

Full wwPDB X-ray Structure Validation Report (i)

Apr 8, 2024 – 04:09 PM EDT

PDB ID : 8GIO

Title : Structure of Ternary Complex of mouse cGAS with dsDNA and Bound ATP:

with 10mM Mg2+ and 0.1mM Mn2+

Authors : Wu, S.; Sohn, J. Deposited on : 2023-03-14

Resolution : 2.67 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.orgA user guide is available at

https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) 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 (1)) 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 : 2.36.1

buster-report : 1.1.7 (2018)

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

 $Refmac \quad : \quad 5.8.0158$

CCP4 : 7.0.044 (Gargrove)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

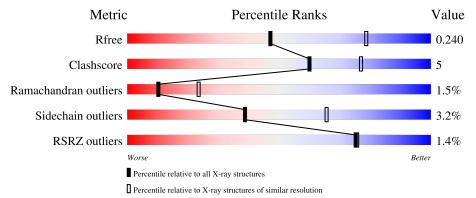
Validation Pipeline (wwPDB-VP) : 2.36.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X-RAY DIFFRACTION

The reported resolution of this entry is 2.67 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 $(\# \mathrm{Entries})$	$\begin{array}{c} {\rm Similar\ resolution} \\ (\#{\rm Entries},{\rm resolution\ range}(\mathring{\rm A})) \end{array}$
R_{free}	130704	3863 (2.70-2.66)
Clashscore	141614	4210 (2.70-2.66)
Ramachandran outliers	138981	4141 (2.70-2.66)
Sidechain outliers	138945	4141 (2.70-2.66)
RSRZ outliers	127900	3780 (2.70-2.66)

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 <=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	364	87%	10%
1	С	364	75% 16%	• 7%
2	Е	18	83%	17%
2	F	18	89%	6% 6%
2	I	18	78%	22%



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Mol	Chain	Length	Quality of chain	
	т	10	6%	
2	J	18	89%	11%



2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 7326 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		At	oms			ZeroOcc	AltConf	Trace
1	A	356	Total 2947	C 1895	- 1	O 539	S 13	0	0	0
1	С	340	Total 2822	_	N 476	O 513	S 13	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

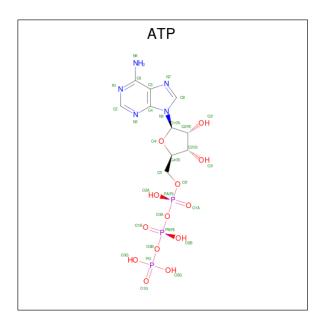
Chain	Residue	Modelled	Actual	Comment	Reference
A	144	GLY	-	expression tag	UNP Q8C6L5
A	145	THR	-	expression tag	UNP Q8C6L5
A	146	GLY	-	expression tag	UNP Q8C6L5
С	144	GLY	-	expression tag	UNP Q8C6L5
С	145	THR	-	expression tag	UNP Q8C6L5
С	146	GLY	-	expression tag	UNP Q8C6L5

• Molecule 2 is a DNA chain called Palindromic DNA18.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
2	Е	18	Total	С	N	О	Р	0	0	0
2	12	10	366	177	66	106	17	U	0	
2	F	18	Total	С	N	О	Р	0	0	0
	Г	10	366	177	66	106	17			
2	Т	18	Total	С	N	О	Р	0	0	0
	1	10	366	177	66	106	17	U	0	
2	Ţ	18	Total	С	N	О	Р	0	0	0
2	J	10	366	177	66	106	17			0

• Molecule 3 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		
9	A	1	Total	С	N	О	Р	0	0
3		1	31	10	5	13	3	U	
9	C	1	Total	С	N	О	Р	0	0
3		$C \mid I$		31	10	5	13	3	

• Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Zn 1 1	0	0
4	С	1	Total Zn 1 1	0	0

• Molecule 5 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	2	Total Mn 2 2	0	0
5	С	2	Total Mn 2 2	0	0

• Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	13	Total O 13 13	0	0



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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	С	11	Total O 11 11	0	0
6	F	1	Total O 1 1	0	0



