



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 06:16 AM UTC

PDB ID : 4PKO / pdb_00004pko
Title : Crystal structure of the Football-shaped GroEL-GroES2-(ADPBeFx)₁₄ complex
Authors : Fei, X.; Ye, X.; Laronde-Leblanc, N.; Lorimer, G.H.
Deposited on : 2014-05-15
Resolution : 3.84 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

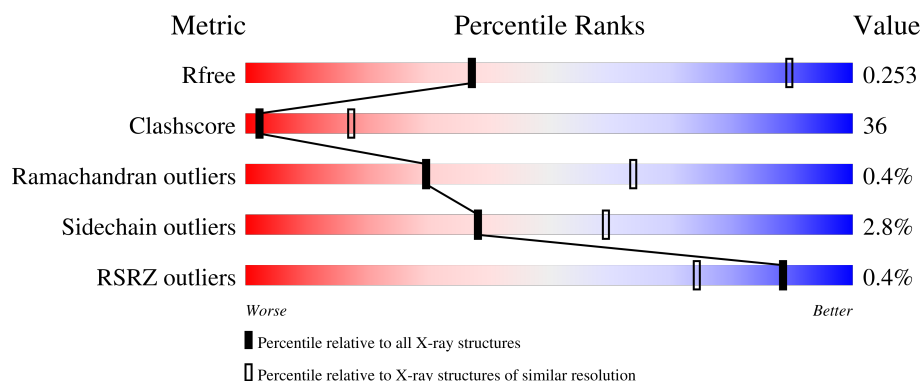
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.84 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	1169 (4.00-3.68)
Clashscore	190562	1211 (4.00-3.68)
Ramachandran outliers	187476	1156 (4.00-3.68)
Sidechain outliers	187428	1149 (4.00-3.68)
RSRZ outliers	180081	1168 (4.00-3.68)

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	 51% 42% ..
1	B	548	 48% 45% . .
1	C	548	 51% 43% ..
1	D	548	 55% 39% . .
1	E	548	 50% 42% . .

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Mol	Chain	Length	Quality of chain
1	F	548	% 50% 42% . .
1	G	548	% 49% 44% . .
1	H	548	50% 43% . .
1	I	548	50% 44% . .
1	J	548	52% 40% . .
1	K	548	% 52% 40% . .
1	L	548	47% 45% . .
1	M	548	51% 42% . .
1	N	548	43% 49% . .
2	1	97	% 44% 45% 6% .
2	2	97	% 49% 41% 9%
2	O	97	41% 54% . .
2	P	97	% 53% 41% 6%
2	Q	97	35% 55% 9% .
2	R	97	42% 51% 6% .
2	S	97	% 39% 53% 5% . .
2	T	97	% 38% 60% .
2	U	97	33% 62% 5%
2	V	97	38% 52% 9% .
2	W	97	% 43% 48% 8%
2	X	97	6% 52% 35% 11% .
2	Y	97	30% 65% . .
2	Z	97	40% 52% 6% .

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	A	602	-	-	X	-
4	BEF	B	602	-	-	X	-
4	BEF	C	602	-	-	X	-
4	BEF	H	602	-	-	X	-
4	BEF	I	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 64559 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.

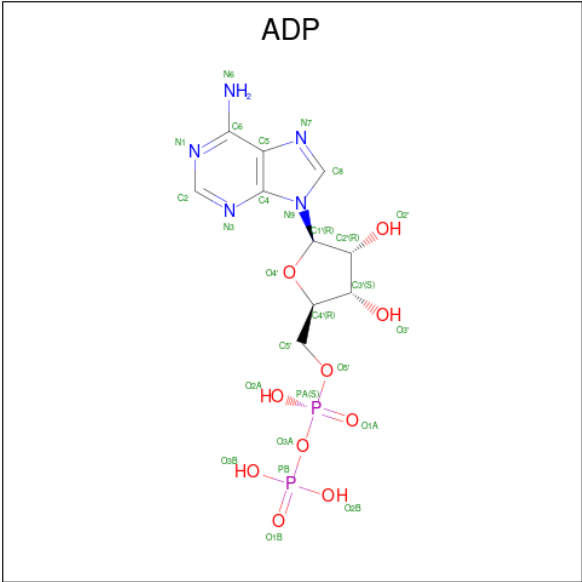
- Molecule 1 is a protein called 60 kDa chaperonin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	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	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	E	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	G	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	I	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	K	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	N	524	Total	C	N	O	S	0	0	0
			3855	2397	665	773	20			

- Molecule 2 is a protein called 10 kDa chaperonin.

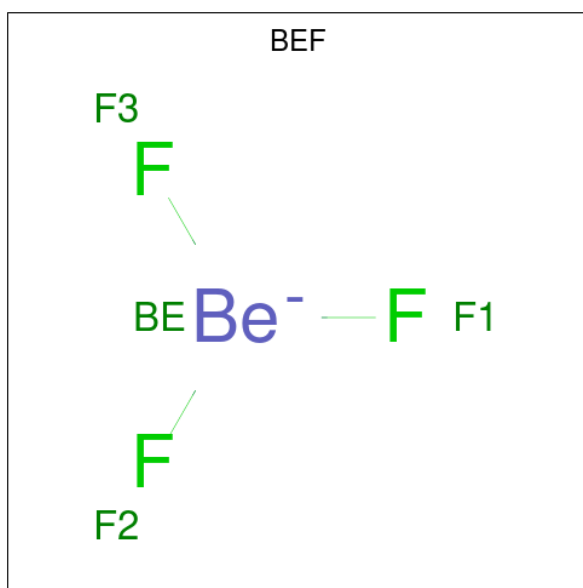
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	O	95	Total	C	N	O	S	0	0	0
			711	445	124	141	1			
2	P	97	Total	C	N	O	S	0	0	0
			727	454	127	144	2			
2	Q	96	Total	C	N	O	S	0	0	0
			719	449	126	143	1			
2	R	97	Total	C	N	O	S	0	0	0
			727	454	127	144	2			
2	S	96	Total	C	N	O	S	0	0	0
			719	449	126	143	1			
2	T	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	V	97	Total	C	N	O	S	0	0	0
			727	454	127	144	2			
2	W	97	Total	C	N	O	S	0	0	0
			727	454	127	144	2			
2	X	97	Total	C	N	O	S	0	0	0
			727	454	127	144	2			
2	Y	96	Total	C	N	O	S	0	0	0
			722	451	126	143	2			
2	Z	95	Total	C	N	O	S	0	0	0
			713	446	125	140	2			
2	1	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			

- 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	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	F	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	G	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	H	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	I	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	J	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	K	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	L	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	M	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	N	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

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



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

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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	A	1	Total	Mg	0	0
			1	1		
5	B	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	E	1	Total	Mg	0	0
			1	1		
5	F	1	Total	Mg	0	0
			1	1		
5	G	1	Total	Mg	0	0
			1	1		
5	H	1	Total	Mg	0	0
			1	1		
5	I	1	Total	Mg	0	0
			1	1		
5	J	1	Total	Mg	0	0
			1	1		
5	K	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	N	1	Total	Mg	0	0
			1	1		

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

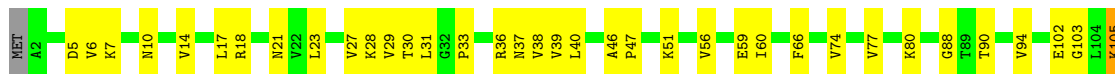
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	K	0	0
			1	1		
6	B	1	Total	K	0	0
			1	1		

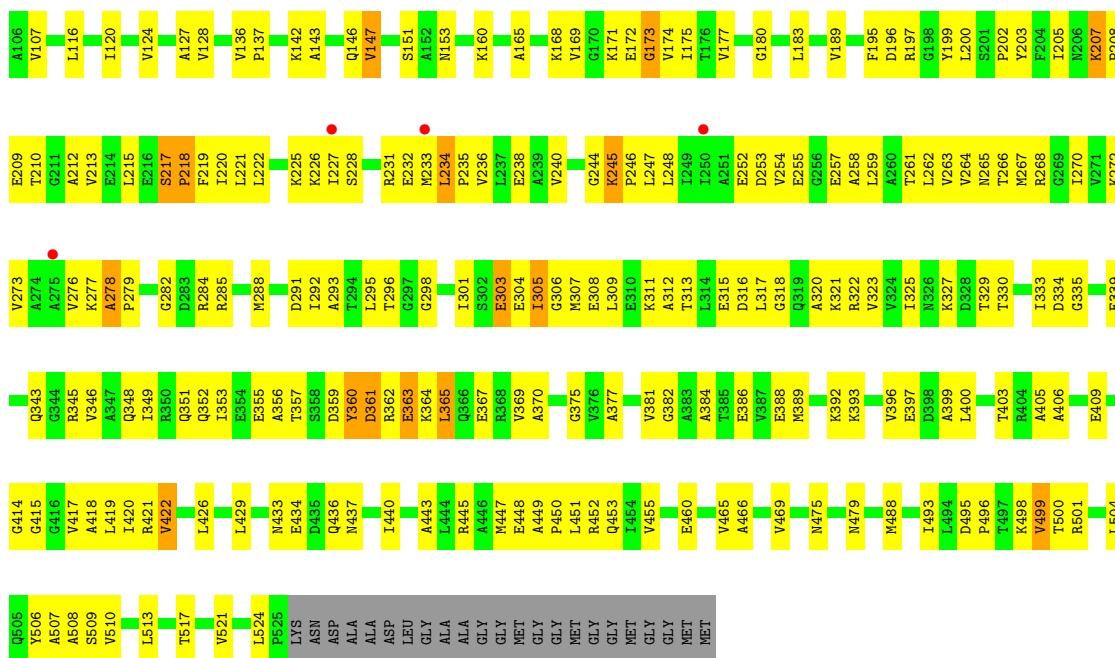
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	1	Total 1	K 1	0	0
6	D	1	Total 1	K 1	0	0
6	E	1	Total 1	K 1	0	0
6	F	1	Total 1	K 1	0	0
6	G	1	Total 1	K 1	0	0
6	H	1	Total 1	K 1	0	0
6	I	1	Total 1	K 1	0	0
6	J	1	Total 1	K 1	0	0
6	K	1	Total 1	K 1	0	0
6	L	1	Total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





