



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:52 PM UTC

PDB ID : 4O6A / pdb_00004o6a
Title : Mouse cyclic GMP-AMP synthase (cGAS) in complex with DNA
Authors : Zhang, X.; Chen, Z.; Zhang, X.W.; Chen, Z.J.
Deposited on : 2013-12-20
Resolution : 1.86 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
Xtriage (Phenix)	:	2.0
EDS	:	3.0
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

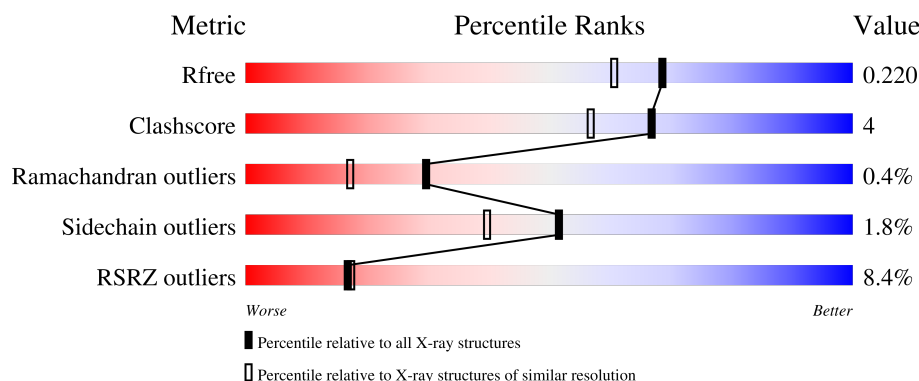
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.86 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	3428 (1.86-1.86)
Clashscore	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)
RSRZ outliers	180081	3429 (1.86-1.86)

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	7% 91% 8%
1	B	362	8% 90% 9%
2	C	17	18% 47% 53%
2	D	17	12% 53% 35% 12%
3	E	17	6% 76% 6% 18%

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Mol	Chain	Length	Quality of chain
3	F	17	24% 53% 47%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8279 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	0	0
			2984	1918	508	544	14			
1	B	358	Total	C	N	O	S	0	0	0
			2961	1904	505	539	13			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	146	MET	-	expression tag	UNP Q8C6L5
B	146	MET	-	expression tag	UNP Q8C6L5

- Molecule 2 is a DNA chain called DNA1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	15	Total	C	N	O	P	0	0	0
			308	147	63	84	14			
2	C	17	Total	C	N	O	P	0	0	0
			350	167	73	94	16			

- Molecule 3 is a DNA chain called DNA2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	14	Total	C	N	O	P	0	0	0
			281	136	47	85	13			
3	F	17	Total	C	N	O	P	0	0	0
			344	166	53	108	17			

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

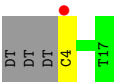
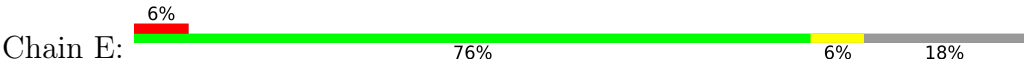
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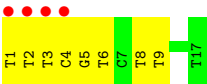
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Zn	0	0
			1	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	429	Total	O	0	0
			429	429		
5	D	64	Total	O	0	0
			64	64		
5	E	43	Total	O	0	0
			43	43		
5	B	369	Total	O	0	0
			369	369		
5	C	73	Total	O	0	0
			73	73		
5	F	71	Total	O	0	0
			71	71		



● Molecule 3: DNA2



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	183.71Å 96.33Å 75.99Å 90.00° 98.28° 90.00°	Depositor
Resolution (Å)	36.66 – 1.86 36.66 – 1.86	Depositor EDS
% Data completeness (in resolution range)	99.1 (36.66-1.86) 97.3 (36.66-1.86)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.12 (at 1.85Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.186 , 0.218 0.187 , 0.220	Depositor DCC
R_{free} test set	2000 reflections (1.19%)	wwPDB-VP
Wilson B-factor (Å ²)	26.7	Xtriage
Anisotropy	0.426	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 51.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8279	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.04% 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: 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 lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.44	0/3049	0.76	2/4093 (0.0%)
1	B	0.41	0/3025	0.72	0/4060
2	C	0.27	0/395	0.97	1/608 (0.2%)
2	D	0.28	0/347	0.88	0/534
3	E	0.26	0/313	0.91	0/481
3	F	0.30	0/382	1.14	4/587 (0.7%)
All	All	0.40	0/7511	0.80	7/10363 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	1	DT	C1'-O4'-C4'	-9.96	94.75	109.70
3	F	1	DT	C2-N1-C1'	-7.14	108.65	119.35
1	A	241	ARG	N-CA-C	6.89	117.74	108.23
3	F	1	DT	O4'-C1'-N1	6.89	118.73	108.40
3	F	1	DT	C6-N1-C1'	6.56	129.19	119.35
1	A	255	GLU	N-CA-C	-5.96	105.58	112.92
2	C	5	DT	O4'-C1'-N1	-5.22	100.57	108.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	228	TYR	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2984	0	3031	21	0
1	B	2961	0	3011	16	0
2	C	350	0	191	7	0
2	D	308	0	169	4	0
3	E	281	0	161	1	0
3	F	344	0	196	5	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	429	0	0	5	0
5	B	369	0	0	1	0
5	C	73	0	0	0	0
5	D	64	0	0	0	0
5	E	43	0	0	0	0
5	F	71	0	0	0	0
All	All	8279	0	6759	52	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 4.

