



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2024 – 11:51 AM EST

PDB ID : 7FTF
Title : Crystal Structure of apo human cyclic GMP-AMP synthase
Authors : Leibrock, L.; Benz, J.; Groebke-Zbinden, K.; Rudolph, M.G.
Deposited on : 2023-02-08
Resolution : 1.51 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (Phenix) : 1.13
EDS : 2.36
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) : 2.36

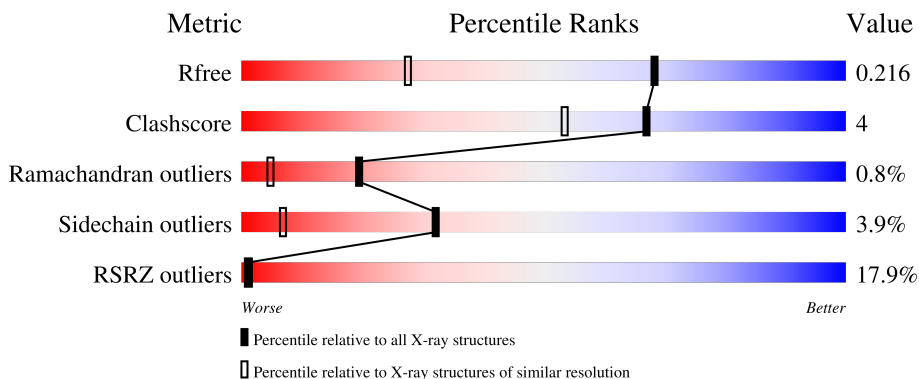
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


The reported resolution of this entry is 1.51 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	2936 (1.50-1.50)
Clashscore	141614	3144 (1.50-1.50)
Ramachandran outliers	138981	3066 (1.50-1.50)
Sidechain outliers	138945	3064 (1.50-1.50)
RSRZ outliers	127900	2884 (1.50-1.50)

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	362	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 3229 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
			Total	C	N	O	S			
1	A	358	3032	1949	520	547	16	0	13	0

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	A	1	4	2	2	0	0

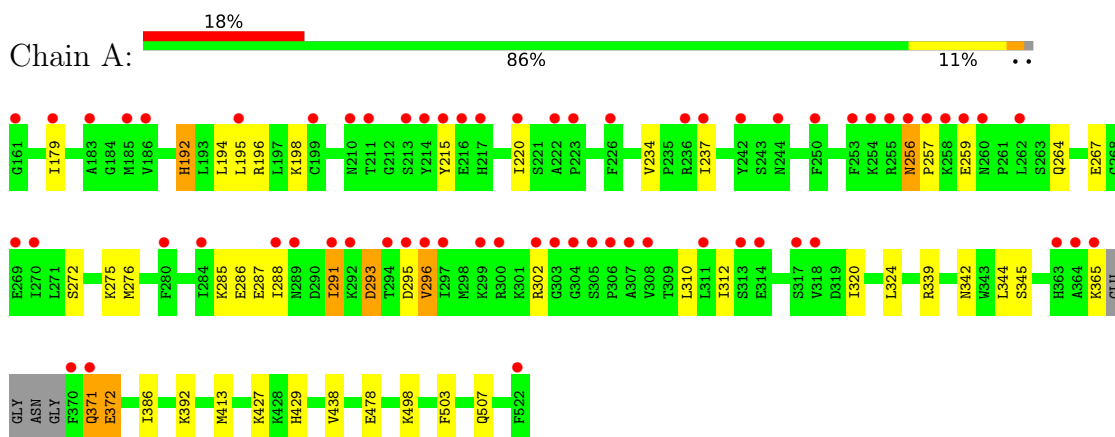
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	190	Total 192	O 192	0	2

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

Property	Value	Source
Space group	P 21 2 21	Depositor
Cell constants a, b, c, α , β , γ	48.37Å 59.90Å 125.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.13 – 1.51 62.73 – 1.51	Depositor EDS
% Data completeness (in resolution range)	81.7 (45.13-1.51) 79.2 (62.73-1.51)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.03 (at 1.51Å)	Xtrriage
Refinement program	PHENIX dev_3139	Depositor
R, R_{free}	0.179 , 0.214 0.181 , 0.216	Depositor DCC
R_{free} test set	2394 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	24.6	Xtrriage
Anisotropy	0.010	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 52.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	3229	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.14% 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: EDO, 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	0.37	0/3125	0.53	0/4188

