	Total	C	N	O	S	0	0	0
			722	451	126	143	2			
2	Z	97	Total	C	N	O	S	0	0	0
			727	454	127	144	2			
2	2	97	Total	C	N	O	S	0	0	0
			727	454	127	144	2			
2	1	97	Total	C	N	O	S	0	0	0
			727	454	127	144	2			

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	G	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	A	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	B	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	F	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	E	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	C	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	D	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	K	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	J	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	I	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	L	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	M	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	H	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	N	1	Total 27	C 10	N 5	O 10	P 2	0	0

- Molecule 4 is BERYLLIUM TRIFLUORIDE ION (CCD ID: BEF) (formula: BeF₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	G	1	Total 4	Be 1	F 3	0	0
4	A	1	Total 4	Be 1	F 3	0	0
4	B	1	Total 4	Be 1	F 3	0	0
4	F	1	Total 4	Be 1	F 3	0	0
4	E	1	Total 4	Be 1	F 3	0	0
4	C	1	Total 4	Be 1	F 3	0	0
4	D	1	Total 4	Be 1	F 3	0	0
4	K	1	Total 4	Be 1	F 3	0	0
4	J	1	Total 4	Be 1	F 3	0	0
4	I	1	Total 4	Be 1	F 3	0	0
4	L	1	Total 4	Be 1	F 3	0	0
4	M	1	Total 4	Be 1	F 3	0	0
4	H	1	Total 4	Be 1	F 3	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	N	1	Total	Be	F	0	0
			4	1	3		

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 6 is POTASSIUM ION (CCD ID: K) (formula: K).

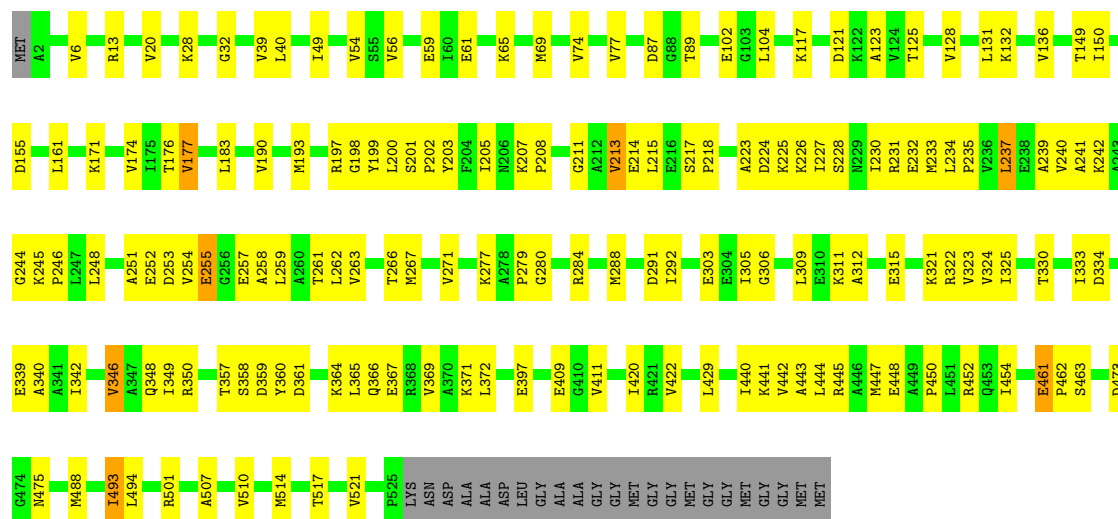
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	G	1	Total	K	0	0
			1	1		
6	A	1	Total	K	0	0
			1	1		

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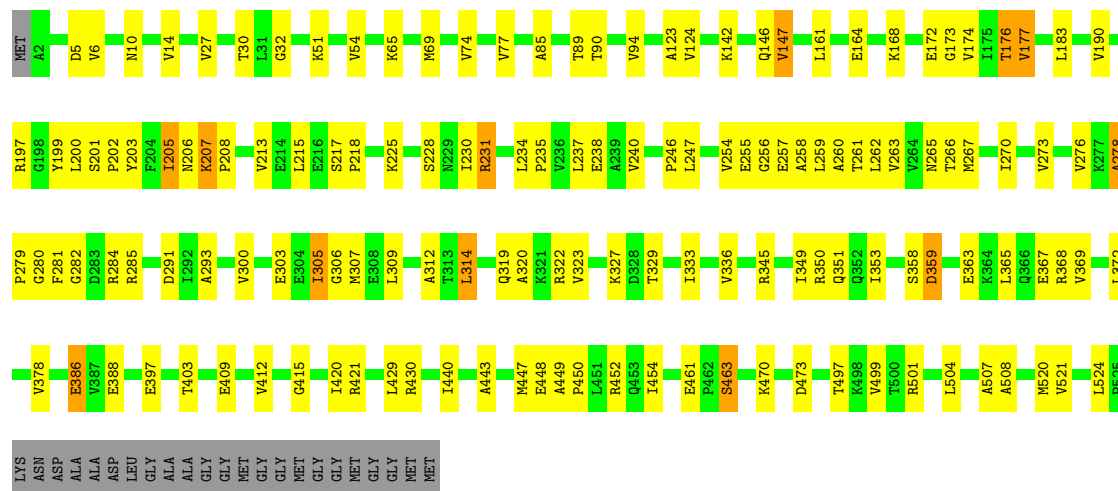
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total 1	K 1	0	0
6	F	1	Total 1	K 1	0	0
6	E	1	Total 1	K 1	0	0
6	C	1	Total 1	K 1	0	0
6	D	1	Total 1	K 1	0	0
6	K	1	Total 1	K 1	0	0
6	J	1	Total 1	K 1	0	0
6	I	1	Total 1	K 1	0	0
6	L	1	Total 1	K 1	0	0
6	M	1	Total 1	K 1	0	0
6	H	1	Total 1	K 1	0	0
6	N	1	Total 1	K 1	0	0

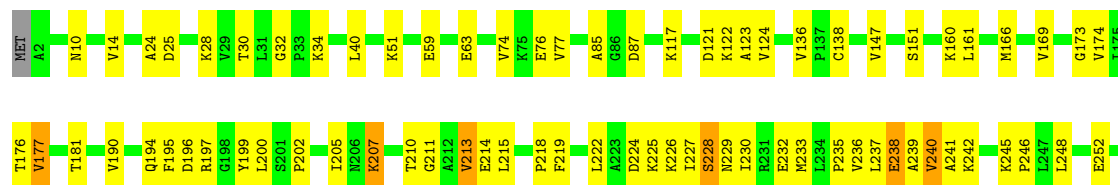
Chain B: 66% 28% ..



Chain F: 69% 24% . .

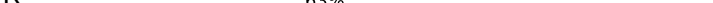


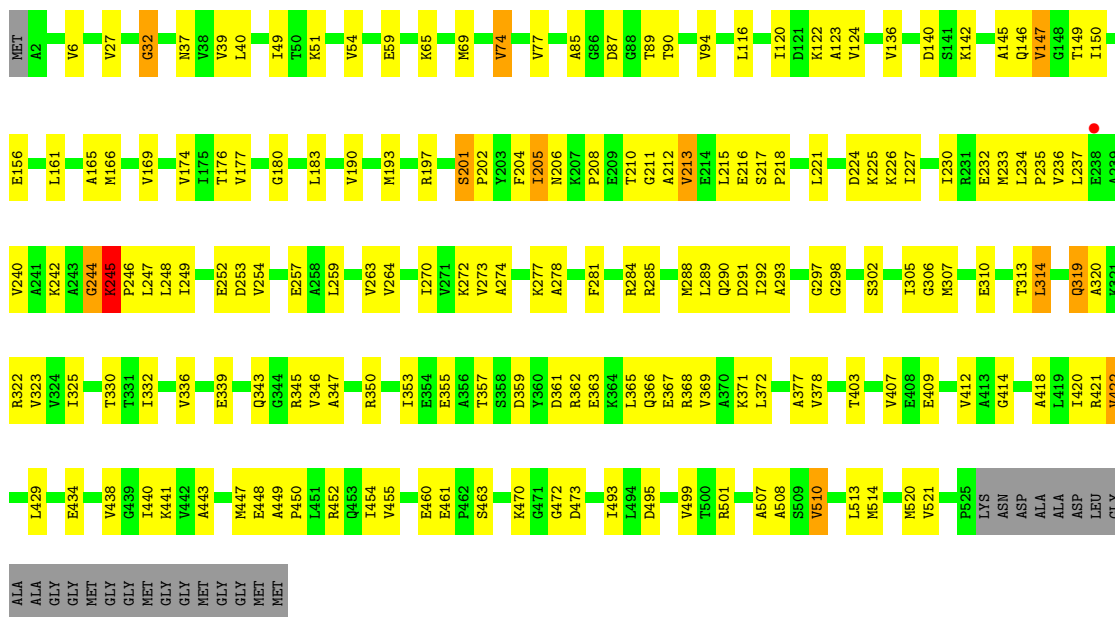
Chain E: 64% 30% . .





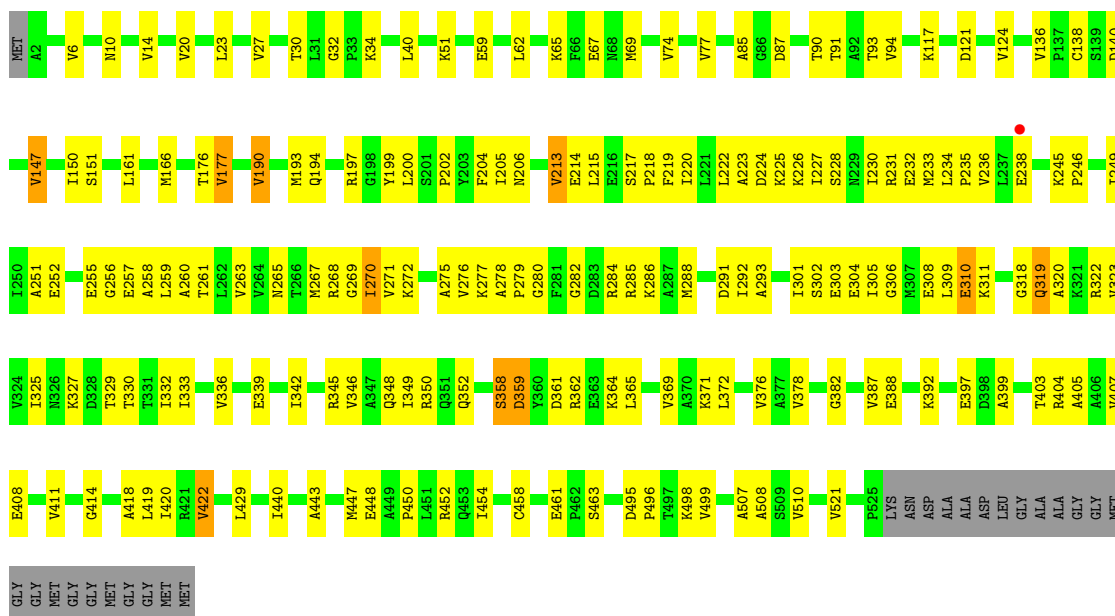
- Molecule 1: 60 kDa chaperonin

Chain K:  63% 30% . .



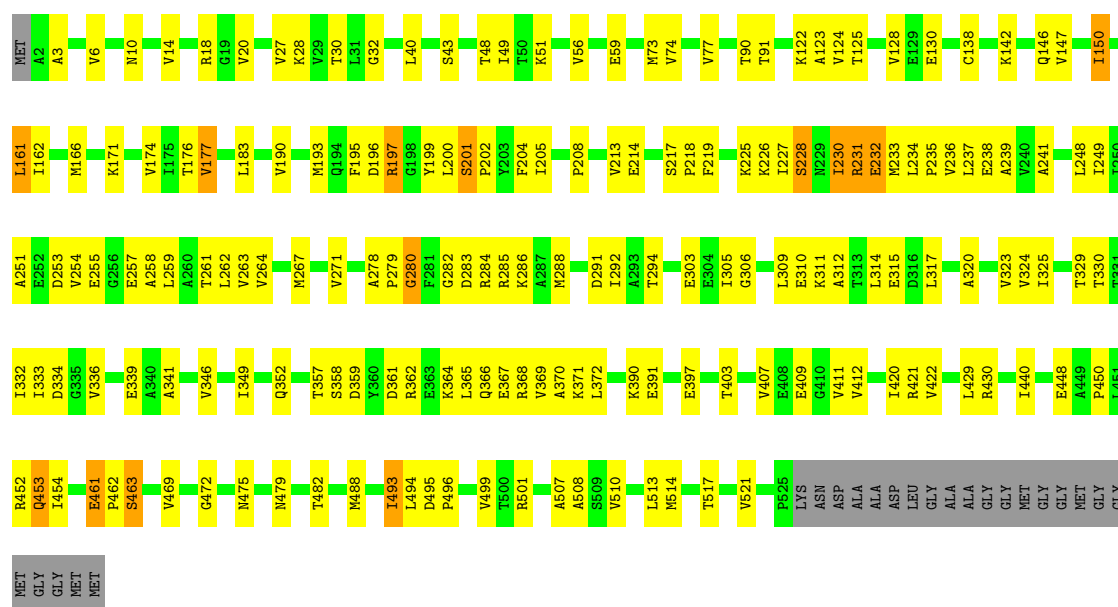
- Molecule 1: 60 kDa chaperonin

Chain J: 63% 31% . .



