



wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 4, 2024 – 12:14 AM JST

PDB ID : 8YN0
Title : Crystal structure of NRG1C in complex with EDS1-SAG101-(ADPr-ATP)
Authors : Huang, S.; Xiao, Y.; Chai, J.
Deposited on : 2024-03-10
Resolution : 2.49 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.21
EDS : 3.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.004 (Gargrove)
Density-Fitness : 1.0.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.40

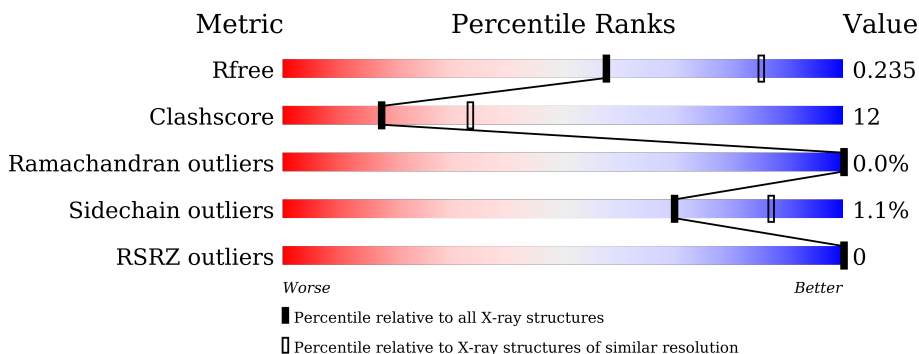
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.49 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}	164625	5504 (2.50-2.50)
Clashscore	180529	6282 (2.50-2.50)
Ramachandran outliers	177936	6191 (2.50-2.50)
Sidechain outliers	177891	6193 (2.50-2.50)
RSRZ outliers	164620	5504 (2.50-2.50)

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	617	76% 24%
1	B	617	73% 27%
2	C	536	72% 26% .
2	E	536	73% 24% ..
3	D	415	75% 24% ..
3	H	415	75% 24% .

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 26107 atoms, of which 62 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 Protein EDS1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	B	617	5008	3184	861	944	19	0	0	0
1	A	617	5013	3188	861	944	20	0	1	0

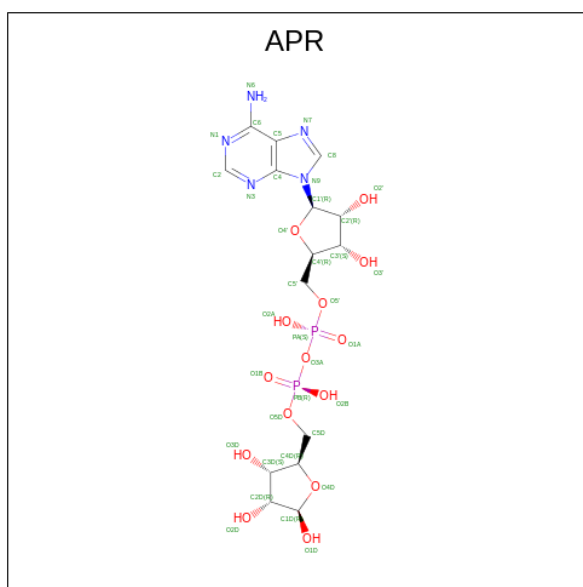
- Molecule 2 is a protein called Senescence-associated carboxylesterase 101.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	E	527	4287	2747	719	798	23	0	0	0
2	C	527	4287	2747	719	798	23	0	0	0

- Molecule 3 is a protein called Probable disease resistance protein At5g66890.

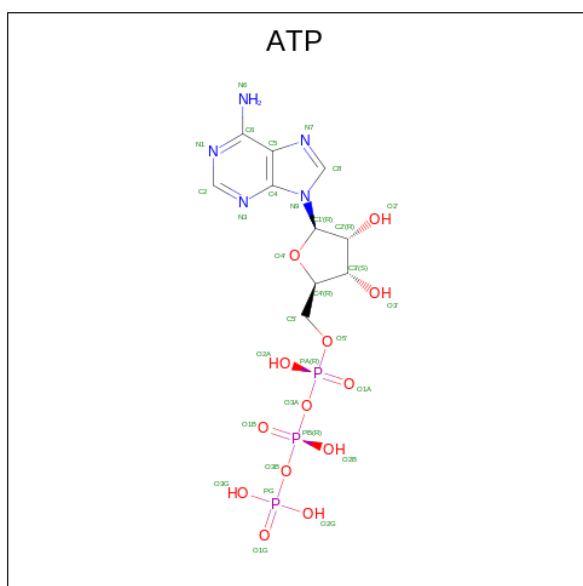
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	H	412	3311	2111	545	635	20	0	0	0
3	D	411	3303	2106	544	634	19	0	0	0

- Molecule 4 is ADENOSINE-5-DIPHOSPHORIBOSE (three-letter code: APR) (formula: $C_{15}H_{23}N_5O_{14}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	H	N	O			P
4	B	1	55	15	20	5	13	2	0	0
4	A	1	55	15	20	5	13	2	0	0

- Molecule 5 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	H	N	O			P
5	E	1	42	10	11	5	13	3	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	H	N	O	P		
5	C	1	42	10	11	5	13	3	0	0