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	3032	0	3114	24	0
2	A	1	0	0	0	0
3	A	4	0	6	1	0
4	A	192	0	0	2	0
All	All	3229	0	3120	24	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 (24) 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:392:LYS:HB3	3:A:602:EDO:H22	1.78	0.65
1:A:196:ARG:HG2	1:A:287:GLU:HG3	1.84	0.58
1:A:371:GLN:O	1:A:372:GLU:HB2	2.03	0.58
1:A:194:LEU:HG	1:A:198:LYS:HE3	1.88	0.55
1:A:285:LYS:HA	1:A:288:ILE:HG22	1.89	0.55
1:A:179:ILE:HG21	1:A:220:ILE:HD11	1.90	0.54
1:A:256:ASN:N	1:A:257:PRO:HD3	2.23	0.53
1:A:291:ILE:HG23	1:A:293:ASP:OD1	2.10	0.52
1:A:427:LYS:HB2	1:A:429:HIS:NE2	2.25	0.51
1:A:413[B]:MET:HE1	4:A:768:HOH:O	2.13	0.48
1:A:310:LEU:HD13	1:A:320:ILE:HD12	1.94	0.48
1:A:503:PHE:O	1:A:507:GLN:HG2	2.15	0.47
1:A:196:ARG:NH2	1:A:286:GLU:OE2	2.47	0.47
1:A:234:VAL:HG21	1:A:324:LEU:HD22	1.97	0.47
1:A:237:ILE:HD12	1:A:237:ILE:HA	1.79	0.47
1:A:296:VAL:HG12	1:A:312:ILE:HG12	1.97	0.45
1:A:196:ARG:HG2	1:A:287:GLU:CG	2.47	0.45
1:A:192:HIS:O	1:A:195:LEU:HG	2.18	0.44
1:A:344:LEU:HD11	1:A:386[B]:ILE:HG23	2.00	0.44
1:A:267:GLU:HG3	1:A:272:SER:HB2	2.00	0.42
1:A:478[A]:GLU:OE1	1:A:498:LYS:NZ	2.49	0.42
1:A:342:ASN:HB2	4:A:730:HOH:O	2.19	0.41
1:A:272:SER:OG	1:A:275:LYS:HG2	2.21	0.40
1:A:276:MET:HE2	1:A:276:MET:HB2	1.93	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	367/362 (101%)	348 (95%)	16 (4%)	3 (1%)	19 5

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	372	GLU
1	A	345	SER
1	A	256	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	345/334 (103%)	331 (96%)	14 (4%)	30 6

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	192	HIS
1	A	215	TYR
1	A	259	GLU
1	A	264	GLN
1	A	291	ILE
1	A	293	ASP
1	A	295	ASP
1	A	296	VAL
1	A	302	ARG
1	A	339	ARG
1	A	365	LYS
1	A	371	GLN
1	A	438[A]	VAL
1	A	438[B]	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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	EDO	A	602	-	3,3,3	0.40	0	2,2,2	0.26	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
3	EDO	A	602	-	-	0/1/1/1	-

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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	602	EDO	1	0

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	358/362 (98%)	0.75	64 (17%) 1 1	20, 49, 121, 175	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	370	PHE	10.5
1	A	255	ARG	7.9
1	A	303	GLY	7.2
1	A	215	TYR	6.8
1	A	296	VAL	6.4
1	A	288	ILE	6.1
1	A	307	ALA	5.7
1	A	258	LYS	5.7
1	A	294	THR	5.6
1	A	236	ARG	5.6
1	A	302	ARG	5.5
1	A	291	ILE	5.4
1	A	292	LYS	5.4
1	A	254	LYS	5.3
1	A	257	PRO	4.8
1	A	311	LEU	4.5
1	A	295	ASP	4.5
1	A	522	PHE	4.4
1	A	179	ILE	4.4
1	A	237	ILE	4.3
1	A	183	ALA	4.1
1	A	289	ASN	3.8
1	A	269	GLU	3.7
1	A	256	ASN	3.6
1	A	313	SER	3.5
1	A	186	VAL	3.3
1	A	222	ALA	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	214	TYR	3.2
1	A	260	ASN	3.2
1	A	210	ASN	3.2
1	A	262	LEU	3.1
1	A	199	CYS	3.1
1	A	244	ASN	3.1
1	A	306	PRO	3.0
1	A	259	GLU	3.0
1	A	308	VAL	3.0
1	A	242	TYR	3.0
1	A	161	GLY	2.9
1	A	195	LEU	2.9
1	A	299	LYS	2.9
1	A	371	GLN	2.9
1	A	185	MET	2.8
1	A	304	GLY	2.8
1	A	305	SER	2.7
1	A	216	GLU	2.7
1	A	223	PRO	2.6
1	A	364	ALA	2.5
1	A	317	SER	2.4
1	A	297	ILE	2.4
1	A	270	ILE	2.4
1	A	365	LYS	2.4
1	A	220	ILE	2.3
1	A	226	PHE	2.3
1	A	318	VAL	2.3
1	A	213	SER	2.2
1	A	280	PHE	2.2
1	A	284	ILE	2.2
1	A	314	GLU	2.2
1	A	253	PHE	2.1
1	A	217	HIS	2.1
1	A	300	ARG	2.1
1	A	211	THR	2.0
1	A	363	HIS	2.0
1	A	250	PHE	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 [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
3	EDO	A	602	4/4	0.97	0.12	29,37,56,57	0
2	ZN	A	601	1/1	1.00	0.10	22,22,22,22	0

6.5 Other polymers [i](#)

There are no such residues in this entry.