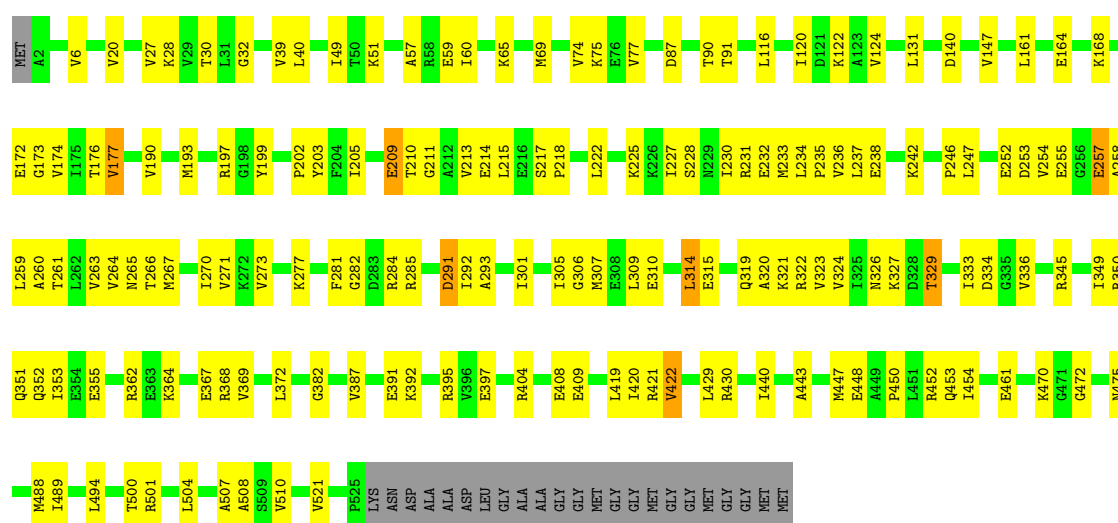
- Molecule 1: 60 kDa chaperonin

Chain I:  63% 30%



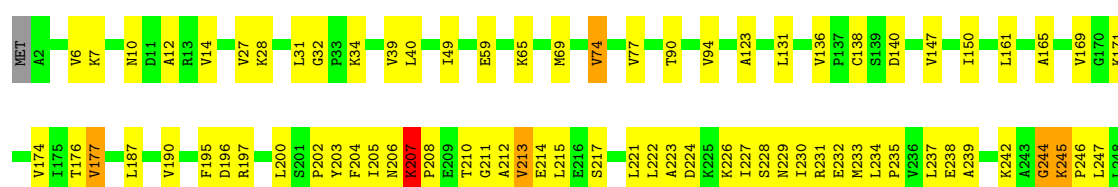
• Molecule 1: 60 kDa chaperonin

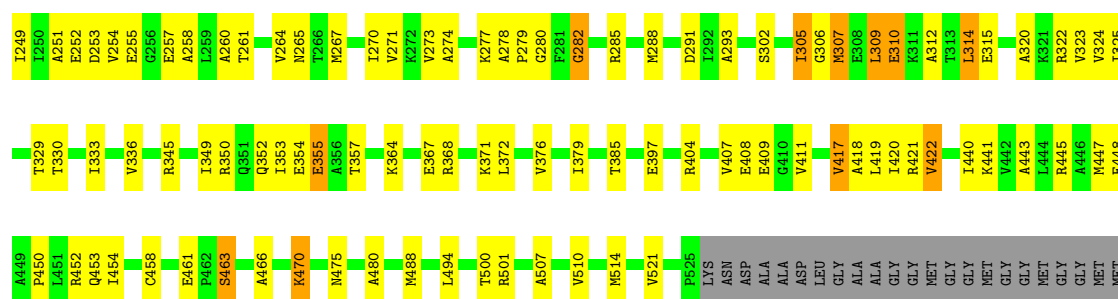
Chain L:  66% 28%



• Molecule 1: 60 kDa chaperonin

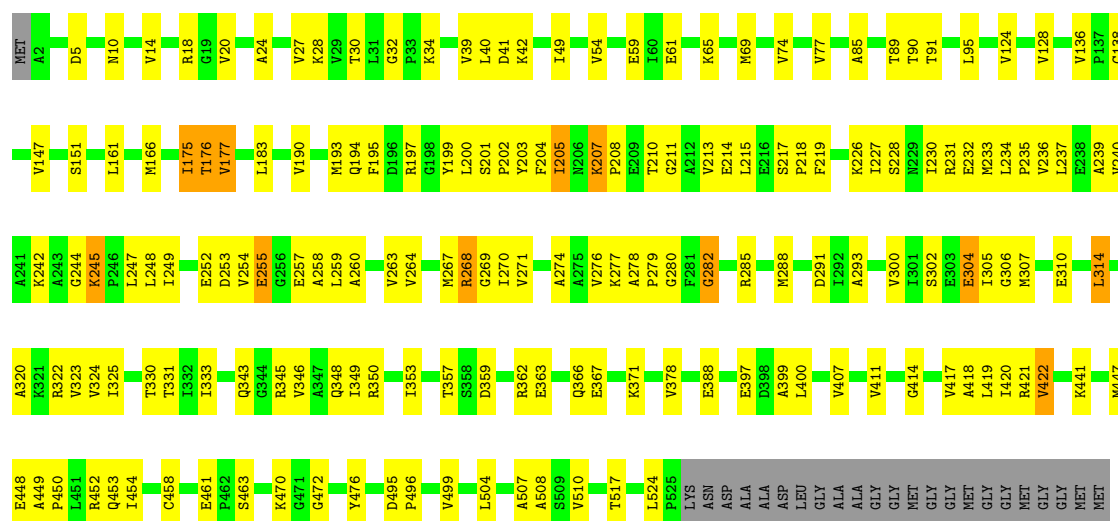
Chain M:  64% 28%





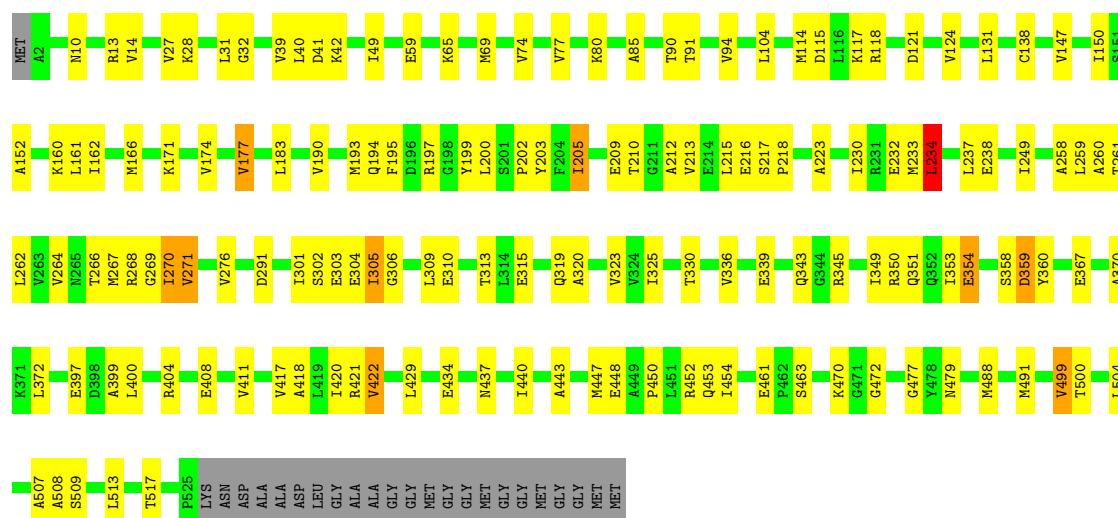
• Molecule 1: 60 kDa chaperonin

Chain H: 64% 30%



• Molecule 1: 60 kDa chaperonin

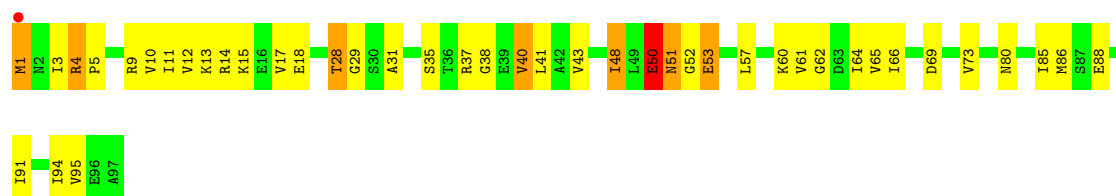
Chain N: 68% 26%



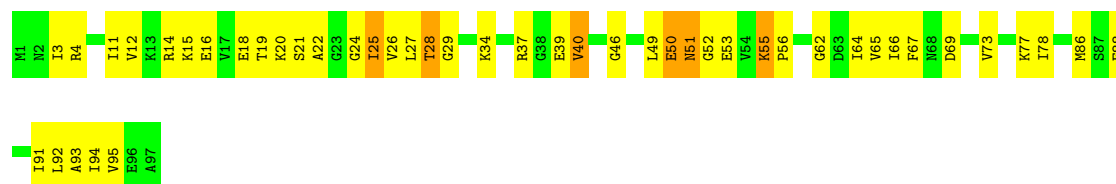
• Molecule 2: 10 kDa chaperonin



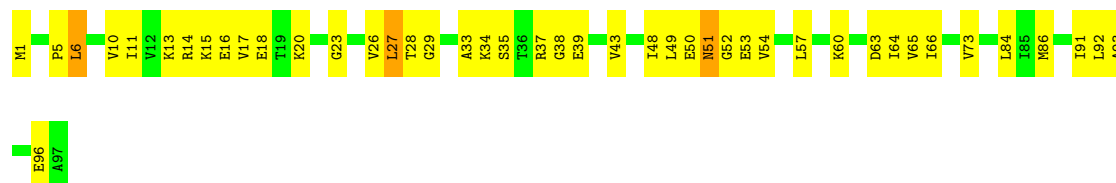
- Molecule 2: 10 kDa chaperonin



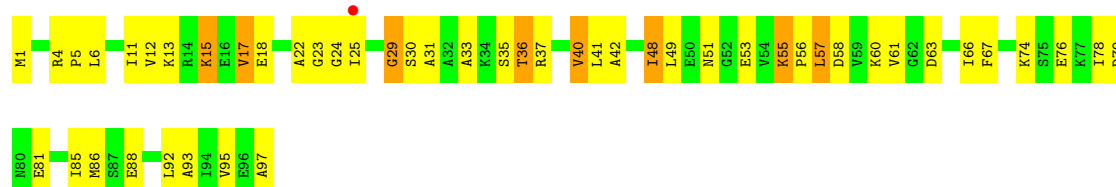
- Molecule 2: 10 kDa chaperonin



- Molecule 2: 10 kDa chaperonin

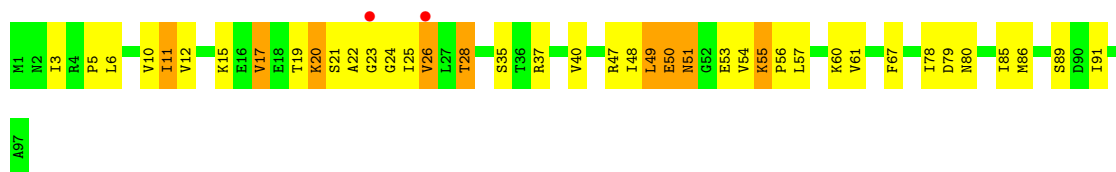


- Molecule 2: 10 kDa chaperonin

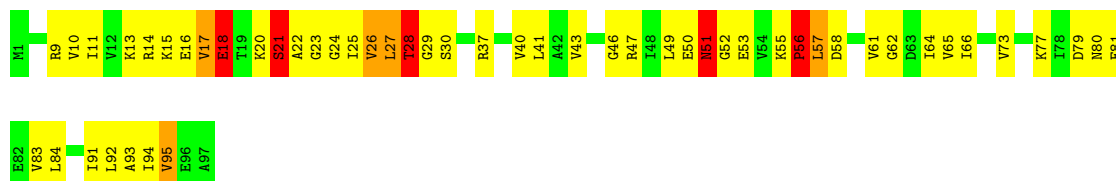


- Molecule 2: 10 kDa chaperonin

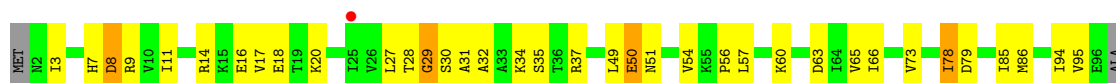




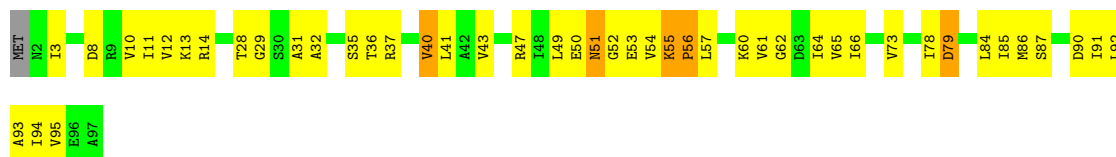
- Molecule 2: 10 kDa chaperonin



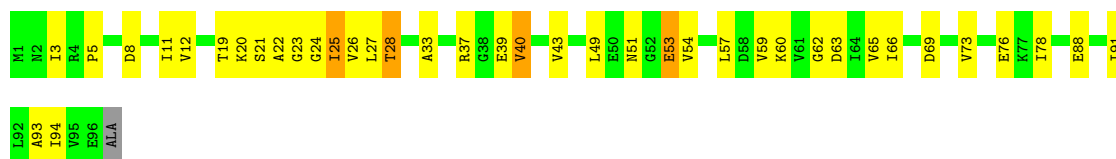
- Molecule 2: 10 kDa chaperonin



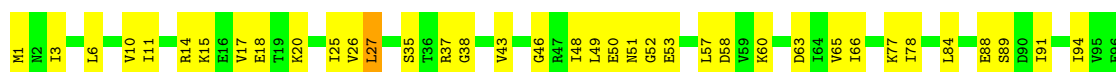
- Molecule 2: 10 kDa chaperonin



- Molecule 2: 10 kDa chaperonin

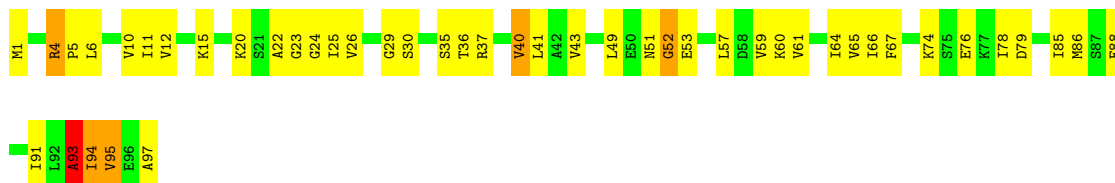


- Molecule 2: 10 kDa chaperonin

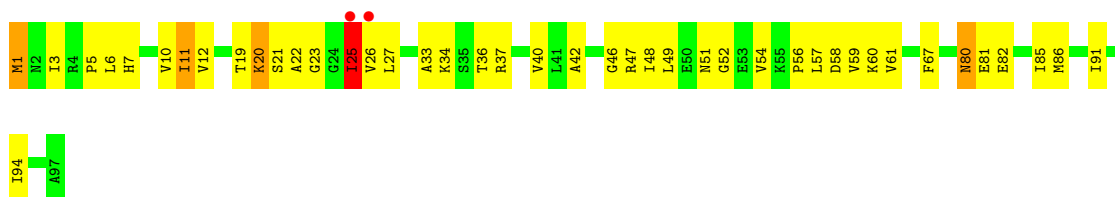


ALA

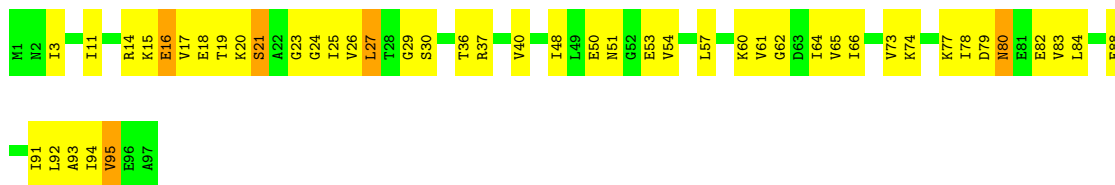
- Molecule 2: 10 kDa chaperonin

Chain Z:  53% 41% 5% •

- Molecule 2: 10 kDa chaperonin

Chain 2:  2% 56% 39% • •

- Molecule 2: 10 kDa chaperonin

Chain 1:  52% 43% 5%

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	171.95Å 173.65Å 411.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	122.19 – 3.66 122.19 – 3.66	Depositor EDS
% Data completeness (in resolution range)	99.5 (122.19-3.66) 99.6 (122.19-3.66)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.34 (at 3.67Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.188 , 0.241 0.198 , 0.253	Depositor DCC
R_{free} test set	2000 reflections (1.47%)	wwPDB-VP
Wilson B-factor (Å ²)	87.5	Xtriage
Anisotropy	0.664	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 93.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.190 for k,h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	64579	wwPDB-VP
Average B, all atoms (Å ²)	106.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.93% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ADP, K, BEF