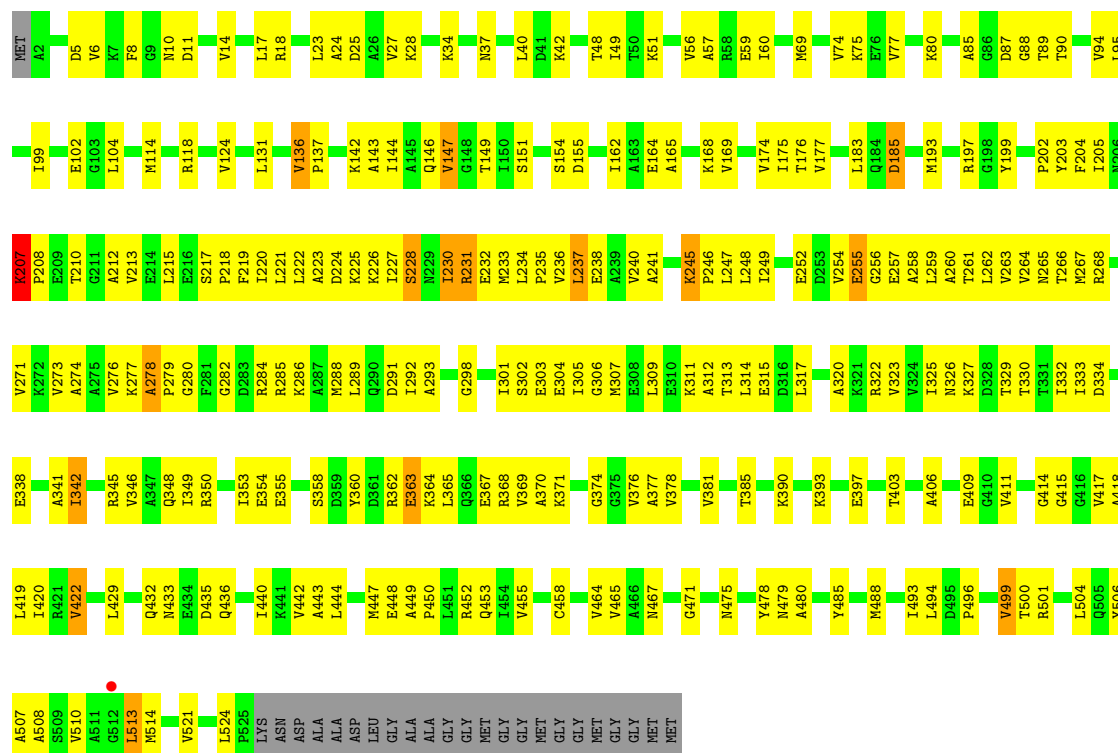


• Molecule 1: 60 kDa chaperonin



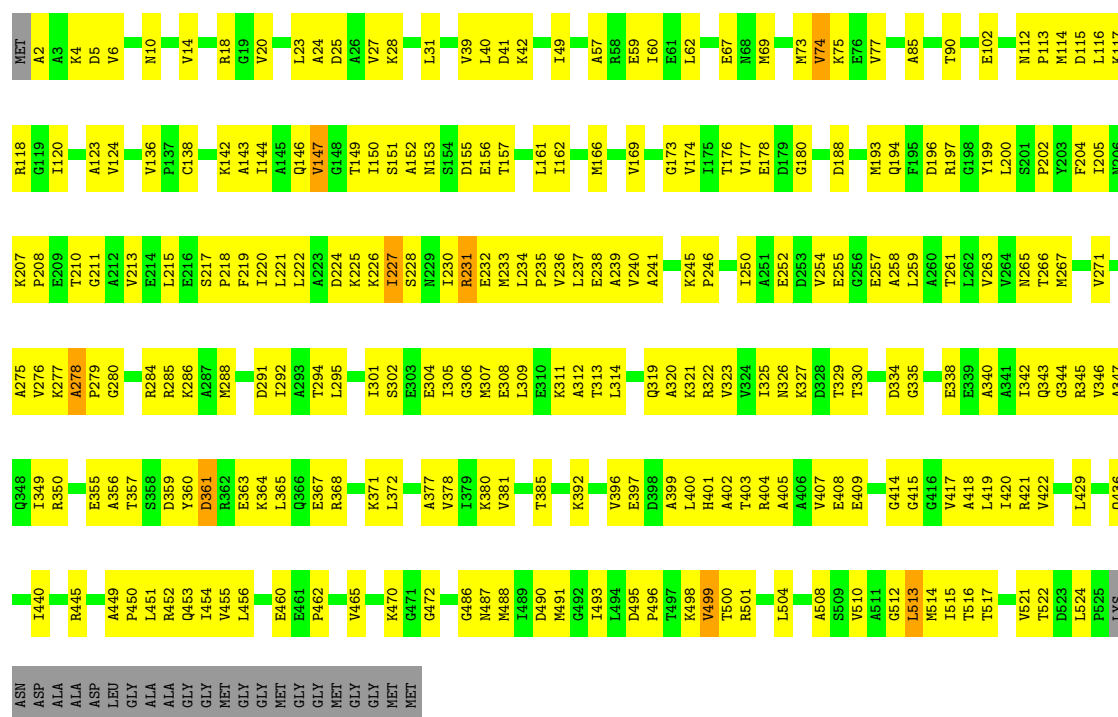
• Molecule 1: 60 kDa chaperonin





● Molecule 1: 60 kDa chaperonin

Chain I: 50% 44%

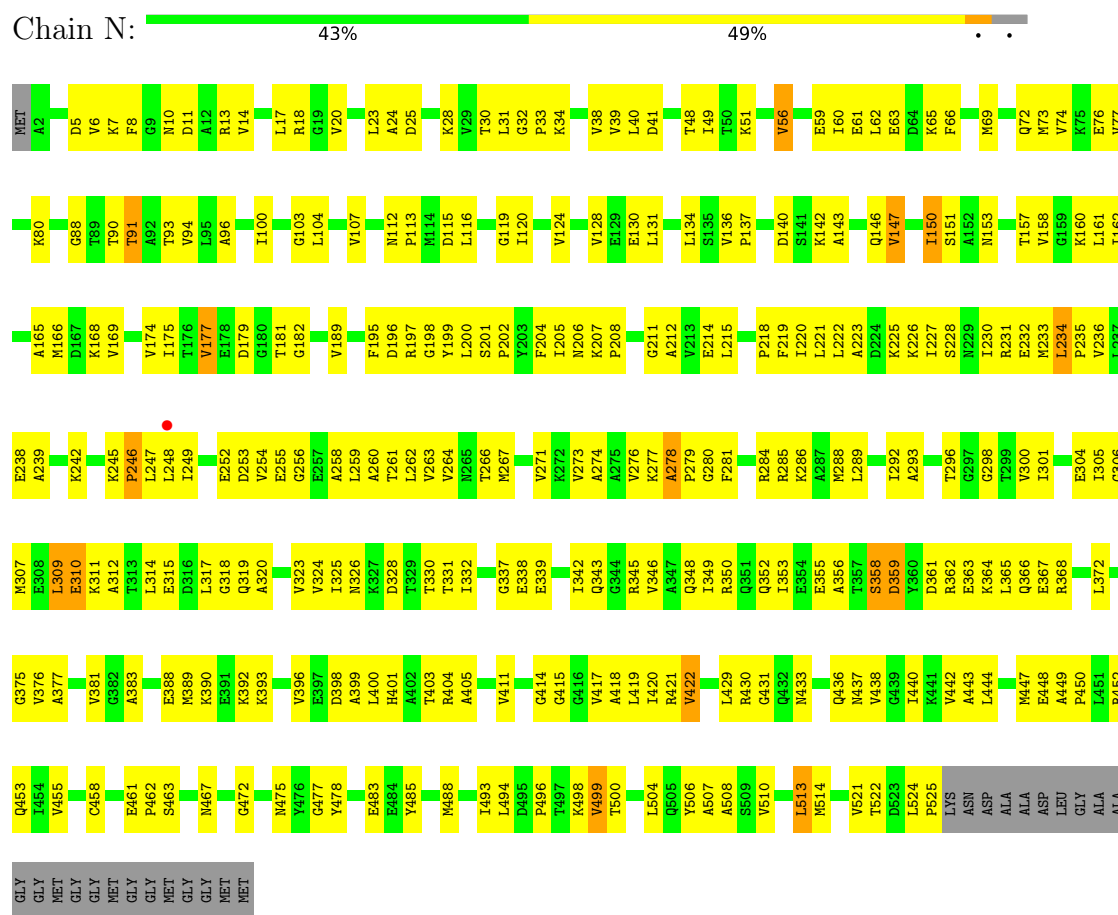


● Molecule 1: 60 kDa chaperonin

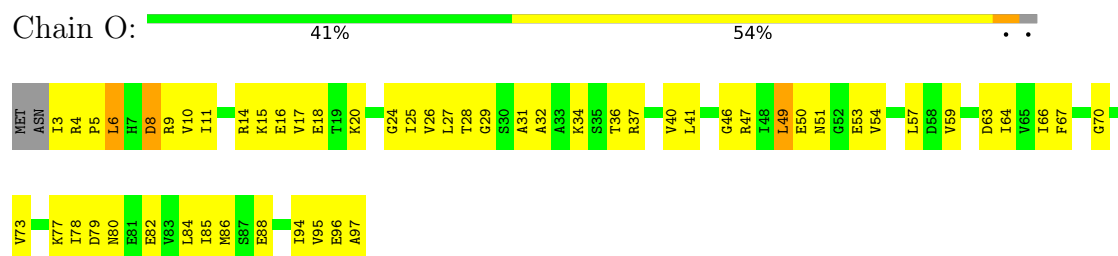




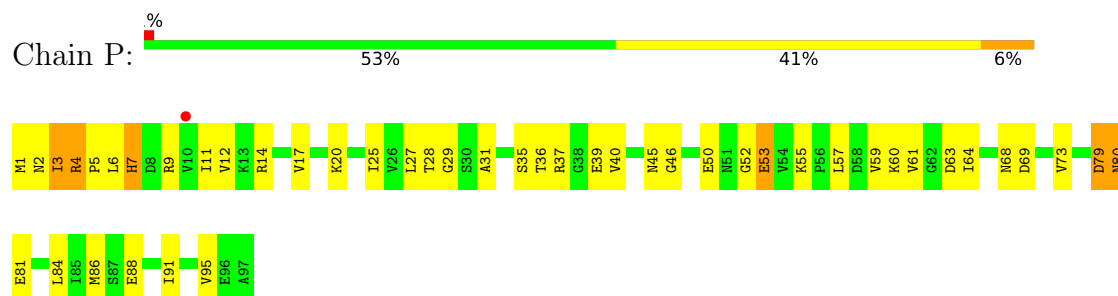
- Molecule 1: 60 kDa chaperonin



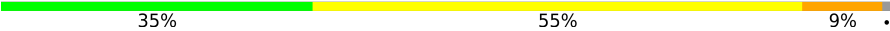
- Molecule 2: 10 kDa chaperonin



- Molecule 2: 10 kDa chaperonin

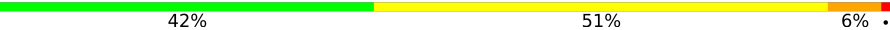


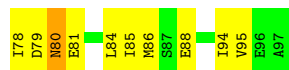
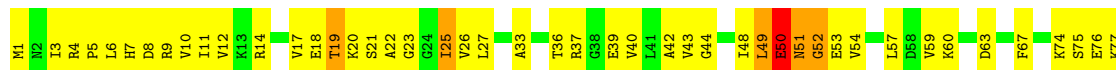
- Molecule 2: 10 kDa chaperonin

Chain Q:  35% 55% 9% .



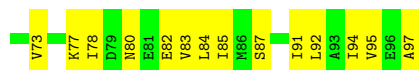
• Molecule 2: 10 kDa chaperonin

Chain R:  42% 51% 6% .



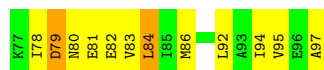
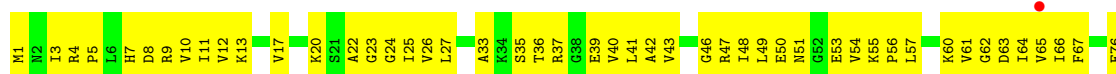
• Molecule 2: 10 kDa chaperonin

Chain S:  39% 53% 5% ..



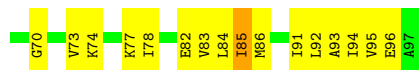
• Molecule 2: 10 kDa chaperonin

Chain T:  38% 60% .

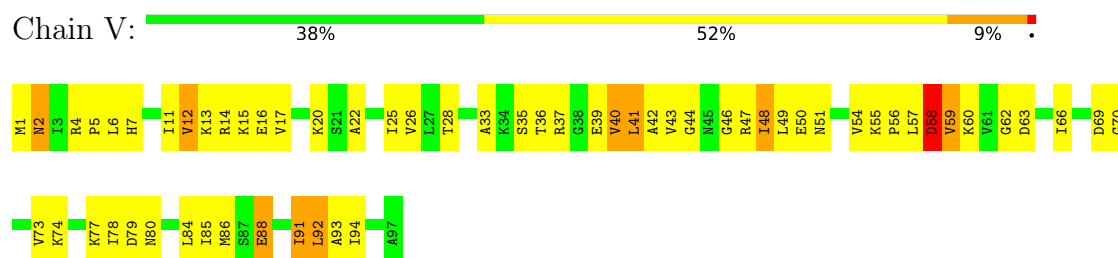


• Molecule 2: 10 kDa chaperonin

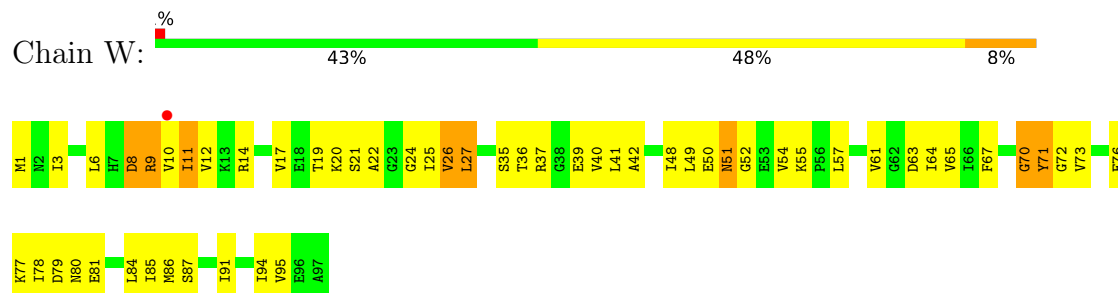
Chain U:  33% 62% 5%



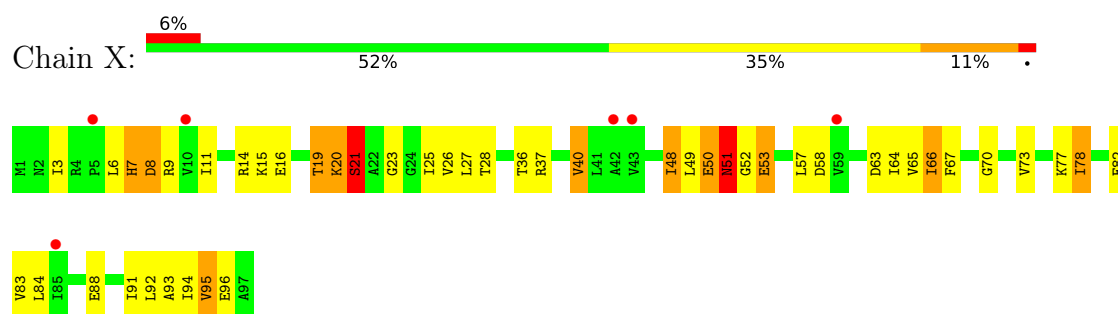
- Molecule 2: 10 kDa chaperonin



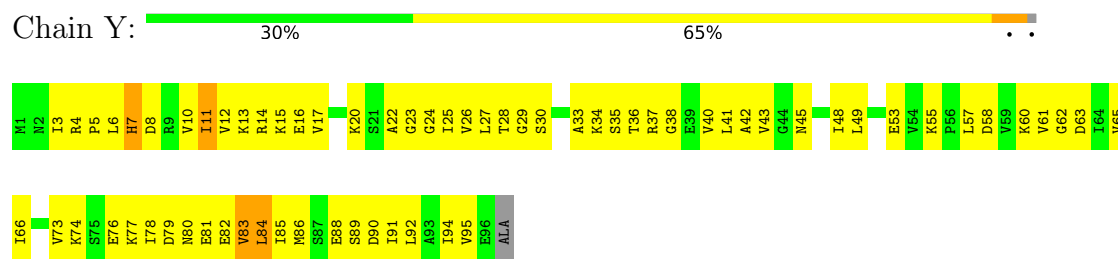
- Molecule 2: 10 kDa chaperonin



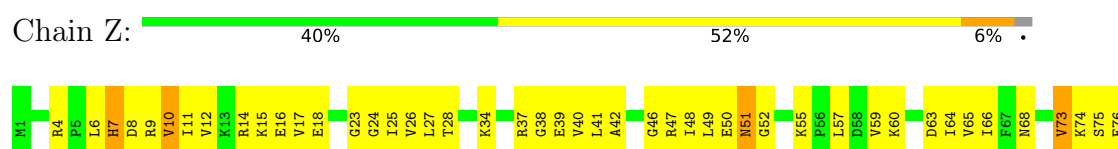
- Molecule 2: 10 kDa chaperonin



- Molecule 2: 10 kDa chaperonin



- Molecule 2: 10 kDa chaperonin

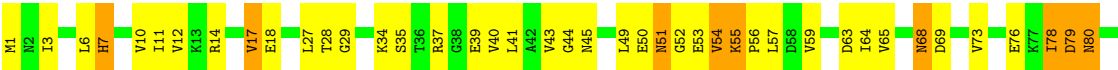




● Molecule 2: 10 kDa chaperonin



● Molecule 2: 10 kDa chaperonin



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	169.79Å 174.49Å 410.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	90.90 – 3.84 90.90 – 3.84	Depositor EDS
% Data completeness (in resolution range)	99.9 (90.90-3.84) 99.9 (90.90-3.84)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.72 (at 3.89Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.183 , 0.248 0.189 , 0.253	Depositor DCC
R_{free} test set	1271 reflections (1.09%)	wwPDB-VP
Wilson B-factor (Å ²)	114.0	Xtriage
Anisotropy	0.331	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 154.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.118 for k,h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	64559	wwPDB-VP
Average B, all atoms (Å ²)	160.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.24% 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: ADP, K, MG, 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	0.43	3/3883 (0.1%)	0.98	18/5243 (0.3%)
1	B	0.37	2/3883 (0.1%)	0.93	17/5243 (0.3%)
1	C	0.39	2/3883 (0.1%)	0.91	11/5243 (0.2%)
1	D	0.35	0/3883	0.90	10/5243 (0.2%)
1	E	0.46	3/3883 (0.1%)	1.00	27/5243 (0.5%)
1	F	0.35	1/3883 (0.0%)	0.93	16/5243 (0.3%)
1	G	0.38	2/3883 (0.1%)	0.92	16/5243 (0.3%)
1	H	0.33	0/3883	0.89	8/5243 (0.2%)
1	I	0.35	0/3883	0.89	4/5243 (0.1%)
1	J	0.38	1/3883 (0.0%)	0.98	20/5243 (0.4%)
1	K	0.37	1/3883 (0.0%)	0.94	15/5243 (0.3%)
1	L	0.36	0/3883	1.01	21/5243 (0.4%)
1	M	0.37	2/3883 (0.1%)	0.92	13/5243 (0.2%)
1	N	0.32	1/3883 (0.0%)	0.80	9/5243 (0.2%)
2	1	0.58	2/731 (0.3%)	1.19	8/983 (0.8%)
2	2	0.35	0/731	0.99	6/983 (0.6%)
2	O	0.34	0/715	0.95	1/962 (0.1%)
2	P	0.39	1/731 (0.1%)	0.98	7/983 (0.7%)
2	Q	0.37	0/723	1.06	7/973 (0.7%)
2	R	0.34	0/731	0.91	3/983 (0.3%)
2	S	0.42	0/723	0.91	1/973 (0.1%)
2	T	0.29	0/731	0.79	1/983 (0.1%)
2	U	0.39	0/731	0.84	1/983 (0.1%)
2	V	0.40	1/731 (0.1%)	1.17	12/983 (1.2%)
2	W	0.42	1/731 (0.1%)	1.05	6/983 (0.6%)
2	X	0.68	3/731 (0.4%)	1.41	12/983 (1.2%)
2	Y	0.36	0/726	1.07	7/976 (0.7%)
2	Z	0.36	0/717	0.82	1/964 (0.1%)
All	All	0.38	26/64545 (0.0%)	0.95	278/87097 (0.3%)