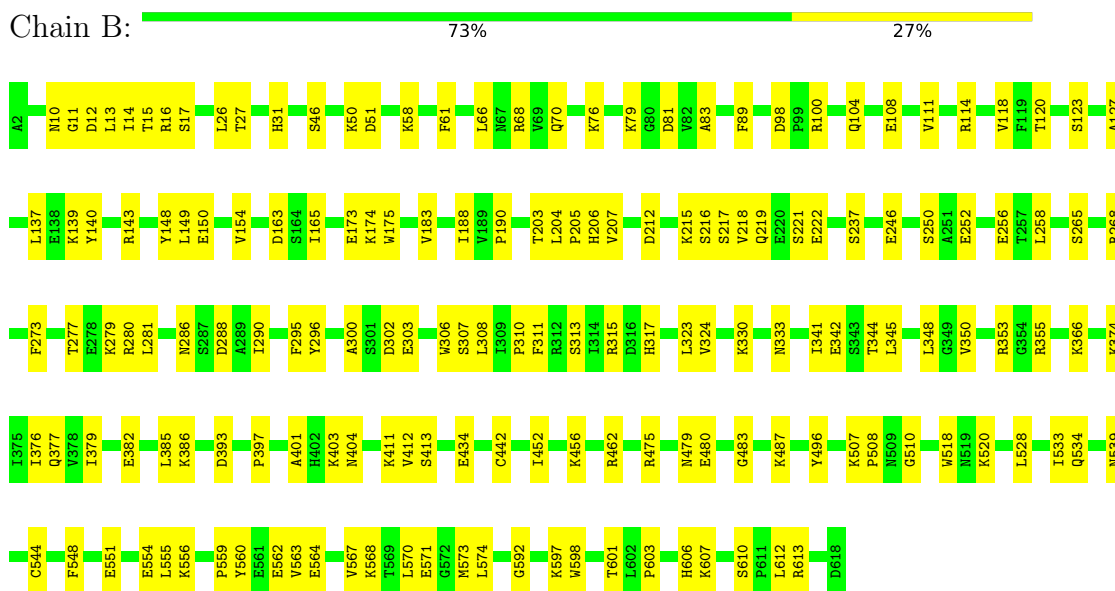
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	B	132	132	132	0	0
6	E	133	133	133	0	0
6	C	127	127	127	0	0
6	H	122	122	122	0	0
6	A	91	91	91	0	0
6	D	99	99	99	0	0

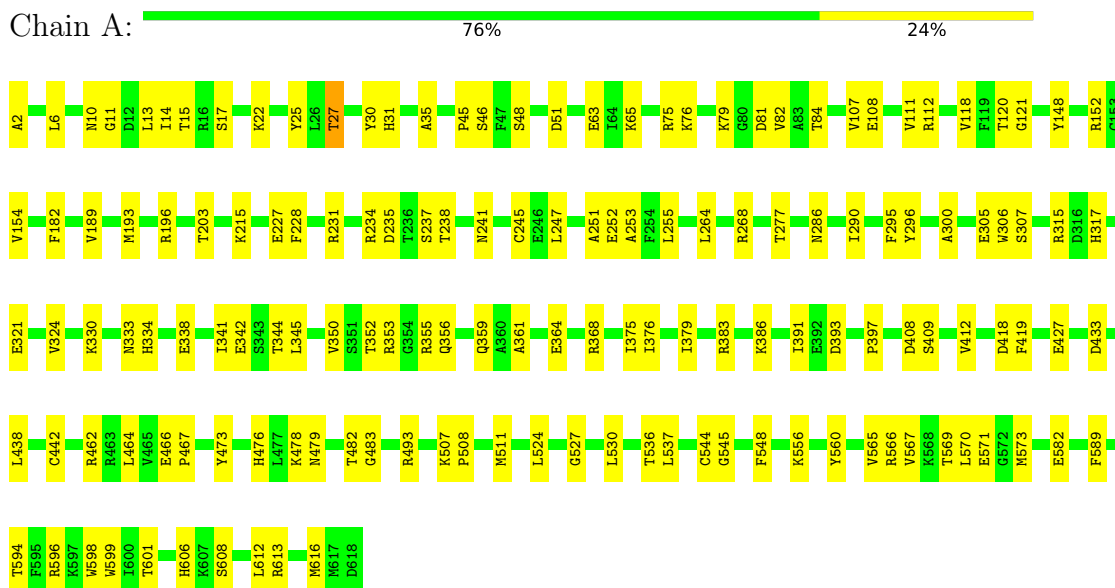
3 Residue-property plots [i](#)

