



wwPDB X-ray Structure Validation Summary Report ⓘ

May 21, 2020 – 08:31 pm BST

PDB ID : 4KI8
Title : Crystal structure of a GroEL-ADP complex in the relaxed allosteric state
Authors : Fei, X.; Yang, D.; LaRonde-LeBlanc, N.; Lorimer, G.H.
Deposited on : 2013-05-01
Resolution : 2.72 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

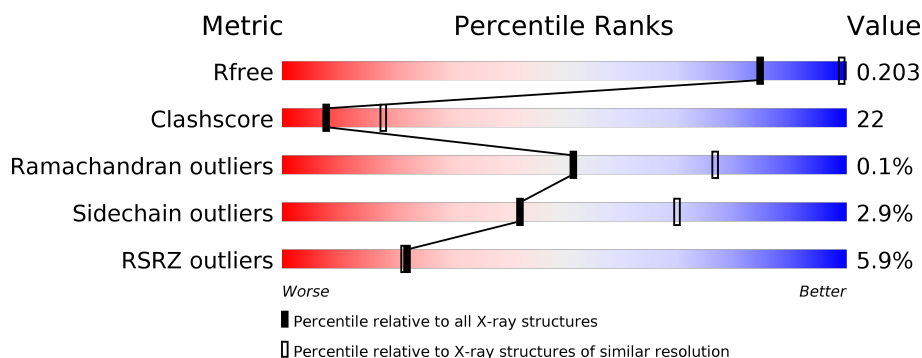
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.72 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}	130704	3359 (2.74-2.70)
Clashscore	141614	3686 (2.74-2.70)
Ramachandran outliers	138981	3622 (2.74-2.70)
Sidechain outliers	138945	3623 (2.74-2.70)
RSRZ outliers	127900	3276 (2.74-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on 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	<div> <div>3%</div> <div> <div></div> <div>68%</div> <div>26%</div> <div>• •</div> </div> </div>
1	B	548	<div> <div>4%</div> <div> <div></div> <div>67%</div> <div>27%</div> <div>• •</div> </div> </div>
1	C	548	<div> <div>12%</div> <div> <div></div> <div>62%</div> <div>32%</div> <div>• •</div> </div> </div>
1	D	548	<div> <div>2%</div> <div> <div></div> <div>68%</div> <div>26%</div> <div>• •</div> </div> </div>
1	E	548	<div> <div>2%</div> <div> <div></div> <div>68%</div> <div>25%</div> <div>• •</div> </div> </div>
1	F	548	<div> <div>6%</div> <div> <div></div> <div>64%</div> <div>30%</div> <div>• •</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	548	

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	K	F	605	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 27977 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.

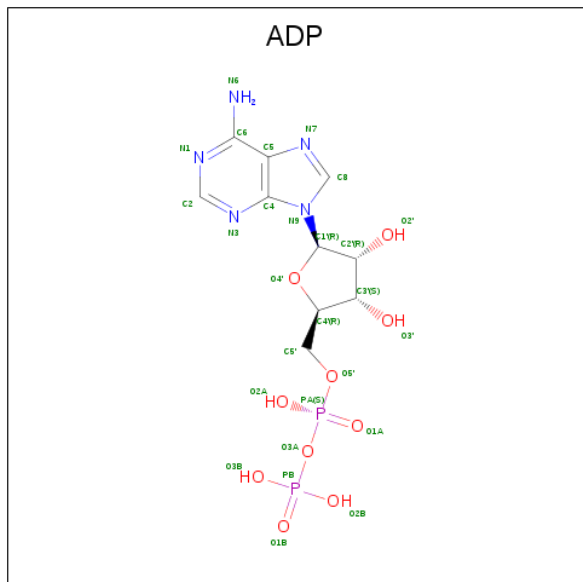
- Molecule 1 is a protein called GroEL protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	524	Total	C	N	O	S	0	1	0
			3854	2398	665	771	20			
1	B	524	Total	C	N	O	S	0	1	0
			3854	2398	665	771	20			
1	C	524	Total	C	N	O	S	0	3	0
			3864	2405	668	771	20			
1	D	524	Total	C	N	O	S	0	2	0
			3862	2403	668	771	20			
1	E	524	Total	C	N	O	S	0	1	0
			3851	2396	663	772	20			
1	F	524	Total	C	N	O	S	0	4	0
			3873	2410	668	775	20			
1	G	524	Total	C	N	O	S	0	1	0
			3854	2398	665	771	20			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	83	ALA	ASP	ENGINEERED MUTATION	UNP Q548M1
A	197	ALA	ARG	ENGINEERED MUTATION	UNP Q548M1
B	83	ALA	ASP	ENGINEERED MUTATION	UNP Q548M1
B	197	ALA	ARG	ENGINEERED MUTATION	UNP Q548M1
C	83	ALA	ASP	ENGINEERED MUTATION	UNP Q548M1
C	197	ALA	ARG	ENGINEERED MUTATION	UNP Q548M1
D	83	ALA	ASP	ENGINEERED MUTATION	UNP Q548M1
D	197	ALA	ARG	ENGINEERED MUTATION	UNP Q548M1
E	83	ALA	ASP	ENGINEERED MUTATION	UNP Q548M1
E	197	ALA	ARG	ENGINEERED MUTATION	UNP Q548M1
F	83	ALA	ASP	ENGINEERED MUTATION	UNP Q548M1
F	197	ALA	ARG	ENGINEERED MUTATION	UNP Q548M1
G	83	ALA	ASP	ENGINEERED MUTATION	UNP Q548M1
G	197	ALA	ARG	ENGINEERED MUTATION	UNP Q548M1

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	F	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	G	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		
3	E	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total 1	Mg 1	0	0
3	C	1	Total 1	Mg 1	0	0
3	A	1	Total 1	Mg 1	0	0
3	F	1	Total 1	Mg 1	0	0

- Molecule 4 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	G	2	Total 2	K 2	0	0
4	D	1	Total 1	K 1	0	0
4	E	1	Total 1	K 1	0	0
4	B	1	Total 1	K 1	0	0
4	C	1	Total 1	K 1	0	0
4	A	1	Total 1	K 1	0	0
4	F	2	Total 2	K 2	0	0

- Molecule 5 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: C₆H₁₄O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			8	6	2		
5	A	1	Total	C	O	0	0
			8	6	2		
5	A	1	Total	C	O	0	0
			8	6	2		
5	A	1	Total	C	O	0	0
			8	6	2		
5	A	1	Total	C	O	0	0
			8	6	2		
5	A	1	Total	C	O	0	0
			8	6	2		
5	B	1	Total	C	O	0	0
			8	6	2		
5	B	1	Total	C	O	0	0
			8	6	2		
5	B	1	Total	C	O	0	0
			8	6	2		
5	B	1	Total	C	O	0	0
			8	6	2		
5	B	1	Total	C	O	0	0
			8	6	2		
5	C	1	Total	C	O	0	0
			8	6	2		
5	D	1	Total	C	O	0	0
			8	6	2		
5	D	1	Total	C	O	0	0
			8	6	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	D	1	Total	C	O	0	0
			8	6	2		
5	E	1	Total	C	O	0	0
			8	6	2		
5	F	1	Total	C	O	0	0
			8	6	2		
5	G	1	Total	C	O	0	0
			8	6	2		
5	G	1	Total	C	O	0	0
			8	6	2		

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	G	3	Total	Ca	0	0
			3	3		
6	D	1	Total	Ca	0	0
			1	1		
6	E	3	Total	Ca	0	0
			3	3		
6	B	1	Total	Ca	0	0
			1	1		
6	A	2	Total	Ca	0	0
			2	2		
6	F	1	Total	Ca	0	0
			1	1		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	90	Total	O	0	0
			90	90		
7	B	112	Total	O	0	0
			112	112		
7	C	88	Total	O	0	0
			88	88		
7	D	90	Total	O	0	0
			90	90		
7	E	65	Total	O	0	0
			65	65		
7	F	67	Total	O	0	0
			67	67		