All (52) 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:173:LYS:HE3	1:B:280:ILE:HD11	1.64	0.79
1:A:177:ARG:HG3	1:A:180:ARG:HH22	1.54	0.72
1:A:358:PHE:O	1:A:362:THR:HG23	1.91	0.71
1:B:267:ARG:NH1	1:B:285:GLU:O	2.24	0.70
1:B:358:PHE:O	1:B:362:THR:HG23	1.93	0.69
1:A:181:ARG:HD2	1:A:185:ARG:HH11	1.59	0.67
1:B:293:ALA:HB2	1:B:309:ILE:HD13	1.82	0.61
1:A:173:LYS:HE3	1:A:280:ILE:HD11	1.84	0.58
1:A:242:ILE:HG12	1:A:243:PRO:HA	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:391:LYS:NZ	1:B:396:GLU:OE1	2.34	0.56
1:B:188:GLU:HG3	1:B:251:PHE:CE2	2.41	0.56
2:C:3:DA:H2''	2:C:4:DT:H72	1.88	0.56
1:A:146:MET:HG3	1:A:149:LYS:H	1.71	0.55
2:D:15:DG:H1	3:E:4:DC:H42	1.53	0.55
2:C:16:DA:H2''	2:C:17:DA:C8	2.42	0.55
3:F:4:DC:H2'	3:F:5:DG:C8	2.42	0.54
1:A:353:LYS:NZ	5:A:917:HOH:O	2.37	0.51
2:C:15:DG:C6	2:C:16:DA:C6	2.99	0.50
1:A:146:MET:CG	1:A:149:LYS:H	2.26	0.48
1:B:155:ASP:HA	1:B:158:ARG:NH1	2.29	0.48
1:A:146:MET:HE3	1:A:149:LYS:HE3	1.95	0.47
2:C:1:DA:H2''	2:C:2:DA:C8	2.50	0.47
1:B:409:LYS:NZ	5:B:958:HOH:O	2.47	0.47
1:B:149:LYS:NZ	1:B:446:SER:OG	2.48	0.47
1:A:183:GLN:O	1:A:190:LYS:HG3	2.15	0.46
1:A:451:LYS:HG3	5:A:1002:HOH:O	2.16	0.45
1:A:156:LYS:NZ	5:A:837:HOH:O	2.48	0.45
1:B:476:PHE:HB3	1:B:486:LYS:HE2	1.97	0.45
1:B:183:GLN:O	1:B:190:LYS:HG3	2.17	0.45
3:F:8:DT:H2''	3:F:9:DT:H5'	1.98	0.45
2:C:16:DA:C5	2:C:17:DA:C6	3.06	0.44
1:A:248:LEU:HA	1:A:251:PHE:CD2	2.53	0.44
2:D:3:DA:H2''	2:D:4:DT:H72	2.00	0.44
1:A:189:PHE:O	1:A:192:VAL:HG22	2.18	0.43
1:A:486:LYS:NZ	5:A:981:HOH:O	2.52	0.43
2:C:16:DA:C5	2:C:17:DA:N1	2.87	0.43
1:B:225:LEU:HD21	1:B:347:LEU:HD11	2.01	0.43
1:B:204:VAL:O	1:B:402:LYS:NZ	2.49	0.43
1:A:248:LEU:HD22	1:A:262:MET:HE3	2.01	0.43
2:D:14:DC:H2''	2:D:15:DG:C8	2.54	0.42
1:B:188:GLU:HG3	1:B:251:PHE:HE2	1.83	0.42
1:B:188:GLU:CD	1:B:188:GLU:H	2.27	0.42
1:A:302:GLU:H	1:A:302:GLU:CD	2.27	0.42
1:A:196:ASN:HB3	1:A:201:TYR:CD2	2.55	0.41
1:A:350:LYS:NZ	5:A:1007:HOH:O	2.53	0.41
1:A:353:LYS:HA	1:A:353:LYS:HD3	1.74	0.41
1:A:177:ARG:HA	1:A:180:ARG:NH2	2.36	0.41
1:B:395:LYS:NZ	2:C:11:DA:OP1	2.46	0.41
3:F:8:DT:H2'	3:F:9:DT:C6	2.56	0.41
3:F:2:DT:H1'	3:F:3:DT:H5'	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1:DA:H2''	2:D:2:DA:C8	2.56	0.41
3:F:5:DG:H2'	3:F:6:DT:H71	2.03	0.41