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

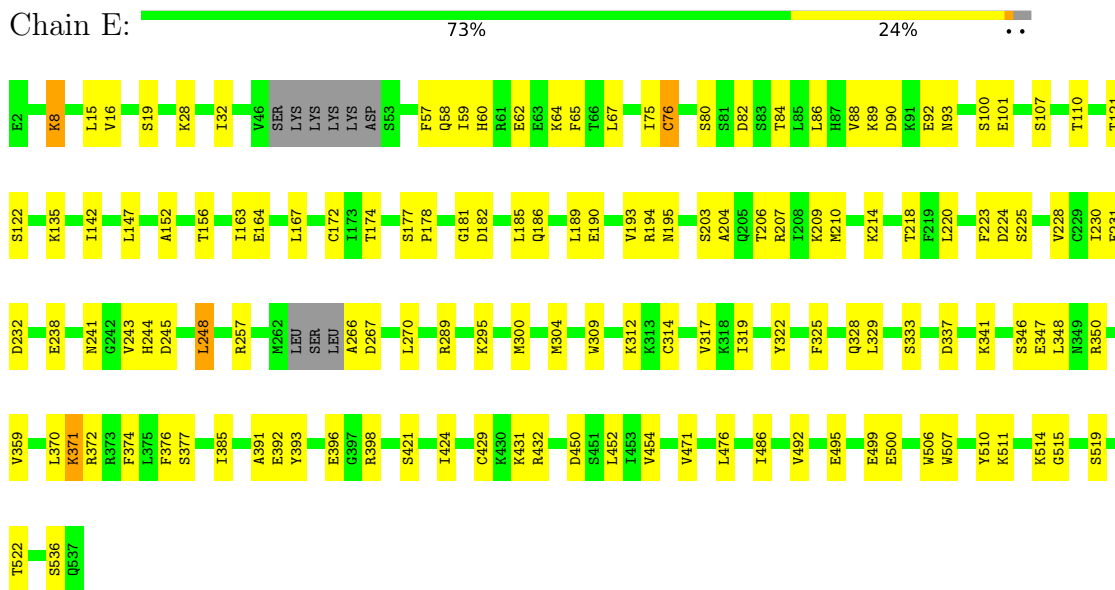
- Molecule 1: Protein EDS1



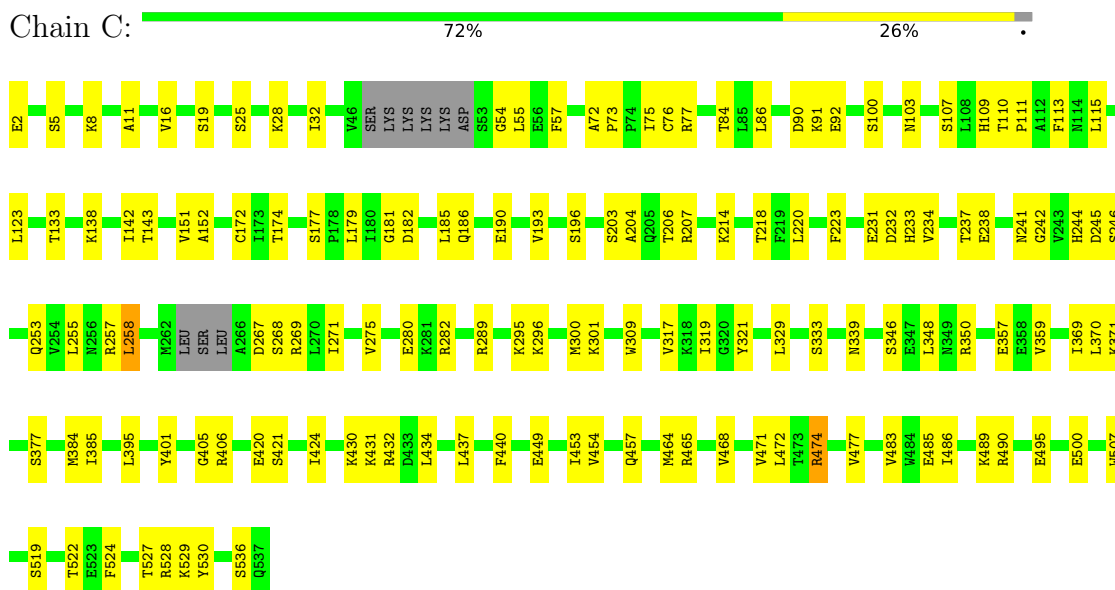
- Molecule 1: Protein EDS1



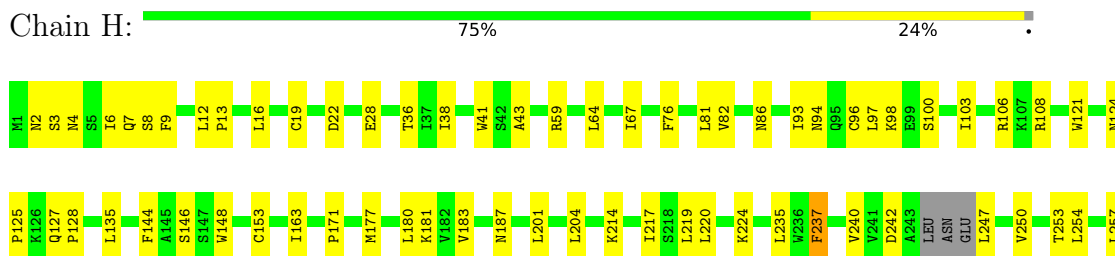
- Molecule 2: Senescence-associated carboxylesterase 101

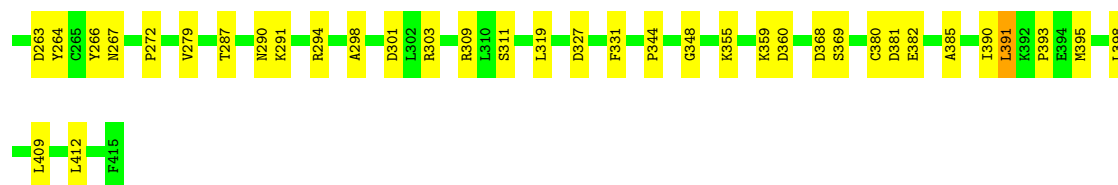


- Molecule 2: Senescence-associated carboxylesterase 101



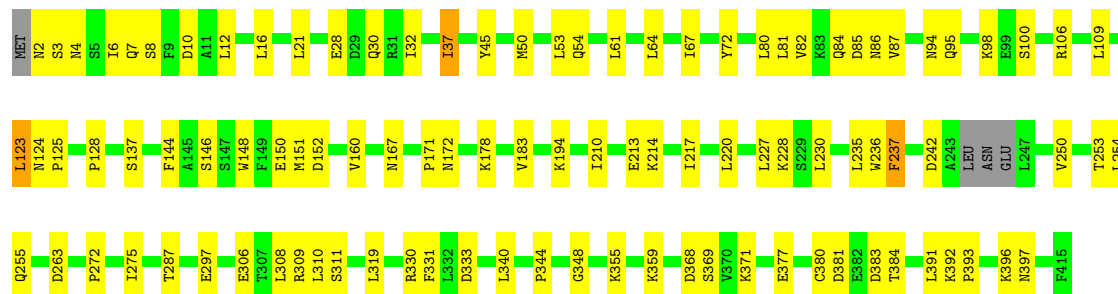
- Molecule 3: Probable disease resistance protein At5g66890





- Molecule 3: Probable disease resistance protein At5g66890

Chain D: 75% 24% ..