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	0.47	0/3883	0.90	6/5243 (0.1%)
1	B	0.43	0/3883	0.88	11/5243 (0.2%)
1	C	0.46	0/3883	0.93	8/5243 (0.2%)
1	D	0.48	0/3883	0.92	8/5243 (0.2%)
1	E	0.46	0/3883	0.91	6/5243 (0.1%)
1	F	0.47	0/3883	0.91	12/5243 (0.2%)
1	G	0.48	0/3883	0.88	3/5243 (0.1%)
1	H	0.46	0/3883	0.92	9/5243 (0.2%)
1	I	0.43	0/3883	0.91	9/5243 (0.2%)
1	J	0.45	0/3883	0.90	4/5243 (0.1%)
1	K	0.46	0/3883	0.93	11/5243 (0.2%)
1	L	0.45	0/3883	0.89	5/5243 (0.1%)
1	M	0.45	0/3883	0.95	12/5243 (0.2%)
1	N	0.48	0/3883	0.92	7/5243 (0.1%)
2	1	0.44	0/731	1.04	2/983 (0.2%)
2	2	0.44	0/731	1.06	6/983 (0.6%)
2	O	0.42	0/731	1.07	4/983 (0.4%)
2	P	0.47	0/731	1.12	6/983 (0.6%)
2	Q	0.43	0/731	1.10	6/983 (0.6%)
2	R	0.44	0/731	1.14	6/983 (0.6%)
2	S	0.55	0/731	1.24	7/983 (0.7%)
2	T	0.42	0/731	1.12	7/983 (0.7%)
2	U	0.40	0/731	0.96	0/983
2	V	0.38	0/726	1.02	5/976 (0.5%)
2	W	0.44	0/723	1.06	1/973 (0.1%)
2	X	0.47	0/718	0.98	1/966 (0.1%)
2	Y	0.41	0/726	1.06	0/976
2	Z	0.42	0/731	1.10	6/983 (0.6%)
All	All	0.46	0/64565	0.94	168/87123 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	E	0	2
1	K	0	1
2	2	0	1
2	O	0	1
2	P	0	1
2	Q	0	1
2	S	0	4
2	T	0	1
2	W	0	1
2	X	0	1
2	Z	0	1
All	All	0	15

There are no bond length outliers.

The worst 5 of 168 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	227	ILE	N-CA-C	-10.46	102.60	111.91
1	H	282	GLY	N-CA-C	10.28	125.08	112.64
1	H	245	LYS	N-CA-C	10.14	120.02	108.25
1	C	282	GLY	N-CA-C	9.37	123.98	112.64
1	D	245	LYS	N-CA-C	8.78	118.23	108.14

There are no chirality outliers.

5 of 15 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	228	SER	Peptide
1	E	305	ILE	Peptide
2	O	29	GLY	Peptide
2	P	50	GLU	Peptide
2	Q	51	ASN	Peptide

5.2 Too-close contacts

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

the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3855	0	3974	112	0
1	B	3855	0	3976	124	0
1	C	3855	0	3975	130	0
1	D	3855	0	3976	108	0
1	E	3855	0	3976	135	0
1	F	3855	0	3975	100	0
1	G	3855	0	3975	119	0
1	H	3855	0	3976	129	0
1	I	3855	0	3975	133	0
1	J	3855	0	3975	137	0
1	K	3855	0	3974	128	0
1	L	3855	0	3975	111	0
1	M	3855	0	3975	133	0
1	N	3855	0	3976	98	0
2	1	727	0	762	43	0
2	2	727	0	762	43	0
2	O	727	0	762	24	0
2	P	727	0	762	43	0
2	Q	727	0	762	40	0
2	R	727	0	762	34	0
2	S	727	0	762	60	0
2	T	727	0	762	40	0
2	U	727	0	762	43	0
2	V	722	0	757	27	0
2	W	719	0	750	38	0
2	X	714	0	745	19	0
2	Y	722	0	757	28	0
2	Z	727	0	762	37	0
3	A	27	0	12	0	0
3	B	27	0	12	1	0
3	C	27	0	12	2	0
3	D	27	0	12	3	0
3	E	27	0	12	1	0
3	F	27	0	12	2	0
3	G	27	0	12	2	0
3	H	27	0	12	2	0
3	I	27	0	12	3	0
3	J	27	0	12	3	0
3	K	27	0	12	2	0
3	L	27	0	12	2	0
3	M	27	0	12	3	0
3	N	27	0	12	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	4	0	0	0	0
4	B	4	0	0	3	0
4	C	4	0	0	1	0
4	D	4	0	0	1	0
4	E	4	0	0	2	0
4	F	4	0	0	1	0
4	G	4	0	0	3	0
4	H	4	0	0	1	0
4	I	4	0	0	1	0
4	J	4	0	0	2	0
4	K	4	0	0	2	0
4	L	4	0	0	2	0
4	M	4	0	0	1	0
4	N	4	0	0	2	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
5	G	1	0	0	0	0
5	H	1	0	0	0	0
5	I	1	0	0	0	0
5	J	1	0	0	0	0
5	K	1	0	0	0	0
5	L	1	0	0	0	0
5	M	1	0	0	0	0
5	N	1	0	0	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
6	E	1	0	0	0	0
6	F	1	0	0	0	0
6	G	1	0	0	0	0
6	H	1	0	0	0	0
6	I	1	0	0	0	0
6	J	1	0	0	0	0
6	K	1	0	0	0	0
6	L	1	0	0	0	0
6	M	1	0	0	0	0
6	N	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	64579	0	66450	2087	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 16.

The worst 5 of 2087 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:226:LYS:HG2	1:C:252:GLU:HG2	1.39	1.03
1:C:239:ALA:HA	2:Q:25:ILE:HD11	1.43	1.01
1:E:238:GLU:HB2	2:S:22:ALA:HB1	1.45	0.97
2:S:28:THR:HG22	2:S:29:GLY:HA3	1.49	0.94
1:B:291:ASP:HB3	1:B:372:LEU:HD21	1.50	0.93

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	522/548 (95%)	506 (97%)	15 (3%)	1 (0%)	43	70
1	B	522/548 (95%)	502 (96%)	20 (4%)	0	100	100
1	C	522/548 (95%)	501 (96%)	20 (4%)	1 (0%)	43	70
1	D	522/548 (95%)	498 (95%)	23 (4%)	1 (0%)	43	70
1	E	522/548 (95%)	505 (97%)	16 (3%)	1 (0%)	43	70
1	F	522/548 (95%)	500 (96%)	21 (4%)	1 (0%)	43	70
1	G	522/548 (95%)	503 (96%)	18 (3%)	1 (0%)	43	70
1	H	522/548 (95%)	501 (96%)	21 (4%)	0	100	100
1	I	522/548 (95%)	503 (96%)	19 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	J	522/548 (95%)	500 (96%)	20 (4%)	2 (0%)	30	58
1	K	522/548 (95%)	505 (97%)	17 (3%)	0	100	100
1	L	522/548 (95%)	508 (97%)	14 (3%)	0	100	100
1	M	522/548 (95%)	502 (96%)	20 (4%)	0	100	100
1	N	522/548 (95%)	505 (97%)	17 (3%)	0	100	100
2	1	95/97 (98%)	83 (87%)	12 (13%)	0	100	100
2	2	95/97 (98%)	82 (86%)	12 (13%)	1 (1%)	11	39
2	O	95/97 (98%)	86 (90%)	8 (8%)	1 (1%)	11	39
2	P	95/97 (98%)	85 (90%)	10 (10%)	0	100	100
2	Q	95/97 (98%)	84 (88%)	11 (12%)	0	100	100
2	R	95/97 (98%)	85 (90%)	8 (8%)	2 (2%)	5	28
2	S	95/97 (98%)	77 (81%)	14 (15%)	4 (4%)	2	16
2	T	95/97 (98%)	87 (92%)	7 (7%)	1 (1%)	11	39
2	U	95/97 (98%)	84 (88%)	10 (10%)	1 (1%)	11	39
2	V	94/97 (97%)	84 (89%)	10 (11%)	0	100	100
2	W	94/97 (97%)	78 (83%)	15 (16%)	1 (1%)	11	39
2	X	93/97 (96%)	81 (87%)	10 (11%)	2 (2%)	5	27
2	Y	94/97 (97%)	86 (92%)	7 (7%)	1 (1%)	11	39
2	Z	95/97 (98%)	88 (93%)	7 (7%)	0	100	100
All	All	8633/9030 (96%)	8209 (95%)	402 (5%)	22 (0%)	36	64

5 of 22 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	270	ILE
1	E	305	ILE
1	C	230	ILE
1	D	230	ILE
2	S	26	VAL

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	404/415 (97%)	386 (96%)	18 (4%)	24	48
1	B	404/415 (97%)	389 (96%)	15 (4%)	30	52
1	C	404/415 (97%)	389 (96%)	15 (4%)	30	52
1	D	404/415 (97%)	391 (97%)	13 (3%)	34	54
1	E	404/415 (97%)	383 (95%)	21 (5%)	21	46
1	F	404/415 (97%)	391 (97%)	13 (3%)	34	54
1	G	404/415 (97%)	388 (96%)	16 (4%)	28	50
1	H	404/415 (97%)	386 (96%)	18 (4%)	24	48
1	I	404/415 (97%)	388 (96%)	16 (4%)	28	50
1	J	404/415 (97%)	387 (96%)	17 (4%)	26	49
1	K	404/415 (97%)	385 (95%)	19 (5%)	23	47
1	L	404/415 (97%)	390 (96%)	14 (4%)	32	53
1	M	404/415 (97%)	381 (94%)	23 (6%)	18	43
1	N	404/415 (97%)	387 (96%)	17 (4%)	26	49
2	1	80/80 (100%)	71 (89%)	9 (11%)	5	24
2	2	80/80 (100%)	75 (94%)	5 (6%)	16	41
2	O	80/80 (100%)	78 (98%)	2 (2%)	42	59
2	P	80/80 (100%)	76 (95%)	4 (5%)	22	46
2	Q	80/80 (100%)	76 (95%)	4 (5%)	22	46
2	R	80/80 (100%)	76 (95%)	4 (5%)	22	46
2	S	80/80 (100%)	73 (91%)	7 (9%)	9	31
2	T	80/80 (100%)	76 (95%)	4 (5%)	22	46
2	U	80/80 (100%)	74 (92%)	6 (8%)	12	37
2	V	80/80 (100%)	77 (96%)	3 (4%)	29	51
2	W	79/80 (99%)	75 (95%)	4 (5%)	21	46
2	X	79/80 (99%)	76 (96%)	3 (4%)	29	51
2	Y	80/80 (100%)	78 (98%)	2 (2%)	42	59
2	Z	80/80 (100%)	77 (96%)	3 (4%)	29	51
All	All	6774/6930 (98%)	6479 (96%)	295 (4%)	25	49

5 of 295 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	30	THR
2	1	11	ILE
1	H	177	VAL
1	N	360	TYR
1	C	463	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 33 such sidechains are listed below:

Mol	Chain	Res	Type
2	V	51	ASN
2	Y	7	HIS
2	Z	51	ASN
1	D	505	GLN
1	C	290	GLN

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 56 ligands modelled in this entry, 28 are monoatomic - leaving 28 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
3	ADP	B	601	5,6	28,29,29	1.37	4 (14%)	43,45,45	1.93	11 (25%)
3	ADP	D	601	5,6	28,29,29	1.42	5 (17%)	43,45,45	1.81	10 (23%)
4	BEF	E	602	-	0,3,3	-	-	-	-	-
4	BEF	H	602	-	0,3,3	-	-	-	-	-
3	ADP	K	601	5,6	28,29,29	1.40	4 (14%)	43,45,45	1.87	8 (18%)
4	BEF	J	602	-	0,3,3	-	-	-	-	-
4	BEF	N	602	-	0,3,3	-	-	-	-	-
3	ADP	L	601	5,6	28,29,29	1.41	4 (14%)	43,45,45	1.83	10 (23%)
4	BEF	G	602	-	0,3,3	-	-	-	-	-
4	BEF	D	602	-	0,3,3	-	-	-	-	-
4	BEF	L	602	-	0,3,3	-	-	-	-	-
3	ADP	E	601	5,6	28,29,29	1.39	4 (14%)	43,45,45	1.84	9 (20%)
3	ADP	J	601	5,6	28,29,29	1.39	4 (14%)	43,45,45	1.86	8 (18%)
4	BEF	M	602	-	0,3,3	-	-	-	-	-
3	ADP	C	601	5,6	28,29,29	1.39	4 (14%)	43,45,45	1.79	7 (16%)
4	BEF	F	602	-	0,3,3	-	-	-	-	-
3	ADP	H	601	5,6	28,29,29	1.39	5 (17%)	43,45,45	1.80	8 (18%)
4	BEF	A	602	-	0,3,3	-	-	-	-	-
3	ADP	G	601	5,6	28,29,29	1.37	4 (14%)	43,45,45	1.91	9 (20%)
3	ADP	N	601	5,6	28,29,29	1.40	5 (17%)	43,45,45	1.84	11 (25%)
4	BEF	B	602	-	0,3,3	-	-	-	-	-
3	ADP	I	601	5,6	28,29,29	1.37	5 (17%)	43,45,45	1.88	10 (23%)
4	BEF	C	602	-	0,3,3	-	-	-	-	-
3	ADP	M	601	5,6	28,29,29	1.46	5 (17%)	43,45,45	1.83	8 (18%)
3	ADP	F	601	5,6	28,29,29	1.34	4 (14%)	43,45,45	1.95	11 (25%)
4	BEF	I	602	-	0,3,3	-	-	-	-	-
4	BEF	K	602	-	0,3,3	-	-	-	-	-
3	ADP	A	601	5,6	28,29,29	1.35	4 (14%)	43,45,45	1.97	10 (23%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ADP	C	601	5,6	-	3/16/32/32	0/3/3/3
3	ADP	M	601	5,6	-	8/16/32/32	0/3/3/3
3	ADP	F	601	5,6	-	4/16/32/32	0/3/3/3
3	ADP	L	601	5,6	-	3/16/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ADP	H	601	5,6	-	5/16/32/32	0/3/3/3
3	ADP	B	601	5,6	-	5/16/32/32	0/3/3/3
3	ADP	G	601	5,6	-	5/16/32/32	0/3/3/3
3	ADP	D	601	5,6	-	3/16/32/32	0/3/3/3
3	ADP	K	601	5,6	-	2/16/32/32	0/3/3/3
3	ADP	N	601	5,6	-	5/16/32/32	0/3/3/3
3	ADP	I	601	5,6	-	3/16/32/32	0/3/3/3
3	ADP	J	601	5,6	-	7/16/32/32	0/3/3/3
3	ADP	E	601	5,6	-	4/16/32/32	0/3/3/3
3	ADP	A	601	5,6	-	4/16/32/32	0/3/3/3

The worst 5 of 61 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	M	601	ADP	C5-C4	4.69	1.47	1.39
3	D	601	ADP	C5-C4	4.67	1.47	1.39
3	L	601	ADP	C5-C4	4.60	1.47	1.39
3	C	601	ADP	C5-C4	4.60	1.47	1.39
3	K	601	ADP	C5-C4	4.54	1.47	1.39

The worst 5 of 130 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	601	ADP	C5-C4-N3	-6.07	118.35	126.72
3	F	601	ADP	C5-C4-N3	-6.07	118.36	126.72
3	A	601	ADP	C5-C4-N3	-6.03	118.41	126.72
3	K	601	ADP	C5-C4-N3	-6.03	118.41	126.72
3	J	601	ADP	C5-C4-N3	-5.94	118.54	126.72

There are no chirality outliers.

5 of 61 torsion outliers are listed below:

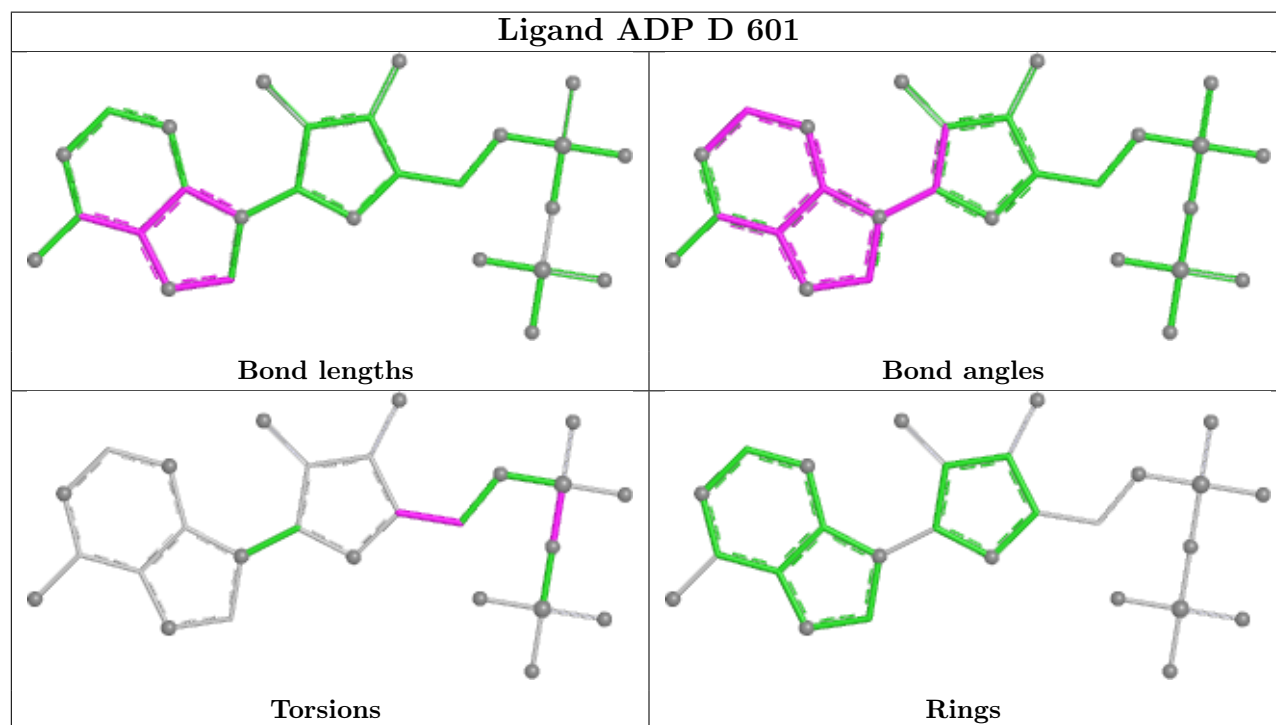
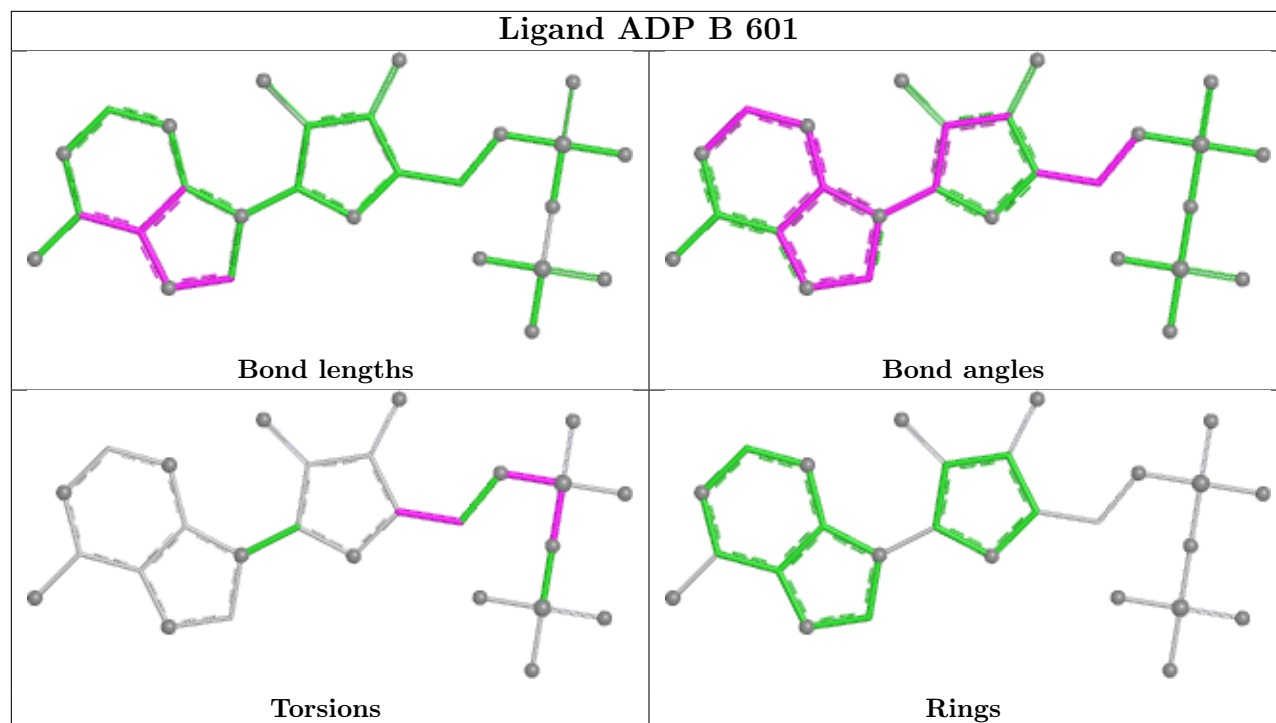
Mol	Chain	Res	Type	Atoms
3	A	601	ADP	C5'-O5'-PA-O1A
3	F	601	ADP	O4'-C4'-C5'-O5'
3	F	601	ADP	C3'-C4'-C5'-O5'
3	E	601	ADP	PA-O3A-PB-O3B
3	E	601	ADP	C5'-O5'-PA-O1A

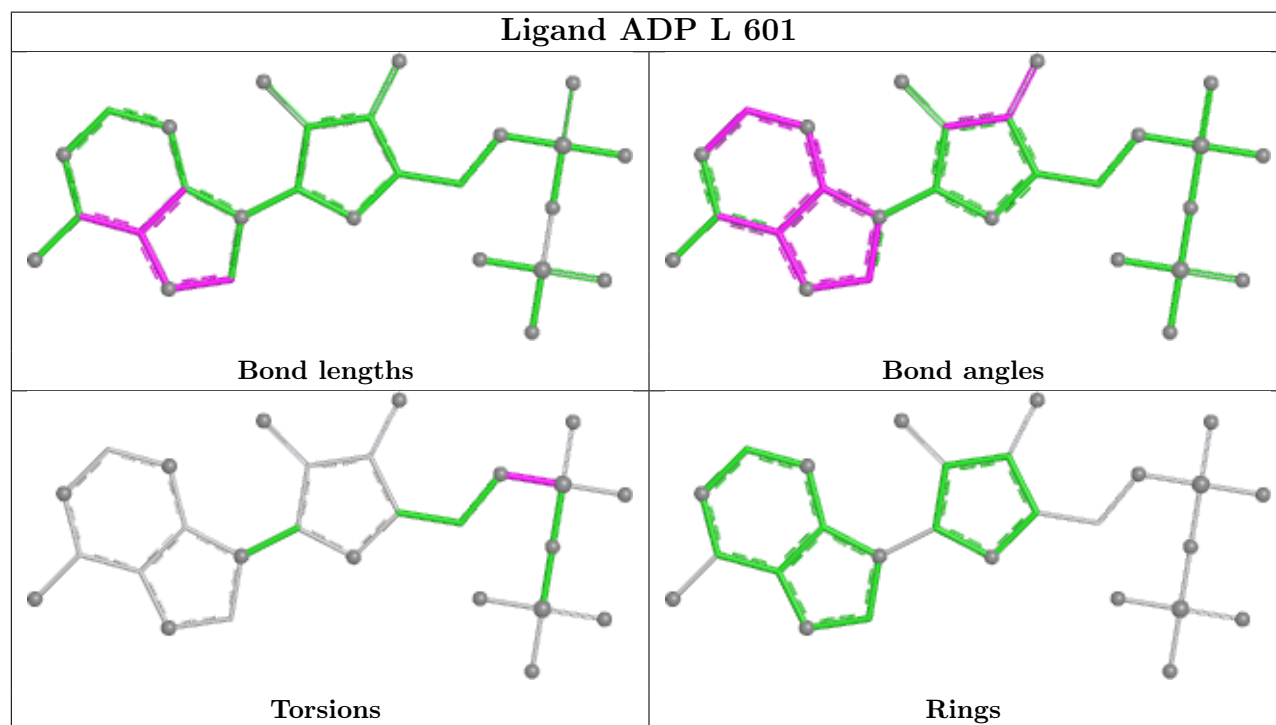
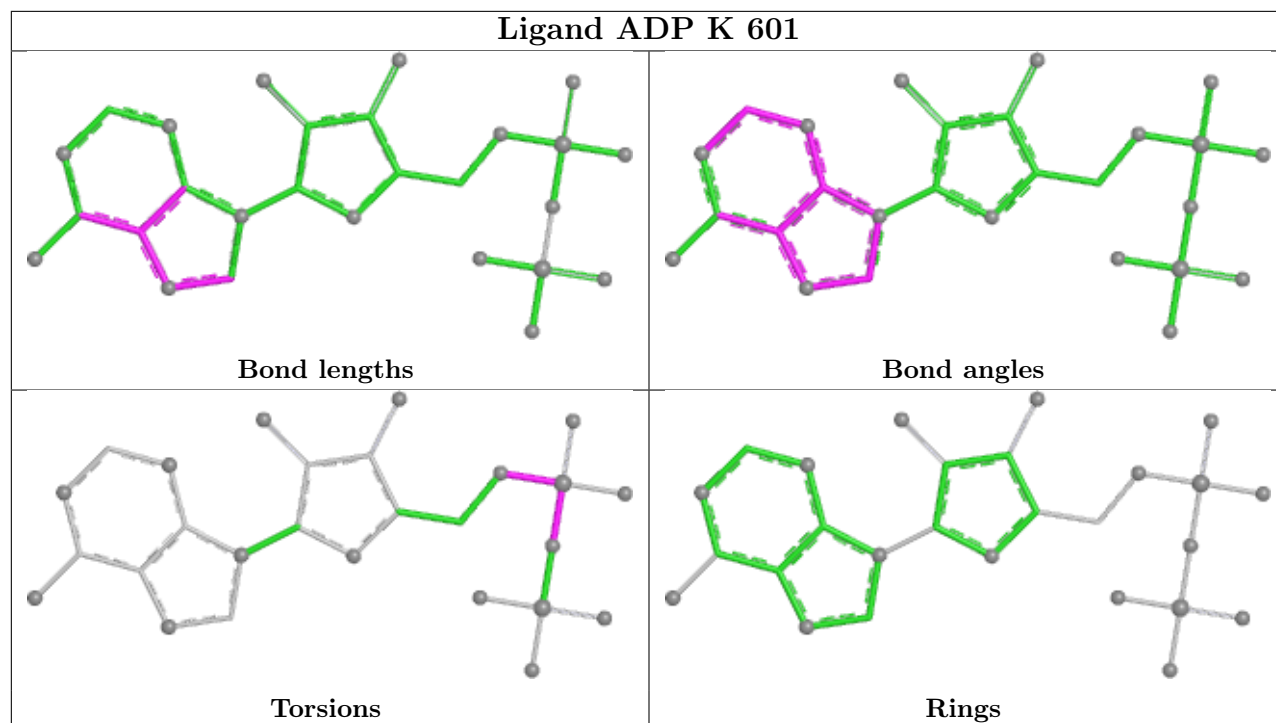
There are no ring outliers.