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

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	D	0	1
2	1	0	2
2	S	0	1
All	All	0	5

The worst 5 of 26 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	171	LYS	CA-C	12.52	1.69	1.52
1	C	171	LYS	CA-C	11.71	1.68	1.52
2	1	8	ASP	CA-C	11.02	1.67	1.52
2	X	51	ASN	CA-C	10.80	1.67	1.52
1	A	246	PRO	N-CD	-10.66	1.32	1.47

The worst 5 of 278 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	X	21	SER	N-CA-C	16.75	146.49	110.80
1	A	310	GLU	N-CA-C	15.55	132.00	113.18
1	E	172	GLU	N-CA-C	14.12	129.96	113.01
2	X	7	HIS	CB-CA-C	-13.38	101.16	116.54
1	E	360	TYR	N-CA-C	12.48	126.30	111.82

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	1	50	GLU	Peptide
2	1	6	LEU	Peptide
1	A	179	ASP	Peptide
1	D	232	GLU	Peptide
2	S	50	GLU	Peptide

5.2 Too-close contacts

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

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3855	0	3974	278	0
1	B	3855	0	3975	296	5
1	C	3855	0	3974	273	0
1	D	3855	0	3975	231	0
1	E	3855	0	3976	285	0
1	F	3855	0	3975	260	0
1	G	3855	0	3975	294	2
1	H	3855	0	3975	294	0
1	I	3855	0	3976	263	0
1	J	3855	0	3976	253	0
1	K	3855	0	3976	238	12
1	L	3855	0	3975	286	1
1	M	3855	0	3974	259	7
1	N	3855	0	3976	325	0
2	1	727	0	762	71	1
2	2	727	0	762	75	1
2	O	711	0	744	91	0
2	P	727	0	762	73	2
2	Q	719	0	750	74	0
2	R	727	0	762	108	0
2	S	719	0	750	88	0
2	T	727	0	762	80	1
2	U	727	0	762	107	0
2	V	727	0	762	92	0
2	W	727	0	762	82	0
2	X	727	0	762	68	0
2	Y	722	0	757	87	0
2	Z	713	0	751	92	0
3	A	27	0	12	1	0
3	B	27	0	12	5	0
3	C	27	0	12	4	0
3	D	27	0	12	4	0
3	E	27	0	12	4	0
3	F	27	0	12	4	0
3	G	27	0	12	5	0
3	H	27	0	12	2	0
3	I	27	0	12	3	0
3	J	27	0	12	1	0
3	K	27	0	12	4	0
3	L	27	0	12	2	0
3	M	27	0	12	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	N	27	0	12	5	0
4	A	4	0	0	2	0
4	B	4	0	0	3	0
4	C	4	0	0	4	0
4	D	4	0	0	1	0
4	E	4	0	0	1	0
4	F	4	0	0	1	0
4	G	4	0	0	1	0
4	H	4	0	0	4	0
4	I	4	0	0	4	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	3	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	N	1	0	0	0	0
All	All	64559	0	66430	4705	16

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 36.

The worst 5 of 4705 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:95:VAL:HA	2:P:3:ILE:CG2	1.26	1.56
1:K:207:LYS:CG	1:K:208:PRO:HD3	1.46	1.42
2:O:95:VAL:CA	2:P:3:ILE:HG22	1.52	1.37
1:F:218:PRO:O	1:F:219:PHE:CD1	1.81	1.33
2:V:56:PRO:O	2:V:57:LEU:HG	1.26	1.32

The worst 5 of 16 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:339:GLU:OE2	1:K:207:LYS:NZ[1_545]	0.50	1.70
1:K:430:ARG:CG	1:M:245:LYS:NZ[4_565]	0.86	1.34
1:B:339:GLU:CD	1:K:207:LYS:NZ[1_545]	1.06	1.14
1:K:430:ARG:CB	1:M:245:LYS:NZ[4_565]	1.09	1.11
1:B:339:GLU:OE2	1:K:207:LYS:CE[1_545]	1.58	0.62

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%)	496 (95%)	23 (4%)	3 (1%)	21 55
1	B	522/548 (95%)	499 (96%)	21 (4%)	2 (0%)	30 64

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	522/548 (95%)	509 (98%)	13 (2%)	0	100	100
1	D	522/548 (95%)	502 (96%)	19 (4%)	1 (0%)	43	74
1	E	522/548 (95%)	500 (96%)	18 (3%)	4 (1%)	16	50
1	F	522/548 (95%)	504 (97%)	16 (3%)	2 (0%)	30	64
1	G	522/548 (95%)	508 (97%)	12 (2%)	2 (0%)	30	64
1	H	522/548 (95%)	502 (96%)	19 (4%)	1 (0%)	43	74
1	I	522/548 (95%)	507 (97%)	14 (3%)	1 (0%)	43	74
1	J	522/548 (95%)	503 (96%)	17 (3%)	2 (0%)	30	64
1	K	522/548 (95%)	507 (97%)	15 (3%)	0	100	100
1	L	522/548 (95%)	504 (97%)	18 (3%)	0	100	100
1	M	522/548 (95%)	503 (96%)	16 (3%)	3 (1%)	21	55
1	N	522/548 (95%)	503 (96%)	19 (4%)	0	100	100
2	1	95/97 (98%)	87 (92%)	4 (4%)	4 (4%)	2	20
2	2	95/97 (98%)	87 (92%)	7 (7%)	1 (1%)	11	43
2	O	93/97 (96%)	89 (96%)	4 (4%)	0	100	100
2	P	95/97 (98%)	86 (90%)	9 (10%)	0	100	100
2	Q	94/97 (97%)	84 (89%)	9 (10%)	1 (1%)	11	43
2	R	95/97 (98%)	88 (93%)	6 (6%)	1 (1%)	11	43
2	S	94/97 (97%)	83 (88%)	10 (11%)	1 (1%)	11	43
2	T	95/97 (98%)	90 (95%)	5 (5%)	0	100	100
2	U	95/97 (98%)	85 (90%)	8 (8%)	2 (2%)	5	32
2	V	95/97 (98%)	89 (94%)	5 (5%)	1 (1%)	11	43
2	W	95/97 (98%)	84 (88%)	10 (10%)	1 (1%)	11	43
2	X	95/97 (98%)	87 (92%)	6 (6%)	2 (2%)	5	32
2	Y	94/97 (97%)	90 (96%)	4 (4%)	0	100	100
2	Z	93/97 (96%)	89 (96%)	4 (4%)	0	100	100
All	All	8631/9030 (96%)	8265 (96%)	331 (4%)	35 (0%)	30	64

5 of 35 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	233	MET
1	E	233	MET

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Mol	Chain	Res	Type
1	E	234	LEU
1	M	270	ILE
2	R	50	GLU

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%)	398 (98%)	6 (2%)	57	69
1	B	404/415 (97%)	396 (98%)	8 (2%)	48	65
1	C	404/415 (97%)	397 (98%)	7 (2%)	53	68
1	D	404/415 (97%)	396 (98%)	8 (2%)	48	65
1	E	404/415 (97%)	397 (98%)	7 (2%)	53	68
1	F	404/415 (97%)	395 (98%)	9 (2%)	45	64
1	G	404/415 (97%)	397 (98%)	7 (2%)	53	68
1	H	404/415 (97%)	392 (97%)	12 (3%)	36	57
1	I	404/415 (97%)	396 (98%)	8 (2%)	48	65
1	J	404/415 (97%)	392 (97%)	12 (3%)	36	57
1	K	404/415 (97%)	395 (98%)	9 (2%)	45	64
1	L	404/415 (97%)	394 (98%)	10 (2%)	42	62
1	M	404/415 (97%)	397 (98%)	7 (2%)	53	68
1	N	404/415 (97%)	387 (96%)	17 (4%)	26	51
2	1	80/80 (100%)	76 (95%)	4 (5%)	22	47
2	2	80/80 (100%)	75 (94%)	5 (6%)	16	43
2	O	78/80 (98%)	75 (96%)	3 (4%)	29	53
2	P	80/80 (100%)	77 (96%)	3 (4%)	29	53
2	Q	79/80 (99%)	75 (95%)	4 (5%)	21	47
2	R	80/80 (100%)	75 (94%)	5 (6%)	16	43
2	S	79/80 (99%)	72 (91%)	7 (9%)	9	32

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	T	80/80 (100%)	77 (96%)	3 (4%)	29	53
2	U	80/80 (100%)	77 (96%)	3 (4%)	29	53
2	V	80/80 (100%)	75 (94%)	5 (6%)	16	43
2	W	80/80 (100%)	75 (94%)	5 (6%)	16	43
2	X	80/80 (100%)	73 (91%)	7 (9%)	9	33
2	Y	80/80 (100%)	76 (95%)	4 (5%)	22	47
2	Z	79/80 (99%)	73 (92%)	6 (8%)	12	38
All	All	6771/6930 (98%)	6580 (97%)	191 (3%)	38	59

5 of 191 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	N	147	VAL
2	S	40	VAL
1	N	234	LEU
2	P	3	ILE
2	T	79	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 42 such sidechains are listed below:

Mol	Chain	Res	Type
1	K	475	ASN
1	N	10	ASN
1	L	82	ASN
1	M	10	ASN
2	O	7	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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
4	BEF	F	602	-	0,3,3	-	-	-		
4	BEF	M	602	-	0,3,3	-	-	-		
3	ADP	I	601	6,5	28,29,29	1.35	5 (17%)	43,45,45	1.87	10 (23%)
4	BEF	C	602	-	0,3,3	-	-	-		
4	BEF	B	602	-	0,3,3	-	-	-		
3	ADP	G	601	6,5	28,29,29	1.45	5 (17%)	43,45,45	1.91	10 (23%)
3	ADP	A	601	6,5,4	28,29,29	1.44	5 (17%)	43,45,45	1.89	11 (25%)
3	ADP	C	601	6,5	28,29,29	1.41	5 (17%)	43,45,45	1.90	8 (18%)
4	BEF	L	602	-	0,3,3	-	-	-		
4	BEF	A	602	3	0,3,3	-	-	-		
4	BEF	K	602	-	0,3,3	-	-	-		
3	ADP	L	601	6,5	28,29,29	1.37	4 (14%)	43,45,45	1.93	12 (27%)
3	ADP	H	601	6,5	28,29,29	1.40	5 (17%)	43,45,45	1.89	11 (25%)
4	BEF	J	602	-	0,3,3	-	-	-		
3	ADP	N	601	6,5	28,29,29	1.41	5 (17%)	43,45,45	1.87	11 (25%)
4	BEF	N	602	-	0,3,3	-	-	-		
3	ADP	M	601	6,5	28,29,29	1.41	5 (17%)	43,45,45	1.88	10 (23%)
4	BEF	E	602	-	0,3,3	-	-	-		
3	ADP	B	601	6,5	28,29,29	1.44	6 (21%)	43,45,45	1.86	9 (20%)
3	ADP	J	601	6,5	28,29,29	1.43	5 (17%)	43,45,45	1.93	12 (27%)
4	BEF	H	602	-	0,3,3	-	-	-		
4	BEF	G	602	-	0,3,3	-	-	-		
4	BEF	D	602	-	0,3,3	-	-	-		
3	ADP	D	601	6,5	28,29,29	1.41	6 (21%)	43,45,45	1.90	11 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ADP	K	601	6,5	28,29,29	1.38	4 (14%)	43,45,45	1.86	11 (25%)
3	ADP	F	601	6,5	28,29,29	1.38	4 (14%)	43,45,45	1.87	11 (25%)
3	ADP	E	601	6,5	28,29,29	1.40	5 (17%)	43,45,45	1.92	11 (25%)
4	BEF	I	602	-	0,3,3	-	-	-		

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	L	601	6,5	-	1/16/32/32	0/3/3/3
3	ADP	H	601	6,5	-	6/16/32/32	0/3/3/3
3	ADP	I	601	6,5	-	4/16/32/32	0/3/3/3
3	ADP	B	601	6,5	-	1/16/32/32	0/3/3/3
3	ADP	D	601	6,5	-	6/16/32/32	0/3/3/3
3	ADP	K	601	6,5	-	5/16/32/32	0/3/3/3
3	ADP	G	601	6,5	-	4/16/32/32	0/3/3/3
3	ADP	N	601	6,5	-	8/16/32/32	0/3/3/3
3	ADP	A	601	6,5,4	-	1/16/32/32	0/3/3/3
3	ADP	J	601	6,5	-	6/16/32/32	0/3/3/3
3	ADP	C	601	6,5	-	5/16/32/32	0/3/3/3
3	ADP	F	601	6,5	-	3/16/32/32	0/3/3/3
3	ADP	M	601	6,5	-	7/16/32/32	0/3/3/3
3	ADP	E	601	6,5	-	3/16/32/32	0/3/3/3

The worst 5 of 69 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	601	ADP	C5-C4	4.65	1.47	1.39
3	H	601	ADP	C5-C4	4.57	1.47	1.39
3	B	601	ADP	C5-C4	4.54	1.47	1.39
3	N	601	ADP	C5-C4	4.53	1.47	1.39
3	A	601	ADP	C5-C4	4.50	1.47	1.39

The worst 5 of 148 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	601	ADP	C5-C4-N3	-6.14	118.26	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	601	ADP	C5-C4-N3	-5.77	118.78	126.72
3	A	601	ADP	C5-C4-N3	-5.65	118.94	126.72
3	N	601	ADP	C5-C4-N3	-5.55	119.08	126.72
3	M	601	ADP	C5-C4-N3	-5.55	119.08	126.72

There are no chirality outliers.

5 of 60 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	601	ADP	C5'-O5'-PA-O2A
3	C	601	ADP	C5'-O5'-PA-O3A
3	D	601	ADP	C5'-O5'-PA-O2A
3	D	601	ADP	C5'-O5'-PA-O3A
3	F	601	ADP	C3'-C4'-C5'-O5'

There are no ring outliers.