4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	91.52Å 154.91Å 171.11Å 90.00° 89.69° 90.00°	Depositor
Resolution (Å)	39.77 – 2.49 39.77 – 2.49	Depositor EDS
% Data completeness (in resolution range)	95.5 (39.77-2.49) 94.5 (39.77-2.49)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.43 (at 2.48Å)	Xtrriage
Refinement program	PHENIX (1.18.2_3874: ???)	Depositor
R, R_{free}	0.199 , 0.238 0.206 , 0.235	Depositor DCC
R_{free} test set	156989 reflections (1.25%)	wwPDB-VP
Wilson B-factor (Å ²)	45.6	Xtrriage
Anisotropy	0.379	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 26.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.388 for h,-k,-l	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	26107	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.06% 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: APR, ATP

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	0.61	0/5129	0.71	4/6922 (0.1%)
1	B	0.58	0/5121	0.68	0/6912
2	C	0.68	0/4383	0.75	2/5906 (0.0%)
2	E	0.62	0/4383	0.74	1/5906 (0.0%)
3	D	0.63	0/3357	0.76	2/4538 (0.0%)
3	H	0.63	0/3365	0.74	0/4548
All	All	0.62	0/25738	0.73	9/34732 (0.0%)

There are no bond length outliers.

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	35	ALA	N-CA-C	-7.92	89.62	111.00
2	C	258	LEU	CA-CB-CG	7.48	132.50	115.30
2	E	515	GLY	N-CA-C	7.14	130.95	113.10
1	A	527	GLY	N-CA-C	6.76	130.01	113.10
1	A	524	LEU	N-CA-C	-6.20	94.26	111.00

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	5013	0	4925	115	0
1	B	5008	0	4916	138	0
2	C	4287	0	4283	112	0
2	E	4287	0	4283	110	0
3	D	3303	0	3353	76	0
3	H	3311	0	3365	75	0
4	A	35	20	19	1	0
4	B	35	20	19	2	0
5	C	31	11	11	1	0
5	E	31	11	11	3	0
6	A	91	0	0	16	0
6	B	132	0	0	18	1
6	C	127	0	0	13	1
6	D	99	0	0	8	1
6	E	133	0	0	15	1
6	H	122	0	0	8	2
All	All	26045	62	25185	615	3

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 12.

The worst 5 of 615 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:17:SER:HB3	1:B:120:THR:HG21	1.16	1.08
1:B:215:LYS:HE2	1:B:217:SER:HB2	1.39	1.02
1:A:599:TRP:HB3	1:A:616:MET:HE1	1.45	0.99
1:B:76:LYS:NZ	1:B:442:CYS:SG	2.36	0.98
2:C:11:ALA:HB1	1:A:241:ASN:HB2	1.46	0.96

All (3) 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)
6:C:720:HOH:O	6:H:556:HOH:O[1_556]	1.97	0.23
6:B:920:HOH:O	6:H:520:HOH:O[2_645]	2.05	0.15
6:E:827:HOH:O	6:D:598:HOH:O[1_654]	2.17	0.03

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	616/617 (100%)	599 (97%)	17 (3%)	0	100	100
1	B	615/617 (100%)	603 (98%)	12 (2%)	0	100	100
2	C	521/536 (97%)	504 (97%)	17 (3%)	0	100	100
2	E	521/536 (97%)	510 (98%)	11 (2%)	0	100	100
3	D	407/415 (98%)	396 (97%)	10 (2%)	1 (0%)	44	64
3	H	408/415 (98%)	399 (98%)	9 (2%)	0	100	100
All	All	3088/3136 (98%)	3011 (98%)	76 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	D	124	ASN

5.3.2 Protein sidechains [i](#)

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	543/542 (100%)	538 (99%)	5 (1%)	75	90
1	B	542/542 (100%)	537 (99%)	5 (1%)	75	90
2	C	486/495 (98%)	482 (99%)	4 (1%)	79	91
2	E	486/495 (98%)	479 (99%)	7 (1%)	62	83
3	D	385/389 (99%)	380 (99%)	5 (1%)	65	85
3	H	386/389 (99%)	381 (99%)	5 (1%)	65	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2828/2852 (99%)	2797 (99%)	31 (1%)	70 87

5 of 31 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	295	LYS
3	D	45	TYR
3	H	237	PHE
3	D	368	ASP
1	A	353	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
3	D	54	GLN
3	D	372	ASN
3	D	255	GLN
2	C	343	HIS
1	A	605	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	ATP	E	601	4	26,33,33	0.88	0	31,52,52	1.89	8 (25%)
4	APR	A	701	5	33,38,39	0.72	0	37,58,60	1.60	6 (16%)
5	ATP	C	601	4	26,33,33	0.81	0	31,52,52	2.02	12 (38%)
4	APR	B	701	5	33,38,39	0.78	1 (3%)	37,58,60	1.66	5 (13%)

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
5	ATP	E	601	4	-	6/18/38/38	0/3/3/3
4	APR	A	701	5	-	3/18/51/54	0/4/4/4
5	ATP	C	601	4	-	2/18/38/38	0/3/3/3
4	APR	B	701	5	-	2/18/51/54	0/4/4/4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	701	APR	C5-C4	2.22	1.46	1.40

