



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 27, 2017 – 02:29 AM EDT

PDB ID : 1G49
Title : A CARBOXYLIC ACID BASED INHIBITOR IN COMPLEX WITH MMP3
Authors : Natchus, M.G.; Bookland, R.G.; De, B.; Almstead, N.G.; Pikul, S.
Deposited on : unknown
Resolution : 1.90 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030345

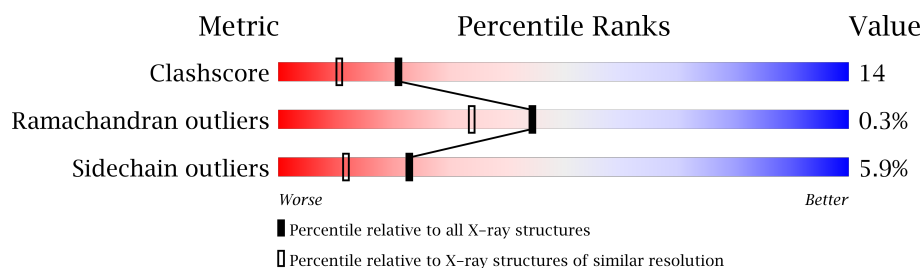
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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 (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	112137	5731 (1.90-1.90)
Ramachandran outliers	110173	5669 (1.90-1.90)
Sidechain outliers	110143	5670 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	173	
1	B	173	

2 Entry composition

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	A	169	Total	C	N	O	S	0	0	0
			1346	865	224	255	2			
1	B	173	Total	C	N	O	S	0	0	0
			1376	882	228	264	2			

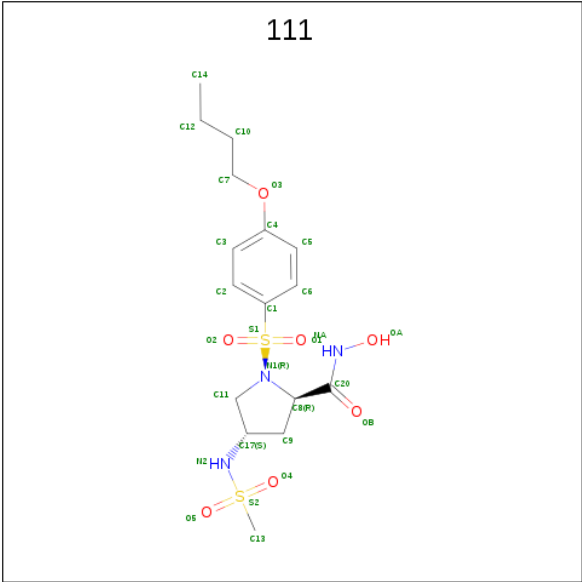
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

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

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

- 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
4	B	1	Total	C	N	O	S	0	0
			28	16	3	7	2		

- Molecule 5 is water.


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

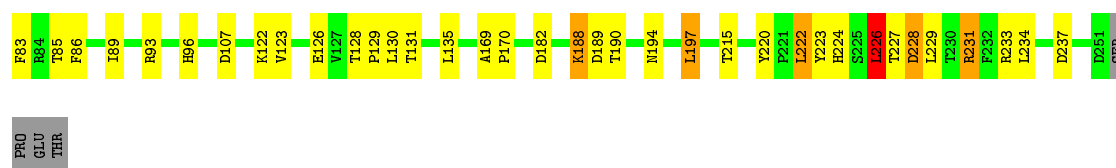
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

Note EDS was not executed.

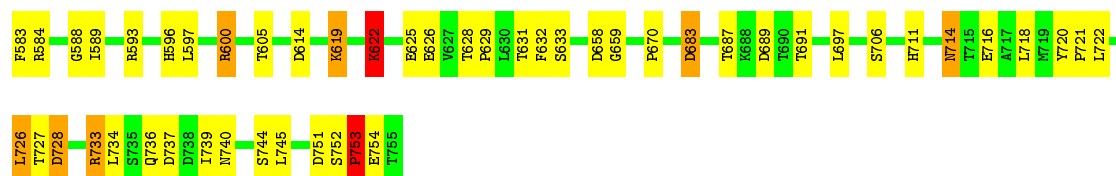
• Molecule 1: MATRIX METALLOPROTEINASE 3

Chain A: 



• Molecule 1: MATRIX METALLOPROTEINASE 3

Chain B: 



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	37.67Å 77.11Å 106.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.70 – 1.90	Depositor
% Data completeness (in resolution range)	(Not available) (19.70-1.90)	Depositor
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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, 111, CA