28 monomers are involved in 65 short contacts:

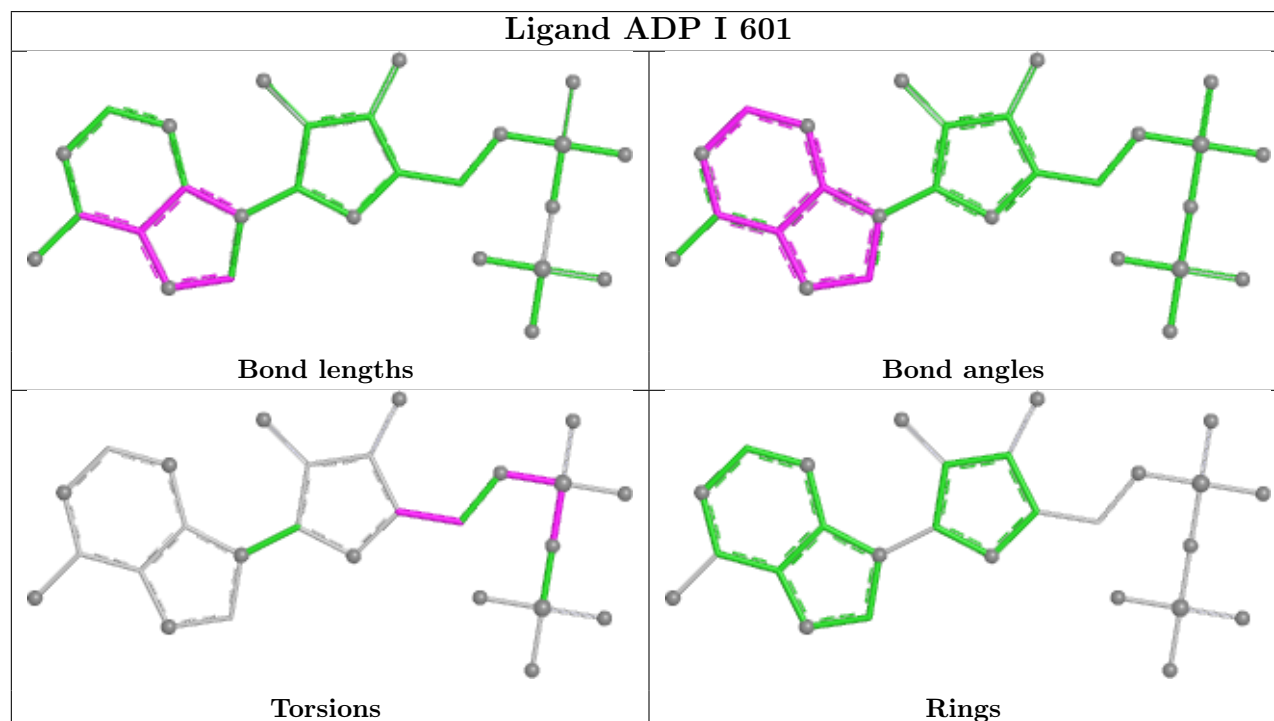
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	602	BEF	1	0
4	M	602	BEF	1	0
3	I	601	ADP	3	0
4	C	602	BEF	4	0
4	B	602	BEF	3	0
3	G	601	ADP	5	0
3	A	601	ADP	1	0
3	C	601	ADP	4	0
4	L	602	BEF	2	0
4	A	602	BEF	2	0
4	K	602	BEF	2	0
3	L	601	ADP	2	0
3	H	601	ADP	2	0
4	J	602	BEF	2	0
3	N	601	ADP	5	0
4	N	602	BEF	3	0
3	M	601	ADP	4	0
4	E	602	BEF	1	0
3	B	601	ADP	5	0
3	J	601	ADP	1	0
4	H	602	BEF	4	0
4	G	602	BEF	1	0

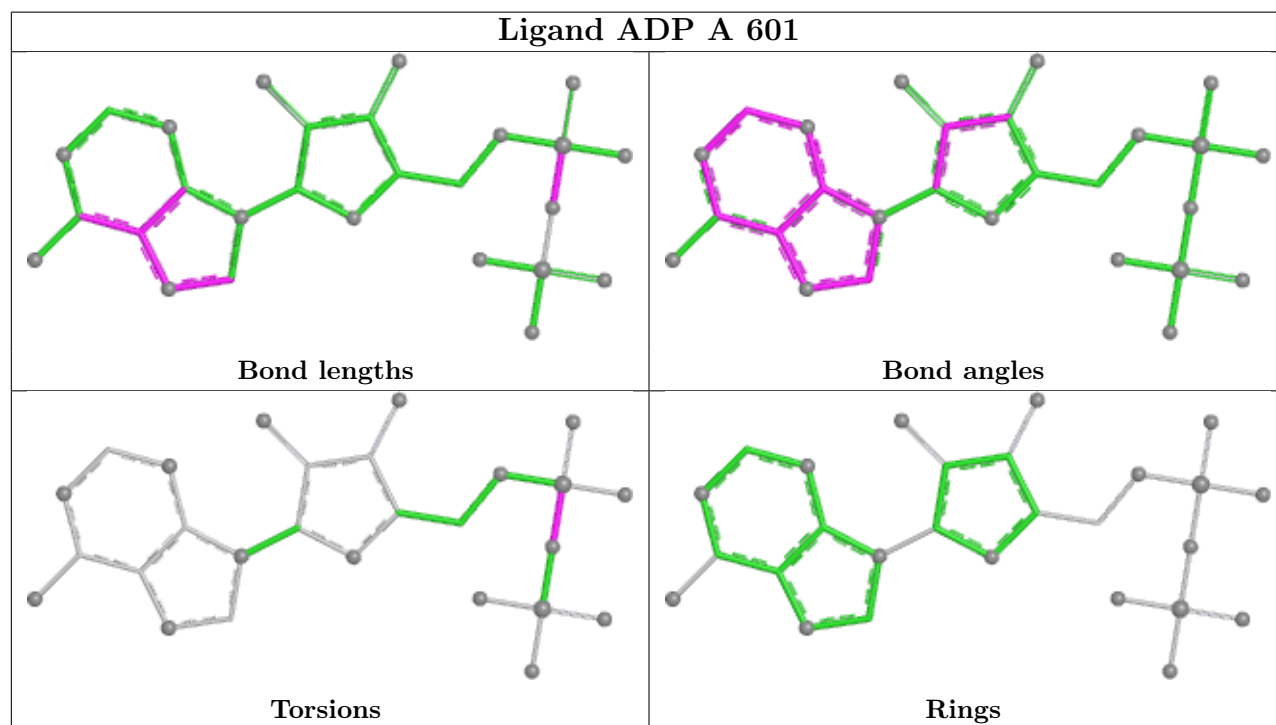
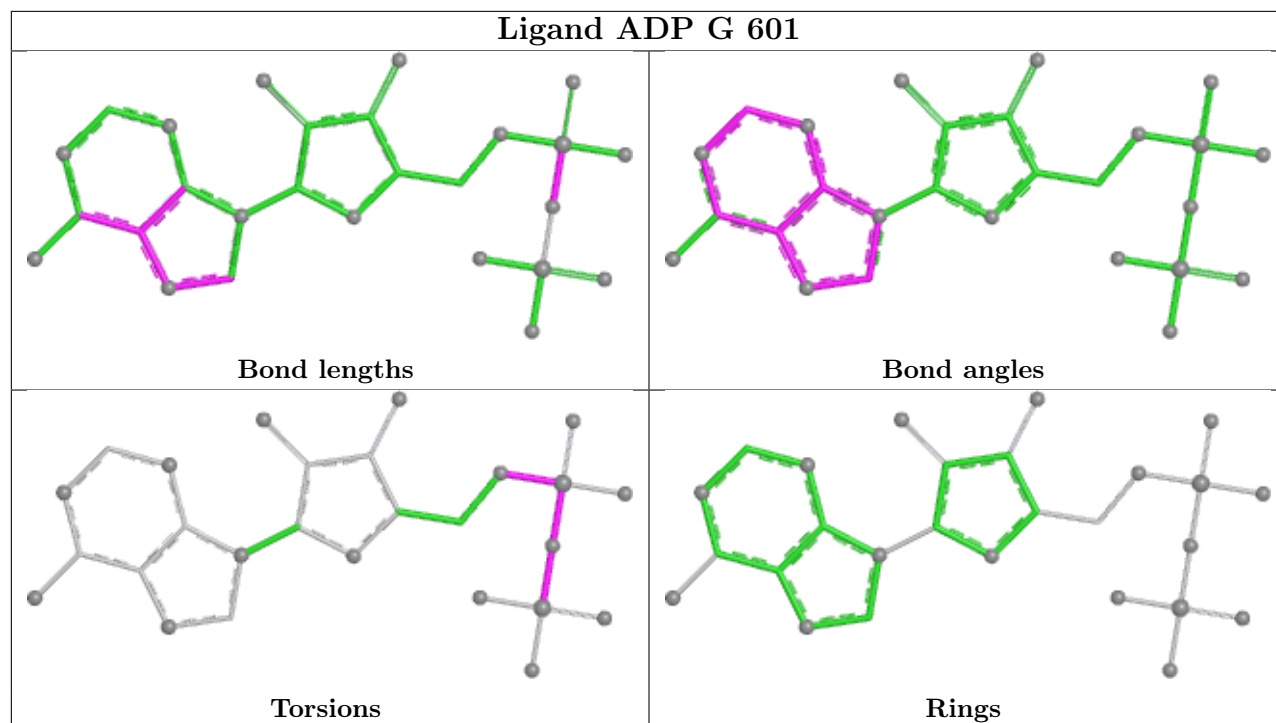
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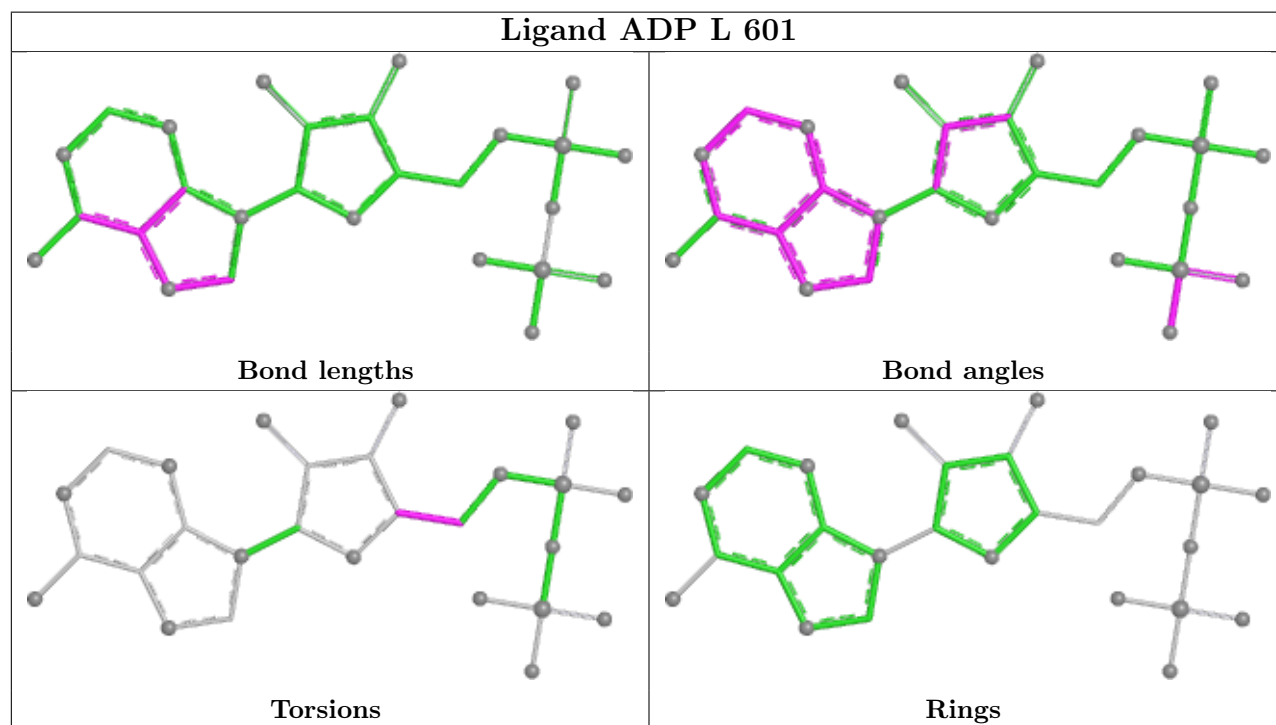
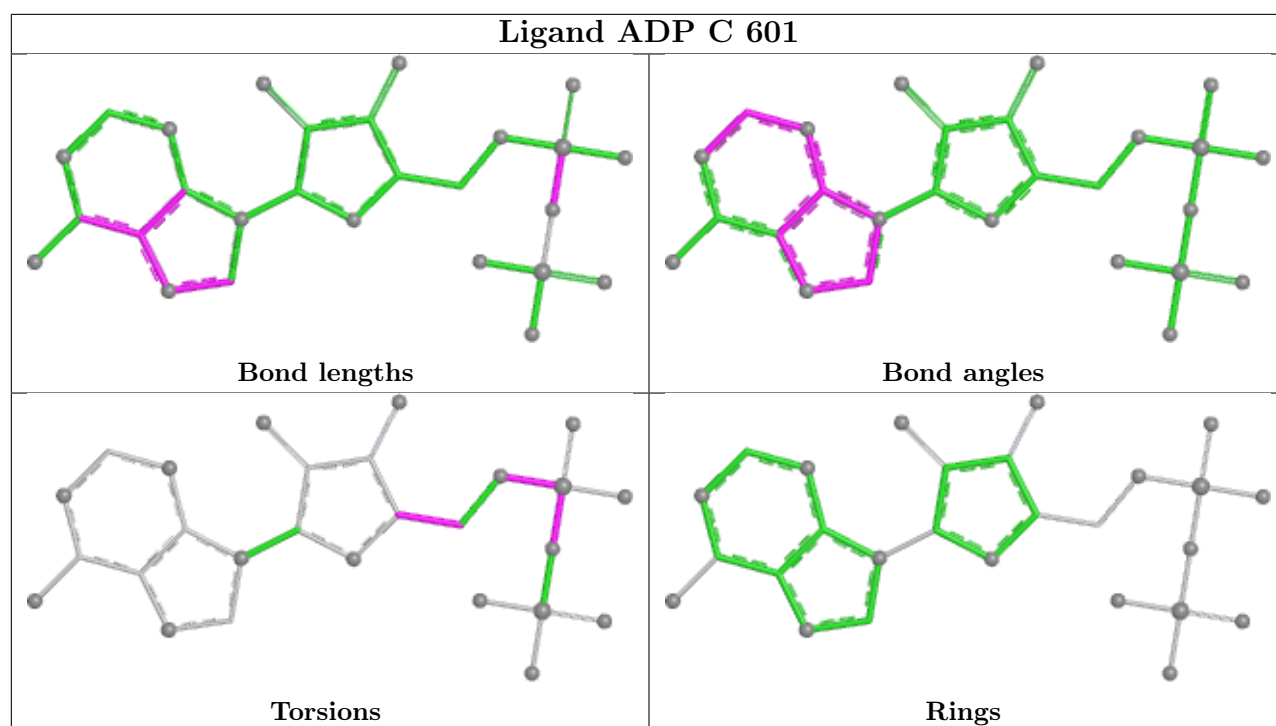
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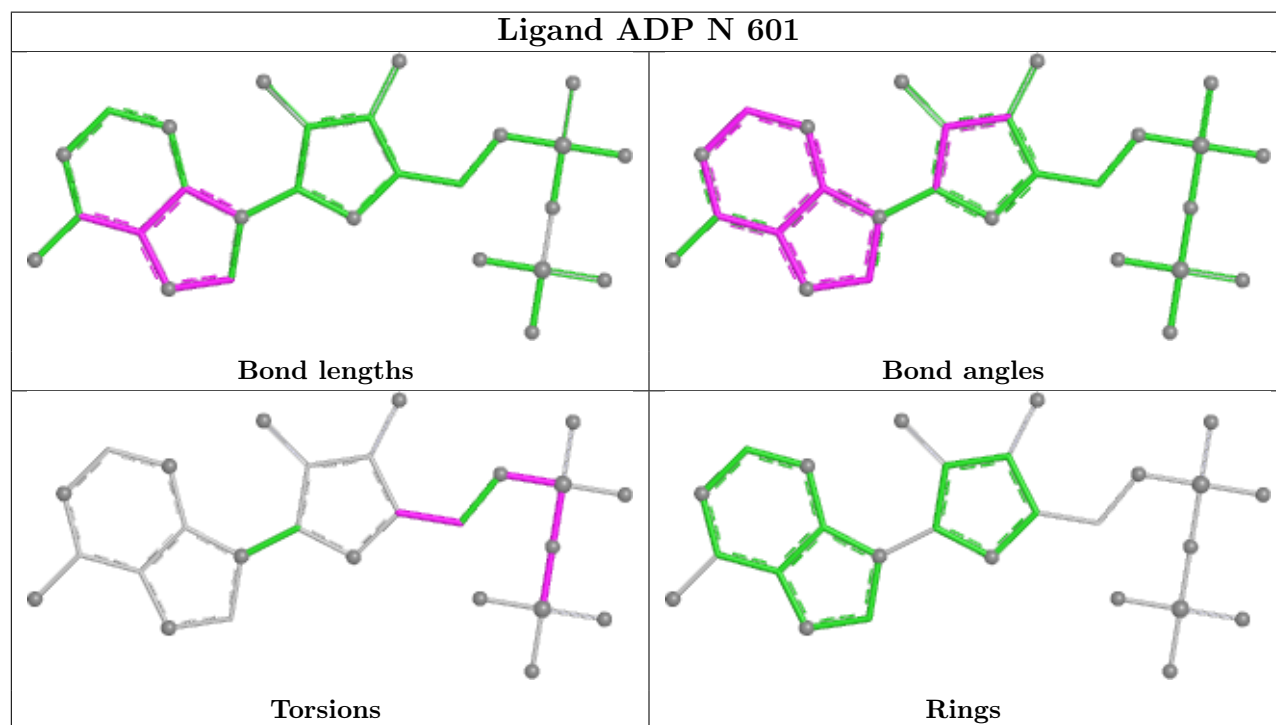
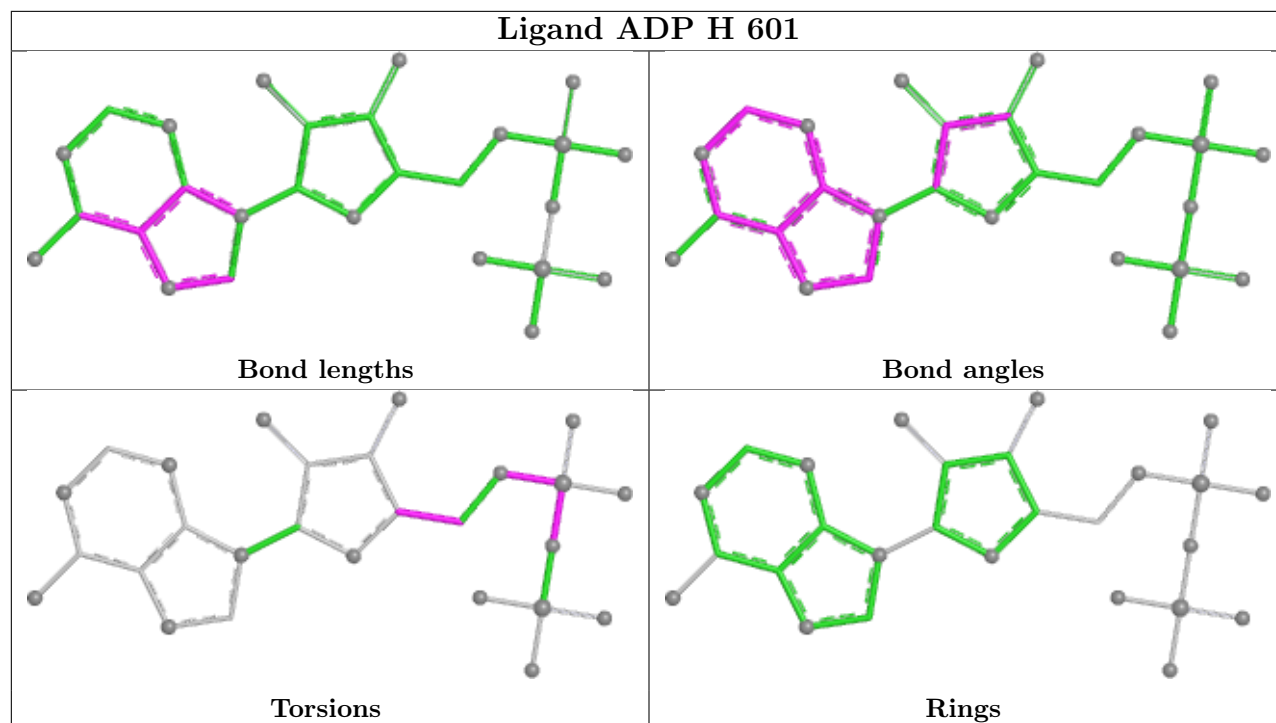
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	602	BEF	1	0
3	D	601	ADP	4	0
3	K	601	ADP	4	0
3	F	601	ADP	4	0
3	E	601	ADP	4	0
4	I	602	BEF	4	0