The worst 5 of 31 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	601	ATP	PA-O3A-PB	-5.22	114.91	132.83
4	B	701	APR	O4D-C4D-C3D	5.15	109.26	104.70
4	A	701	APR	N3-C2-N1	-3.78	122.78	128.68
5	E	601	ATP	O3B-PG-O1G	-3.75	90.38	111.19
5	C	601	ATP	C1'-N9-C4	-3.75	120.06	126.64

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	701	APR	PB-O3A-PA-O5'

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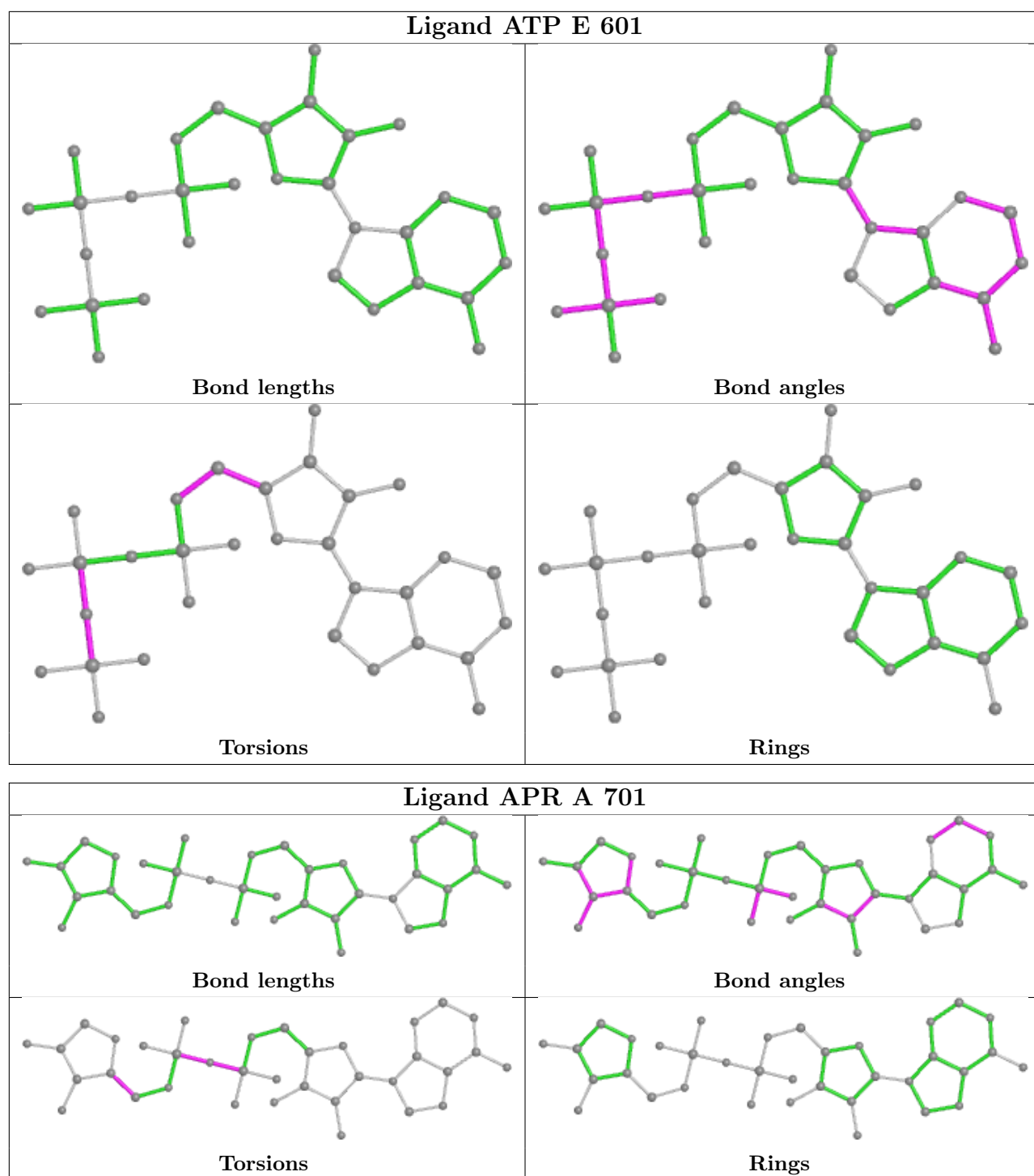
Mol	Chain	Res	Type	Atoms
4	A	701	APR	PB-O3A-PA-O5'
5	E	601	ATP	PB-O3B-PG-O2G
5	E	601	ATP	C4'-C5'-O5'-PA
5	C	601	ATP	C4'-C5'-O5'-PA