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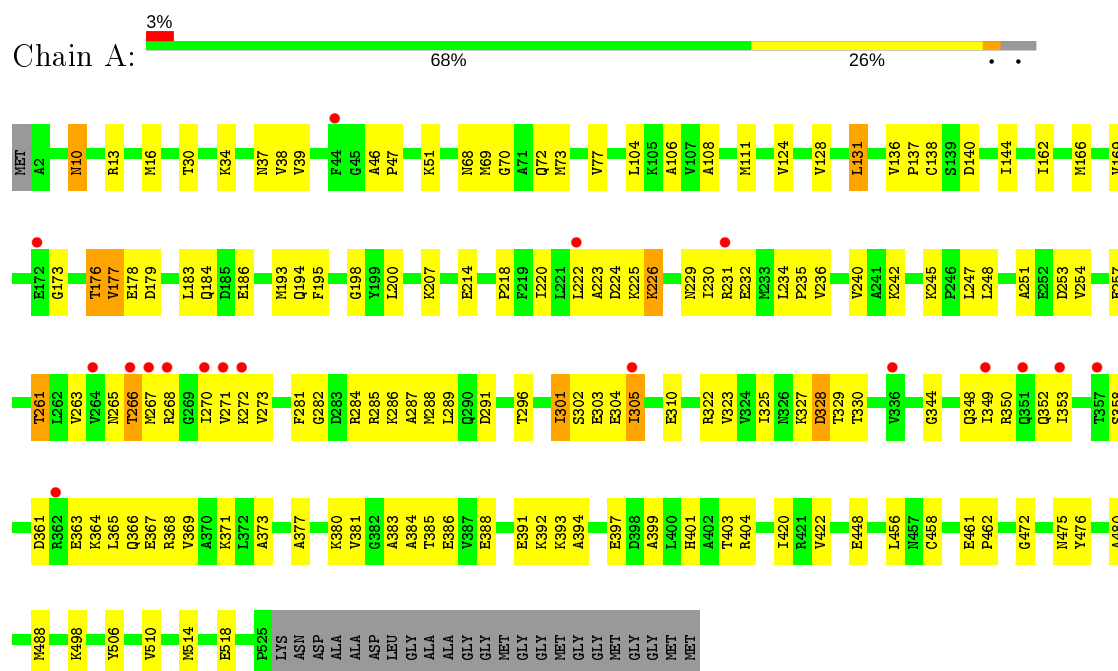
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	G	85	Total	O	0	0
			85	85		

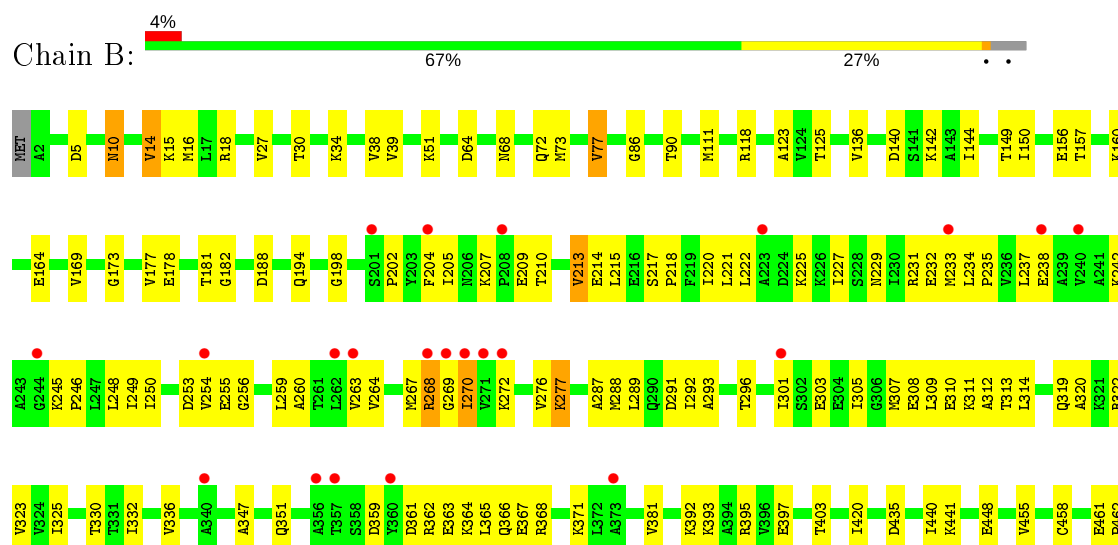
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: GroEL protein



• Molecule 1: GroEL protein



P525	A223	A287	D861	
LYS	D224	P288	R362	
ASN	K225	L289	E363	
ASP	K226	Q290	K364	
ALA	I227	D291	L365	
ALA	S228	L295	Q366	
ASP	N229	T299	E367	
LEU	I230	V300	R368	
GLY	R231	V301	V369	
ALA	E232	I301	A370	
ALA	N233	S302	K371	
GLY	L234	E303	L372	
GLY	P235	E304	V378	
MET	V240	I305	R379	
GLY	A241	G306	K380	
GLY	K242	N307	E381	
MET	A243	E308	G382	
GLY	G244	L309	G383	
GLY	K245	E310	A384	
MET	P246	K311	T385	
GLY	L247	A312	E386	
GLY	L248	T313	V387	
MET	I249	L314	E388	
MET	I250	E315	K392	
A251	A251	D816	R393	
E252	E252	L317	A394	
D253	D253	G318	K395	
V254	V254	Q319	R396	
E257	E257	A320	H401	
A258	A258	K321	R404	
L259	L259	R322	V407	
A260	A260	V323	L420	
T261	T261	I325	K433	
L262	L262	N326	E448	
V263	V263	K327	V455	
V264	V264	D328	L456	
N265	N265	T329	C458	
T266	T266	T330	E461	
N267	N267	T331	P462	
R268	R268	I332	A480	
G269	G269	I333	L493	
I270	I270	D334	V499	
V271	V271	E335	M514	
E272	E272	G336	L524	
V273	V273	V336		
A274	A274	V346		
A275	A275	R350		
V276	V276	Q351		
K277	K277	Q352		
A278	A278	I353		
P279	P279	E354		
G280	G280	E355		
F281	F281	A356		
G282	G282	T357		
D283	D283	S358		
R284	R284	D359		
K285	K285	Y360		
K286	K286			

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	235.22Å 141.66Å 156.69Å 90.00° 113.84° 90.00°	Depositor
Resolution (Å)	46.17 – 2.72 46.17 – 2.72	Depositor EDS
% Data completeness (in resolution range)	95.6 (46.17-2.72) 95.6 (46.17-2.72)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.10 (at 2.73Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.166 , 0.203 0.167 , 0.203	Depositor DCC
R_{free} test set	2000 reflections (1.66%)	wwPDB-VP
Wilson B-factor (Å ²)	45.2	Xtriage
Anisotropy	0.465	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 61.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	27977	wwPDB-VP
Average B, all atoms (Å ²)	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.12% 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: K, MG, MPD, CA, ADP

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	0.28	0/3885	0.48	0/5246
1	B	0.29	0/3885	0.47	0/5246
1	C	0.32	0/3907	0.50	0/5274
1	D	0.28	0/3896	0.47	0/5260
1	E	0.27	0/3882	0.47	0/5243
1	F	0.28	0/3913	0.47	0/5284
1	G	0.27	0/3885	0.49	0/5246
All	All	0.29	0/27253	0.48	0/36799

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3854	0	3982	154	0
1	B	3854	0	3982	147	0
1	C	3864	0	3994	249	1
1	D	3862	0	3995	126	0
1	E	3851	0	3975	121	0
1	F	3873	0	4005	180	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	3854	0	3982	259	0
2	A	27	0	12	0	0
2	B	27	0	12	0	0
2	C	27	0	12	0	0
2	D	27	0	12	0	0
2	E	27	0	12	2	0
2	F	27	0	12	0	0
2	G	27	0	12	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	2	0	0	0	0
4	G	2	0	0	0	0
5	A	48	0	84	13	0
5	B	40	0	70	5	0
5	C	8	0	14	1	0
5	D	24	0	42	2	0
5	E	8	0	14	2	0
5	F	8	0	14	0	0
5	G	16	0	28	3	0
6	A	2	0	0	0	0
6	B	1	0	0	0	0
6	D	1	0	0	0	0
6	E	3	0	0	0	0
6	F	1	0	0	0	0
6	G	3	0	0	0	0
7	A	90	0	0	4	0
7	B	112	0	0	7	0
7	C	88	0	0	6	0
7	D	90	0	0	4	0
7	E	65	0	0	8	0
7	F	67	0	0	2	0
7	G	85	0	0	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	27977	0	28265	1210	1

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 22.