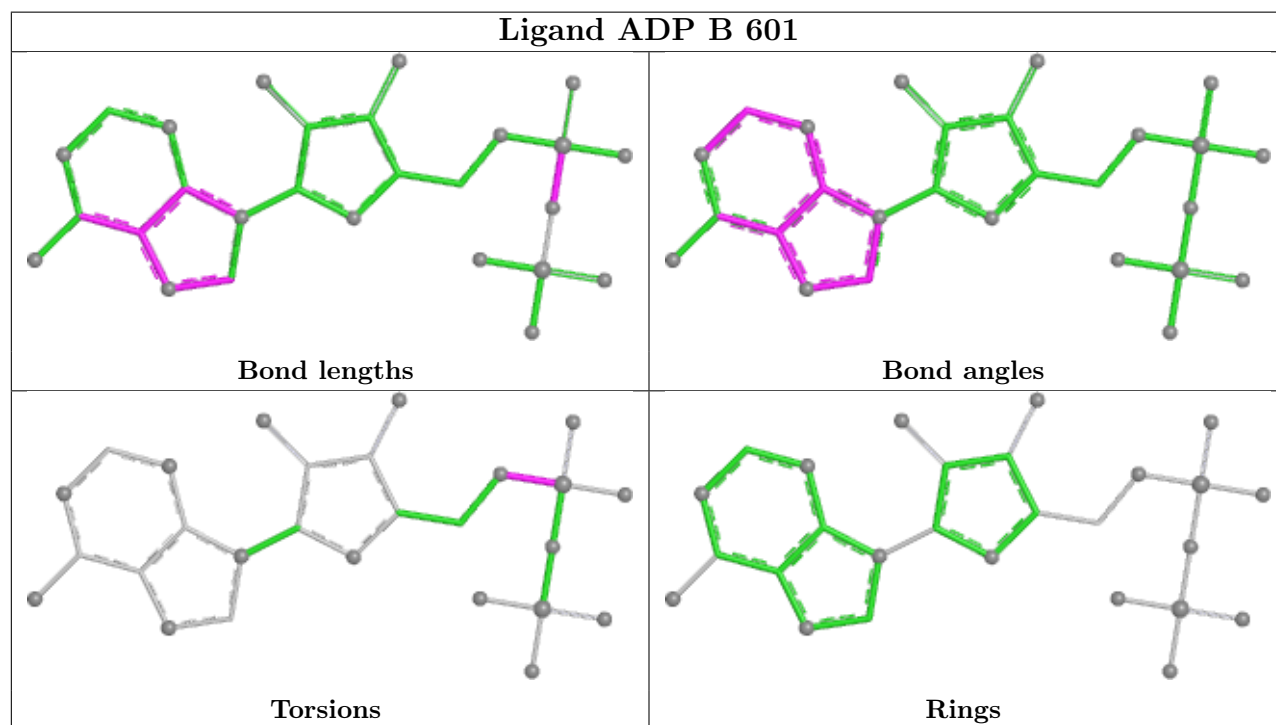
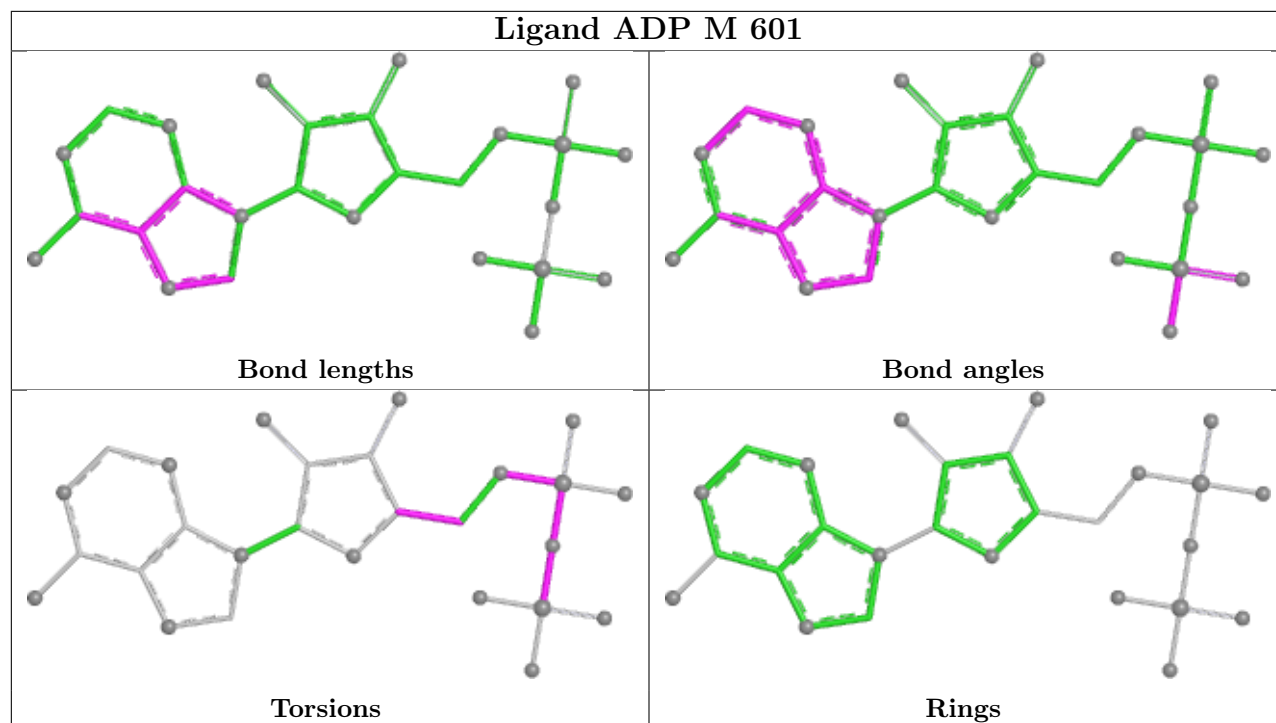
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



