



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:24 PM UTC

PDB ID : 7FUB / pdb_00007fub
Title : Crystal Structure of human cyclic GMP-AMP synthase in complex with 6-(2-chloro-4-methylphenyl)-3-(pyridin-4-ylmethyl)benzimidazole-4-carboxylic acid
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Deposited on : 2023-02-08
Resolution : 1.98 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

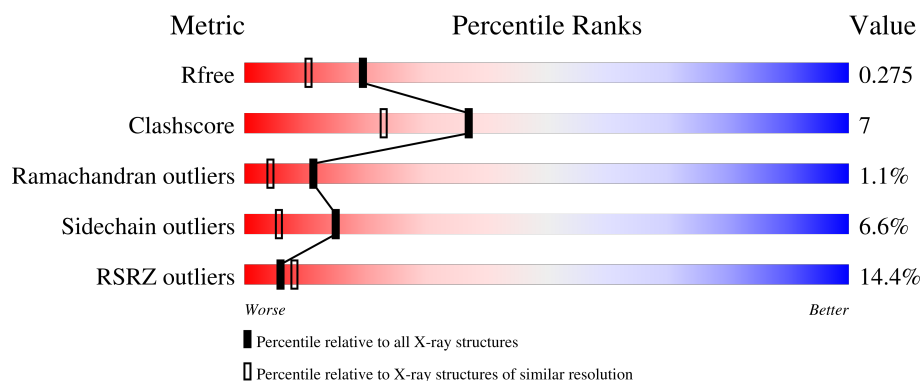
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.98 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	1506 (1.98-1.98)
Clashscore	190562	1534 (1.98-1.98)
Ramachandran outliers	187476	1518 (1.98-1.98)
Sidechain outliers	187428	1518 (1.98-1.98)
RSRZ outliers	180081	1506 (1.98-1.98)

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	362	14% 79% 17% .

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 3104 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.

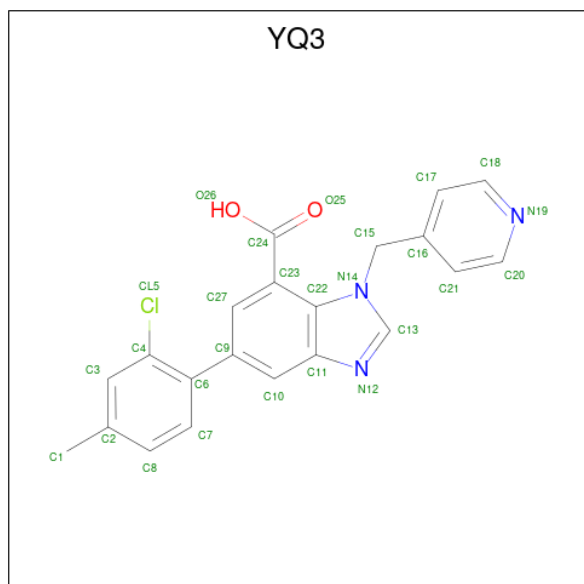
- Molecule 1 is a protein called Cyclic GMP-AMP synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	361	Total	C	N	O	S	0	1	0
			2973	1899	514	544	16			

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

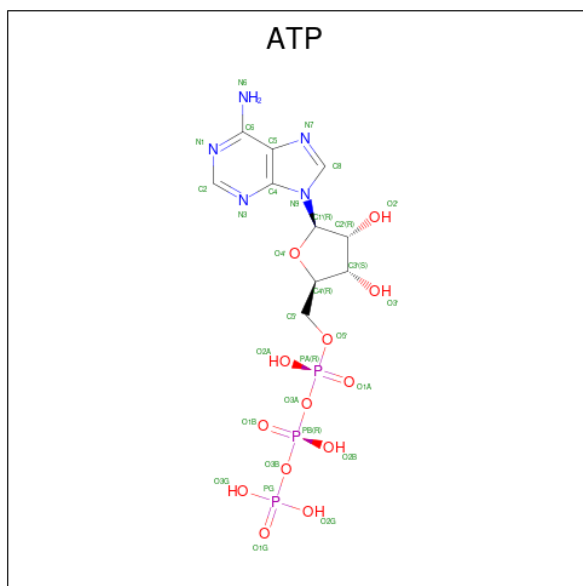
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		