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	0.75	0/1390	1.00	5/1899 (0.3%)
1	B	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.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	600	ARG	NE-CZ-NH2	-7.58	116.51	120.30
1	B	683	ASP	CB-CG-OD2	7.00	124.60	118.30
1	B	753	PRO	CB-CA-C	-6.63	95.42	112.00
1	B	728	ASP	CB-CG-OD2	6.48	124.13	118.30
1	B	614	ASP	CB-CG-OD2	5.98	123.68	118.30
1	A	228	ASP	CB-CG-OD1	5.74	123.47	118.30
1	A	189	ASP	CB-CG-OD2	5.73	123.46	118.30
1	B	737	ASP	CB-CG-OD2	5.70	123.43	118.30
1	B	733	ARG	N-CA-C	-5.69	95.65	111.00
1	B	622	LYS	CD-CE-NZ	-5.51	99.02	111.70
1	A	233	ARG	NE-CZ-NH2	-5.45	117.57	120.30
1	B	658	ASP	CB-CG-OD2	5.43	123.18	118.30
1	A	85	THR	N-CA-C	-5.18	97.00	111.00
1	A	107	ASP	CB-CG-OD2	5.14	122.92	118.30

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	1346	0	1270	27	1
1	B	1376	0	1295	45	1
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	3	0	0	0	0
3	B	3	0	0	0	0
4	B	28	0	24	4	0
5	A	66	0	0	1	0
5	B	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.

All (73) 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: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
1:B:754:GLU:OE1	5:B:103:HOH:O	2.00	0.79
1:A:222:LEU:HD22	1:A:224:HIS:CD2	2.17	0.79
1:B:619:LYS:HE3	1:B:622:LYS:NZ	2.02	0.74
1:B:726:LEU:HD22	1:B:727:THR:H	1.51	0.73
1:B:619:LYS:HE2	1:B:622:LYS:NZ	2.05	0.71
1:A:123:VAL:HG13	1:A:234:LEU:HG	1.73	0.70
1:B:716:GLU:OE1	1:B:716:GLU:HA	1.94	0.67
1:A:197:LEU:HD12	1:A:223:TYR:CE1	2.31	0.66
1:B:622:LYS:O	1:B:626:GLU:HG3	1.95	0.66
1:B:588:GLY:O	1:B:589:ILE:CG2	2.44	0.65
1:B:619:LYS:HE3	1:B:622:LYS:HZ1	1.55	0.64
1:A:190:THR:HG21	1:A:227:THR:HA	1.80	0.64
1:A:222:LEU:CD2	1:A:224:HIS:CD2	2.82	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:718:LEU:O	4:B:901:111:H101	1.98	0.63
1:B:596:HIS:CE1	1:B:633:SER:HB2	2.36	0.61
1:B:628:THR:HB	1:B:629:PRO:CD	2.32	0.59
1:A:222:LEU:HD22	1:A:224:HIS:NE2	2.18	0.57
1:B:726:LEU:HD22	1:B:727:THR:N	2.19	0.57
1:A:93:ARG:HD2	1:A:93:ARG:C	2.24	0.57
1:A:231:ARG:NH2	1:A:231:ARG:HB3	2.21	0.56
1:A:96:HIS:HD2	1:A:131:THR:OG1	1.89	0.55
1:A:215:THR:HG22	1:A:215:THR:O	2.07	0.54
1:A:231:ARG:HH21	1:A:231:ARG:HB3	1.72	0.54
1:A:194:ASN:HD22	1:A:197:LEU:H	1.56	0.54
1:B:720:TYR:CD1	1:B:721:PRO:HD2	2.42	0.53
1:A:128:THR:HB	1:A:129:PRO:CD	2.39	0.53
1:B:619:LYS:CE	1:B:622:LYS:HZ2	2.21	0.52
1:B:697:LEU:HB3	4:B:901:111:H141	1.91	0.52
1:A:188:LYS:NZ	1:A:188:LYS:HB3	2.25	0.52
1:B:720:TYR:HE2	1:B:722:LEU:HD12	1.76	0.51
1:A:220:TYR:CD2	1:A:222:LEU:HB2	2.45	0.51
1:B:596:HIS:NE2	1:B:633:SER:HB2	2.26	0.51
1:B:736:GLN:HA	1:B:739:ILE:HD12	1.93	0.50
1:B:619:LYS:NZ	1:B:622:LYS:HZ1	2.08	0.50
1:B:589:ILE:HG23	1:B:589:ILE:O	2.10	0.50
1:B:596:HIS:HD2	1:B:631:THR:OG1	1.93	0.49
1:A:215:THR:CG2	1:A:215:THR:O	2.60	0.49
1:A:169:ALA:HB1	1:A:170:PRO:HD2	1.95	0.48
1:B:625:GLU:HG3	1:B:632:PHE:CD1	2.48	0.48
1:B:687:THR:HG21	1:B:691:THR:HG23	1.96	0.47
1:B:752:SER:HB2	1:B:753:PRO:HD2	1.95	0.47
1:A:226:LEU:HD23	1:A:228:ASP:OD1	2.15	0.46
1:B:625:GLU:HG3	1:B:632:PHE:HD1	1.81	0.46
1:B:740:ASN:O	1:B:744:SER:HB3	2.15	0.46
1:B:622:LYS:HB2	1:B:622:LYS:HE3	1.55	0.46
1:A:83:PHE:N	1:A:237:ASP:OD1	2.49	0.46
1:B:726:LEU:HD11	1:B:728:ASP:O	2.17	0.45
1:B:711:HIS:CE1	4:B:901:111:OB	2.70	0.44
1:A:194:ASN:OD1	1:A:229:LEU:HD11	2.16	0.44
1:B:714:ASN:HD22	1:B:716:GLU:H	1.65	0.44
1:B:726:LEU:HD13	1:B:727:THR:N	2.33	0.44
4:B:901:111:C14	4:B:901:111:O3	2.65	0.44
1:B:588:GLY:C	1:B:589:ILE:HG22	2.36	0.43
1:A:220:TYR:CE2	1:A:222:LEU:HB2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:659:GLY:HA2	1:B:683:ASP:OD2	2.19	0.43
1:A:194:ASN:ND2	1:A:197:LEU:H	2.16	0.43
1:B:670:PRO:HG3	1:B:706:SER:O	2.18	0.43
1:B:733:ARG:HG2	1:B:734:LEU:N	2.34	0.42
1:A:123:VAL:CG1	1:A:234:LEU:HG	2.46	0.42
1:A:86:PHE:HB2	5:A:365:HOH:O	2.18	0.42
1:A:188:LYS:HB3	1:A:188:LYS:HZ3	1.84	0.41
1:B:751:ASP:OD1	1:B:751:ASP:N	2.53	0.41
1:A:194:ASN:CG	1:A:229:LEU:HD11	2.40	0.41
1:B:619:LYS:HE3	1:B:622:LYS:HZ2	1.81	0.41
1:A:122:LYS:O	1:A:126:GLU:HG3	2.20	0.41
1:B:733:ARG:HG2	1:B:734:LEU:H	1.86	0.41
1:B:593:ARG:NH1	5:B:13:HOH:O	2.34	0.41
1:B:583:PHE:CD1	1:B:583:PHE:C	2.94	0.41