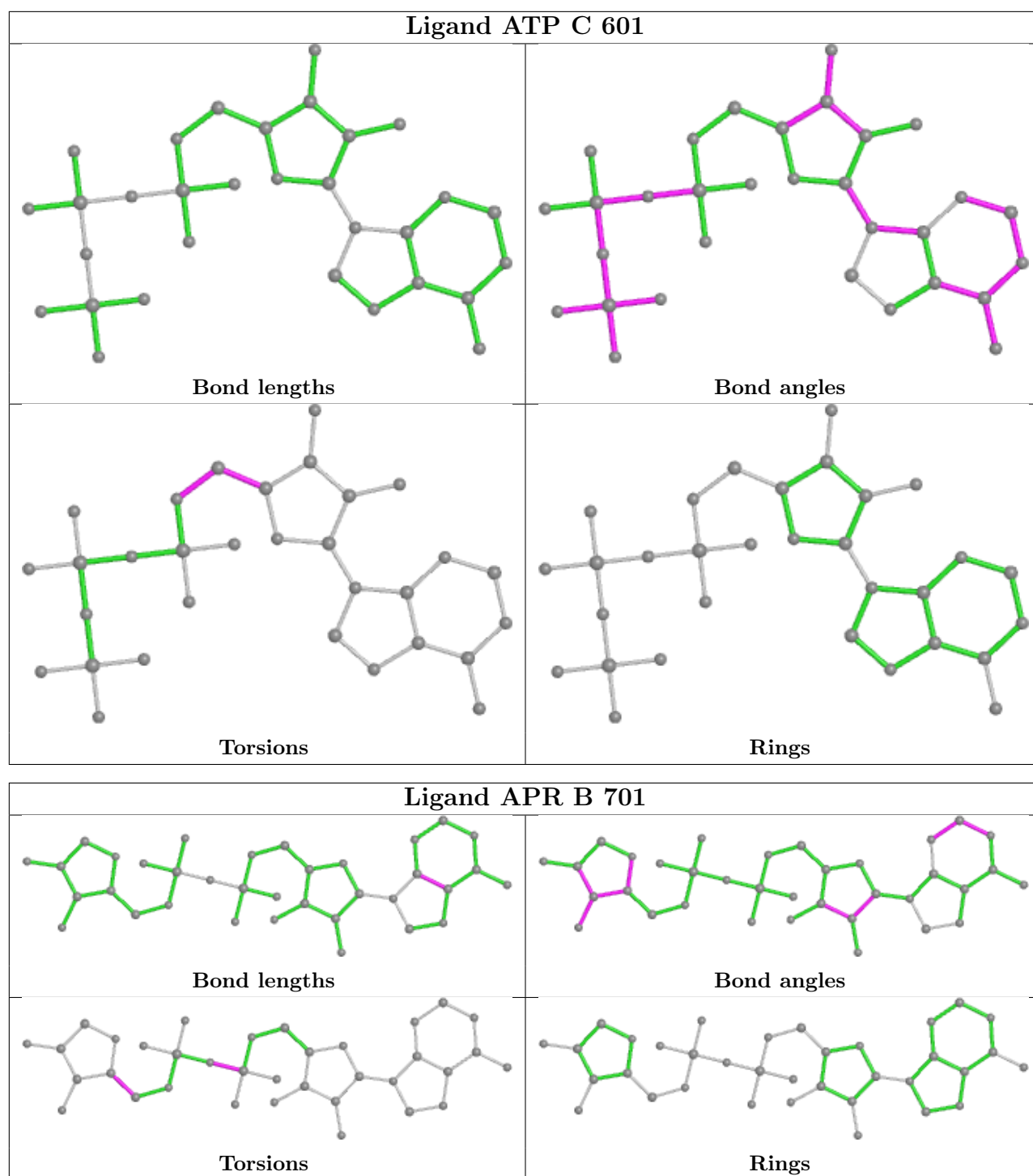
There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	601	ATP	3	0
4	A	701	APR	1	0
5	C	601	ATP	1	0
4	B	701	APR	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.





5.7 Other polymers [\(i\)](#)

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	617/617 (100%)	-1.40	0 100 100	37, 54, 86, 106	1 (0%)
1	B	617/617 (100%)	-1.45	0 100 100	35, 54, 81, 103	0
2	C	527/536 (98%)	-1.36	0 100 100	35, 57, 88, 114	0
2	E	527/536 (98%)	-1.38	0 100 100	32, 55, 88, 114	0
3	D	411/415 (99%)	-1.44	0 100 100	32, 47, 83, 115	0
3	H	412/415 (99%)	-1.41	0 100 100	34, 47, 81, 113	0
All	All	3111/3136 (99%)	-1.41	0 100 100	32, 53, 86, 115	1 (0%)

There are no RSRZ outliers to report.

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 monosaccharides 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.

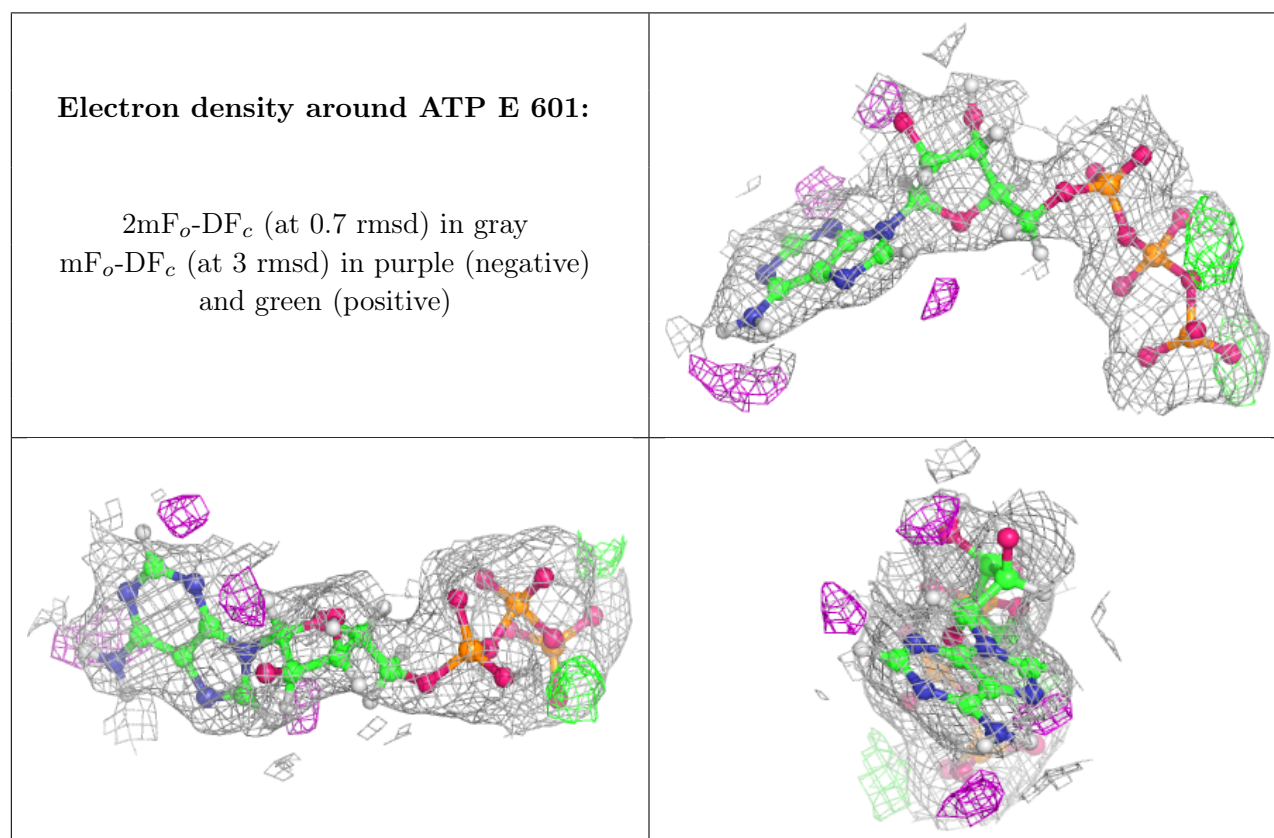
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	ATP	E	601	31/31	0.99	0.04	31,38,54,62	0