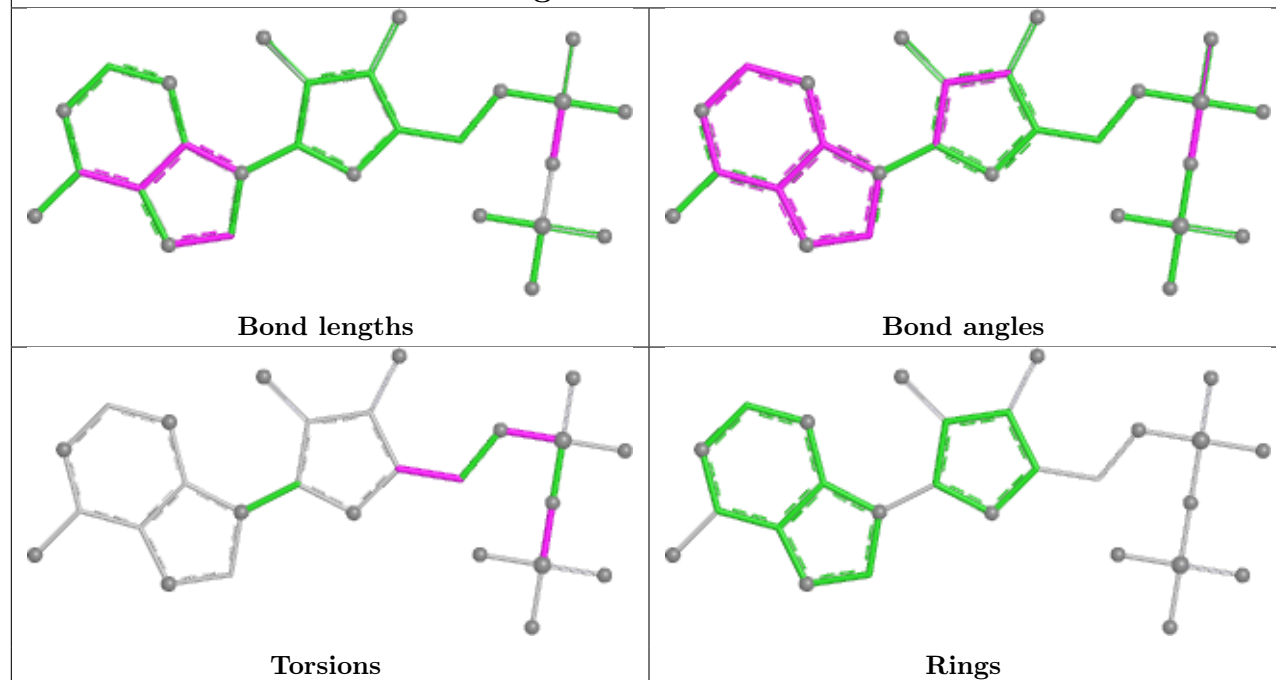




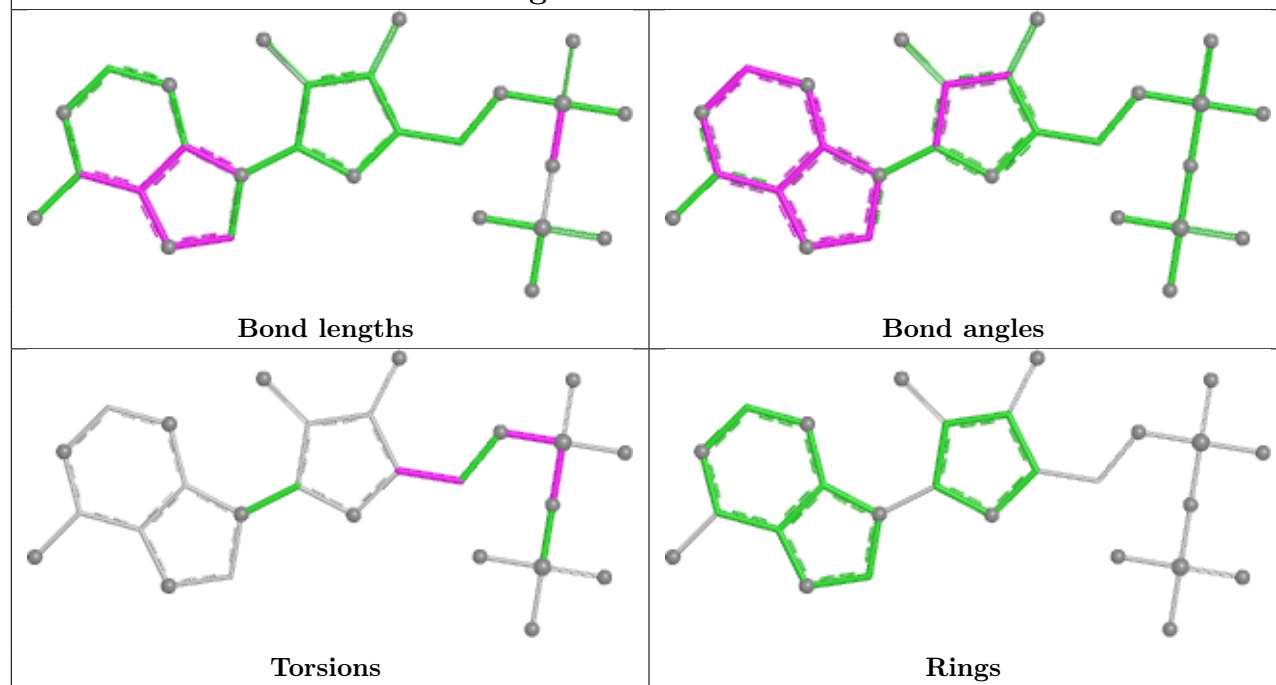


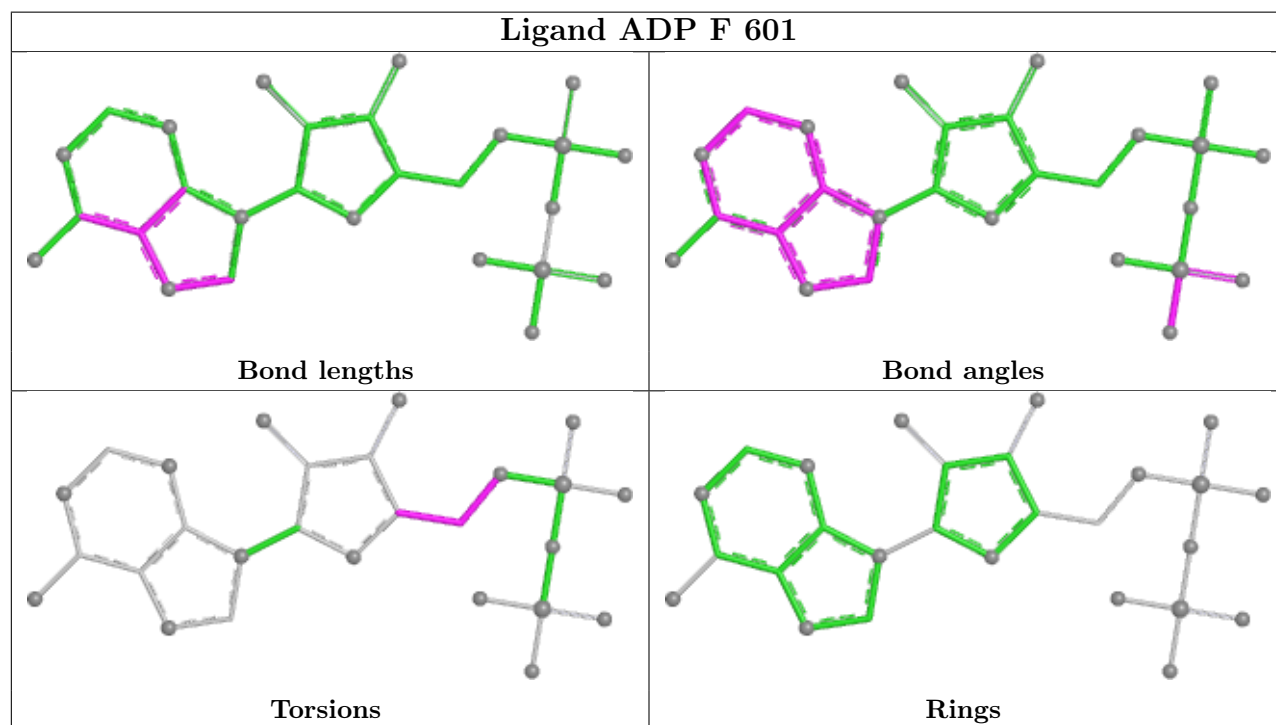
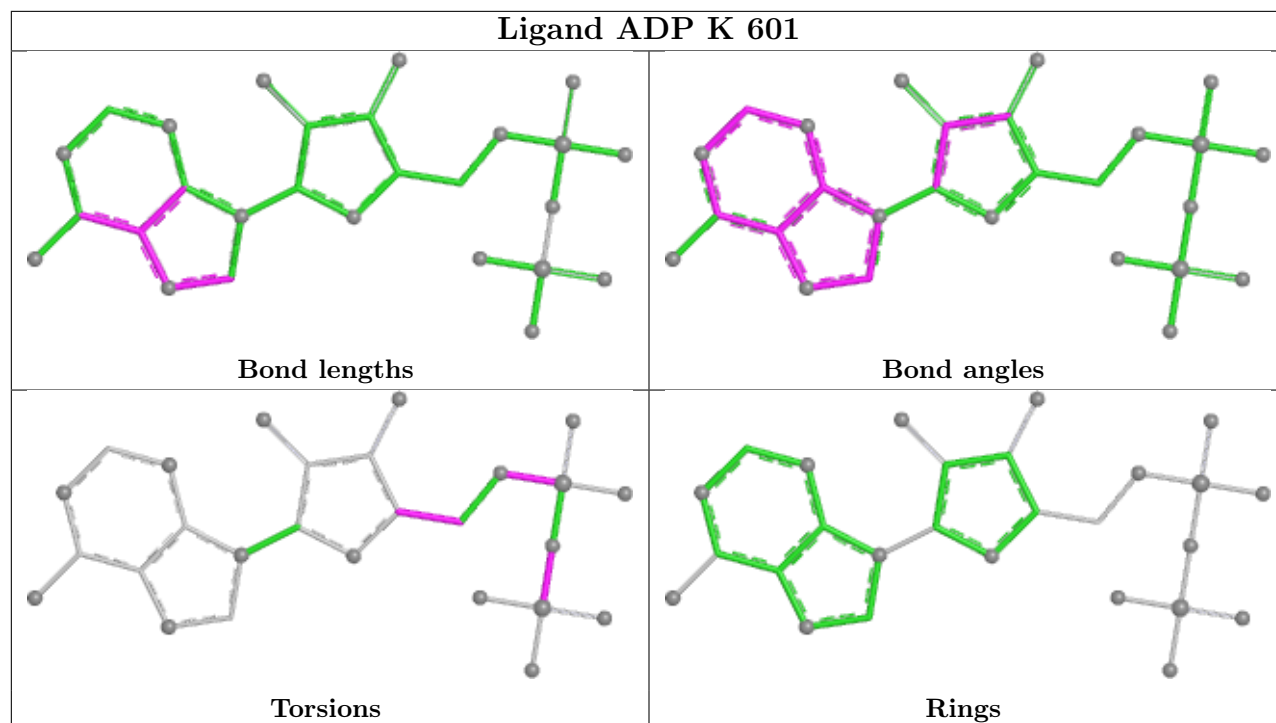


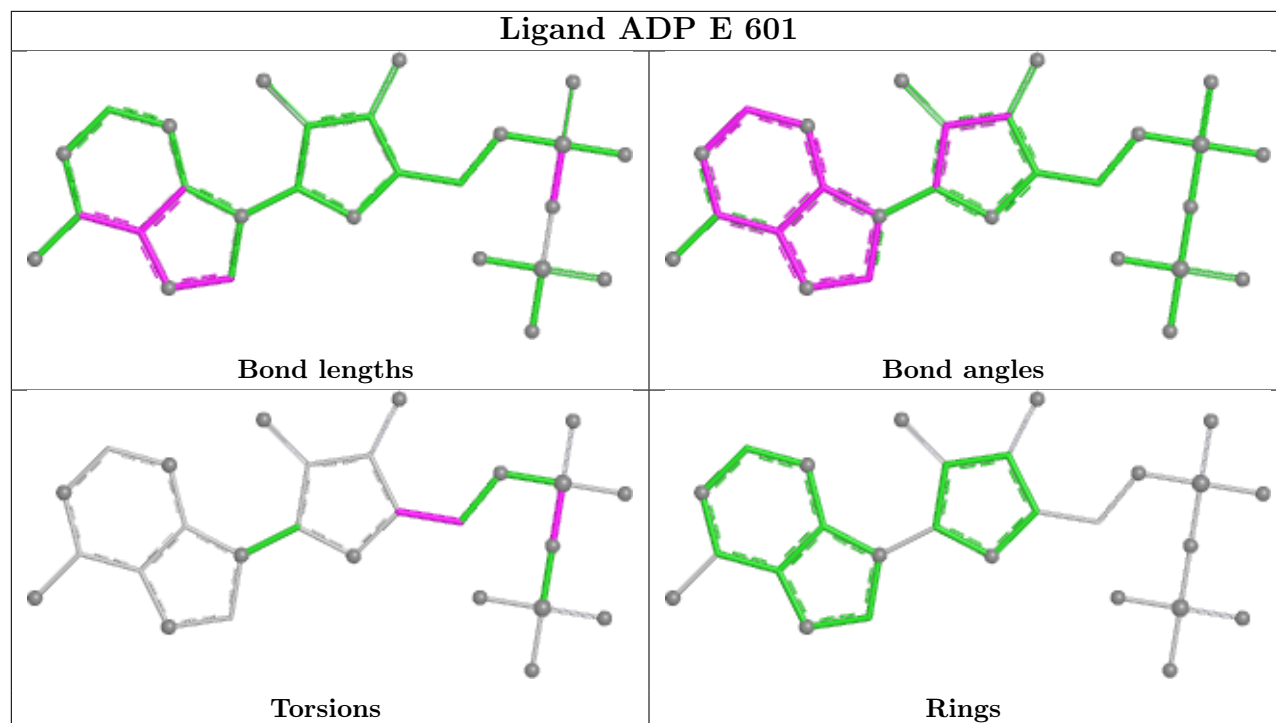
Ligand ADP J 601



Ligand ADP D 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	524/548 (95%)	-0.38	1 (0%) 91 82	54, 121, 305, 467	0
1	B	524/548 (95%)	-0.41	1 (0%) 91 82	57, 135, 293, 355	0
1	C	524/548 (95%)	-0.43	1 (0%) 91 82	54, 126, 274, 415	0
1	D	524/548 (95%)	-0.41	1 (0%) 91 82	53, 113, 212, 321	0
1	E	524/548 (95%)	-0.38	1 (0%) 91 82	62, 139, 293, 376	0
1	F	524/548 (95%)	-0.31	4 (0%) 82 63	51, 122, 288, 363	0
1	G	524/548 (95%)	-0.35	3 (0%) 85 68	43, 111, 278, 398	0
1	H	524/548 (95%)	-0.43	1 (0%) 91 82	61, 150, 325, 459	0
1	I	524/548 (95%)	-0.40	0 100 100	49, 117, 213, 354	0
1	J	524/548 (95%)	-0.43	0 100 100	63, 139, 287, 398	0
1	K	524/548 (95%)	-0.36	3 (0%) 85 68	59, 141, 293, 379	0
1	L	524/548 (95%)	-0.37	2 (0%) 88 74	53, 130, 298, 397	0
1	M	524/548 (95%)	-0.37	1 (0%) 91 82	71, 146, 330, 456	0
1	N	524/548 (95%)	-0.41	1 (0%) 91 82	70, 159, 306, 375	0
2	1	97/97 (100%)	-0.20	1 (1%) 79 58	93, 149, 321, 352	0
2	2	97/97 (100%)	-0.10	1 (1%) 79 58	98, 162, 314, 350	0
2	O	95/97 (97%)	-0.21	0 100 100	88, 136, 315, 390	0
2	P	97/97 (100%)	-0.17	1 (1%) 79 58	74, 152, 323, 361	0
2	Q	96/97 (98%)	-0.22	0 100 100	113, 182, 322, 375	0
2	R	97/97 (100%)	-0.06	0 100 100	112, 168, 267, 319	0
2	S	96/97 (98%)	0.10	1 (1%) 79 58	106, 165, 341, 367	0
2	T	97/97 (100%)	-0.13	1 (1%) 79 58	116, 178, 338, 434	0
2	U	97/97 (100%)	-0.14	0 100 100	88, 156, 354, 422	0
2	V	97/97 (100%)	-0.21	0 100 100	119, 183, 325, 378	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
2	W	97/97 (100%)	-0.04	1 (1%) 79 58	106, 161, 248, 306	0
2	X	97/97 (100%)	0.10	6 (6%) 26 22	101, 153, 297, 380	0
2	Y	96/97 (98%)	-0.20	0 100 100	104, 155, 304, 366	0
2	Z	95/97 (97%)	-0.18	0 100 100	108, 160, 312, 358	0
All	All	8687/9030 (96%)	-0.35	32 (0%) 88 74	43, 139, 302, 467	0

The worst 5 of 32 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	227	ILE	5.4
2	S	59	VAL	3.6
1	K	249	ILE	3.5
1	M	273	VAL	3.4
2	X	59	VAL	3.4

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
4	BEF	F	602	4/4	0.84	0.21	53,80,165,206	0
4	BEF	A	602	4/4	0.88	0.12	62,131,196,204	0
4	BEF	K	602	4/4	0.90	0.14	54,86,101,160	0
4	BEF	N	602	4/4	0.91	0.10	98,99,105,118	0
4	BEF	B	602	4/4	0.92	0.16	45,60,96,100	0
4	BEF	J	602	4/4	0.93	0.09	40,132,142,204	0
5	MG	B	603	1/1	0.93	0.14	66,66,66,66	0