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-2	Interatomic distance (Å)	Clash overlap (Å)
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	Allowed	Outliers	Percentiles	
1	A	167/173 (96%)	159 (95%)	7 (4%)	1 (1%)	28	16
1	B	171/173 (99%)	163 (95%)	8 (5%)	0	100	100
All	All	338/346 (98%)	322 (95%)	15 (4%)	1 (0%)	44	34

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	226	LEU

5.3.2 Protein sidechains ⓘ

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	143/147 (97%)	135 (94%)	8 (6%)	25	13
1	B	147/147 (100%)	138 (94%)	9 (6%)	22	11
All	All	290/294 (99%)	273 (94%)	17 (6%)	23	12

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	130	LEU
1	A	135	LEU
1	A	182	ASP
1	A	188	LYS
1	A	197	LEU
1	A	222	LEU
1	A	226	LEU
1	A	231	ARG
1	B	597	LEU
1	B	600	ARG
1	B	605	THR
1	B	619	LYS
1	B	622	LYS
1	B	714	ASN
1	B	726	LEU
1	B	745	LEU
1	B	753	PRO

Some 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

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Mol	Chain	Res	Type
1	A	194	ASN
1	B	596	HIS
1	B	714	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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	111	B	901	2	29,29,29	4.12	8 (27%)	36,42,42	2.02	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.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	111	B	901	2	-	0/28/40/40	0/2/2/2

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	901	111	O3-C4	-5.41	1.24	1.37
4	B	901	111	S2-N2	5.19	1.73	1.62
4	B	901	111	OB-C20	6.08	1.35	1.23
4	B	901	111	S1-N1	6.90	1.73	1.63
4	B	901	111	O5-S2	7.51	1.57	1.43
4	B	901	111	O4-S2	7.66	1.58	1.43
4	B	901	111	O2-S1	10.53	1.56	1.43
4	B	901	111	O1-S1	10.69	1.56	1.43

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	901	111	O2-S1-O1	-7.48	106.88	119.46
4	B	901	111	O4-S2-O5	-5.11	111.04	118.78
4	B	901	111	C9-C8-C20	-3.63	103.74	111.40
4	B	901	111	C6-C1-S1	2.87	122.91	119.78
4	B	901	111	C1-S1-N1	3.48	113.44	107.37

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	901	111	4	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 ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.