The worst 5 of 1210 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:A:230:ILE:HD12	1:A:261:THR:HG21	1.23	1.15
1:G:281:PHE:HB3	1:G:285:ARG:HB3	1.18	1.14
1:A:183:LEU:HA	1:A:383:ALA:HB2	1.14	1.09
1:B:255:GLU:HA	1:B:259:LEU:HD23	1.28	1.07
1:C:225:LYS:HB2	1:C:251:ALA:HB1	1.31	1.07

All (1) 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:C:461:GLU:OE2	1:F:463:SER:OG[2_959]	2.11	0.09

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	523/548 (95%)	512 (98%)	11 (2%)	0	100	100
1	B	523/548 (95%)	509 (97%)	13 (2%)	1 (0%)	47	72
1	C	525/548 (96%)	505 (96%)	19 (4%)	1 (0%)	47	72
1	D	524/548 (96%)	509 (97%)	15 (3%)	0	100	100
1	E	523/548 (95%)	512 (98%)	10 (2%)	1 (0%)	47	72

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	526/548 (96%)	512 (97%)	13 (2%)	1 (0%)	47	72
1	G	523/548 (95%)	502 (96%)	21 (4%)	0	100	100
All	All	3667/3836 (96%)	3561 (97%)	102 (3%)	4 (0%)	51	77

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	270	ILE
1	F	270	ILE
1	E	270	ILE
1	C	227	ILE

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	403/413 (98%)	391 (97%)	12 (3%)	41	69
1	B	403/413 (98%)	395 (98%)	8 (2%)	55	80
1	C	405/413 (98%)	393 (97%)	12 (3%)	41	69
1	D	404/413 (98%)	392 (97%)	12 (3%)	41	69
1	E	403/413 (98%)	390 (97%)	13 (3%)	39	67
1	F	406/413 (98%)	397 (98%)	9 (2%)	52	78
1	G	403/413 (98%)	385 (96%)	18 (4%)	27	53
All	All	2827/2891 (98%)	2743 (97%)	84 (3%)	42	69

5 of 84 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	188	ASP
1	E	169	VAL
1	G	253	ASP
1	D	228	SER
1	D	389	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	10	ASN
1	E	146	GLN
1	F	401	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 53 ligands modelled in this entry, 27 are monoatomic - leaving 26 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	ADP	A	601	3,4	24,29,29	0.95	1 (4%)	29,45,45	1.43	4 (13%)
5	MPD	D	606	-	7,7,7	0.43	0	9,10,10	0.69	0
5	MPD	C	604	-	7,7,7	0.41	0	9,10,10	0.81	0
5	MPD	G	604	-	7,7,7	0.36	0	9,10,10	0.53	0
5	MPD	B	604	-	7,7,7	0.39	0	9,10,10	0.43	0
2	ADP	B	601	3,4	24,29,29	1.04	2 (8%)	29,45,45	1.47	4 (13%)
5	MPD	G	605	-	7,7,7	0.80	0	9,10,10	0.92	0
5	MPD	D	604	-	7,7,7	0.33	0	9,10,10	0.30	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ADP	C	601	3,4	24,29,29	0.96	1 (4%)	29,45,45	1.38	5 (17%)
5	MPD	F	604	-	7,7,7	0.32	0	9,10,10	0.47	0
2	ADP	F	601	3,4	24,29,29	0.98	1 (4%)	29,45,45	1.46	3 (10%)
5	MPD	A	607	-	7,7,7	0.34	0	9,10,10	0.35	0
5	MPD	D	605	-	7,7,7	0.32	0	9,10,10	0.52	0
5	MPD	B	606	-	7,7,7	0.38	0	9,10,10	0.52	0
2	ADP	E	601	3,4	24,29,29	0.96	1 (4%)	29,45,45	1.41	3 (10%)
5	MPD	B	608	-	7,7,7	0.37	0	9,10,10	0.42	0
5	MPD	A	609	-	7,7,7	0.24	0	9,10,10	0.48	0
5	MPD	E	604	-	7,7,7	0.38	0	9,10,10	0.50	0
5	MPD	A	608	-	7,7,7	0.32	0	9,10,10	0.77	0
2	ADP	D	601	3,4	24,29,29	0.97	2 (8%)	29,45,45	1.51	5 (17%)
5	MPD	A	606	-	7,7,7	0.37	0	9,10,10	0.75	0
5	MPD	A	605	-	7,7,7	0.37	0	9,10,10	0.63	0
2	ADP	G	601	3,4	24,29,29	1.03	2 (8%)	29,45,45	1.51	5 (17%)
5	MPD	B	607	-	7,7,7	0.31	0	9,10,10	0.44	0
5	MPD	A	604	-	7,7,7	0.41	0	9,10,10	0.36	0
5	MPD	B	605	-	7,7,7	0.32	0	9,10,10	0.61	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ADP	A	601	3,4	-	2/12/32/32	0/3/3/3
5	MPD	D	606	-	-	3/5/5/5	-
5	MPD	C	604	-	-	2/5/5/5	-
5	MPD	G	604	-	-	0/5/5/5	-
5	MPD	B	604	-	-	1/5/5/5	-
2	ADP	B	601	3,4	-	6/12/32/32	0/3/3/3
5	MPD	G	605	-	-	0/5/5/5	-
5	MPD	D	604	-	-	2/5/5/5	-
2	ADP	C	601	3,4	-	2/12/32/32	0/3/3/3
5	MPD	F	604	-	-	2/5/5/5	-
2	ADP	F	601	3,4	-	7/12/32/32	0/3/3/3
5	MPD	A	607	-	-	0/5/5/5	-
5	MPD	D	605	-	-	0/5/5/5	-
5	MPD	B	606	-	-	0/5/5/5	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ADP	E	601	3,4	-	6/12/32/32	0/3/3/3
5	MPD	B	608	-	-	3/5/5/5	-
5	MPD	A	609	-	-	2/5/5/5	-
5	MPD	E	604	-	-	2/5/5/5	-
5	MPD	A	608	-	-	5/5/5/5	-
2	ADP	D	601	3,4	-	2/12/32/32	0/3/3/3
5	MPD	A	606	-	-	1/5/5/5	-
5	MPD	A	605	-	-	2/5/5/5	-
2	ADP	G	601	3,4	-	3/12/32/32	0/3/3/3
5	MPD	B	607	-	-	2/5/5/5	-
5	MPD	A	604	-	-	0/5/5/5	-
5	MPD	B	605	-	-	2/5/5/5	-

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	ADP	C5-C4	2.37	1.47	1.40
2	F	601	ADP	C5-C4	2.35	1.47	1.40
2	G	601	ADP	C2-N3	2.31	1.35	1.32
2	G	601	ADP	C5-C4	2.31	1.47	1.40
2	E	601	ADP	C5-C4	2.28	1.47	1.40

The worst 5 of 29 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	ADP	PA-O3A-PB	-3.99	119.13	132.83
2	A	601	ADP	N3-C2-N1	-3.73	122.85	128.68
2	E	601	ADP	PA-O3A-PB	-3.64	120.32	132.83
2	E	601	ADP	N3-C2-N1	-3.64	122.98	128.68
2	F	601	ADP	PA-O3A-PB	-3.56	120.59	132.83

There are no chirality outliers.

