

wwPDB X-ray Structure Validation Summary Report (i)

Jan 27, 2024 – 10:50 PM EST

PDB ID : 1G49

Title : A CARBOXYLIC ACID BASED INHIBITOR IN COMPLEX WITH MMP3

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Deposited on : 2000-10-26

Resolution : 1.90 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 (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) : NOT EXECUTED

EDS : NOT EXECUTED

buster-report : 1.1.7 (2018)

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

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

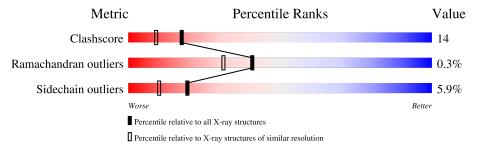
Validation Pipeline (wwPDB-VP) : 2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.90 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	Similar resolution
Metric	$(\# \mathrm{Entries})$	$(\# ext{Entries}, ext{ resolution range}(ext{Å}))$
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)

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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain				
1	A	173	77%	17%	• • • •		
1	В	173	71%	24%			



2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 2871 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 MATRIX METALLOPROTEINASE 3.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	Λ	169	Total	С	N	О	S	0	0	0
1	A	109	1346	865	224	255	2	0	U	U
1	D	173	Total	С	N	О	S	0	0	0
1	Б	173	1376	882	228	264	2	0	0	U

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

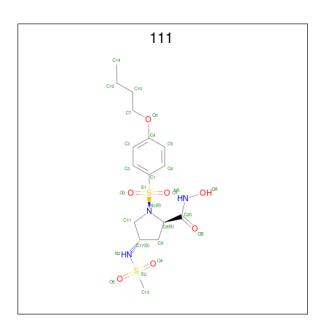
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Zn 2 2	0	0
2	В	2	Total Zn 2 2	0	0

• Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	3	Total Ca 3 3	0	0
3	В	3	Total Ca 3 3	0	0

• Molecule 4 is (1N)-4-N-BUTOXYPHENYLSULFONYL-(2R)-N-HYDROXYCARBOX AMIDO-(4S)-METHANESULFONYLAMINO-PYRROLIDINE (three-letter code: 111) (formula: C₁₆H₂₅N₃O₇S₂).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf		
1	D	1	Total	С	N	О	S	0	0
4	Б	1	28	16	3	7	2	0	

• Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	66	Total O 66 66	0	0
5	В	45	Total O 45 45	0	0

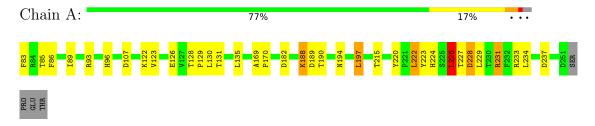


3 Residue-property plots (i)

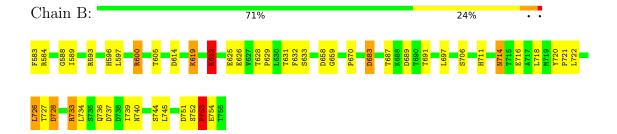
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

Note EDS was not executed.

• Molecule 1: MATRIX METALLOPROTEINASE 3



• Molecule 1: MATRIX METALLOPROTEINASE 3





4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	37.67Å 77.11Å 106.14Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.70 - 1.90	Depositor
% Data completeness	(Not available) (19.70-1.90)	Depositor
(in resolution range)	(13.70 1.30)	Берозног
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.210 , 0.253	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2871	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP



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: CA, 111, 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		
IVIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	A	0.75	0/1390	1.00	5/1899 (0.3%)	
1	В	0.79	0/1421	1.03	9/1941 (0.5%)	
All	All	0.77	0/2811	1.02	14/3840 (0.4%)	

There are no bond length outliers.

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
1	В	600	ARG	NE-CZ-NH2	-7.58	116.51	120.30
1	В	683	ASP	CB-CG-OD2	7.00	124.60	118.30
1	В	753	PRO	CB-CA-C	-6.63	95.42	112.00
1	В	728	ASP	CB-CG-OD2	6.48	124.13	118.30
1	В	614	ASP	CB-CG-OD2	5.98	123.68	118.30

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	1346	0	1270	27	1
1	В	1376	0	1295	45	1
2	A	2	0	0	0	0
2	В	2	0	0	0	0

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COHABABACA		DIEUIUU	DUIUE
0 0 1000100000			

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	3	0	0	0	0
3	В	3	0	0	0	0
4	В	28	0	24	4	0
5	A	66	0	0	1	0
5	В	45	0	0	3	0
All	All	2871	0	2589	73	1

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 14.