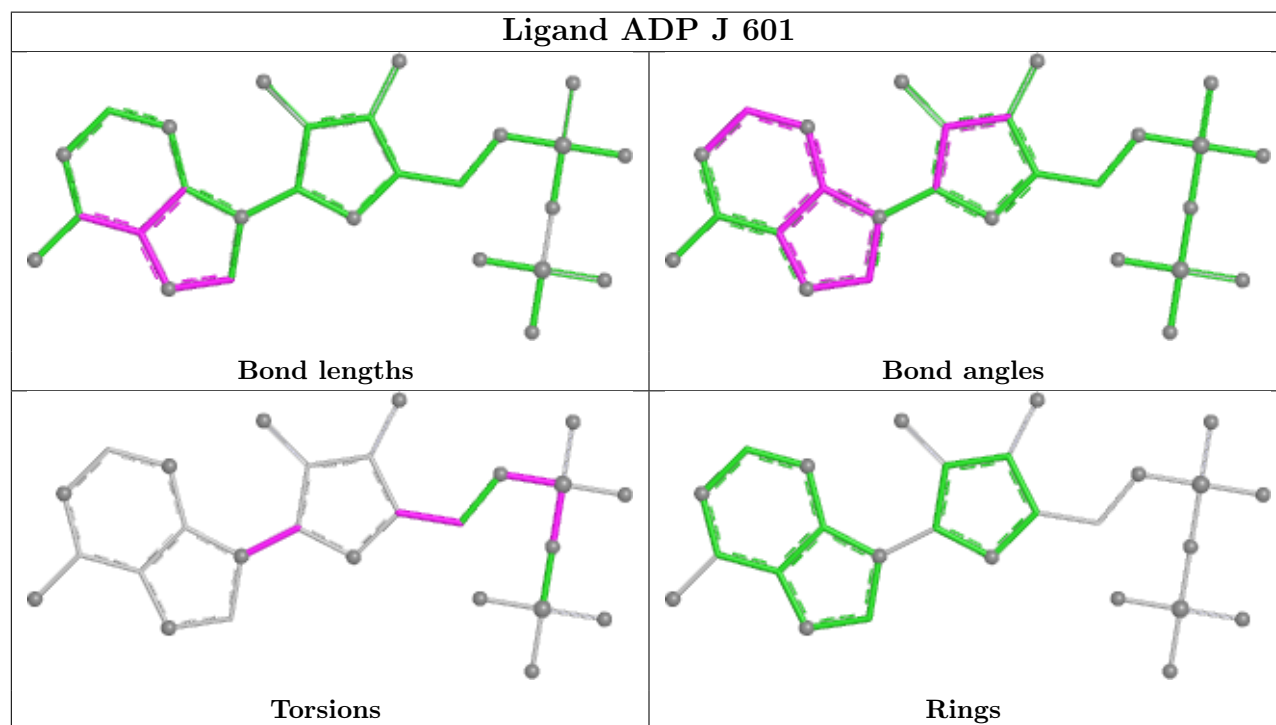
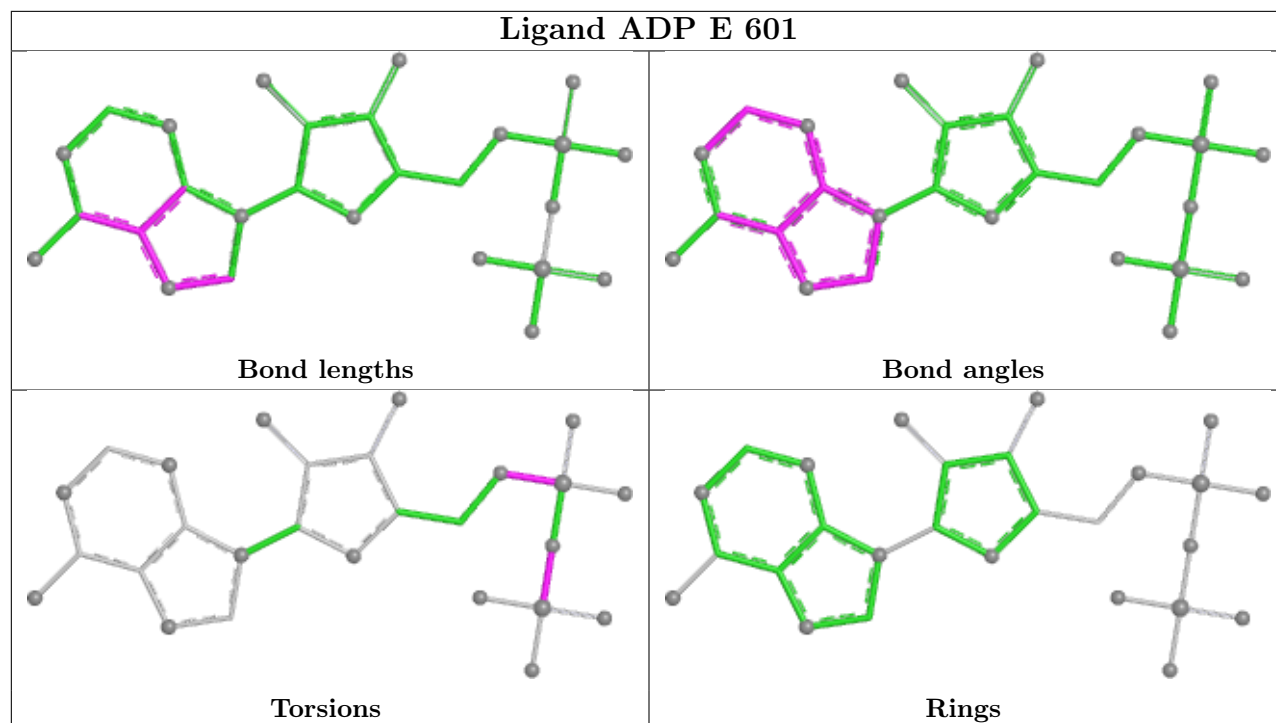
26 monomers are involved in 36 short contacts:

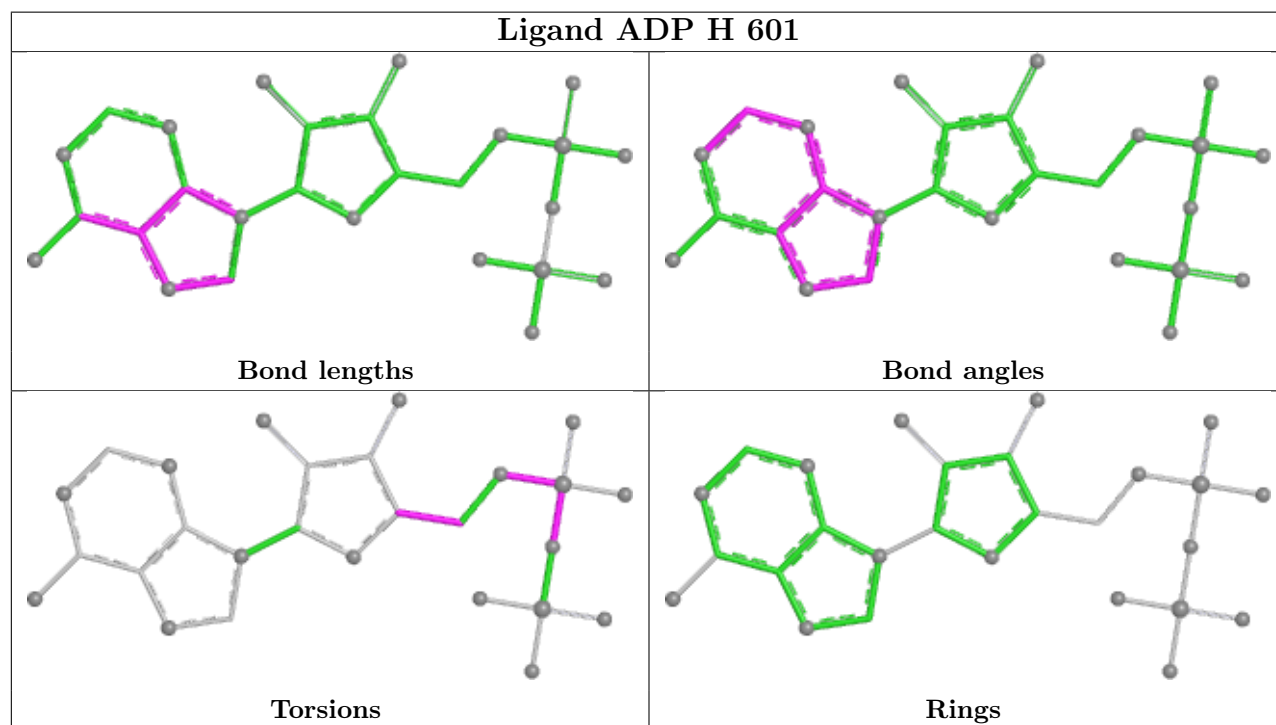
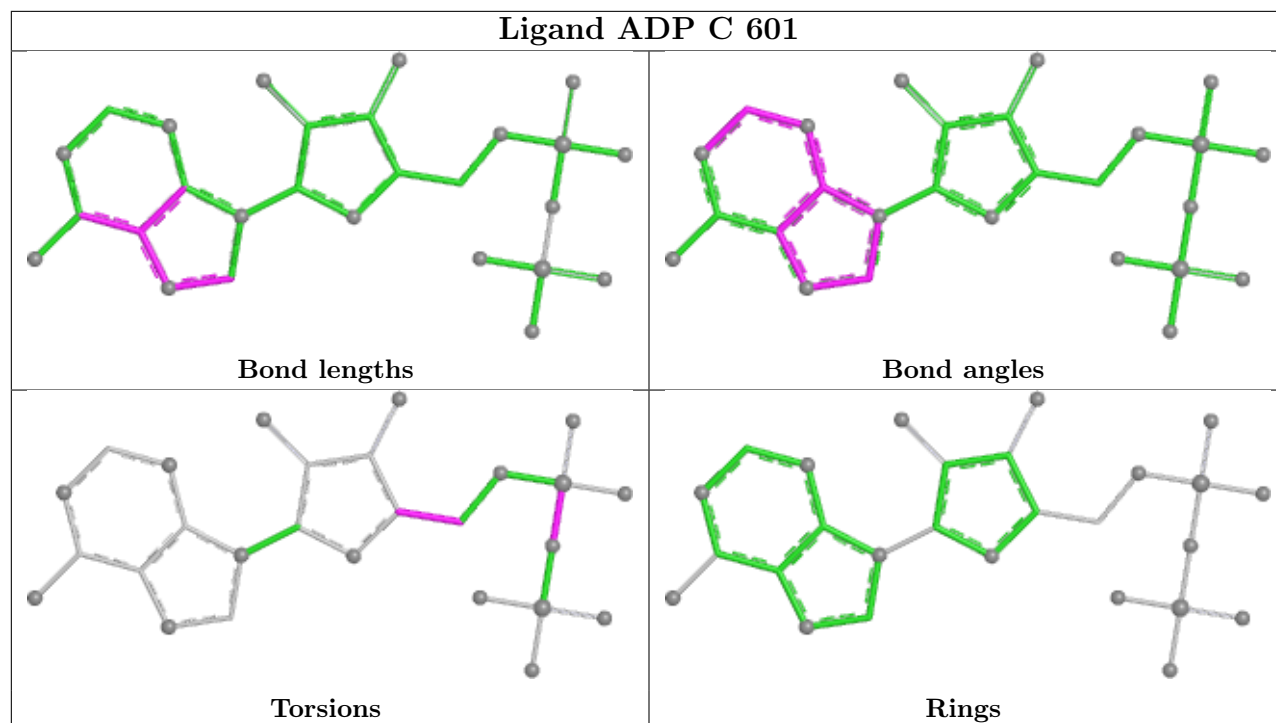
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	601	ADP	1	0
3	D	601	ADP	3	0
4	E	602	BEF	2	0
4	H	602	BEF	1	0
3	K	601	ADP	2	0
4	J	602	BEF	2	0
4	N	602	BEF	2	0
3	L	601	ADP	2	0
4	G	602	BEF	3	0
4	D	602	BEF	1	0
4	L	602	BEF	2	0
3	E	601	ADP	1	0
3	J	601	ADP	3	0
4	M	602	BEF	1	0
3	C	601	ADP	2	0
4	F	602	BEF	1	0
3	H	601	ADP	2	0
3	G	601	ADP	2	0
3	N	601	ADP	2	0
4	B	602	BEF	3	0
3	I	601	ADP	3	0
4	C	602	BEF	1	0
3	M	601	ADP	3	0
3	F	601	ADP	2	0
4	I	602	BEF	1	0
4	K	602	BEF	2	0