5 of 57 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	604	MPD	C2-C3-C4-C5
5	B	604	MPD	C2-C3-C4-C5
2	B	601	ADP	PA-O3A-PB-O2B
2	B	601	ADP	C5'-O5'-PA-O1A

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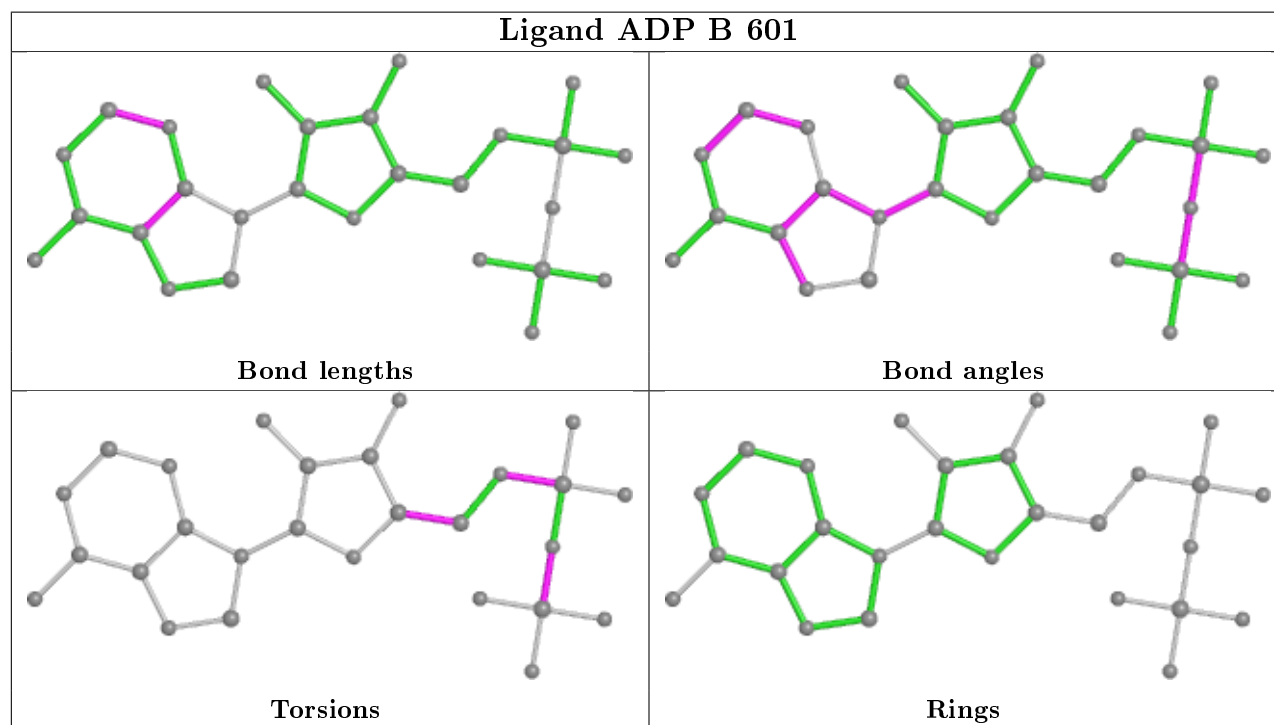
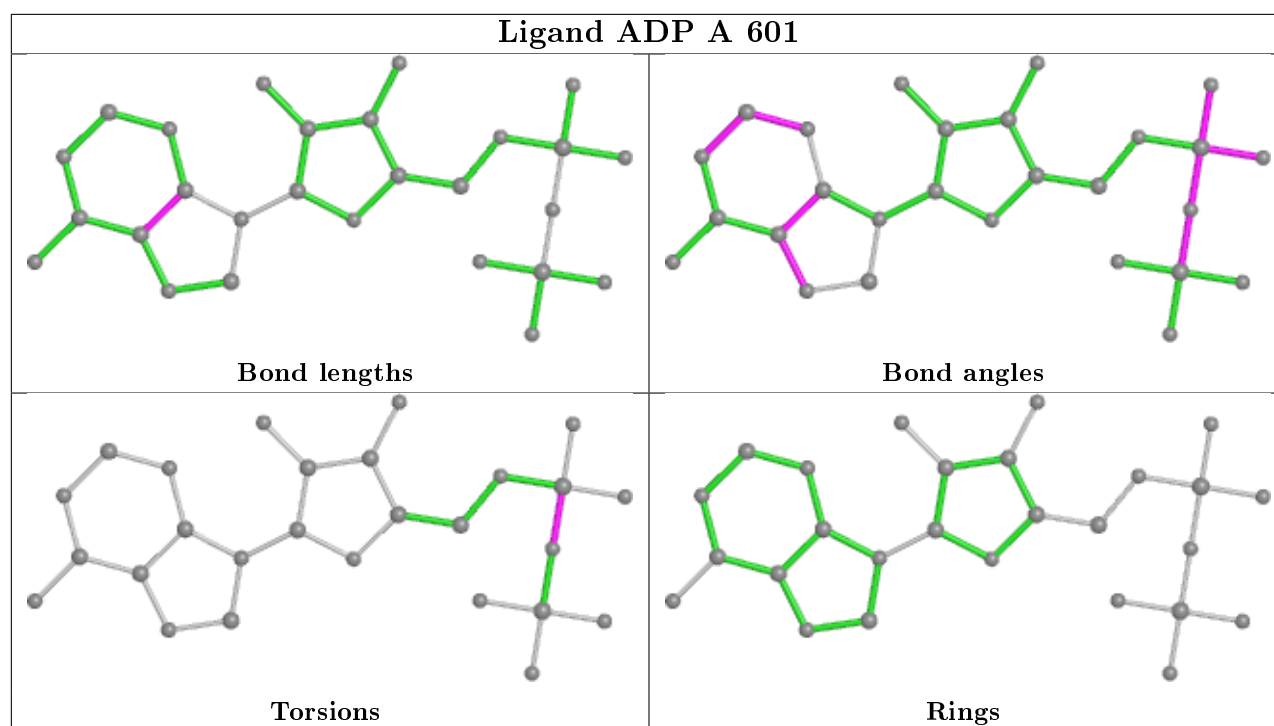
Mol	Chain	Res	Type	Atoms
2	B	601	ADP	C5'-O5'-PA-O2A