- Molecule 3 is (5M)-5-(2-chloro-4-methylphenyl)-1-[(pyridin-4-yl)methyl]-1H-benzimidazole-7-carboxylic acid (CCD ID: YQ3) (formula: C₂₁H₁₆ClN₃O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	O	0	0
			27	21	1	3	2		

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	P	0	0
			13	10	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		

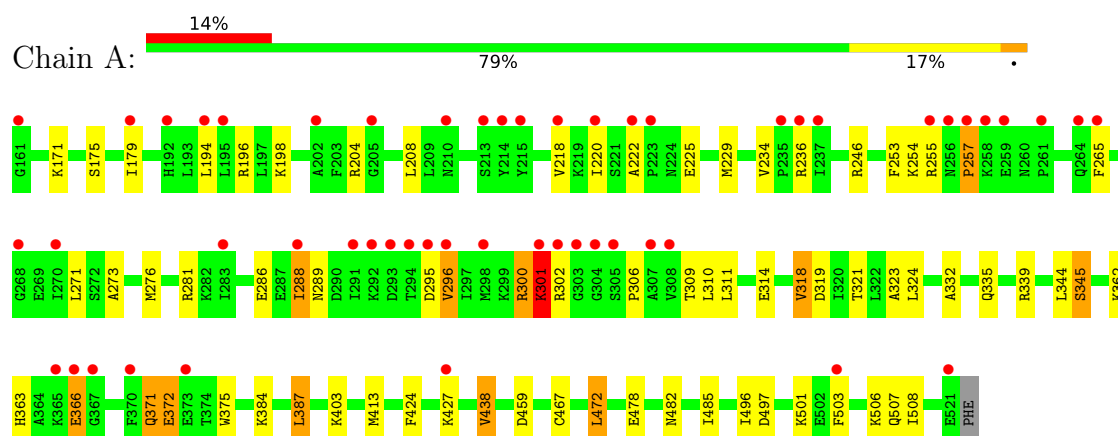
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	89	Total	O	0	0
			89	89		

3 Residue-property plots

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: Cyclic GMP-AMP synthase



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2 ₁	Depositor
Cell constants a, b, c, α , β , γ	47.59Å 60.28Å 126.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	63.26 – 1.98 63.26 – 1.98	Depositor EDS
% Data completeness (in resolution range)	59.4 (63.26-1.98) 57.0 (63.26-1.98)	Depositor EDS
R_{merge}	0.23	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.36 (at 1.98Å)	Xtriage
Refinement program	PHENIX 1.15rc1_3423	Depositor
R, R_{free}	0.188 , 0.273 0.193 , 0.275	Depositor DCC
R_{free} test set	787 reflections (3.01%)	wwPDB-VP
Wilson B-factor (Å ²)	27.0	Xtriage
Anisotropy	0.070	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 44.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	3104	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.07% 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: MG, ATP, ZN, YQ3