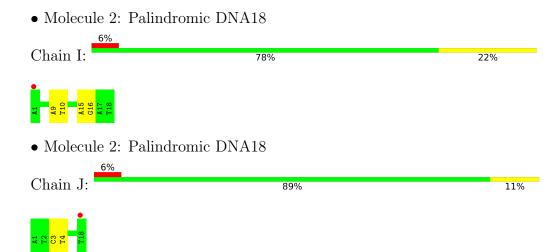
3 Residue-property plots (i)

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: Cyclic GMP-AMP synthase









4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	77.59Å 98.62Å 141.93Å	Donogitor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.80 - 2.67	Depositor
resolution (A)	28.80 - 2.67	EDS
% Data completeness	99.2 (28.80-2.67)	Depositor
(in resolution range)	95.1 (28.80-2.67)	EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	2.06 (at 2.68Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.183 , 0.241	Depositor
it, it free	0.185 , 0.240	DCC
R_{free} test set	1549 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	52.7	Xtriage
Anisotropy	0.145	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.32, 36.3	EDS
L-test for twinning ²	$ < L > = 0.50, < L^2> = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7326	wwPDB-VP
Average B, all atoms $(Å^2)$	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The analyses of the Patterson function reveals a significant off-origin peak that is 28.67 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.7702e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.

²Theoretical values of <|L|>, $<L^2>$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



¹Intensities estimated from amplitudes.

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: MN, ATP, ZN

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	Bond lengths		ond angles
MIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5
1	A	0.50	0/3009	0.65	2/4037~(0.0%)
1	С	0.46	0/2881	0.62	0/3863
2	Е	0.93	0/410	1.05	0/631
2	F	0.89	0/410	1.03	$1/631 \ (0.2\%)$
2	I	0.92	0/410	1.00	0/631
2	J	0.91	0/410	1.05	0/631
All	All	0.60	0/7530	0.75	3/10424 (0.0%)

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 maintenain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	С	0	1
All	All	0	2

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$\mathbf{Ideal}(^o)$
1	A	195	LEU	CA-CB-CG	5.38	127.68	115.30
2	F	2	DT	O5'-P-OP2	-5.19	101.03	105.70
1	A	300	ASN	C-N-CD	-5.05	109.49	120.60

There are no chirality outliers.

All (2) planarity outliers are listed below:



Mol	Chain	Res	Type	Group
1	A	300		Peptide
1	С	299	ARG	Peptide

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	2947	0	2991	20	0
1	С	2822	0	2870	36	0
2	Е	366	0	206	3	0
2	F	366	0	206	1	0
2	I	366	0	206	3	0
2	J	366	0	206	1	0
3	A	31	0	12	0	0
3	С	31	0	12	0	0
4	A	1	0	0	0	0
4	С	1	0	0	0	0
5	A	2	0	0	0	0
5	С	2	0	0	0	0
6	A	13	0	0	0	0
6	С	11	0	0	0	0
6	F	1	0	0	0	0
All	All	7326	0	6709	63	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 5.

All (63) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	Clash overlap (Å)
1:C:183:GLN:HA	1:C:190:LYS:HA	1.53	0.88
1:A:436:GLN:HB2	1:A:439:GLN:HE21	1.42	0.83
1:C:228:TYR:O	1:C:231:THR:HG23	1.98	0.63
1:C:152:LYS:HE3	1:C:152:LYS:HA	1.83	0.61
1:C:204:VAL:HG11	1:C:398:LEU:HD23	1.82	0.61
1:C:483:ARG:O	1:C:487:GLU:HG3	2.00	0.61
1:C:238:LYS:HZ3	1:C:256:VAL:N	1.99	0.60