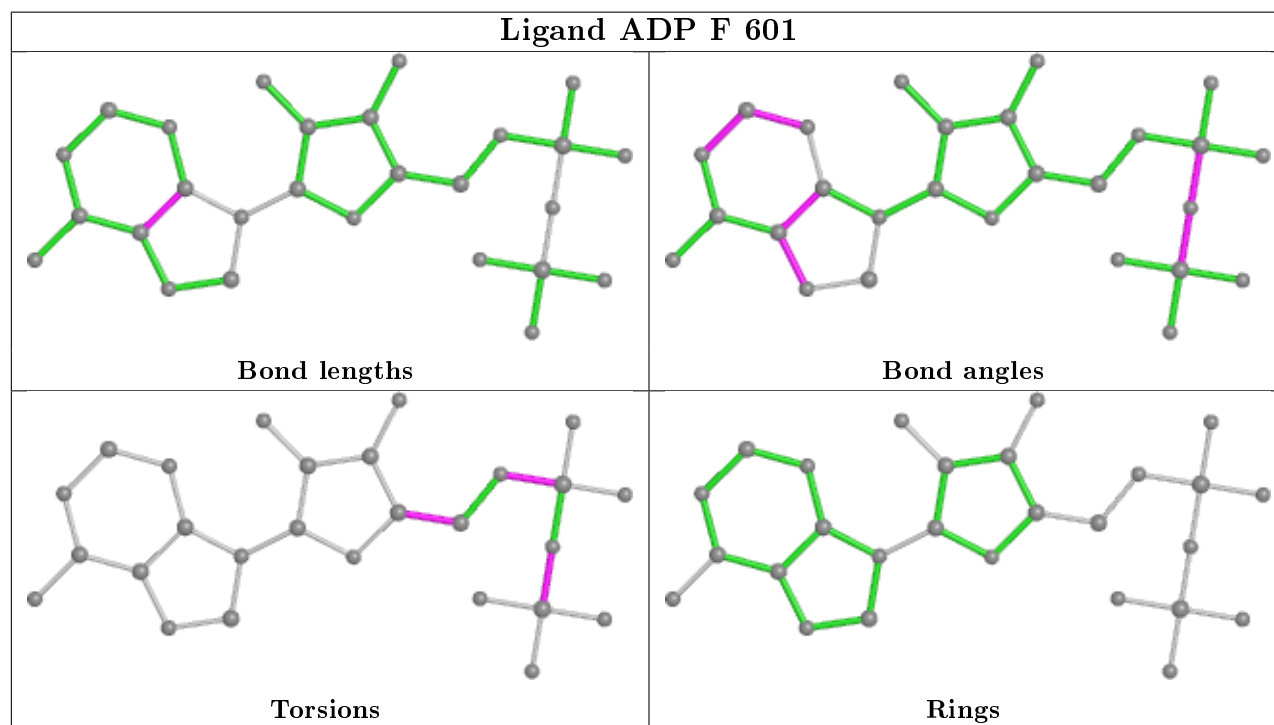
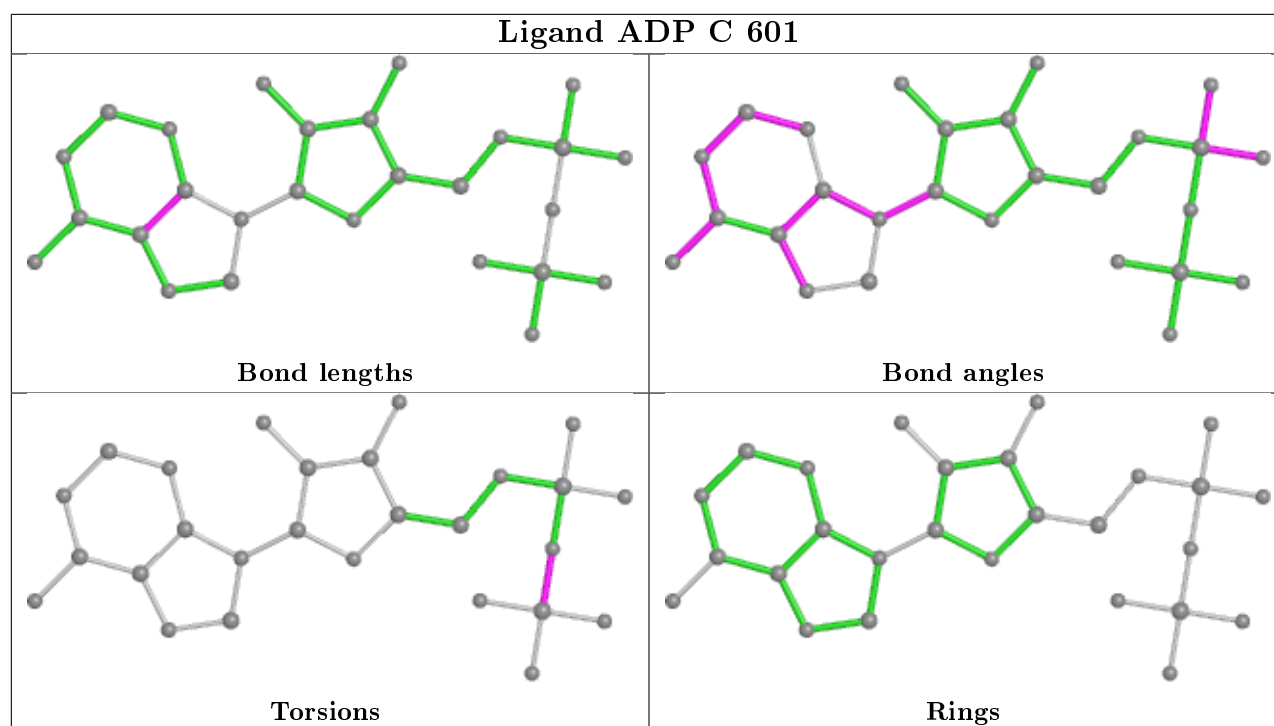
There are no ring outliers.

15 monomers are involved in 29 short contacts:

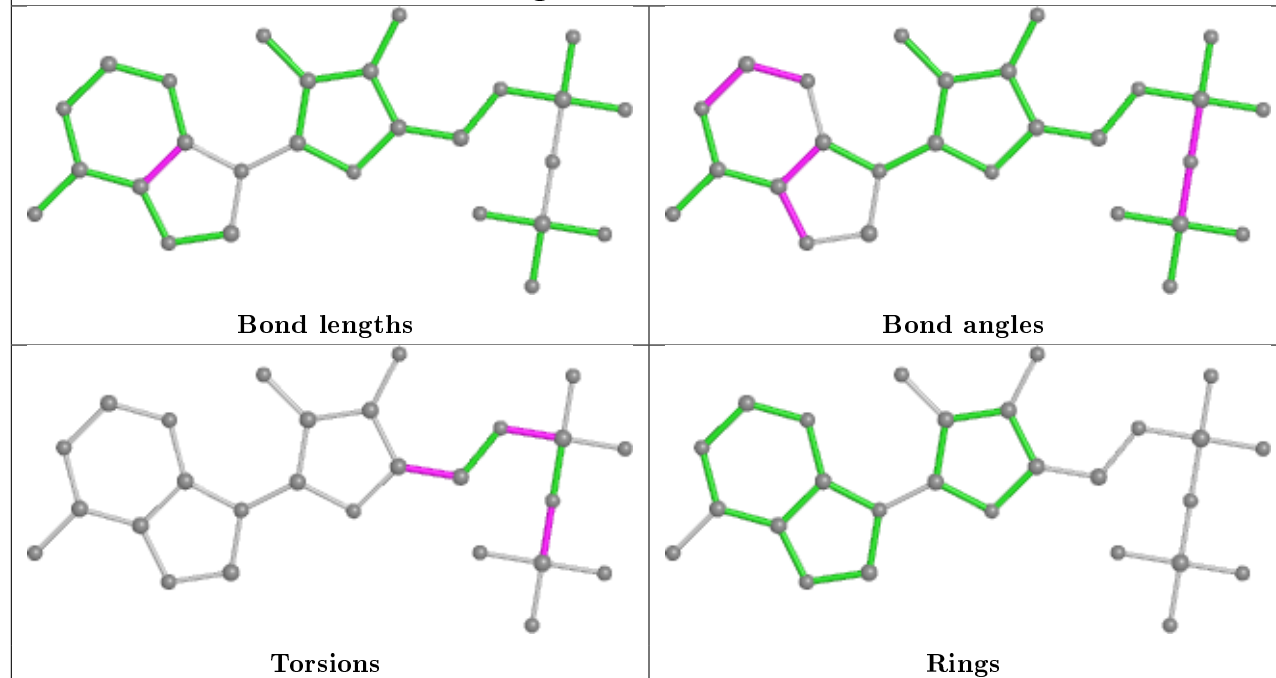
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	604	MPD	1	0
5	G	604	MPD	3	0
5	B	604	MPD	2	0
5	D	604	MPD	1	0
5	D	605	MPD	1	0
2	E	601	ADP	2	0
5	B	608	MPD	2	0
5	A	609	MPD	4	0
5	E	604	MPD	2	0
5	A	608	MPD	3	0
5	A	606	MPD	3	0
5	A	605	MPD	2	0
2	G	601	ADP	1	0
5	A	604	MPD	1	0
5	B	605	MPD	1	0

