



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2018 – 05:42 pm GMT

PDB ID : 1SOJ  
Title : CATALYTIC DOMAIN OF HUMAN PHOSPHODIESTERASE 3B IN COMPLEX WITH IBMX  
Authors : Scapin, G.; Patel, S.B.; Chung, C.; Varnerin, J.P.; Edmondson, S.D.; Mastracchio, A.; Parmee, E.R.; Becker, J.W.; Singh, S.B.; Van Der Ploeg, L.H.; Tota, M.R.  
Deposited on : 2004-03-15  
Resolution : 2.90 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](mailto: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.

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

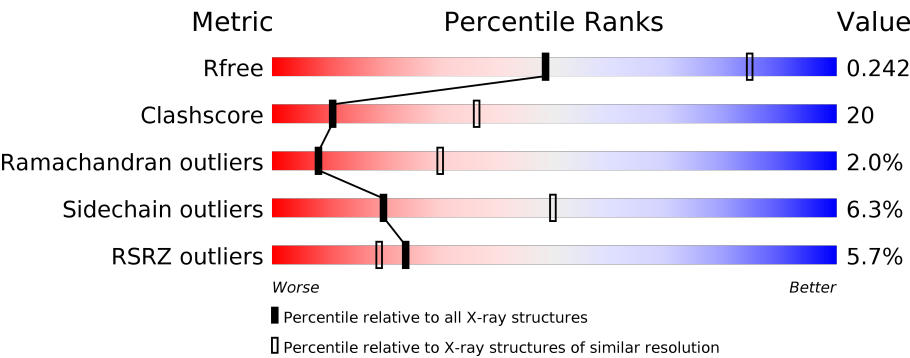
MolProbity : 4.02b-467  
Mogul : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : 1.13  
EDS : trunk30967  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk30967

# 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 2.90 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))
$R_{free}$	111664	1716 (2.90-2.90)
Clashscore	122126	1924 (2.90-2.90)
Ramachandran outliers	120053	1884 (2.90-2.90)
Sidechain outliers	120020	1886 (2.90-2.90)
RSRZ outliers	108989	1669 (2.90-2.90)

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  $\geq 3$ , 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.

Mol	Chain	Length	Quality of chain
1	A	420	<div><div>2%</div><div><div></div><div>56%</div><div>27%</div><div>•</div><div>13%</div></div></div>
1	B	420	<div><div>7%</div><div><div></div><div>55%</div><div>30%</div><div>5%</div><div>9%</div></div></div>
1	C	420	<div><div>3%</div><div><div></div><div>55%</div><div>29%</div><div>•</div><div>13%</div></div></div>
1	D	420	<div><div>6%</div><div><div></div><div>55%</div><div>31%</div><div>5%</div><div>9%</div></div></div>
1	E	420	<div><div>3%</div><div><div></div><div>55%</div><div>28%</div><div>•</div><div>13%</div></div></div>
1	F	420	<div><div>3%</div><div><div></div><div>58%</div><div>29%</div><div>5%</div><div>9%</div></div></div>

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Mol	Chain	Length	Quality of chain
1	G	420	
1	H	420	
1	I	420	
1	J	420	
1	K	420	
1	L	420	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 36048 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 cGMP-inhibited 3',5'-cyclic phosphodiesterase B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	364	Total	C	N	O	S	0	0	0
			2907	1862	496	535	14			
1	B	381	Total	C	N	O	S	0	0	0
			3017	1922	519	562	14			
1	C	364	Total	C	N	O	S	0	0	0
			2907	1862	496	535	14			
1	D	381	Total	C	N	O	S	0	0	0
			3017	1922	519	562	14			
1	E	364	Total	C	N	O	S	0	0	0
			2907	1862	496	535	14			
1	F	381	Total	C	N	O	S	0	0	0
			3017	1922	519	562	14			
1	G	364	Total	C	N	O	S	0	0	0
			2907	1862	496	535	14			
1	H	381	Total	C	N	O	S	0	0	0
			3017	1922	519	562	14			
1	I	364	Total	C	N	O	S	0	0	0
			2907	1862	496	535	14			
1	J	381	Total	C	N	O	S	0	0	0
			3017	1922	519	562	14			
1	K	364	Total	C	N	O	S	0	0	0
			2907	1862	496	535	14			
1	L	381	Total	C	N	O	S	0	0	0
			3017	1922	519	562	14			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

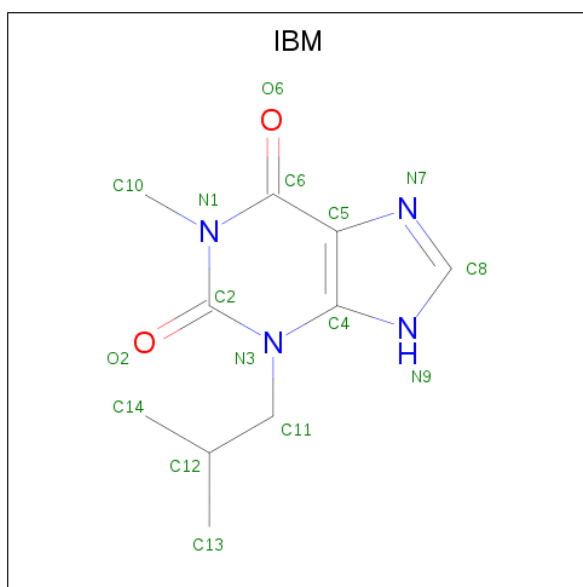
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	2	Total	Mg	0	0
			2	2		
2	J	2	Total	Mg	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	2	Total	Mg	0	0
			2	2		
2	K	2	Total	Mg	0	0
			2	2		
2	E	2	Total	Mg	0	0
			2	2		
2	H	2	Total	Mg	0	0
			2	2		
2	B	2	Total	Mg	0	0
			2	2		
2	I	2	Total	Mg	0	0
			2	2		
2	C	2	Total	Mg	0	0
			2	2		
2	A	2	Total	Mg	0	0
			2	2		
2	L	2	Total	Mg	0	0
			2	2		
2	F	2	Total	Mg	0	0
			2	2		