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	0.36	0/3035	0.58	0/4069

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

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	2973	0	3018	43	0
2	A	1	0	0	0	0
3	A	27	0	0	0	0
4	A	13	0	0	0	0
5	A	1	0	0	0	0
6	A	89	0	0	3	0
All	All	3104	0	3018	43	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (43) 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:222:ALA:HB3	1:A:225:GLU:HB2	1.71	0.73
1:A:366:GLU:HG3	1:A:371:GLN:HB2	1.75	0.69
1:A:236:ARG:HH11	1:A:257:PRO:HG2	1.58	0.69
1:A:271:LEU:HD21	1:A:276:MET:HE1	1.75	0.68
1:A:234:VAL:HG21	1:A:324:LEU:HD22	1.83	0.61
1:A:413[B]:MET:SD	1:A:467:CYS:HB3	2.40	0.61
1:A:196:ARG:NH2	1:A:286:GLU:OE1	2.33	0.61
1:A:288:ILE:HG23	1:A:296:VAL:HG22	1.84	0.59
1:A:478:GLU:HG2	1:A:501:LYS:HD2	1.86	0.57
1:A:306:PRO:HB2	1:A:321:THR:HG23	1.85	0.57
1:A:413[B]:MET:HE2	1:A:438:VAL:HG13	1.87	0.55
1:A:309:THR:OG1	1:A:319:ASP:OD1	2.22	0.54
1:A:301:LYS:O	1:A:302:ARG:HG3	2.09	0.53
1:A:194:LEU:HD22	1:A:208:LEU:HG	1.91	0.52
1:A:236:ARG:NH1	1:A:257:PRO:HG2	2.24	0.51
1:A:175:SER:O	1:A:179:ILE:HG23	2.13	0.48
1:A:246:ARG:HA	1:A:246:ARG:HD2	1.65	0.48
1:A:459:ASP:OD2	6:A:701:HOH:O	2.20	0.47
1:A:413[B]:MET:HB3	1:A:438:VAL:HG13	1.96	0.47
1:A:296:VAL:HA	1:A:311:LEU:O	2.14	0.47
1:A:363:HIS:CD2	1:A:372:GLU:HA	2.50	0.46
1:A:344:LEU:O	1:A:345:SER:OG	2.34	0.46
1:A:424:PHE:CD1	1:A:503:PHE:HE2	2.34	0.45
1:A:255:ARG:C	1:A:257:PRO:HD3	2.41	0.45
1:A:265:PHE:CD2	1:A:276:MET:HE2	2.52	0.45
1:A:306:PRO:HG3	1:A:362:LYS:HB2	1.99	0.45
1:A:171:LYS:HE2	1:A:171:LYS:HB3	1.61	0.44
1:A:503:PHE:O	1:A:507:GLN:HG2	2.17	0.44
1:A:472:LEU:HD23	1:A:472:LEU:HA	1.77	0.44
1:A:363:HIS:CG	1:A:372:GLU:HA	2.53	0.43
1:A:229:MET:HE3	1:A:323:ALA:HB2	2.00	0.43
1:A:253:PHE:N	6:A:713:HOH:O	2.52	0.43
1:A:387:LEU:HD23	1:A:387:LEU:HA	1.79	0.43
1:A:482:ASN:HB3	1:A:485:ILE:O	2.19	0.42
1:A:310:LEU:HB2	1:A:318:VAL:HG13	2.02	0.42
1:A:300:ARG:HB3	1:A:301:LYS:H	1.67	0.41
1:A:198:LYS:HA	1:A:204:ARG:HA	2.02	0.41
1:A:273:ALA:HA	1:A:375:TRP:CZ2	2.55	0.41
1:A:413[A]:MET:HB3	1:A:438:VAL:HG13	2.02	0.41
1:A:506:LYS:NZ	6:A:715:HOH:O	2.53	0.41
1:A:332:ALA:O	1:A:335:GLN:HB2	2.21	0.41
1:A:496:ILE:O	1:A:501:LYS:HE2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:472:LEU:HG	1:A:508:ILE:HG22	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	360/362 (99%)	337 (94%)	19 (5%)	4 (1%)	11 4

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	300	ARG
1	A	301	LYS
1	A	345	SER
1	A	257	PRO

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	334/334 (100%)	312 (93%)	22 (7%)	15 6

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	218	VAL
1	A	220	ILE
1	A	254	LYS
1	A	281	ARG
1	A	288	ILE
1	A	289	ASN
1	A	295	ASP
1	A	296	VAL
1	A	301	LYS
1	A	314	GLU
1	A	318	VAL
1	A	339	ARG
1	A	366	GLU
1	A	371	GLN
1	A	372	GLU
1	A	384	LYS
1	A	387	LEU
1	A	403	LYS
1	A	427	LYS
1	A	438	VAL
1	A	472	LEU
1	A	497	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	238	GLN
1	A	289	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