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

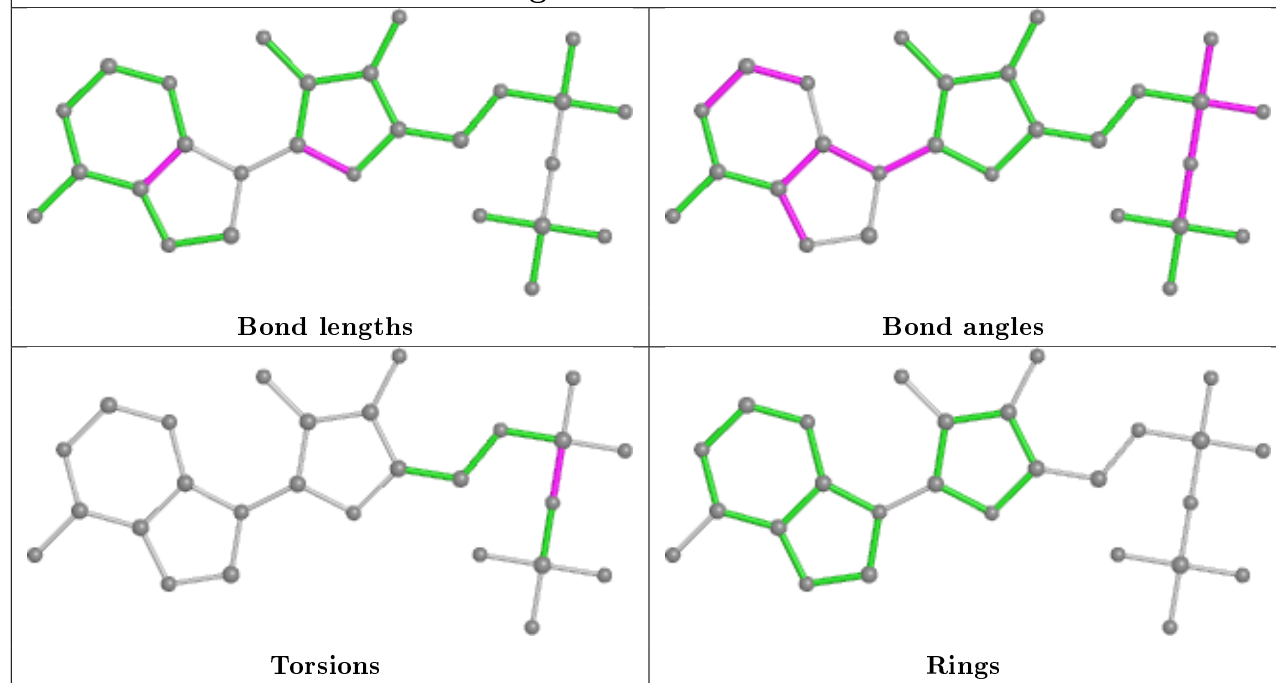


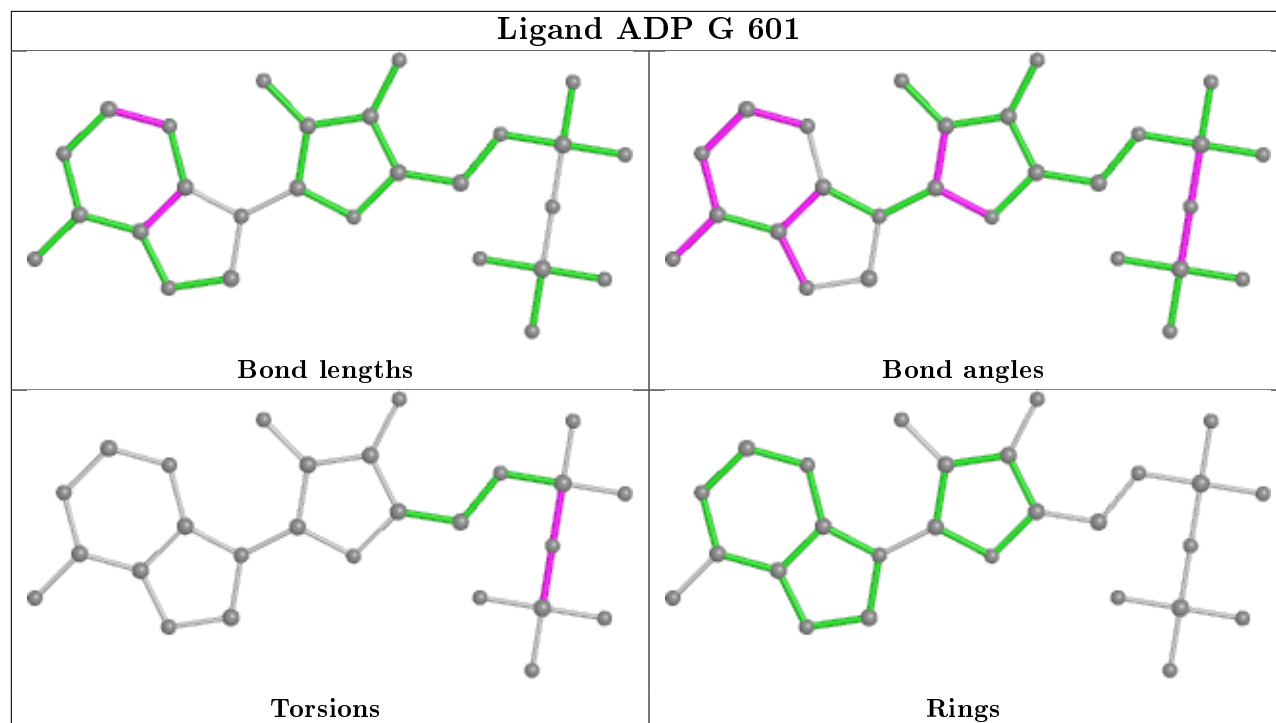


Ligand ADP E 601



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 [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%)	0.03	18 (3%) 45 45	27, 69, 168, 196	0
1	B	524/548 (95%)	0.03	22 (4%) 36 35	24, 60, 160, 190	0
1	C	524/548 (95%)	0.37	65 (12%) 4 3	26, 68, 202, 243	0
1	D	524/548 (95%)	-0.13	9 (1%) 70 72	30, 71, 155, 181	0
1	E	524/548 (95%)	-0.05	13 (2%) 57 59	31, 79, 141, 187	0
1	F	524/548 (95%)	0.06	34 (6%) 18 18	33, 75, 178, 223	0
1	G	524/548 (95%)	0.40	57 (10%) 5 4	30, 71, 211, 243	0
All	All	3668/3836 (95%)	0.10	218 (5%) 22 21	24, 72, 181, 243	0

The worst 5 of 218 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	225	LYS	9.8
1	G	251	ALA	8.5
1	G	233	MET	8.1
1	E	271	VAL	8.1
1	G	301	ILE	7.3

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 carbohydrates in this entry.