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Continued from prev		Interatomic	Clash
Atom-1	Atom-2	${\rm distance}\ (\rm \mathring{A})$	overlap (Å)
1:A:285:GLU:HG3	1:A:297:LEU:HD21	1.83	0.59
1:A:436:GLN:HB2	1:A:439:GLN:NE2	2.17	0.58
1:C:183:GLN:HG2	1:C:184:LYS:H	1.70	0.57
1:A:188:GLU:OE2	1:A:265:LYS:NZ	2.38	0.56
2:I:9:DA:H2'	2:I:10:DT:C6	2.42	0.55
1:C:182:MET:O	1:C:184:LYS:N	2.39	0.55
1:C:183:GLN:HA	1:C:190:LYS:HG3	1.90	0.54
1:A:221:PRO:O	1:A:223:ILE:HG22	2.06	0.54
1:C:458:GLU:OE2	1:C:461:ARG:NH2	2.40	0.53
1:A:461:ARG:NH1	1:A:487:GLU:OE1	2.44	0.51
1:A:177:ARG:HH11	1:A:277:ILE:HG12	1.76	0.51
1:C:196:ASN:HB3	1:C:201:TYR:CD2	2.46	0.50
1:C:220:VAL:HG21	1:C:223:ILE:HD13	1.93	0.50
1:C:350:LYS:HD2	1:C:362:THR:OG1	2.12	0.50
1:C:436:GLN:HB2	1:C:439:GLN:HG3	1.93	0.50
1:C:196:ASN:HB3	1:C:201:TYR:CE2	2.46	0.49
2:E:2:DT:H2"	2:E:3:DC:H6	1.78	0.49
1:C:299:ARG:C	1:C:300:ASN:O	2.51	0.49
1:C:183:GLN:CG	1:C:184:LYS:H	2.26	0.48
1:C:327:PRO:HD2	1:C:468:TYR:CZ	2.49	0.48
1:C:211:GLU:HG2	1:C:305:SER:HB2	1.95	0.48
1:C:162:LYS:O	1:C:166:GLU:HG3	2.14	0.48
1:C:310:LEU:HD22	1:C:311:ALA:H	1.79	0.47
1:C:300:ASN:HB3	1:C:301:PRO:HD2	1.96	0.47
1:C:310:LEU:HD22	1:C:311:ALA:N	2.29	0.47
2:E:1:DA:H2'	2:E:2:DT:C6	2.49	0.47
1:A:353:LYS:HD3	1:A:359:GLN:NE2	2.29	0.47
1:C:359:GLN:HG3	1:C:360:GLY:N	2.29	0.46
2:I:15:DA:H2"	2:I:16:DG:C8	2.50	0.46
1:C:458:GLU:OE2	1:C:461:ARG:NE	2.46	0.46
1:A:448:CYS:HA	1:A:451:LYS:HE2	1.98	0.45
1:C:329:GLN:O	1:C:333:GLY:HA2	2.17	0.45
1:C:463:GLU:HG2	1:C:486:LYS:HD2	1.98	0.44
1:A:204:VAL:O	1:A:402:LYS:HE2	2.18	0.44
1:A:353:LYS:HD3	1:A:359:GLN:HE22	1.83	0.44
1:A:334:THR:HB	2:I:9:DA:OP1	2.19	0.43
1:A:188:GLU:CD	1:A:265:LYS:HZ3	2.21	0.43
1:A:267:ARG:NH2	1:A:285:GLU:O	2.50	0.43
1:C:401:MET:CE	1:C:404:LEU:HD23	2.48	0.43
1:A:288:LYS:HE2	1:A:288:LYS:HB2	1.76	0.42
1:A:354:ASP:OD1	1:A:354:ASP:N	2.51	0.42



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Atom-1	Atom-2	Interatomic	Clash
Atom-1	Atom-2	${f distance} ({f A})$	overlap (Å)
1:C:346:TYR:HE1	1:C:369:HIS:CD2	2.37	0.42
2:E:2:DT:H2"	2:E:3:DC:C6	2.55	0.42
2:J:3:DC:C2'	2:J:4:DT:H71	2.50	0.42
1:A:275:LYS:HE3	1:A:275:LYS:HB3	1.76	0.41
1:C:159:LEU:HB2	1:C:164:ILE:HD11	2.02	0.41
1:A:410:LYS:HB3	1:A:410:LYS:HE2	1.89	0.41
1:C:458:GLU:O	1:C:462:THR:OG1	2.33	0.41
1:C:407:GLN:HB3	1:C:503:ILE:HG12	2.02	0.41
1:A:239:PHE:O	1:A:255:GLU:HG2	2.21	0.41
1:A:219:GLU:CD	1:A:315:LYS:HE3	2.41	0.41
1:C:177:ARG:NH2	1:C:276:GLU:O	2.54	0.41
1:C:251:PHE:HB2	1:C:257:LEU:HD12	2.03	0.41
2:F:1:DA:H2'	2:F:2:DT:C6	2.56	0.41
1:C:292:PRO:HB3	1:C:349:PRO:O	2.20	0.40
1:C:398:LEU:HD13	1:C:427:ILE:HG21	2.04	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	Perc	entiles
1	A	352/364~(97%)	337 (96%)	9 (3%)	6 (2%)	9	20
1	\mathbf{C}	332/364~(91%)	321 (97%)	7 (2%)	4 (1%)	13	29
All	All	$684/728 \; (94\%)$	658 (96%)	16 (2%)	10 (2%)	10	23