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	YQ3	A	602	-	30,30,30	0.15	0	41,43,43	0.74	1 (2%)
4	ATP	A	603	5	10,12,33	1.55	2 (20%)	17,20,52	1.03	2 (11%)

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	YQ3	A	602	-	-	5/12/12/12	0/4/4/4
4	ATP	A	603	5	-	3/12/12/38	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	603	ATP	PB-O3B	3.30	1.63	1.59
4	A	603	ATP	PB-O3A	2.57	1.62	1.59

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	602	YQ3	C16-C15-N14	3.15	117.56	112.78
4	A	603	ATP	O2A-PA-O1A	2.34	119.96	110.83
4	A	603	ATP	O3G-PG-O2G	2.02	115.38	107.80

There are no chirality outliers.

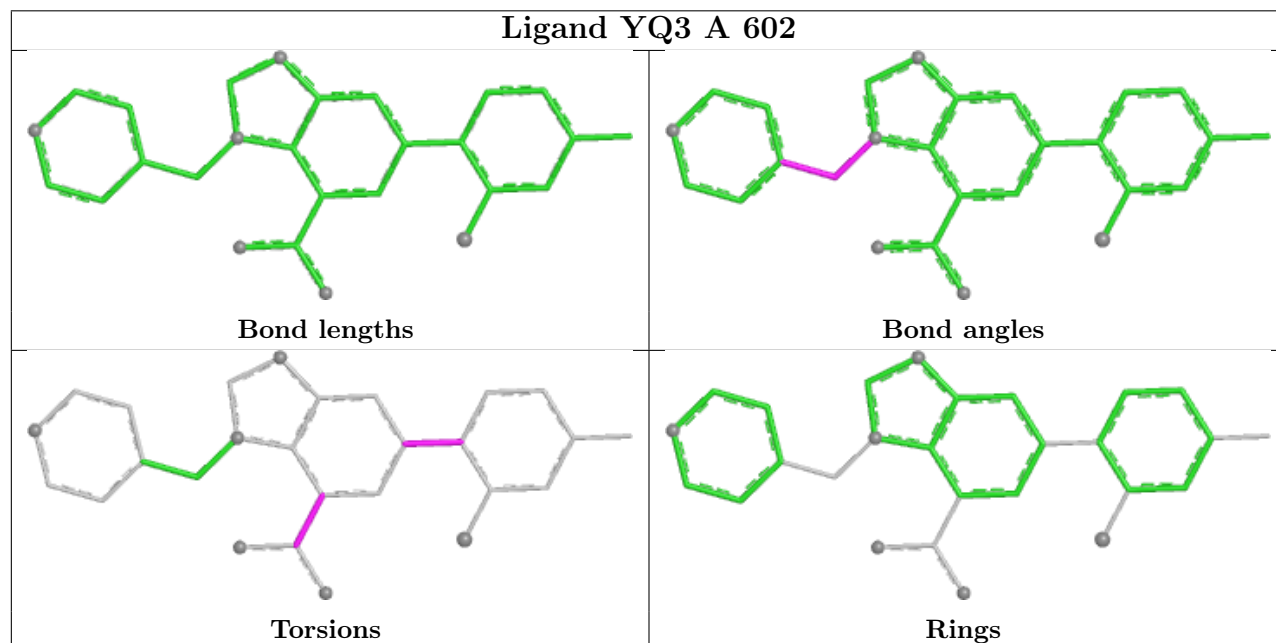
All (8) torsion outliers are listed below:

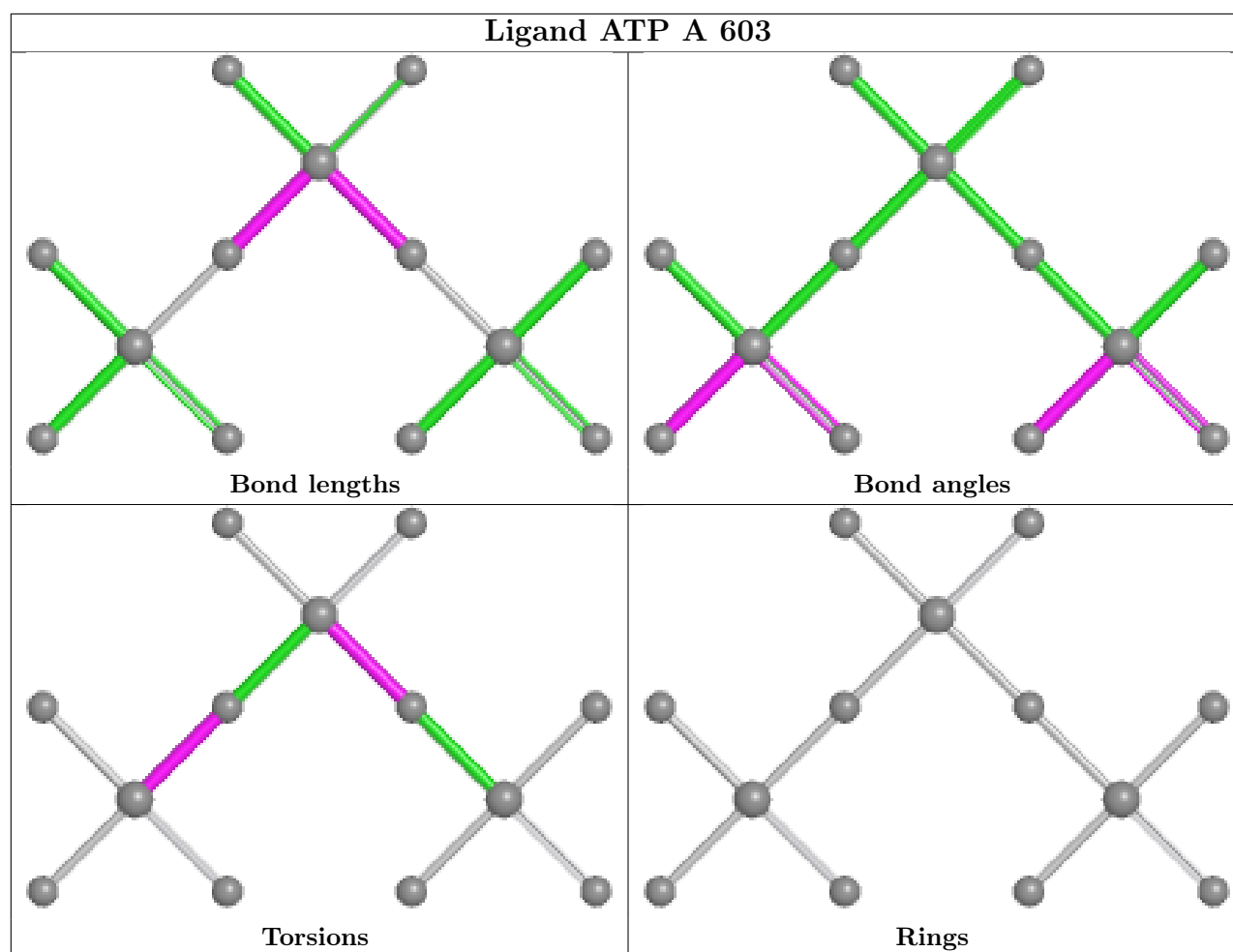
Mol	Chain	Res	Type	Atoms
4	A	603	ATP	PB-O3B-PG-O3G
3	A	602	YQ3	C22-C23-C24-O25
3	A	602	YQ3	C22-C23-C24-O26
3	A	602	YQ3	C4-C6-C9-C27
3	A	602	YQ3	C27-C23-C24-O25
3	A	602	YQ3	C27-C23-C24-O26
4	A	603	ATP	PB-O3B-PG-O1G
4	A	603	ATP	PA-O3A-PB-O2B

There are no ring outliers.

No monomer is involved in short contacts.