6.4 Ligands ⓘ

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

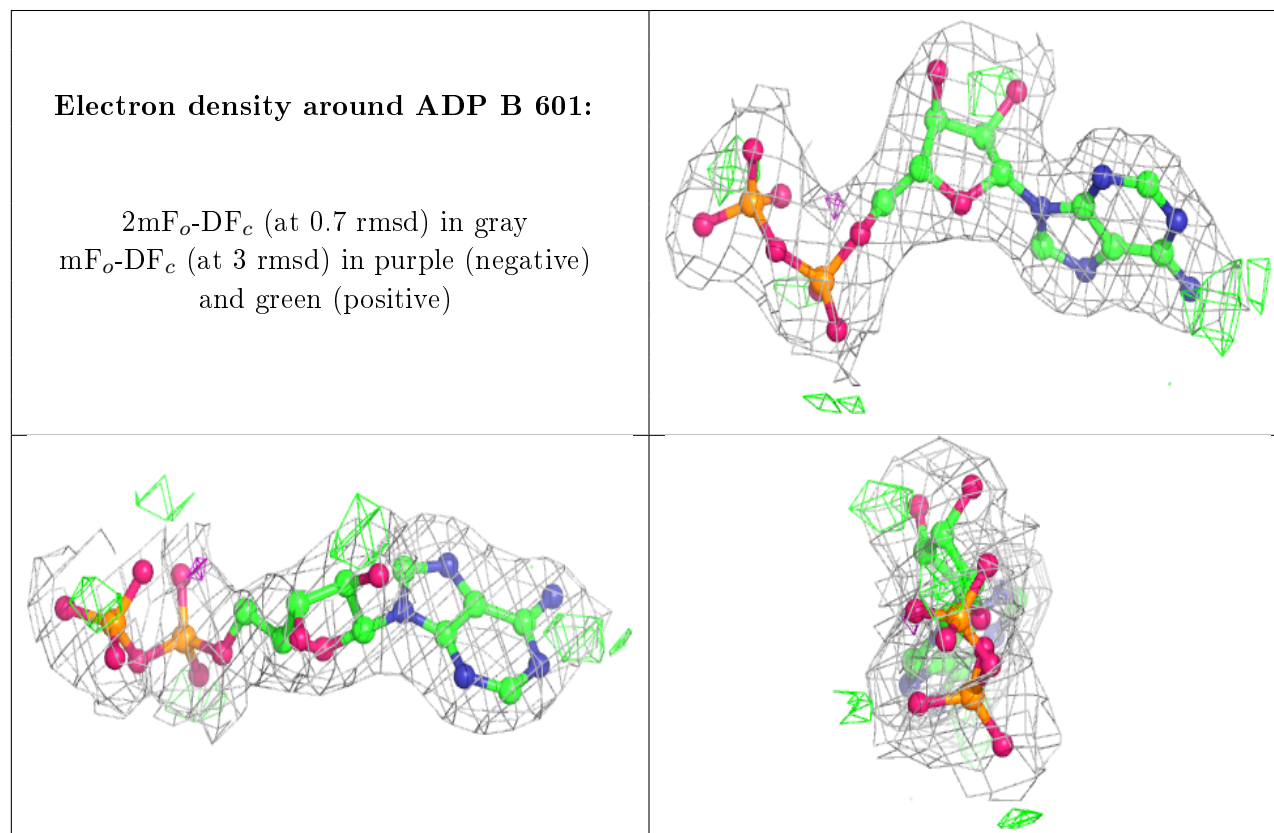
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	K	F	605	1/1	0.40	0.48	166,166,166,166	0
4	K	G	608	1/1	0.71	0.22	154,154,154,154	0
5	MPD	E	604	8/8	0.76	0.39	120,123,127,127	0
6	CA	E	607	1/1	0.78	0.20	126,126,126,126	0
5	MPD	B	608	8/8	0.80	0.28	93,98,109,118	0
5	MPD	D	605	8/8	0.80	0.36	108,112,116,116	0
5	MPD	A	604	8/8	0.80	0.20	106,109,115,123	0
5	MPD	G	604	8/8	0.80	0.37	78,99,109,117	0
6	CA	G	609	1/1	0.81	0.36	123,123,123,123	0
6	CA	G	607	1/1	0.82	0.20	114,114,114,114	0
5	MPD	D	606	8/8	0.85	0.28	79,99,108,113	0
5	MPD	G	605	8/8	0.85	0.32	114,117,141,153	0
6	CA	B	609	1/1	0.86	0.13	141,141,141,141	0
5	MPD	F	604	8/8	0.86	0.30	119,124,125,130	0
5	MPD	A	606	8/8	0.87	0.37	98,111,115,115	0
5	MPD	A	609	8/8	0.87	0.41	110,122,129,134	0
5	MPD	B	606	8/8	0.88	0.23	74,90,103,111	0
5	MPD	D	604	8/8	0.88	0.26	95,110,115,123	0
5	MPD	B	607	8/8	0.89	0.31	92,108,124,126	0
5	MPD	B	604	8/8	0.89	0.24	52,80,90,92	0
5	MPD	A	607	8/8	0.90	0.23	83,95,97,104	0
3	MG	B	602	1/1	0.90	0.18	29,29,29,29	0
5	MPD	A	608	8/8	0.90	0.38	103,110,120,123	0
5	MPD	C	604	8/8	0.90	0.31	102,107,112,117	0
6	CA	E	605	1/1	0.91	0.12	108,108,108,108	0
5	MPD	A	605	8/8	0.91	0.26	90,96,105,107	0
5	MPD	B	605	8/8	0.91	0.33	89,107,112,123	0
6	CA	A	611	1/1	0.93	0.38	107,107,107,107	0
6	CA	E	606	1/1	0.93	0.07	111,111,111,111	0
3	MG	A	602	1/1	0.94	0.15	33,33,33,33	0
6	CA	A	610	1/1	0.95	0.20	129,129,129,129	0
4	K	C	603	1/1	0.96	0.22	79,79,79,79	0
4	K	E	603	1/1	0.96	0.14	89,89,89,89	0
6	CA	F	606	1/1	0.97	0.11	110,110,110,110	0
3	MG	C	602	1/1	0.97	0.13	34,34,34,34	0
6	CA	G	606	1/1	0.97	0.21	88,88,88,88	0
2	ADP	B	601	27/27	0.97	0.19	30,48,62,127	0

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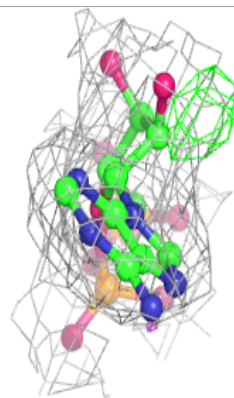
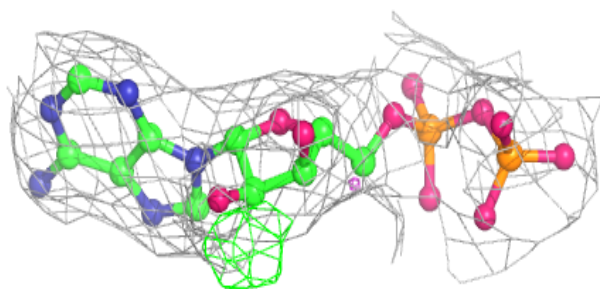
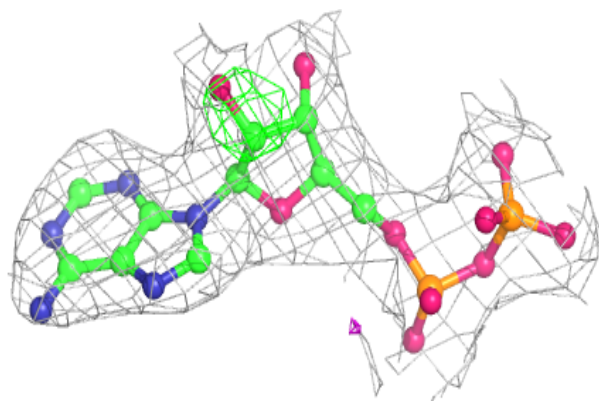
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	MG	E	602	1/1	0.97	0.11	38,38,38,38	0
3	MG	F	602	1/1	0.97	0.11	28,28,28,28	0
6	CA	D	607	1/1	0.97	0.18	118,118,118,118	0
2	ADP	E	601	27/27	0.97	0.15	57,70,80,250	0
2	ADP	A	601	27/27	0.98	0.16	39,56,64,75	0
3	MG	G	602	1/1	0.98	0.14	25,25,25,25	0
2	ADP	G	601	27/27	0.98	0.17	41,50,65,94	0
2	ADP	C	601	27/27	0.98	0.17	43,55,64,66	0
4	K	B	603	1/1	0.98	0.22	62,62,62,62	0
2	ADP	D	601	27/27	0.98	0.17	36,57,70,80	0
4	K	D	603	1/1	0.98	0.16	64,64,64,64	0
2	ADP	F	601	27/27	0.98	0.19	38,62,74,86	0
3	MG	D	602	1/1	0.99	0.13	30,30,30,30	0
4	K	A	603	1/1	0.99	0.22	58,58,58,58	0
4	K	G	603	1/1	0.99	0.19	65,65,65,65	0
4	K	F	603	1/1	1.00	0.27	60,60,60,60	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.