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	185	ARG
1	A	221	PRO
1	A	301	PRO



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Mol	Chain	Res	Type
1	С	183	GLN
1	A	222	ARG
1	A	359	GLN
1	С	222	ARG
1	С	182	MET
1	С	300	ASN
1	A	300	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	330/335 (98%)	321 (97%)	9 (3%)	44 71
1	С	317/335~(95%)	305 (96%)	12 (4%)	33 59
All	All	647/670 (97%)	626 (97%)	21 (3%)	39 65

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	149	LYS
1	A	162	LYS
1	A	165	SER
1	A	214	VAL
1	A	299	ARG
1	A	305	SER
1	A	353	LYS
1	A	359	GLN
1	A	484	LYS
1	С	151	LYS
1	С	183	GLN
1	С	185	ARG
1	С	192	VAL
1	С	238	LYS
1	С	278	LYS
1	С	317	SER



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Mol	Chain	Res	Type
1	С	359	GLN
1	С	388	SER
1	С	391	LYS
1	С	482	ASP
1	С	490	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	359	GLN
1	A	439	GLN
1	A	498	ASN
1	С	226	GLN
1	С	376	ASN
1	С	478	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 6 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).



7	Mol	Tuna	Chain	Chain	Dog	Dag	Pag	Link	Bo	ond leng	$ ag{ths}$	В	ond ang	cles
IVIOI	Type	Chain	Res	LINK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2				
	3	ATP	С	601	5	26,33,33	0.61	0	31,52,52	0.78	1 (3%)			
	3	ATP	A	601	5	26,33,33	0.59	0	31,52,52	0.81	1 (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	ATP	С	601	5	-	5/18/38/38	0/3/3/3
3	ATP	A	601	5	-	3/18/38/38	0/3/3/3

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^o)$	$Ideal(^{o})$
3	С	601	ATP	C5-C6-N6	2.45	124.08	120.35
3	A	601	ATP	C5-C6-N6	2.12	123.58	120.35

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	601	ATP	PB-O3B-PG-O2G
3	A	601	ATP	PB-O3B-PG-O3G
3	С	601	ATP	C5'-O5'-PA-O2A
3	A	601	ATP	PA-O3A-PB-O2B
3	С	601	ATP	PB-O3B-PG-O2G
3	С	601	ATP	PA-O3A-PB-O1B
3	С	601	ATP	PA-O3A-PB-O2B
3	С	601	ATP	C5'-O5'-PA-O1A

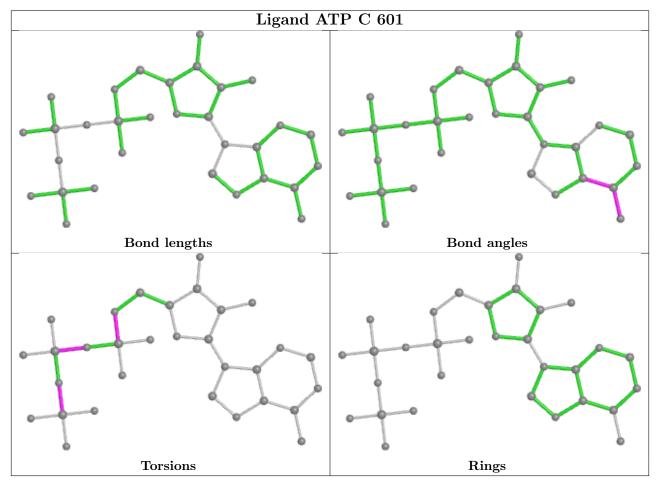
There are no ring outliers.

No monomer is involved in short contacts.