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 [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	361/362 (99%)	0.63	52 (14%) 6 8	15, 46, 94, 136	1 (0%)

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	303	GLY	4.3
1	A	291	ILE	4.2
1	A	257	PRO	4.0
1	A	222	ALA	3.9
1	A	302	ARG	3.6
1	A	237	ILE	3.5
1	A	370	PHE	3.3
1	A	192	HIS	3.2
1	A	236	ARG	3.1
1	A	304	GLY	3.1
1	A	255	ARG	3.0
1	A	214	TYR	2.9
1	A	223	PRO	2.9
1	A	294	THR	2.8
1	A	259	GLU	2.8
1	A	179	ILE	2.8
1	A	308	VAL	2.7
1	A	301	LYS	2.7
1	A	235	PRO	2.7
1	A	215	TYR	2.7
1	A	261	PRO	2.6
1	A	194	LEU	2.6
1	A	521	GLU	2.6
1	A	258	LYS	2.6
1	A	202	ALA	2.6
1	A	220	ILE	2.5
1	A	161	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	367	GLY	2.4
1	A	210	ASN	2.4
1	A	292	LYS	2.4
1	A	365	LYS	2.4
1	A	265	PHE	2.3
1	A	256	ASN	2.3
1	A	305	SER	2.3
1	A	298	MET	2.3
1	A	270	ILE	2.2
1	A	283	ILE	2.2
1	A	213	SER	2.2
1	A	307	ALA	2.2
1	A	427	LYS	2.2
1	A	264	GLN	2.2
1	A	503	PHE	2.1
1	A	218	VAL	2.1
1	A	366	GLU	2.1
1	A	293	ASP	2.1
1	A	295	ASP	2.1
1	A	288	ILE	2.0
1	A	205	GLY	2.0
1	A	268	GLY	2.0
1	A	195	LEU	2.0
1	A	373	GLU	2.0
1	A	296	VAL	2.0

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

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

6.3 Carbohydrates ⓘ

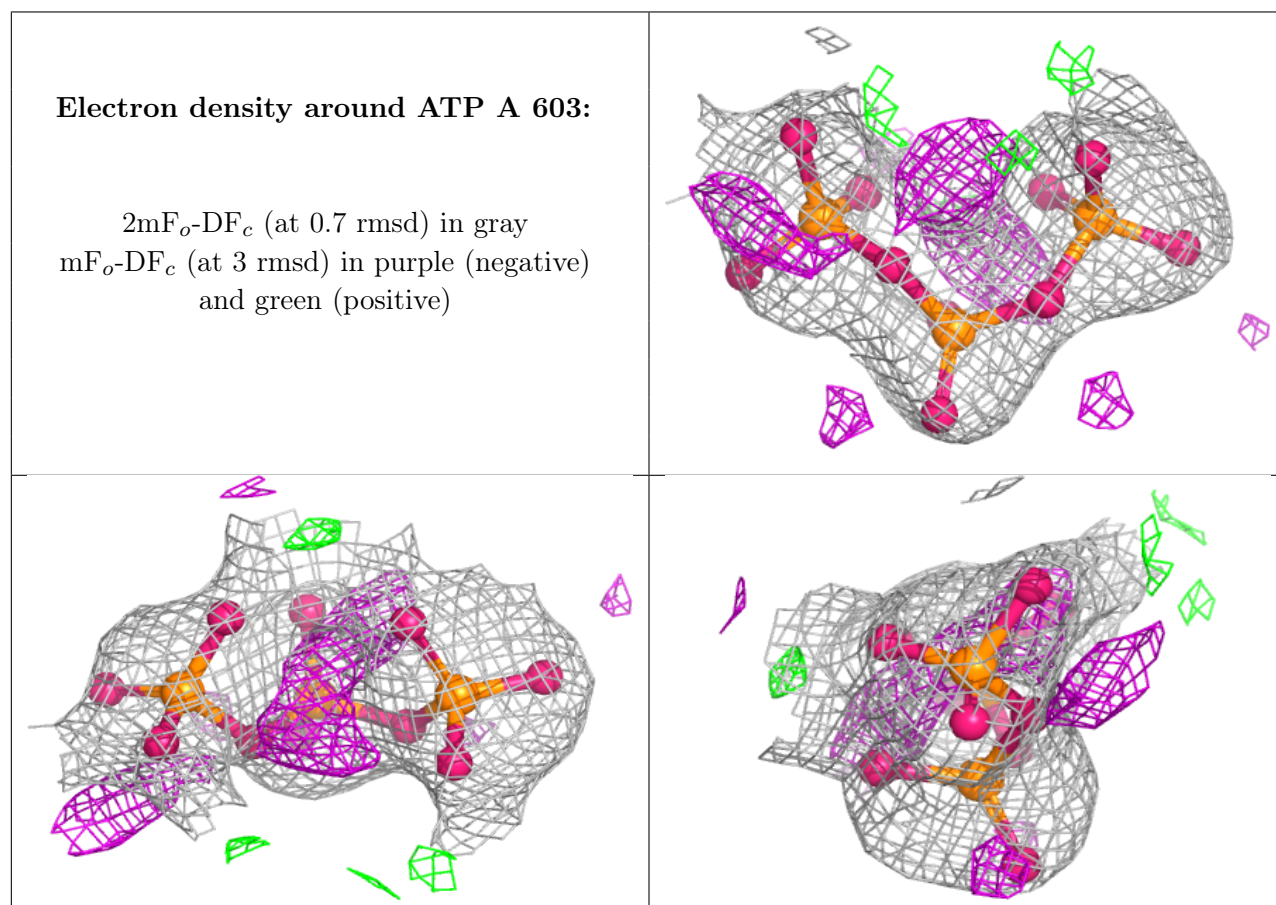
There are no oligosaccharides in this entry.