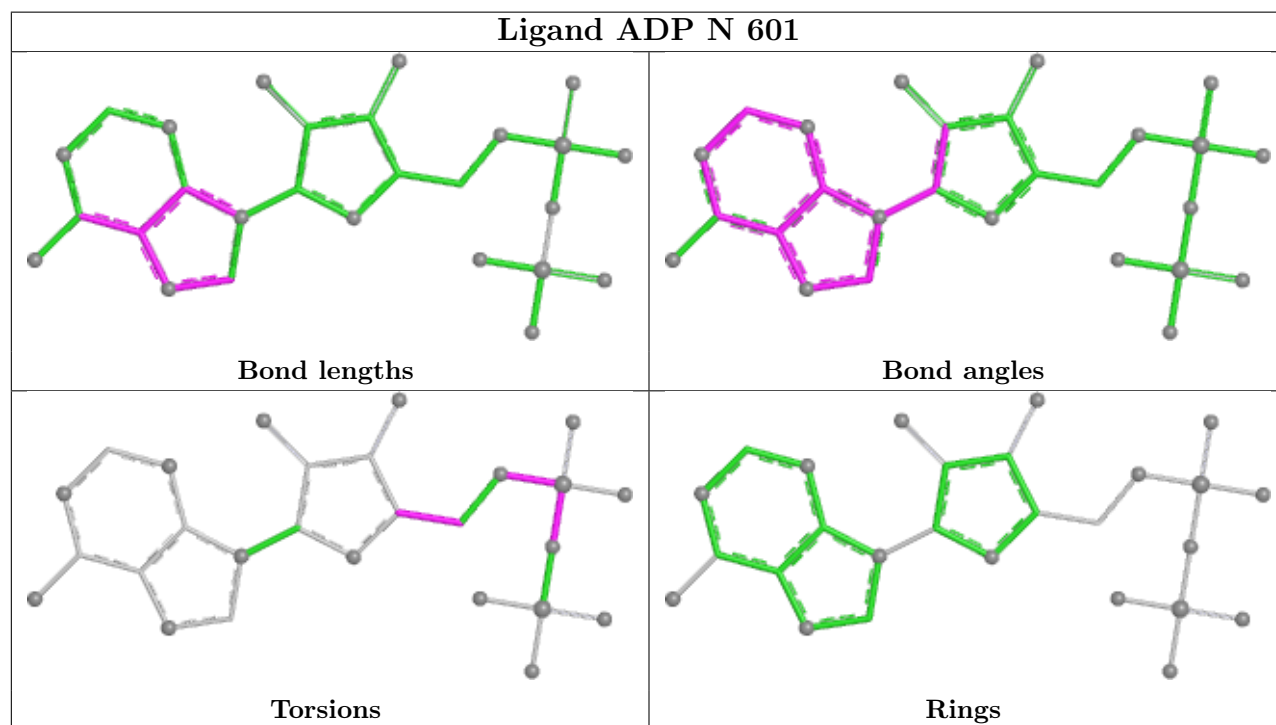
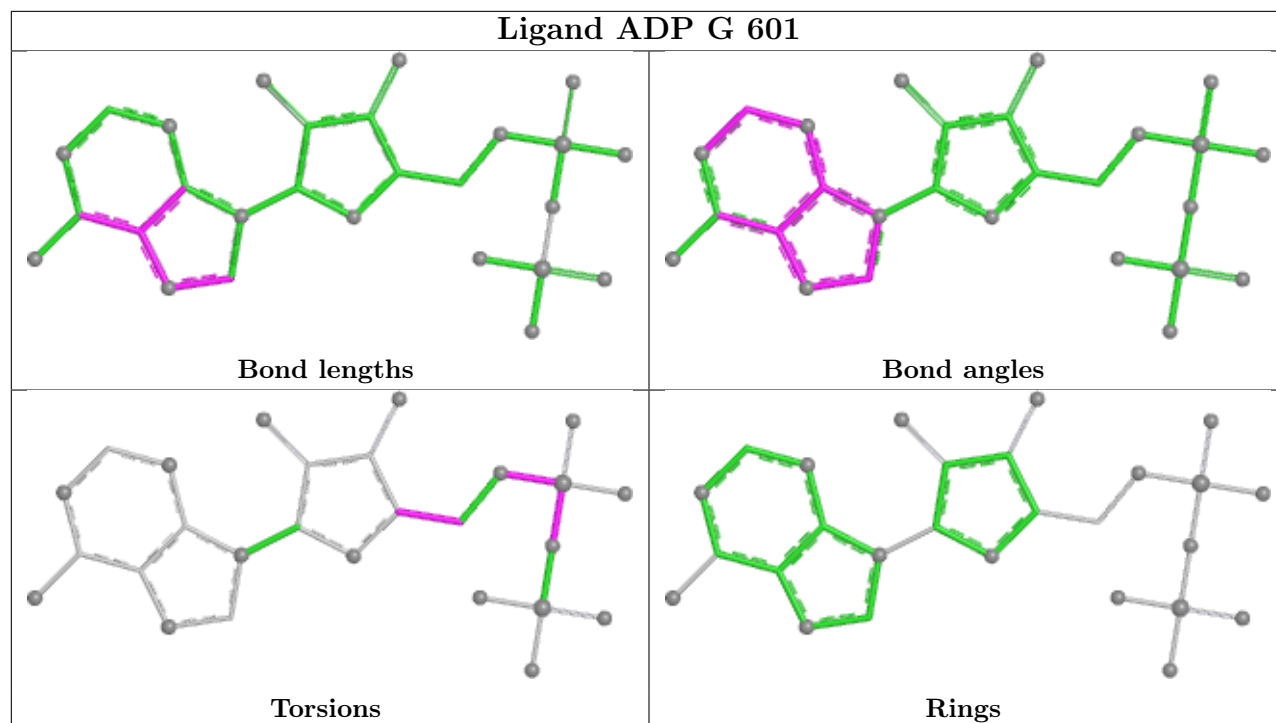
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