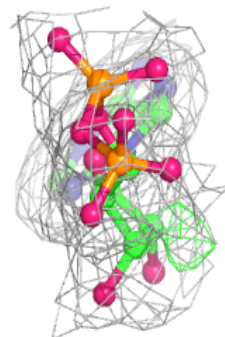
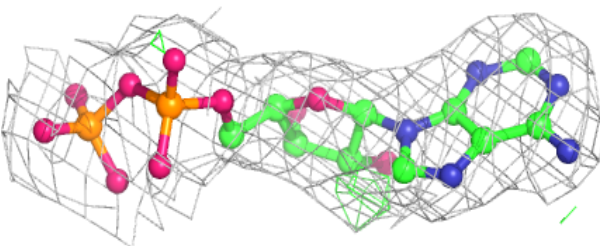
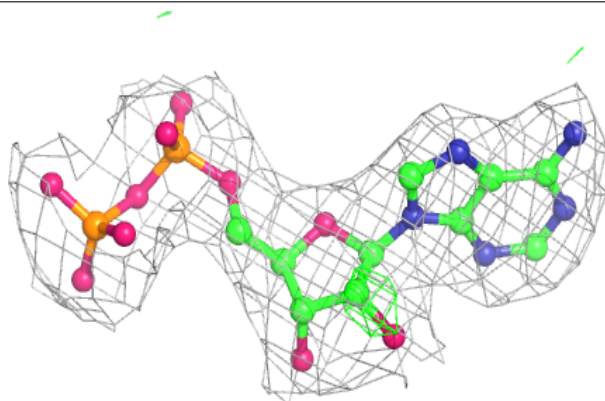


Electron density around ADP E 601:

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

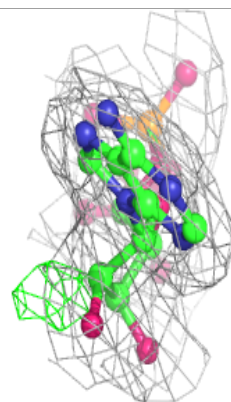
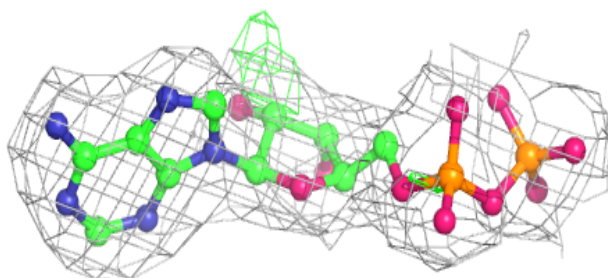
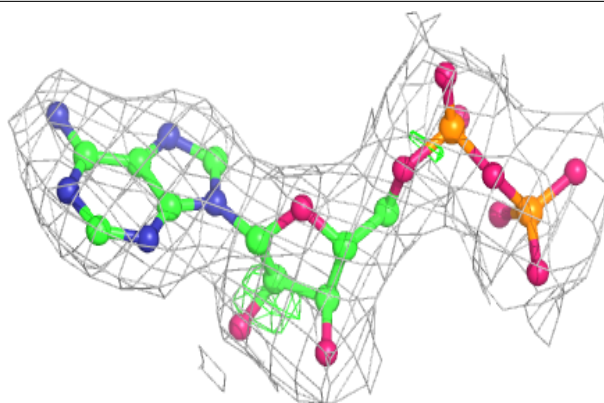
**Electron density around ADP A 601:**

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

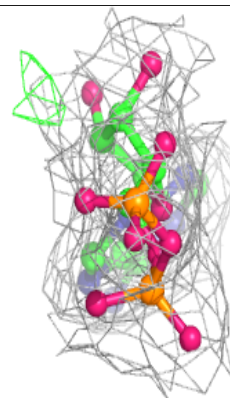
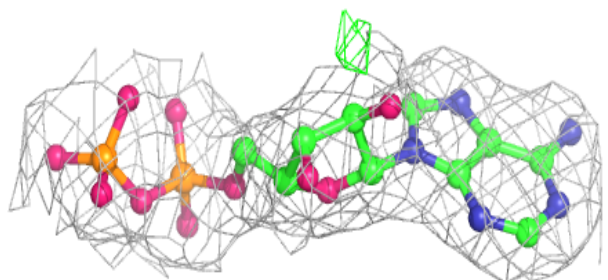
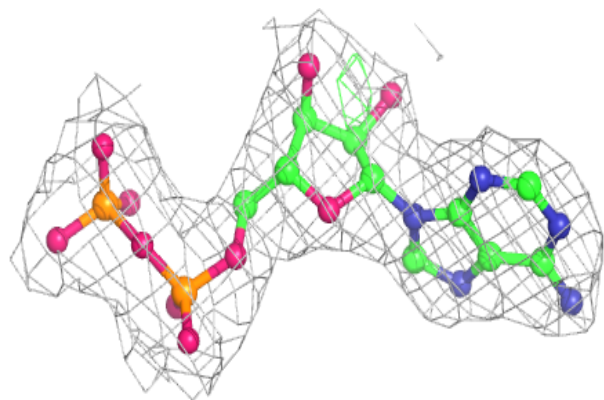


Electron density around ADP G 601:

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

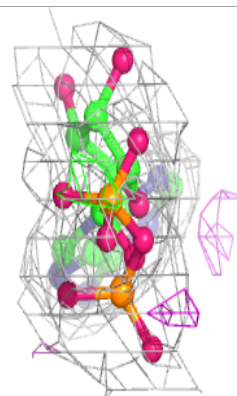
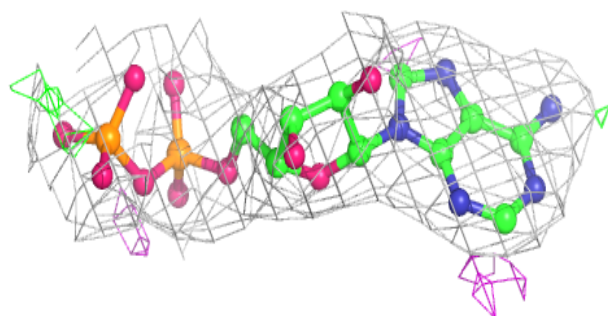
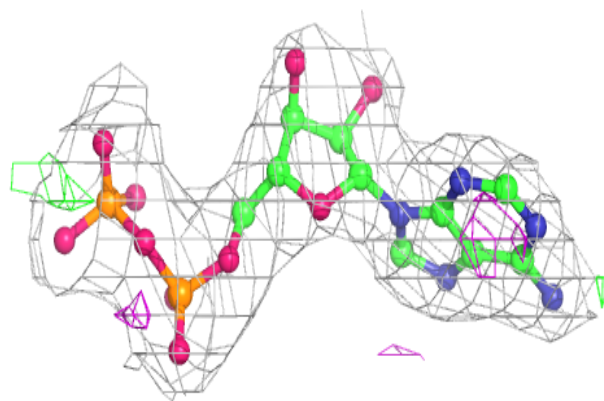
**Electron density around ADP C 601:**

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

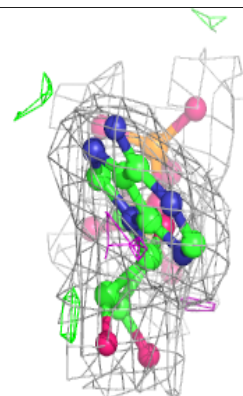
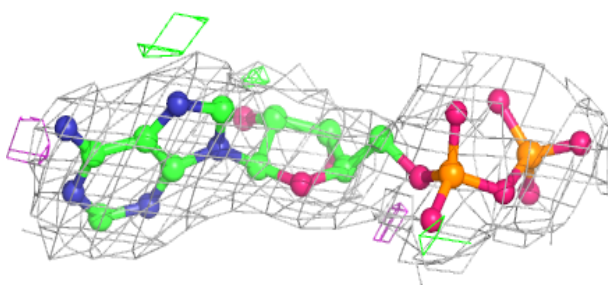
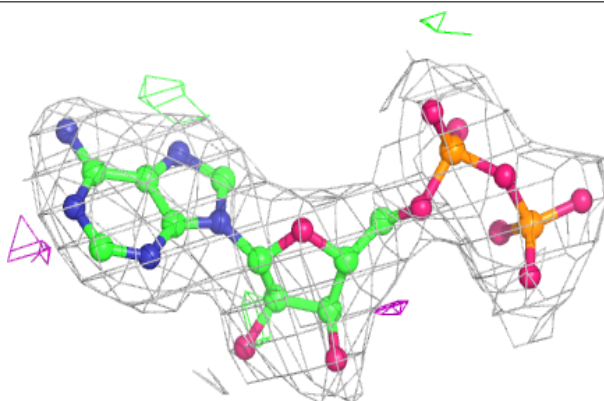


Electron density around ADP D 601:

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

**Electron density around ADP 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.