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	359/362 (99%)	348 (97%)	10 (3%)	1 (0%)	36	25
1	B	356/362 (98%)	348 (98%)	6 (2%)	2 (1%)	21	10
All	All	715/724 (99%)	696 (97%)	16 (2%)	3 (0%)	30	17

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	243	PRO
1	A	300	ASN
1	B	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	334/335 (100%)	326 (98%)	8 (2%)	43	28

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	331/335 (99%)	327 (99%)	4 (1%)	63	55
All	All	665/670 (99%)	653 (98%)	12 (2%)	51	40

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	180	ARG
1	A	218	LEU
1	A	241	ARG
1	A	242	ILE
1	A	250	HIS
1	A	302	GLU
1	A	353	LYS
1	A	414	GLU
1	B	188	GLU
1	B	230	GLU
1	B	242	ILE
1	B	302	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	203	HIS
1	A	356	ASN
1	A	433	GLN
1	B	444	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

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

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%)	0.06	27 (7%) 20 22	16, 26, 59, 134	0
1	B	358/362 (98%)	0.38	29 (8%) 18 19	17, 32, 72, 141	0
2	C	17/17 (100%)	0.31	3 (17%) 4 3	20, 27, 103, 125	0
2	D	15/17 (88%)	0.37	2 (13%) 7 6	22, 33, 85, 96	0
3	E	14/17 (82%)	0.44	1 (7%) 22 24	24, 38, 76, 91	0
3	F	17/17 (100%)	0.66	4 (23%) 2 2	21, 33, 118, 137	0
All	All	782/792 (98%)	0.24	66 (8%) 17 17	16, 29, 73, 141	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	242	ILE	6.3
1	B	229	TYR	5.4
1	A	185	ARG	5.2
1	B	149	LYS	4.8
1	A	184	LYS	4.4
3	F	1	DT	4.3
2	C	17	DA	4.3
1	B	254	GLY	4.0
1	B	231	THR	3.9
1	A	254	GLY	3.9
1	A	245	GLY	3.7
2	C	16	DA	3.7
1	A	229	TYR	3.6
1	A	247	PRO	3.5
1	A	249	SER	3.5
1	A	146	MET	3.5
1	B	243	PRO	3.4
1	A	186	GLU	3.3
1	A	255	GLU	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	256	VAL	3.2
1	A	250	HIS	3.2
3	F	3	DT	3.2
1	A	243	PRO	3.2
1	A	248	LEU	3.2
1	B	245	GLY	3.1
3	F	2	DT	3.0
2	C	15	DG	3.0
1	B	241	ARG	3.0
1	B	244	ARG	3.0
1	B	255	GLU	2.9
1	A	242	ILE	2.9
1	B	495	TYR	2.8
1	B	230	GLU	2.8
1	B	181	ARG	2.8
1	A	256	VAL	2.7
2	D	1	DA	2.7
1	A	353	LYS	2.7
1	B	228	TYR	2.6
1	A	231	THR	2.6
1	A	506	LYS	2.6
1	B	239	PHE	2.6
2	D	15	DG	2.6
1	A	241	ARG	2.6
1	A	230	GLU	2.6
1	B	250	HIS	2.5
1	B	252	LEU	2.5
1	B	160	LYS	2.5
1	B	506	LYS	2.5
1	A	228	TYR	2.5
1	B	412	PHE	2.4
1	B	430	MET	2.4
1	A	181	ARG	2.4
1	A	161	ARG	2.3
1	B	352	ALA	2.3
1	B	498	ASN	2.3
1	A	413	GLN	2.3
1	A	288	LYS	2.3
1	B	483	ARG	2.3
3	E	4	DC	2.3
1	A	239	PHE	2.2
1	A	180	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	353	LYS	2.2
3	F	4	DC	2.1
1	B	487	GLU	2.1
1	B	499	ASN	2.0
1	B	479	GLU	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	ZN	A	601	1/1	0.99	0.02	21,21,21,21	0
4	ZN	B	601	1/1	0.99	0.03	25,25,25,25	0

6.5 Other polymers [i](#)

There are no such residues in this entry.