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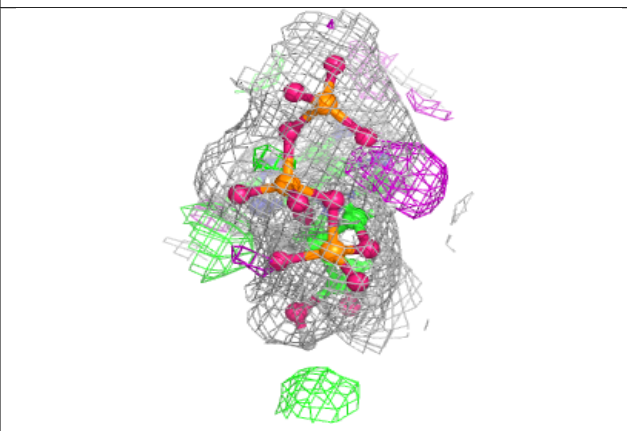
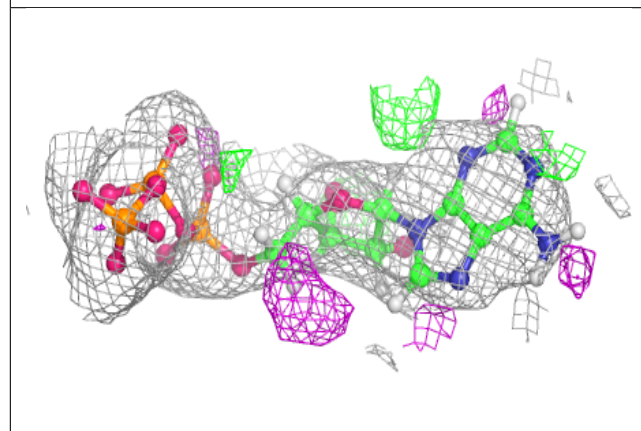
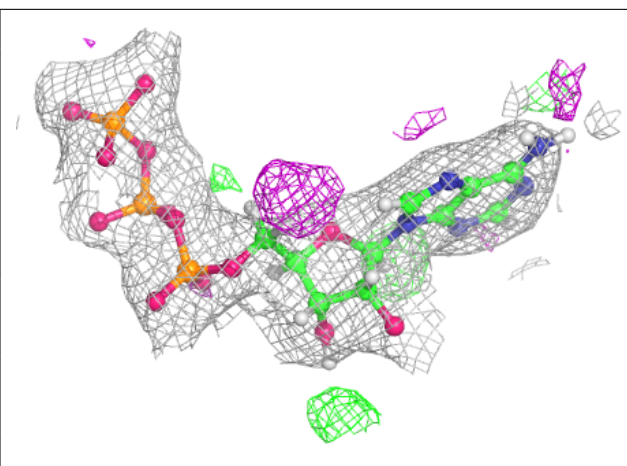
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	ATP	C	601	31/31	0.99	0.04	34,42,57,60	0
4	APR	B	701	35/36	1.00	0.03	28,38,45,47	0
4	APR	A	701	35/36	1.00	0.03	33,40,49,53	0

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.