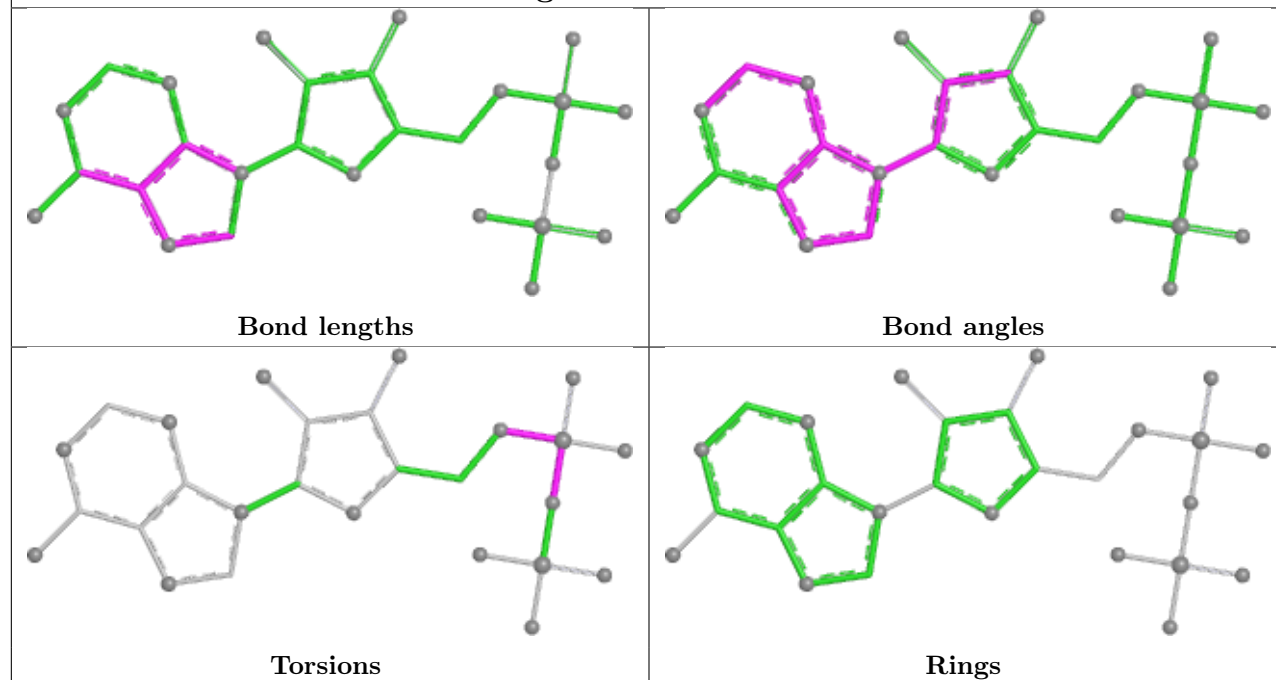




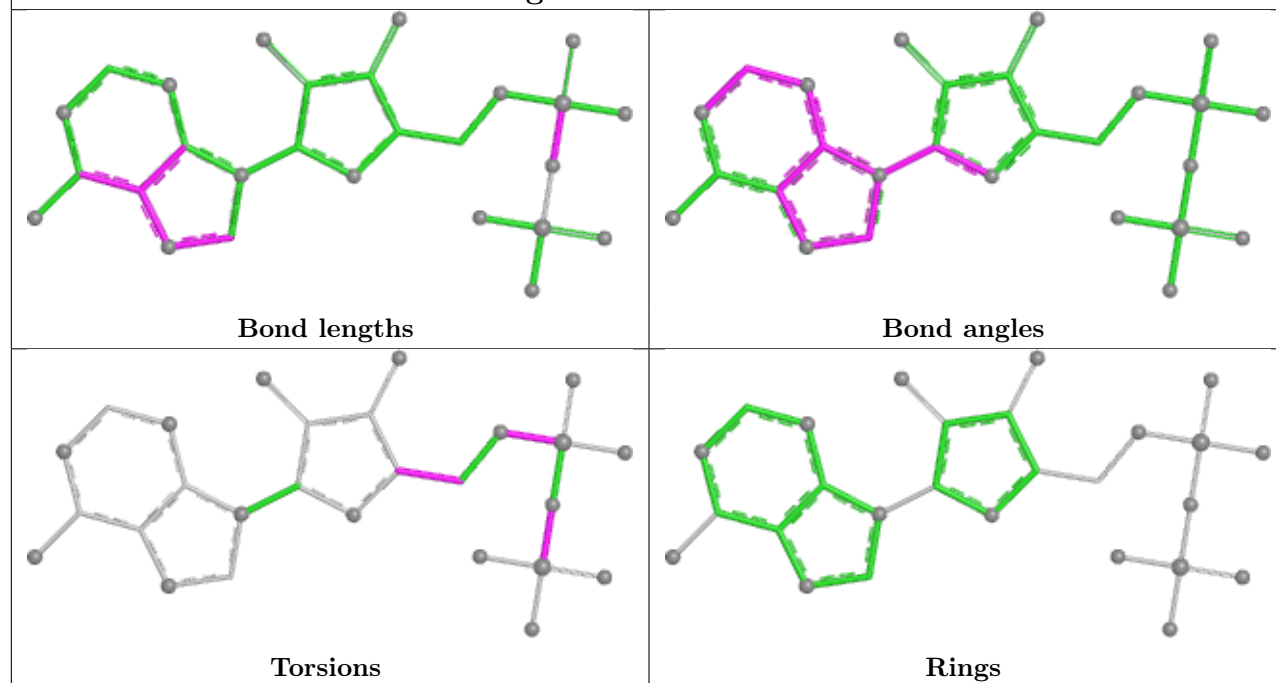


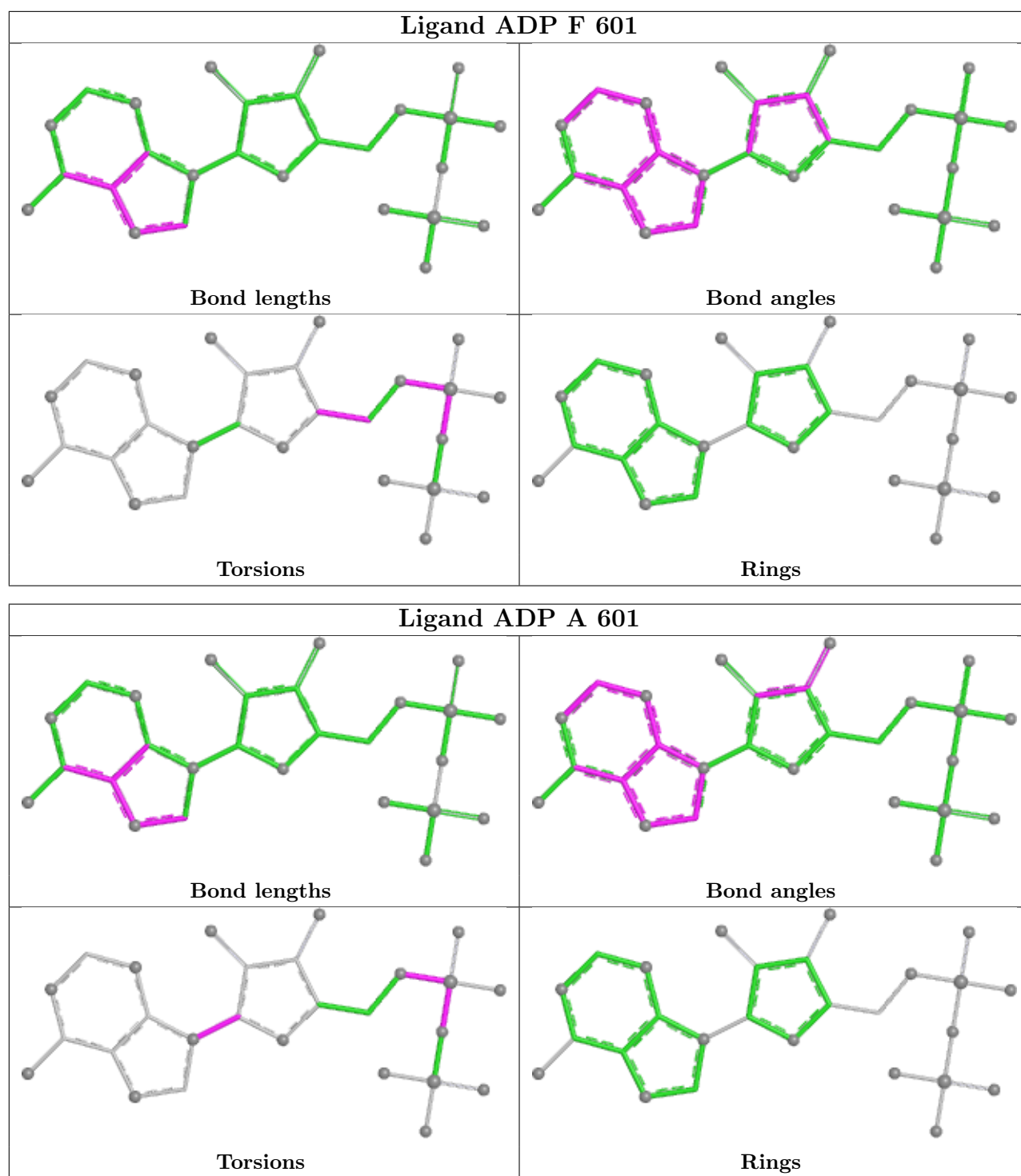


Ligand ADP I 601



Ligand ADP M 601





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	524/548 (95%)	-0.15	2 (0%) 88 71	48, 77, 200, 288	0
1	B	524/548 (95%)	-0.25	0 100 100	52, 85, 190, 249	0
1	C	524/548 (95%)	-0.25	1 (0%) 91 80	42, 86, 191, 259	0
1	D	524/548 (95%)	-0.23	1 (0%) 91 80	47, 75, 147, 200	0
1	E	524/548 (95%)	-0.25	0 100 100	51, 88, 197, 270	0
1	F	524/548 (95%)	-0.26	0 100 100	42, 81, 185, 243	0
1	G	524/548 (95%)	-0.24	0 100 100	36, 72, 192, 265	0
1	H	524/548 (95%)	-0.25	0 100 100	43, 89, 210, 243	0
1	I	524/548 (95%)	-0.22	0 100 100	55, 97, 207, 273	0
1	J	524/548 (95%)	-0.15	1 (0%) 91 80	50, 86, 206, 254	0
1	K	524/548 (95%)	-0.21	1 (0%) 91 80	43, 80, 200, 293	0
1	L	524/548 (95%)	-0.30	0 100 100	46, 86, 193, 240	0
1	M	524/548 (95%)	-0.26	0 100 100	45, 85, 198, 281	0
1	N	524/548 (95%)	-0.25	0 100 100	40, 75, 135, 186	0
2	1	97/97 (100%)	-0.01	0 100 100	81, 119, 204, 255	0
2	2	97/97 (100%)	-0.10	2 (2%) 63 38	73, 112, 188, 247	0
2	O	97/97 (100%)	0.01	2 (2%) 63 38	63, 100, 224, 270	0
2	P	97/97 (100%)	-0.09	1 (1%) 79 54	67, 102, 214, 254	0
2	Q	97/97 (100%)	-0.18	0 100 100	84, 122, 244, 275	0
2	R	97/97 (100%)	-0.02	2 (2%) 63 38	82, 121, 182, 198	0
2	S	97/97 (100%)	0.04	0 100 100	82, 132, 211, 243	0
2	T	97/97 (100%)	-0.01	1 (1%) 79 54	91, 144, 202, 233	0
2	U	97/97 (100%)	-0.07	0 100 100	88, 128, 223, 240	0
2	V	96/97 (98%)	-0.15	0 100 100	71, 125, 230, 288	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
2	W	96/97 (98%)	-0.11	0 100 100	63, 104, 204, 227	0
2	X	95/97 (97%)	-0.10	1 (1%) 78 52	56, 105, 213, 250	0
2	Y	96/97 (98%)	-0.18	0 100 100	83, 123, 214, 292	0
2	Z	97/97 (100%)	0.01	0 100 100	85, 127, 212, 253	0
All	All	8689/9030 (96%)	-0.21	15 (0%) 91 80	36, 91, 200, 293	0

The worst 5 of 15 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	O	97	ALA	3.7
1	K	238	GLU	3.5
2	2	25	ILE	3.0
2	T	25	ILE	2.9
2	2	26	VAL	2.8

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(Å ²)	Q<0.9
6	K	B	604	1/1	0.82	0.11	115,115,115,115	0
6	K	H	604	1/1	0.88	0.12	162,162,162,162	0
6	K	N	604	1/1	0.90	0.11	123,123,123,123	0
4	BEF	A	602	4/4	0.92	0.09	41,46,52,62	0
4	BEF	M	602	4/4	0.93	0.08	37,56,59,69	0
4	BEF	L	602	4/4	0.94	0.10	31,60,69,211	0
6	K	J	604	1/1	0.94	0.06	99,99,99,99	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	K	A	604	1/1	0.95	0.07	76,76,76,76	0
4	BEF	F	602	4/4	0.95	0.07	44,58,60,65	0
6	K	E	604	1/1	0.95	0.07	87,87,87,87	0
4	BEF	I	602	4/4	0.95	0.08	39,77,92,141	0
5	MG	A	603	1/1	0.95	0.10	27,27,27,27	0
5	MG	L	603	1/1	0.95	0.11	53,53,53,53	0
4	BEF	J	602	4/4	0.96	0.07	18,31,49,90	0
3	ADP	L	601	27/27	0.96	0.08	45,70,77,85	0
3	ADP	M	601	27/27	0.96	0.07	26,47,57,70	0
4	BEF	E	602	4/4	0.97	0.07	13,27,53,65	0
4	BEF	C	602	4/4	0.97	0.06	9,45,68,69	0
3	ADP	C	601	27/27	0.97	0.05	29,55,68,72	0
3	ADP	D	601	27/27	0.97	0.06	33,44,59,63	0
3	ADP	K	601	27/27	0.97	0.06	29,50,57,71	0
3	ADP	J	601	27/27	0.97	0.07	11,46,74,80	0
3	ADP	I	601	27/27	0.97	0.06	2,60,73,75	0
3	ADP	A	601	27/27	0.97	0.07	31,50,65,75	0
3	ADP	B	601	27/27	0.97	0.07	26,57,65,66	0
3	ADP	N	601	27/27	0.97	0.07	35,42,48,61	0
4	BEF	G	602	4/4	0.97	0.08	19,29,42,121	0
3	ADP	F	601	27/27	0.97	0.06	30,53,62,71	0
6	K	I	604	1/1	0.97	0.06	67,67,67,67	0
6	K	L	604	1/1	0.97	0.04	65,65,65,65	0
6	K	M	604	1/1	0.97	0.04	51,51,51,51	0
4	BEF	B	602	4/4	0.97	0.06	7,12,25,66	0
3	ADP	E	601	27/27	0.97	0.06	29,50,59,69	0
5	MG	M	603	1/1	0.98	0.06	8,8,8,8	0
6	K	G	604	1/1	0.98	0.04	51,51,51,51	0
4	BEF	D	602	4/4	0.98	0.05	30,30,35,51	0
4	BEF	K	602	4/4	0.98	0.07	19,25,82,105	0
6	K	F	604	1/1	0.98	0.05	81,81,81,81	0
4	BEF	H	602	4/4	0.98	0.05	12,21,33,89	0
6	K	D	604	1/1	0.98	0.07	63,63,63,63	0
4	BEF	N	602	4/4	0.98	0.07	12,28,34,74	0
5	MG	G	603	1/1	0.98	0.04	41,41,41,41	0
3	ADP	H	601	27/27	0.98	0.05	36,58,64,84	0
5	MG	D	603	1/1	0.98	0.05	16,16,16,16	0
5	MG	J	603	1/1	0.98	0.07	51,51,51,51	0
3	ADP	G	601	27/27	0.98	0.05	20,43,54,57	0
6	K	C	604	1/1	0.99	0.04	64,64,64,64	0
5	MG	H	603	1/1	0.99	0.02	44,44,44,44	0
6	K	K	604	1/1	0.99	0.04	47,47,47,47	0

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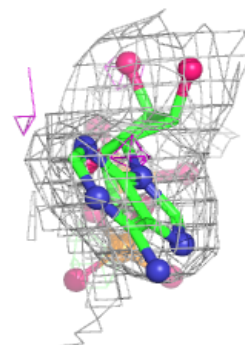
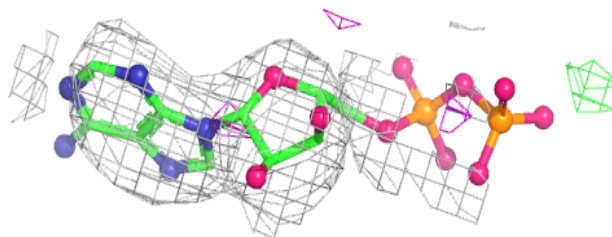
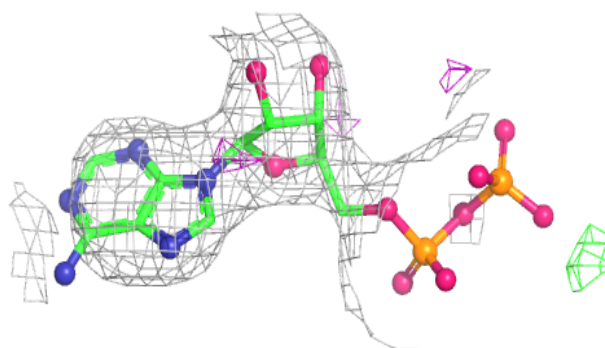
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	MG	N	603	1/1	0.99	0.07	11,11,11,11	0
5	MG	K	603	1/1	0.99	0.05	44,44,44,44	0
5	MG	E	603	1/1	0.99	0.04	11,11,11,11	0
5	MG	I	603	1/1	0.99	0.03	17,17,17,17	0
5	MG	C	603	1/1	0.99	0.04	21,21,21,21	0
5	MG	B	603	1/1	0.99	0.04	32,32,32,32	0
5	MG	F	603	1/1	1.00	0.03	33,33,33,33	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.

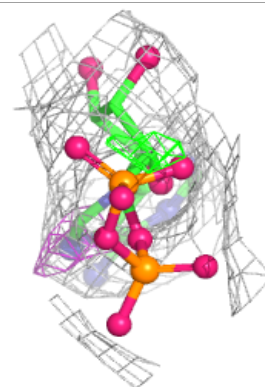
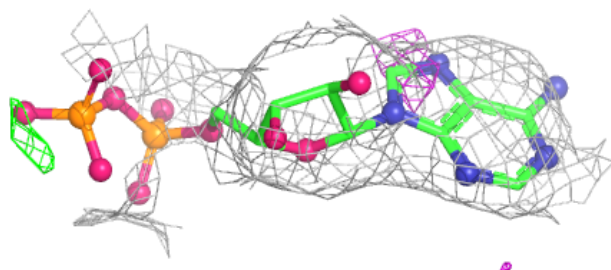
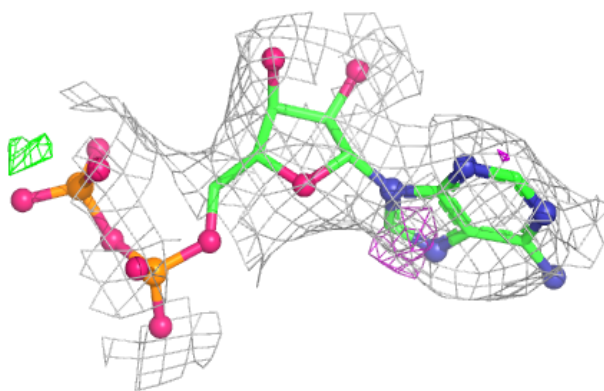
Electron density around ADP L 601:

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

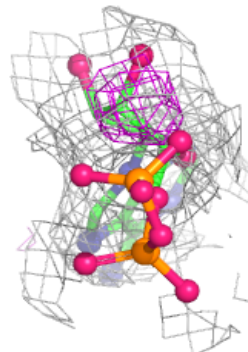
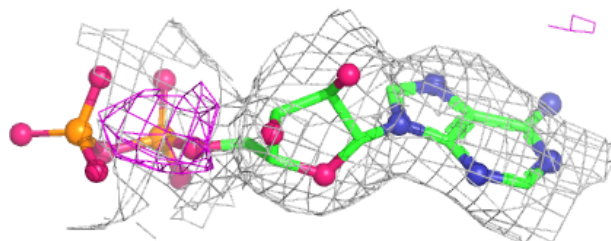
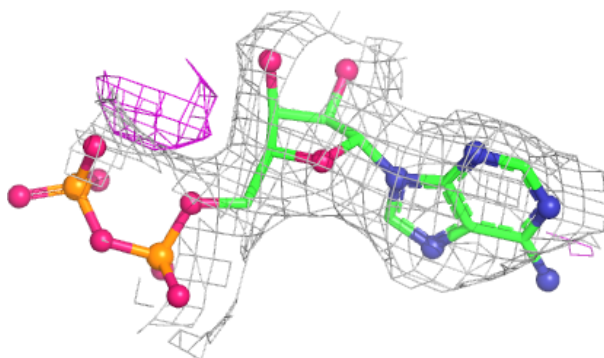


Electron density around ADP M 601:

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

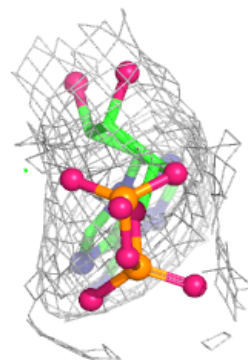
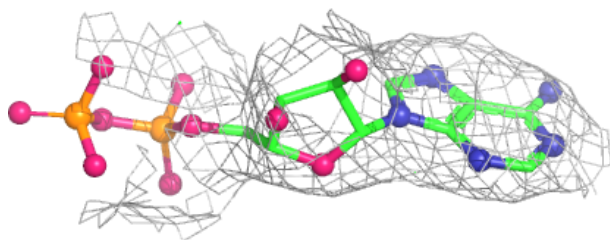
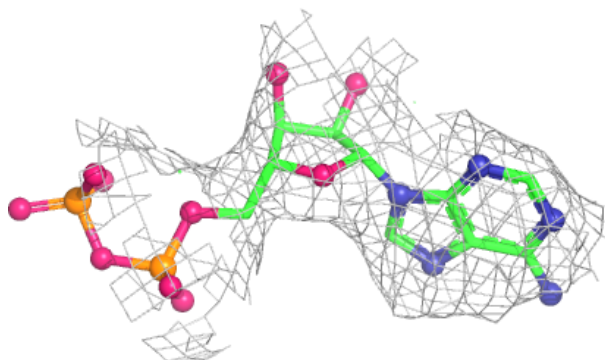
**Electron density around ADP C 601:**

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and green (positive)

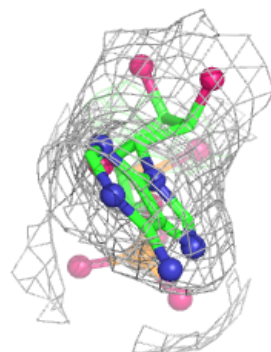
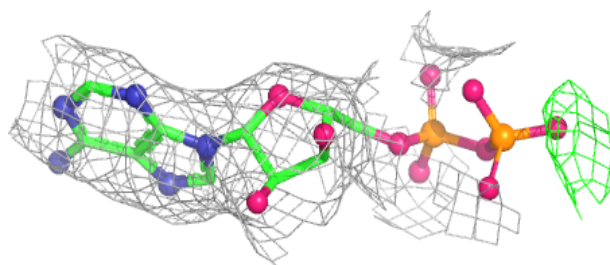
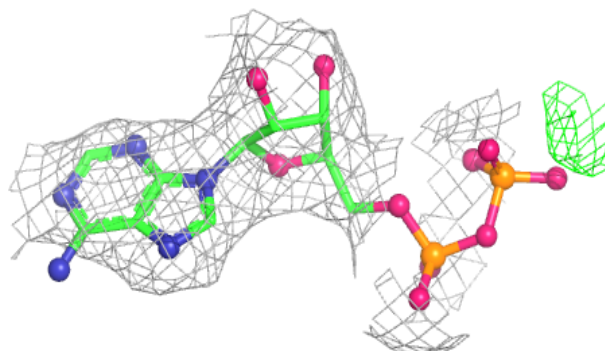