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.

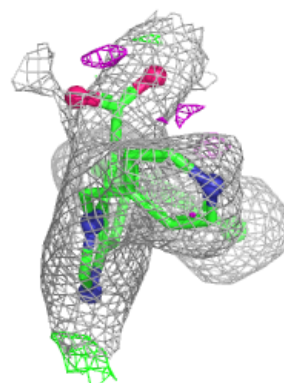
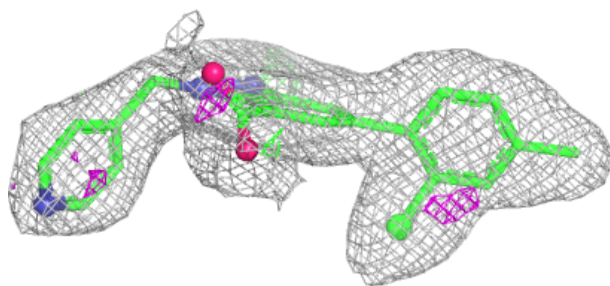
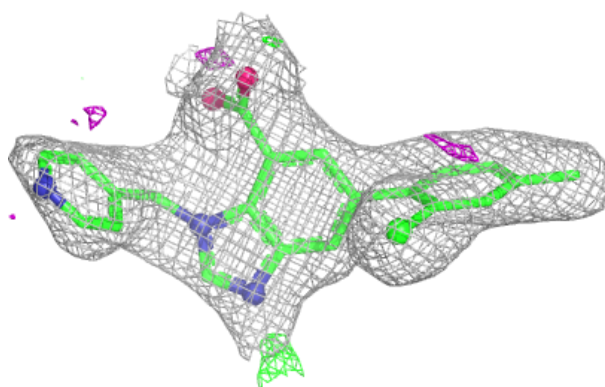
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	MG	A	604	1/1	0.73	0.15	86,86,86,86	1
4	ATP	A	603	13/31	0.82	0.11	74,83,91,97	0
3	YQ3	A	602	27/27	0.94	0.10	10,38,57,73	0
2	ZN	A	601	1/1	0.99	0.01	24,24,24,24	0

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 YQ3 A 602:

$2mF_o-DF_c$ (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.