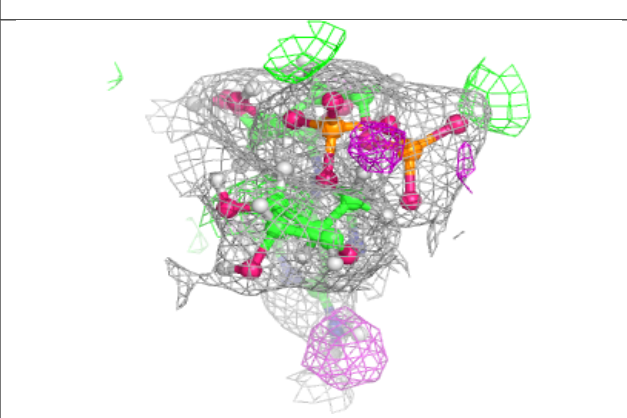
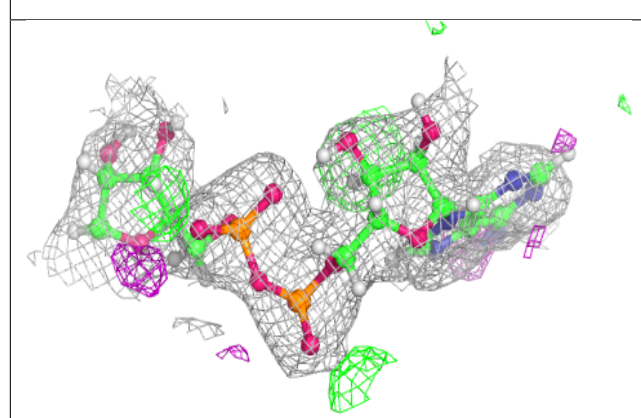
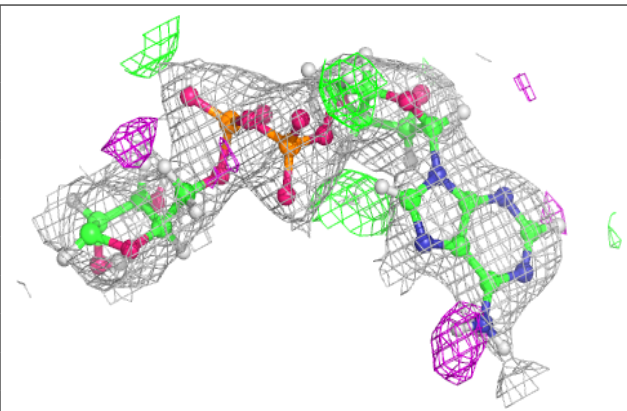


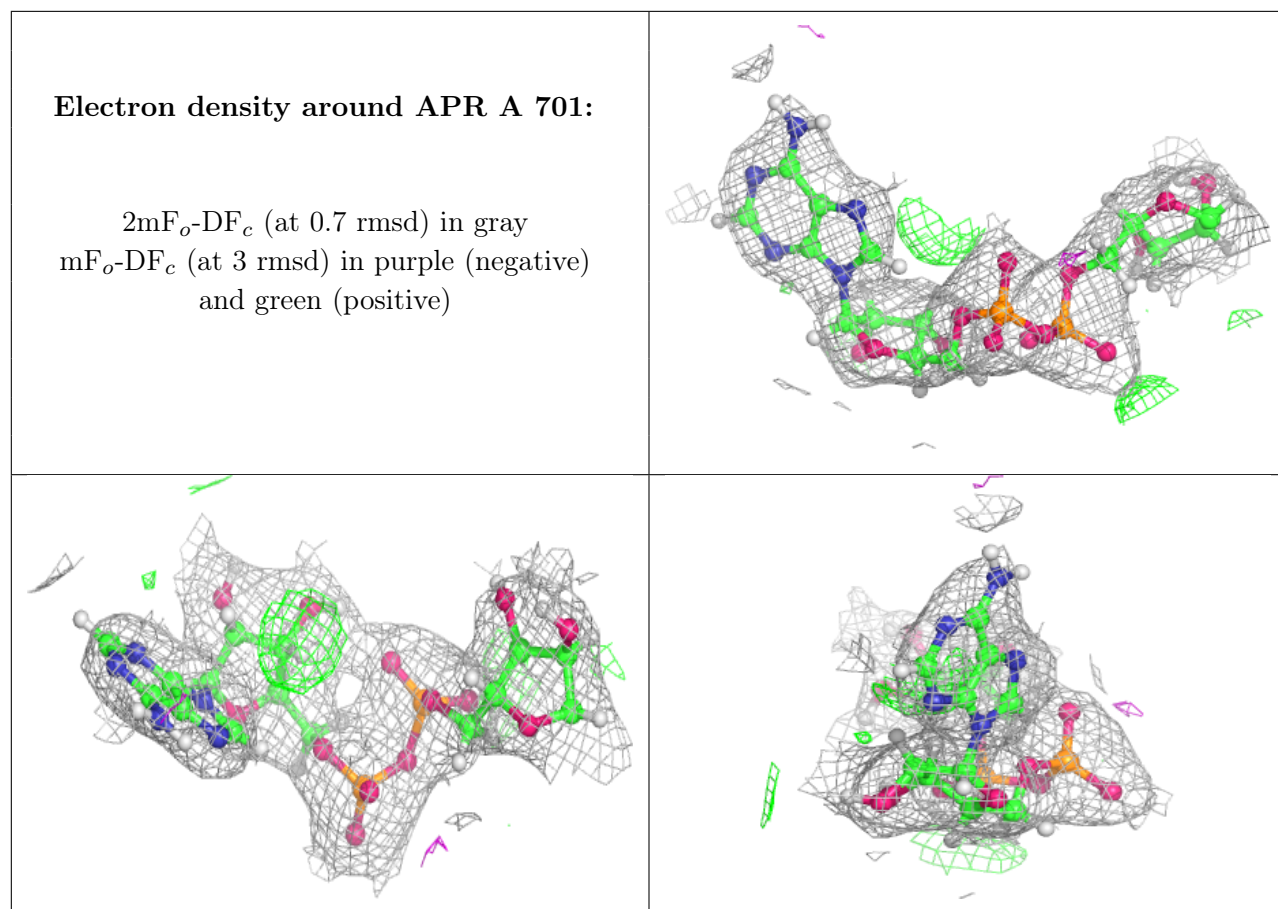
Electron density around ATP C 601:

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

**Electron density around APR B 701:**

$2mF_o-DF_c$ (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.