Electron density around ADP D 601:

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

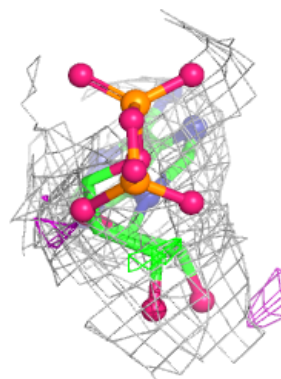
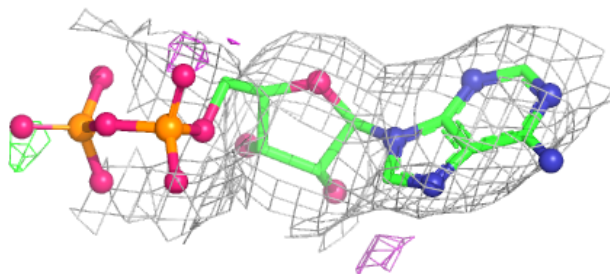
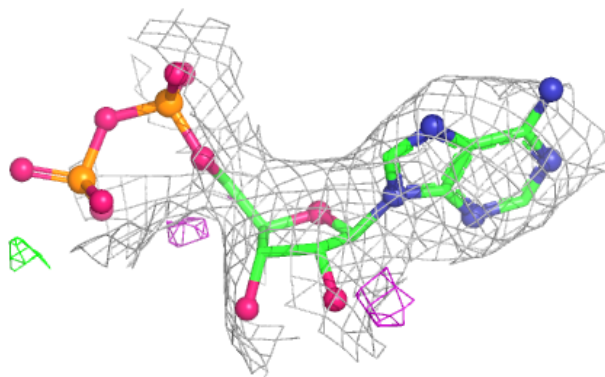
**Electron density around ADP K 601:**

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

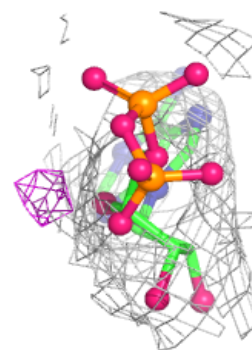
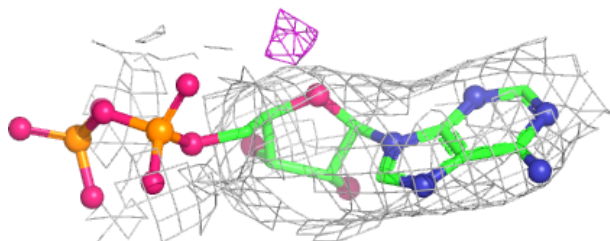
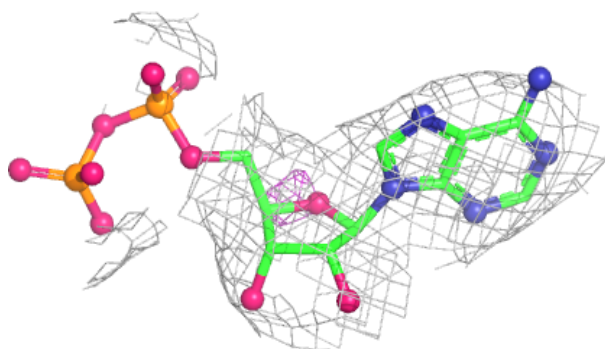


Electron density around ADP J 601:

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

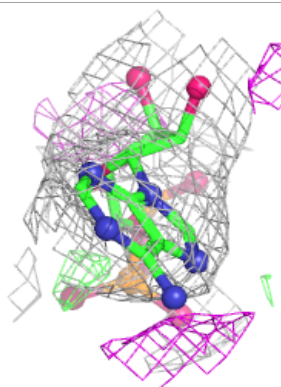
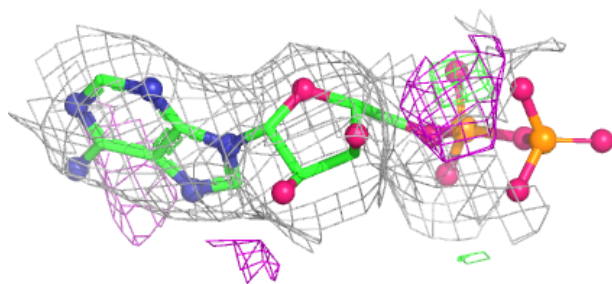
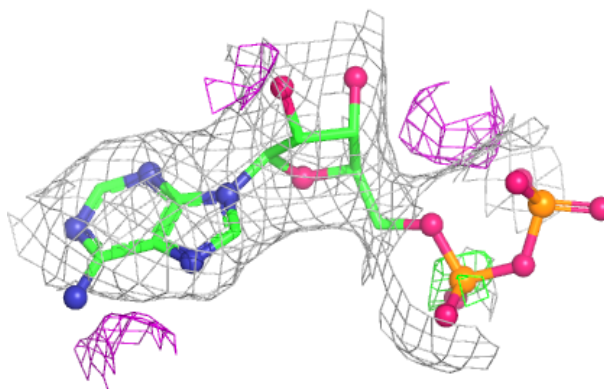
**Electron density around ADP I 601:**

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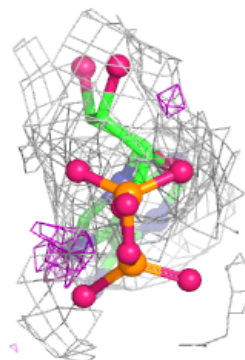
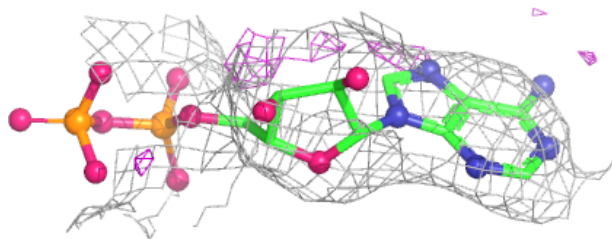
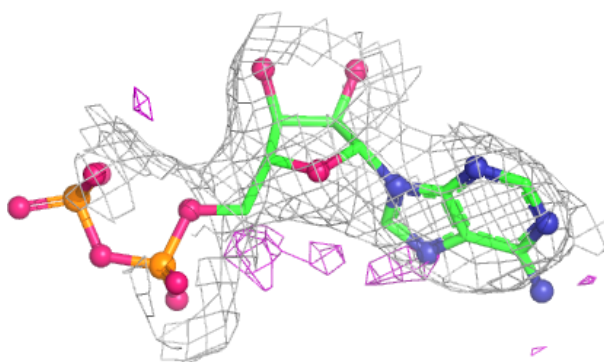


Electron density around ADP A 601:

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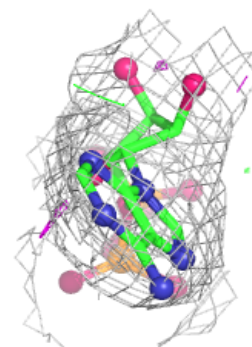
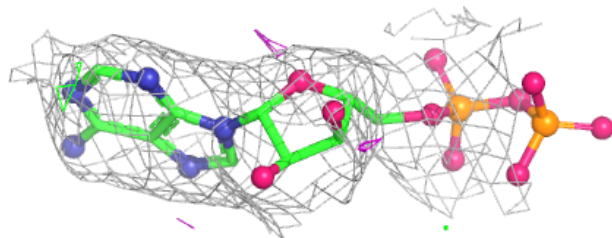
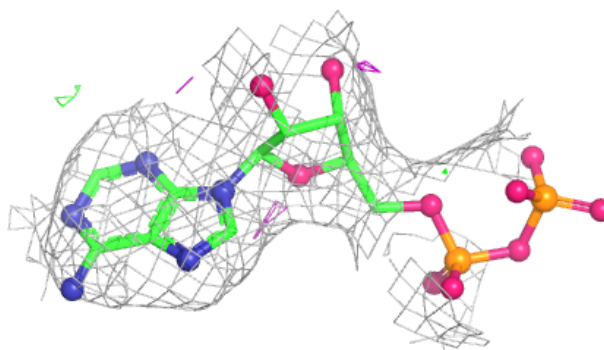
**Electron density around ADP B 601:**

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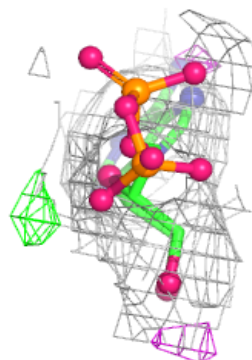
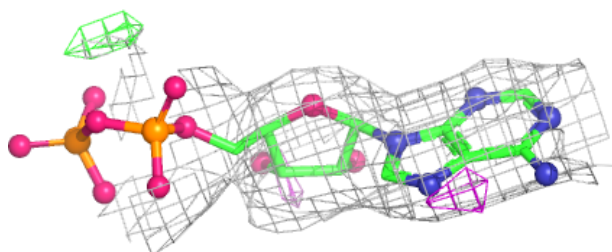
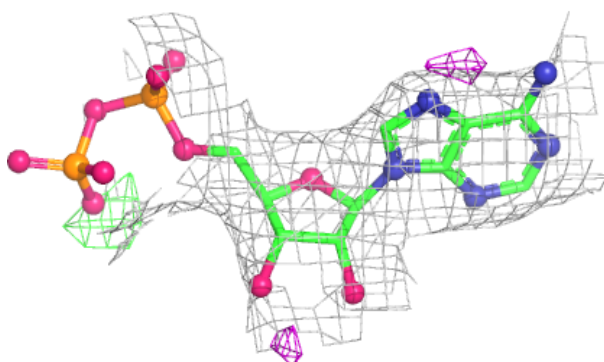


Electron density around ADP N 601:

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and green (positive)

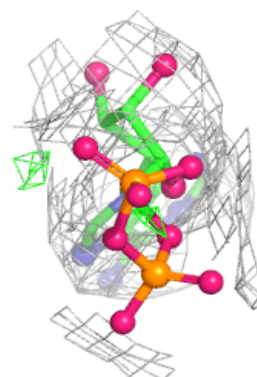
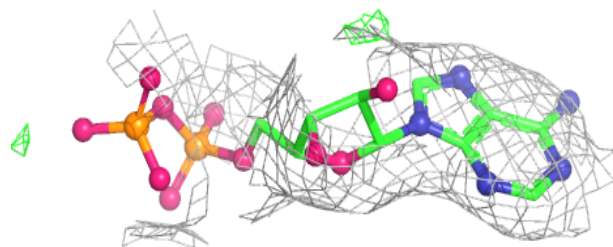
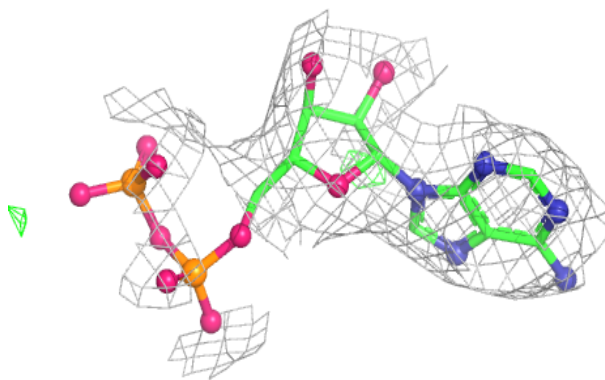
**Electron density around ADP F 601:**

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

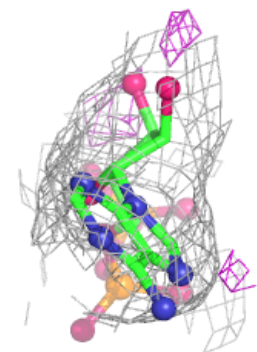
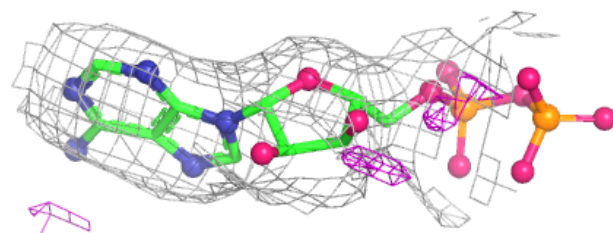
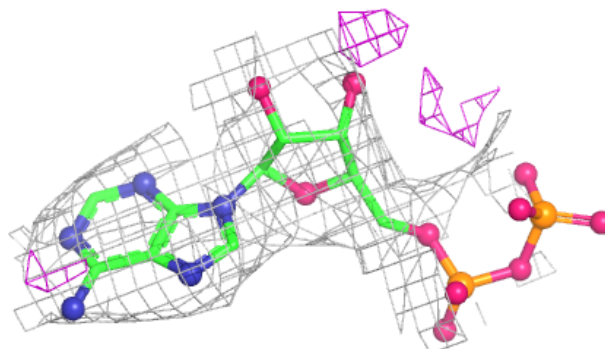


Electron density around ADP E 601:

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

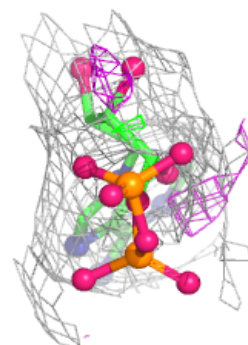
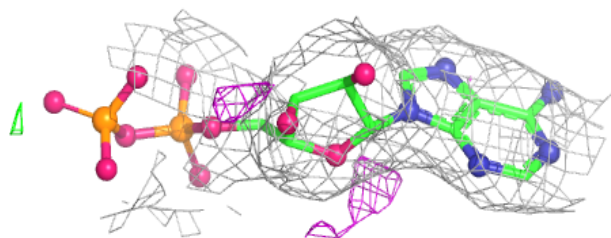
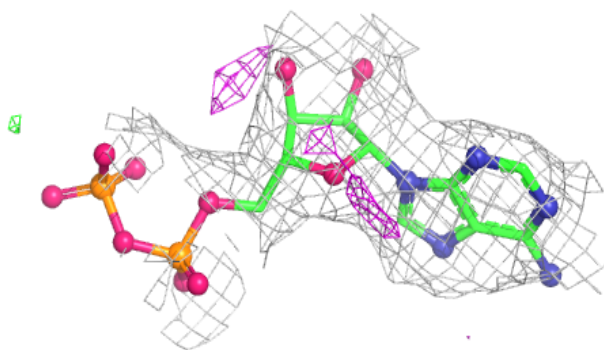
**Electron density around ADP H 601:**

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



Electron density around ADP 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.