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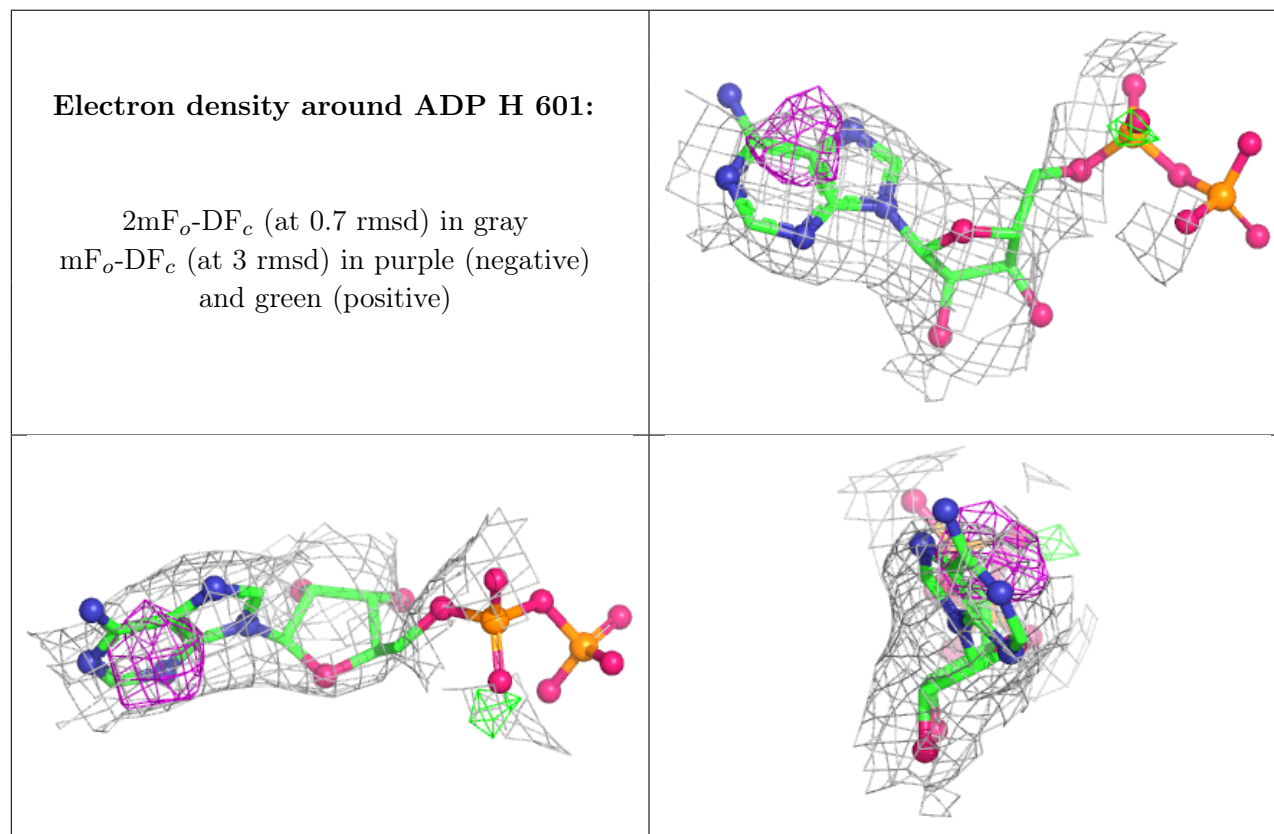
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	BEF	D	602	4/4	0.94	0.09	31,64,104,109	0
3	ADP	H	601	27/27	0.94	0.10	72,93,142,191	0
3	ADP	K	601	27/27	0.94	0.11	80,97,118,125	0
5	MG	L	603	1/1	0.94	0.11	66,66,66,66	0
4	BEF	M	602	4/4	0.95	0.12	119,139,180,221	0
3	ADP	J	601	27/27	0.95	0.11	35,90,137,139	0
3	ADP	C	601	27/27	0.95	0.08	66,83,148,156	0
5	MG	I	603	1/1	0.95	0.17	81,81,81,81	0
3	ADP	M	601	27/27	0.95	0.10	25,77,196,198	0
6	K	J	604	1/1	0.95	0.11	122,122,122,122	0
3	ADP	I	601	27/27	0.96	0.09	47,72,117,158	0
4	BEF	I	602	4/4	0.96	0.09	59,65,81,85	0
5	MG	G	603	1/1	0.96	0.17	48,48,48,48	0
3	ADP	F	601	27/27	0.96	0.10	44,79,128,140	0
3	ADP	A	601	27/27	0.96	0.10	34,80,131,147	0
6	K	C	604	1/1	0.96	0.05	126,126,126,126	0
6	K	F	604	1/1	0.96	0.07	103,103,103,103	0
3	ADP	L	601	27/27	0.96	0.09	69,83,118,128	0
6	K	K	604	1/1	0.96	0.05	110,110,110,110	0
3	ADP	G	601	27/27	0.97	0.08	3,59,88,94	0
4	BEF	L	602	4/4	0.97	0.06	43,102,141,206	0
5	MG	M	603	1/1	0.97	0.09	73,73,73,73	0
4	BEF	E	602	4/4	0.97	0.06	55,87,89,89	0
3	ADP	N	601	27/27	0.97	0.07	66,106,128,133	0
3	ADP	D	601	27/27	0.97	0.07	25,73,84,87	0
3	ADP	B	601	27/27	0.97	0.08	16,86,98,110	0
6	K	N	604	1/1	0.97	0.04	107,107,107,107	0
4	BEF	C	602	4/4	0.98	0.09	2,4,92,93	0
5	MG	K	603	1/1	0.98	0.11	50,50,50,50	0
3	ADP	E	601	27/27	0.98	0.07	36,84,99,115	0
5	MG	A	603	1/1	0.98	0.08	78,78,78,78	0
6	K	A	604	1/1	0.98	0.07	84,84,84,84	0
6	K	B	604	1/1	0.98	0.03	79,79,79,79	0
4	BEF	G	602	4/4	0.98	0.07	36,46,68,99	0
6	K	D	604	1/1	0.98	0.04	82,82,82,82	0
6	K	E	604	1/1	0.98	0.07	89,89,89,89	0
5	MG	D	603	1/1	0.98	0.08	44,44,44,44	0
6	K	H	604	1/1	0.98	0.03	110,110,110,110	0
5	MG	F	603	1/1	0.98	0.12	51,51,51,51	0
4	BEF	H	602	4/4	0.98	0.05	13,85,125,156	0
5	MG	H	603	1/1	0.98	0.07	103,103,103,103	0
6	K	G	604	1/1	0.99	0.04	67,67,67,67	0

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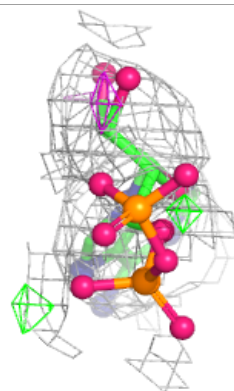
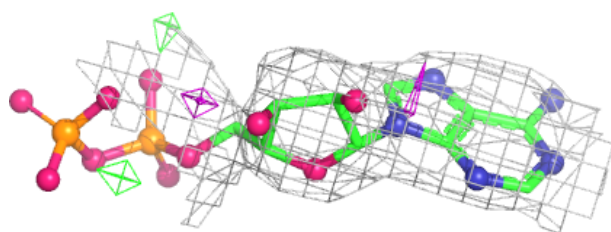
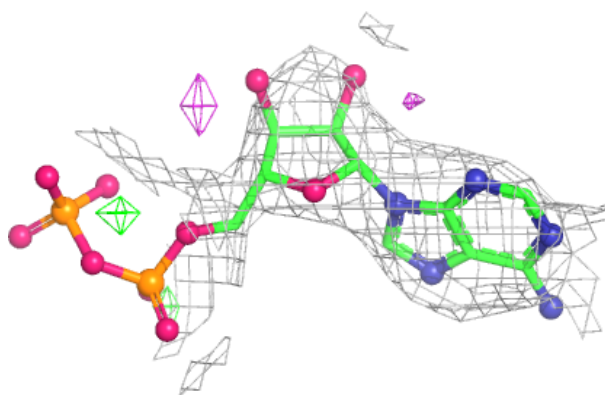
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	MG	J	603	1/1	0.99	0.08	56,56,56,56	0
6	K	I	604	1/1	0.99	0.06	75,75,75,75	0
5	MG	N	603	1/1	0.99	0.04	71,71,71,71	0
5	MG	C	603	1/1	0.99	0.07	57,57,57,57	0
6	K	L	604	1/1	0.99	0.04	87,87,87,87	0
6	K	M	604	1/1	0.99	0.05	94,94,94,94	0
5	MG	E	603	1/1	0.99	0.07	45,45,45,45	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.

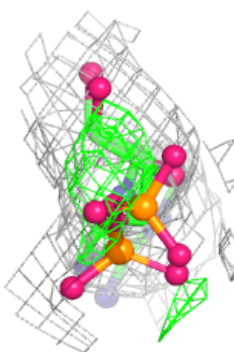
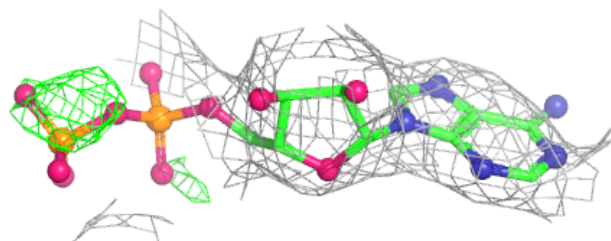
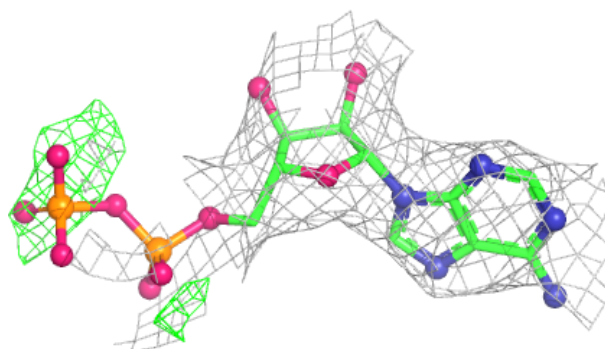


Electron density around ADP K 601:

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

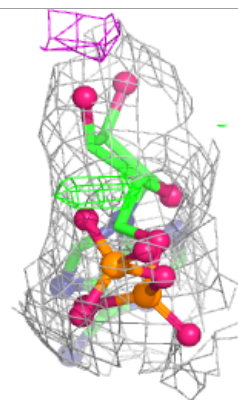
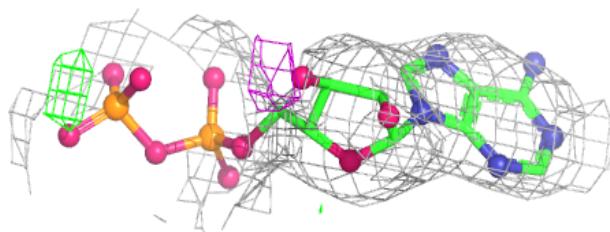
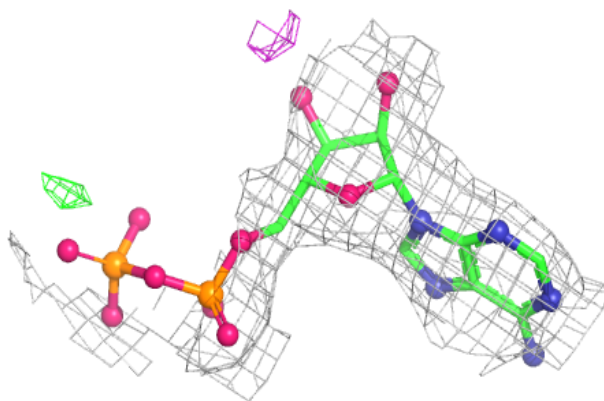
**Electron density around ADP J 601:**

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

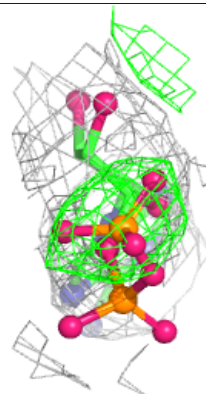
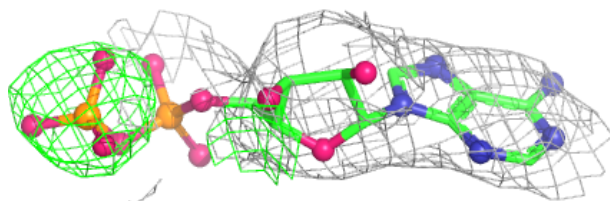
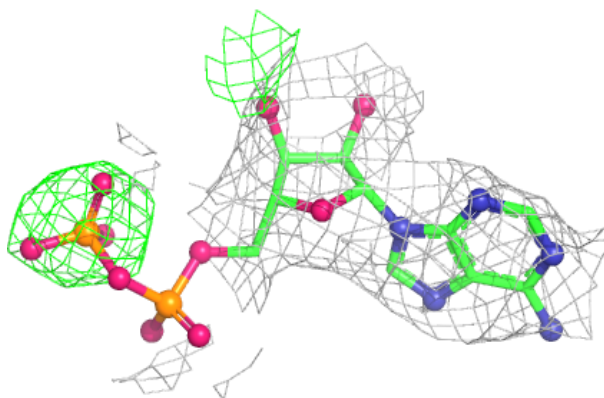


Electron density around ADP C 601:

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

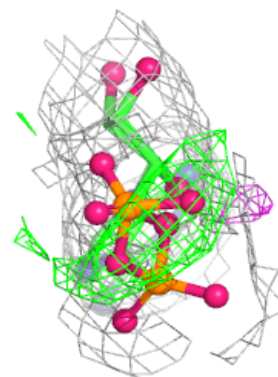
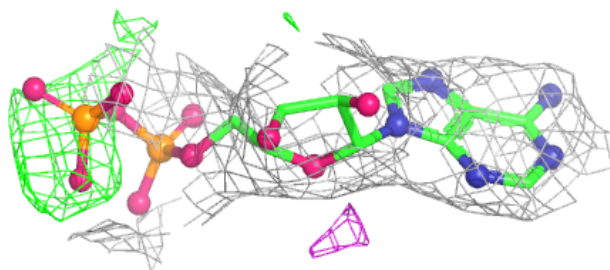
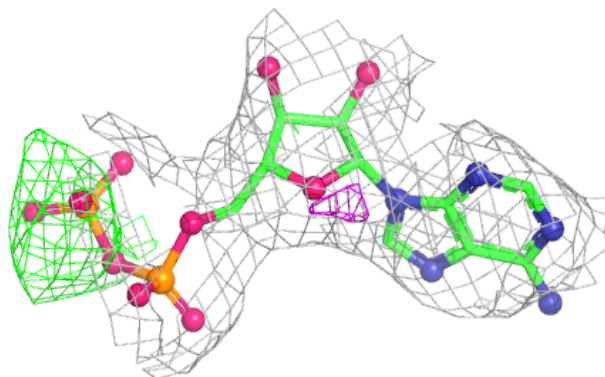
**Electron density around ADP M 601:**

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and green (positive)