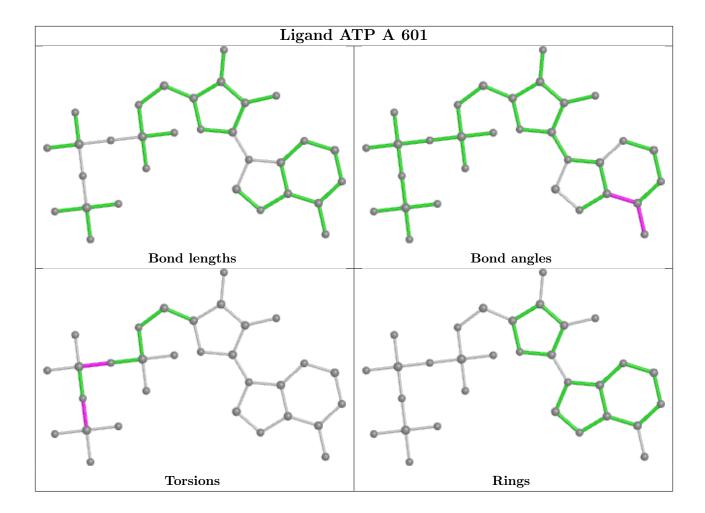
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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 (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, 95^{th} 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>	$\#\mathrm{RSRZ}{>}2$	$\mathbf{OWAB}(\mathbf{\mathring{A}}^2)$	Q < 0.9
1	A	356/364~(97%)	-0.25	4 (1%) 80 81	36, 55, 92, 119	0
1	С	340/364 (93%)	-0.20	5 (1%) 73 74	38, 63, 96, 130	0
2	E	18/18 (100%)	-0.02	0 100 100	45, 72, 144, 147	0
2	F	18/18 (100%)	0.02	0 100 100	47, 76, 143, 162	0
2	I	18/18 (100%)	0.08	1 (5%) 24 22	47, 72, 132, 136	0
2	J	18/18 (100%)	-0.12	1 (5%) 24 22	50, 78, 131, 137	0
All	All	768/800 (96%)	-0.21	11 (1%) 75 76	36, 60, 101, 162	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	С	250	HIS	3.1
1	A	242	ILE	2.9
1	С	222	ARG	2.5
1	A	413	GLN	2.5
2	J	18	DT	2.5
1	С	239	PHE	2.2
2	I	1	DA	2.2
1	A	185	ARG	2.1
1	С	230	GLU	2.0
1	A	222	ARG	2.0
1	С	301	PRO	2.0

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, 95^{th} 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.

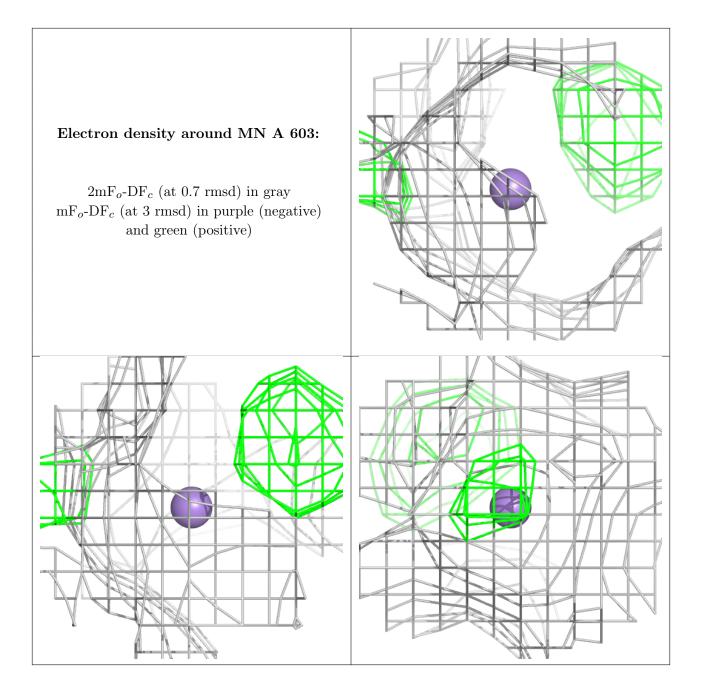
Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q<0.9
5	MN	A	604	1/1	0.89	0.08	76,76,76,76	0
5	MN	A	603	1/1	0.95	0.09	68,68,68,68	0
5	MN	С	603	1/1	0.96	0.07	72,72,72,72	0
3	ATP	С	601	31/31	0.98	0.14	44,50,55,58	0
3	ATP	A	601	31/31	0.98	0.17	40,44,48,49	0
5	MN	С	604	1/1	0.98	0.05	79,79,79,79	0
4	ZN	A	602	1/1	0.99	0.15	50,50,50,50	0
4	ZN	С	602	1/1	0.99	0.12	49,49,49,49	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.