The worst 5 of 73 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:B:584:ARG:NH1	5:B:85:HOH:O	1.92	1.00
1:B:619:LYS:CE	1:B:622:LYS:HZ1	1.85	0.89
1:B:619:LYS:CE	1:B:622:LYS:NZ	2.38	0.88
1:B:588:GLY:O	1:B:589:ILE:HG22	1.79	0.81
1:B:689:ASP:OD1	1:B:691:THR:HG22	1.82	0.79

All (1) 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-1 Atom-2		$\begin{array}{c} \text{Clash} \\ \text{overlap } (\text{\AA}) \end{array}$
1:A:89:ILE:O	1:B:716:GLU:OE2[2_564]	2.18	0.02

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 A		Allowed	Outliers	Perce	entiles
1	A	167/173 (96%)	159 (95%)	7 (4%)	1 (1%)	25	15
1	В	171/173 (99%)	163 (95%)	8 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	338/346 (98%)	322 (95%)	15 (4%)	1 (0%)	41 31	

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	226	LEU

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	Perce	ntiles
1	A	143/147 (97%)	135 (94%)	8 (6%)	21	11
1	В	147/147 (100%)	138 (94%)	9 (6%)	18	9
All	All	290/294 (99%)	273 (94%)	17 (6%)	19	10

5 of 17 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	В	726	LEU
1	В	753	PRO
1	A	231	ARG
1	В	597	LEU
1	В	600	ARG

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	96	HIS
1	A	194	ASN
1	В	596	HIS
1	В	714	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 11 ligands modelled in this entry, 10 are 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	ype Chain	Res	Link	Bond lengths		Bond angles			
IVIOI	туре		nes	Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	111	В	901	2	29,29,29	4.41	8 (27%)	36,42,42	2.07	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.

\mathbf{Mol}	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	111	В	901	2	-	10/28/40/40	0/2/2/2

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	Observed(A)	$\operatorname{Ideal}(ext{\AA})$
4	В	901	111	O1-S1	11.88	1.56	1.43
4	В	901	111	O2-S1	11.71	1.56	1.43
4	В	901	111	O4-S2	8.28	1.58	1.43

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Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(\AA)$	$\operatorname{Ideal}(ext{\AA})$
4	В	901	111	O5-S2	8.12	1.57	1.43
4	В	901	111	S1-N1	6.72	1.73	1.63

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
4	В	901	111	O2-S1-O1	-7.80	106.88	119.52
4	В	901	111	O4-S2-O5	-5.43	111.04	118.85
4	В	901	111	C9-C8-C20	-3.80	103.74	111.32
4	В	901	111	C1-S1-N1	3.42	113.44	107.36
4	В	901	111	C6-C1-S1	2.99	122.91	119.76

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	В	901	111	OB-C20-C8-N1
4	В	901	111	C7-C10-C12-C14
4	В	901	111	OB-C20-C8-C9
4	В	901	111	NA-C20-C8-C9
4	В	901	111	C17-N2-S2-O5

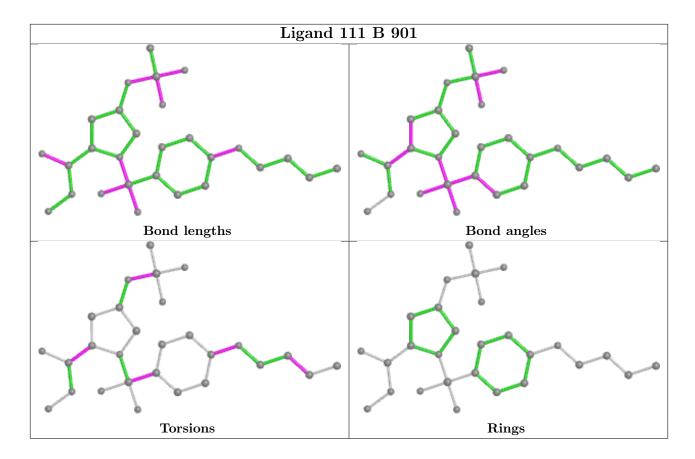
There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	В	901	111	4	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 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)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.