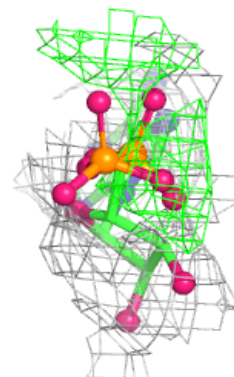
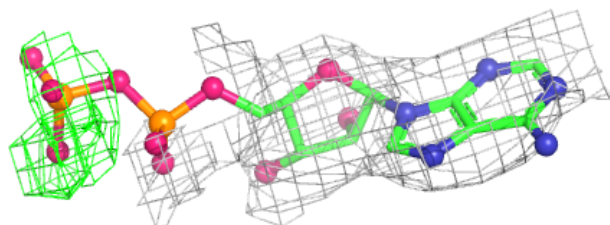
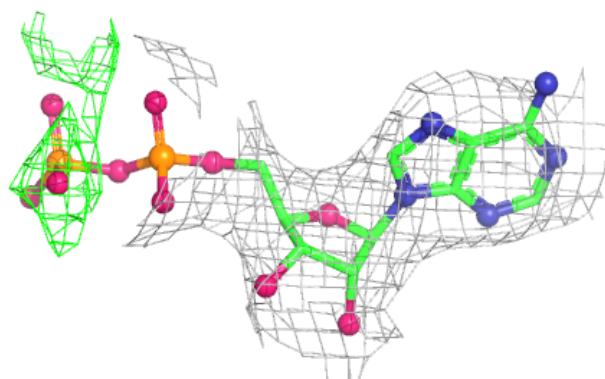


Electron density around ADP I 601:

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and green (positive)

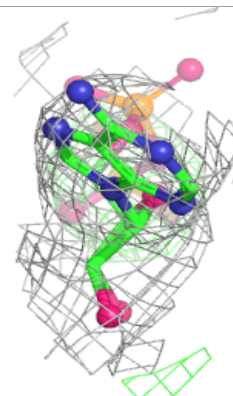
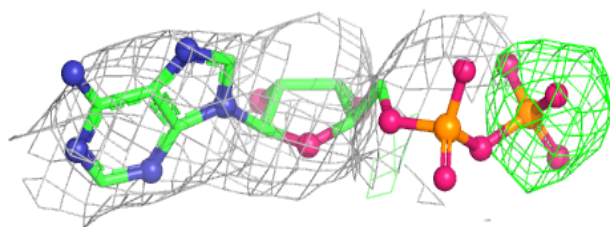
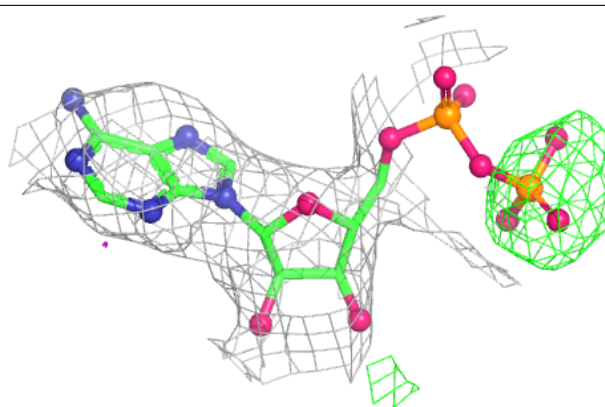
**Electron density around ADP F 601:**

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

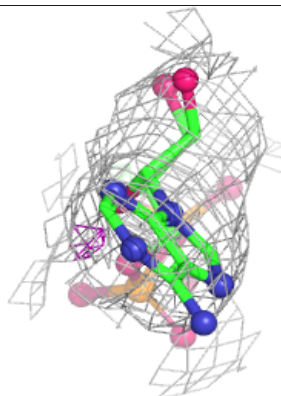
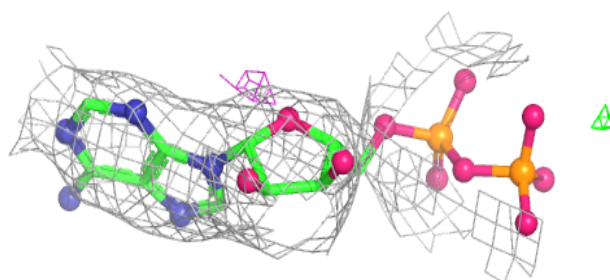
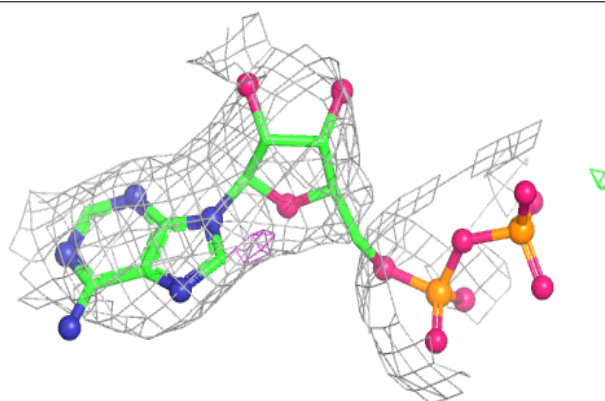


Electron density around ADP A 601:

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

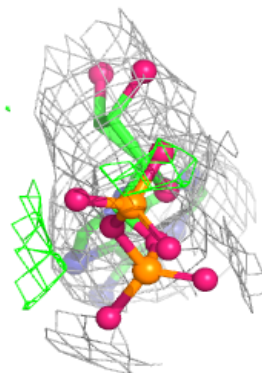
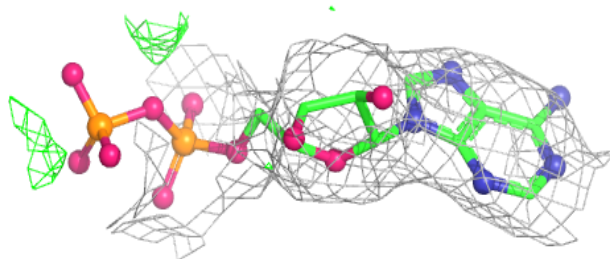
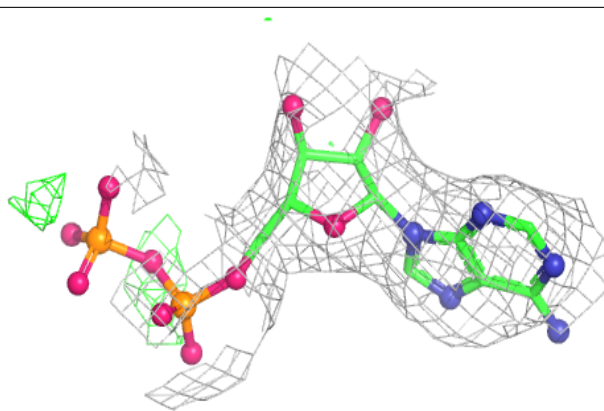
**Electron density around ADP L 601:**

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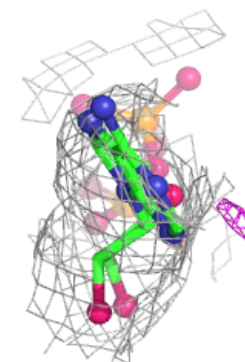
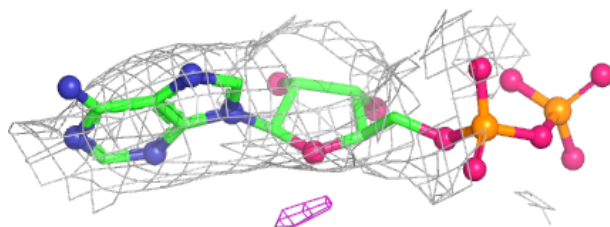
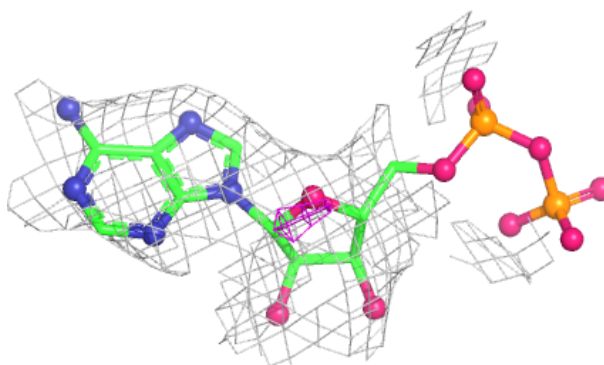


Electron density around ADP G 601:

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and green (positive)

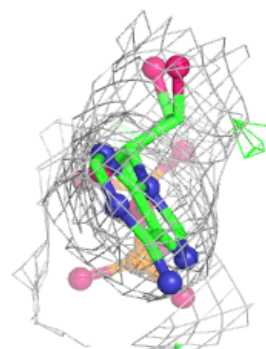
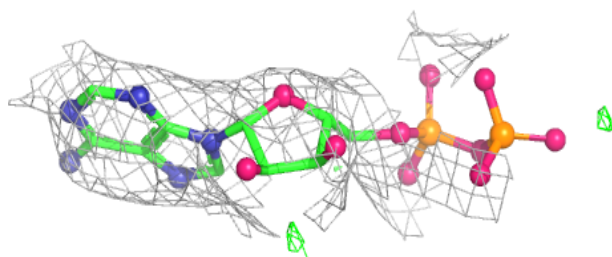
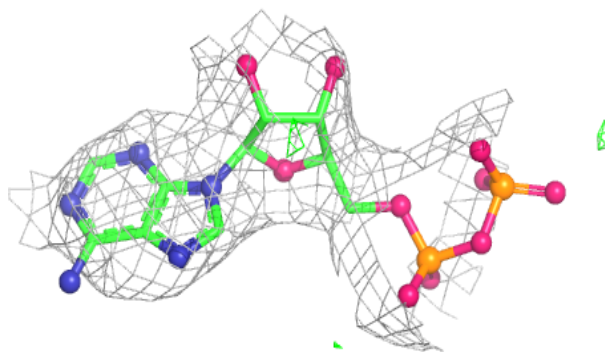
**Electron density around ADP N 601:**

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and green (positive)

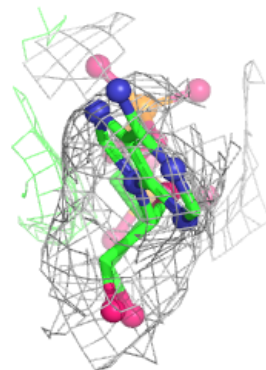
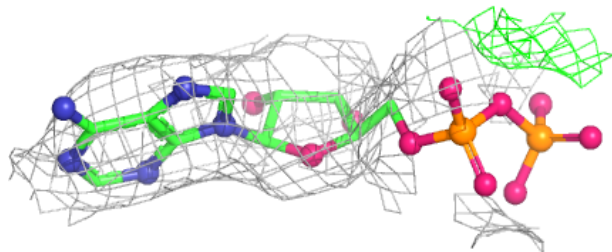
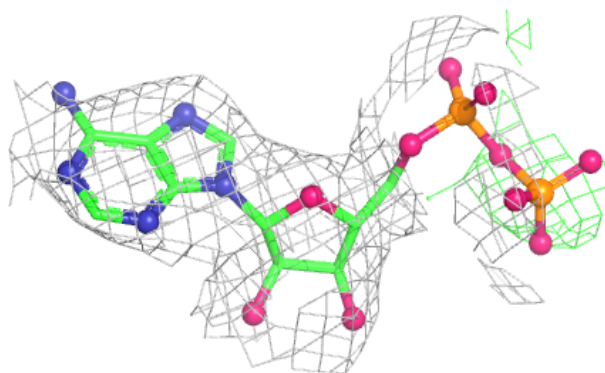


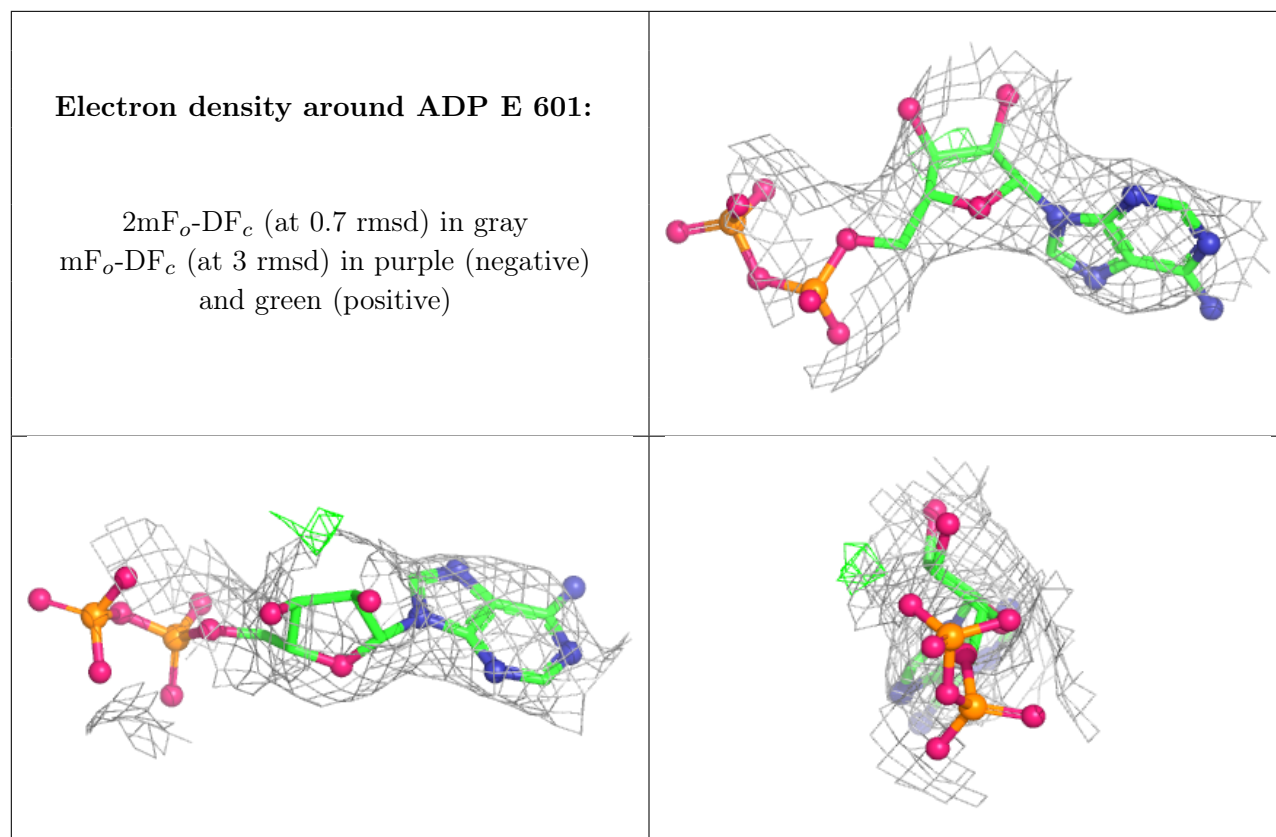
Electron density around ADP D 601:

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

**Electron density around ADP B 601:**

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





6.5 Other polymers [i](#)

There are no such residues in this entry.