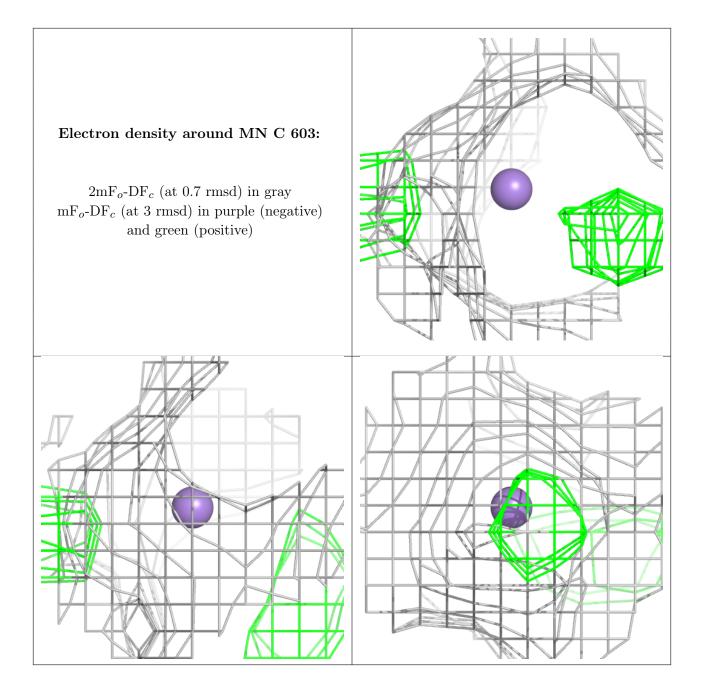


Electron density around MN A 604: $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 0.7 rmsd) in gray ${\rm mF}_o\text{-}{\rm DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)





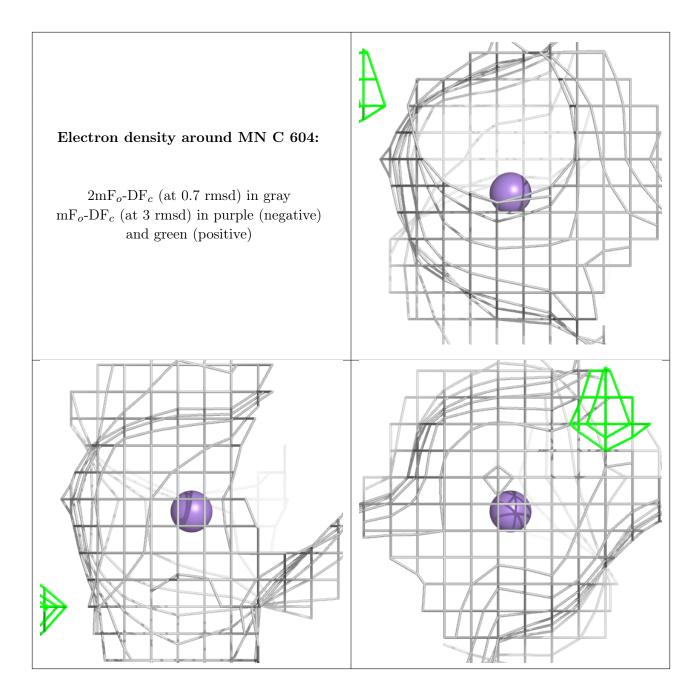






Electron density around ATP C 601: $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 0.7 rmsd) in gray ${\rm mF}_o\text{-}{\rm DF}_c$ (at 3 rmsd) in purple (negative) and green (positive) Electron density around ATP A 601: $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 0.7 rmsd) in gray mF_o -DF_c (at 3 rmsd) in purple (negative) and green (positive)





6.5 Other polymers (i)

There are no such residues in this entry.