- Molecule 3 is 3-ISOBUTYL-1-METHYLNANTHINE (three-letter code: IBM) (formula:  $C_{10}H_{14}N_4O_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			16	10	4	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	O	0	0
			16	10	4	2		
3	C	1	Total	C	N	O	0	0
			16	10	4	2		
3	D	1	Total	C	N	O	0	0
			16	10	4	2		
3	E	1	Total	C	N	O	0	0
			16	10	4	2		
3	F	1	Total	C	N	O	0	0
			16	10	4	2		
3	G	1	Total	C	N	O	0	0
			16	10	4	2		
3	H	1	Total	C	N	O	0	0
			16	10	4	2		
3	I	1	Total	C	N	O	0	0
			16	10	4	2		
3	J	1	Total	C	N	O	0	0
			16	10	4	2		
3	K	1	Total	C	N	O	0	0
			16	10	4	2		
3	L	1	Total	C	N	O	0	0
			16	10	4	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	24	Total	O	0	0
			24	24		
4	B	24	Total	O	0	0
			24	24		
4	C	24	Total	O	0	0
			24	24		
4	D	24	Total	O	0	0
			24	24		
4	E	23	Total	O	0	0
			23	23		
4	F	25	Total	O	0	0
			25	25		
4	G	23	Total	O	0	0
			23	23		
4	H	25	Total	O	0	0
			25	25		

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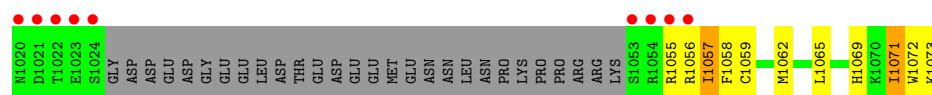
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	I	24	Total 24	O 24	0	0
4	J	24	Total 24	O 24	0	0
4	K	24	Total 24	O 24	0	0
4	L	24	Total 24	O 24	0	0

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.

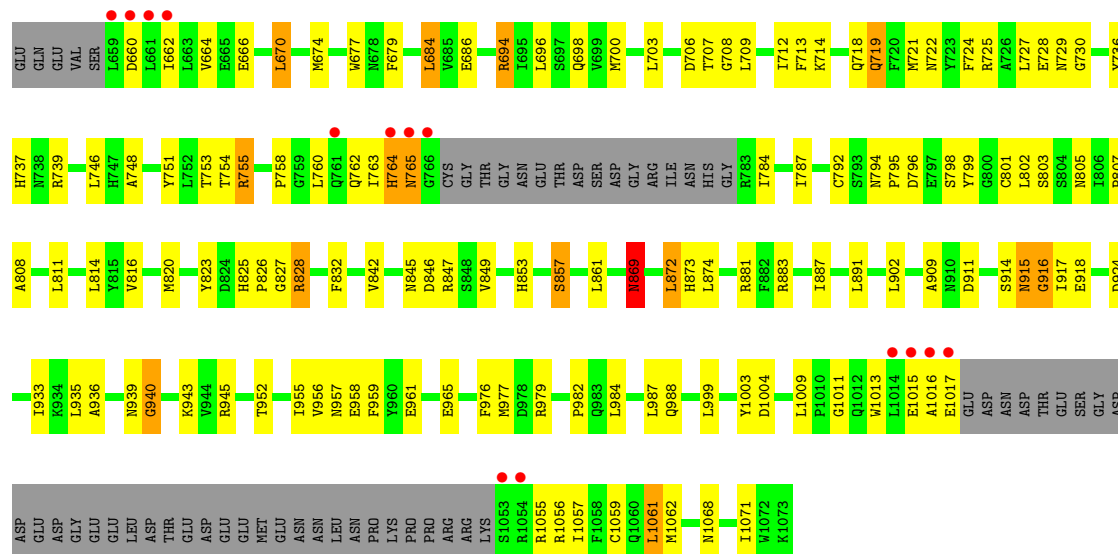
- Chain A:

- Chain B:
- 
- 7% 55% 30% 5% 9%
- GLU  
GLN  
V657  
V658  
L659  
D660  
L661  
L662  
L663  
V664  
V665  
E666  
Y667  
D668  
S669  
L670  
K673  
M674  
S675  
N676  
F679  
P680  
L681  
L684  
V685  
M688  
G689  
S692  
G693  
R694  
L695  
L696  
S697  
Q698  
V699  
M700  
L703  
F704  
Q705  
L710  
F713  
K714  
I715  
Y716  
Q719  
F720  
M721  
N722  
Y723  
F724  
R725  
E728  
N729  
G730  
Y731  
R732  
D733  
P734  
Y735  
Y736  
H737  
N738  
R739  
L746  
Y747  
A748  
Y749  
W750  
Y751  
I754  
R755  
P758  
Q761  
Q762  
I763  
H764  
N765  
Q766  
CYS  
GLY  
THR  
GLY  
ASN  
GLU  
THR  
ASP  
SER  
D776  
C792  
D796  
E797  
S798  
Y799  
L802  
S803  
S804  
N805  
E810  
L811  
N812  
V816  
M820  
Y823  
D824  
H825  
P826  
G827  
R828  
F832  
N845  
D846  
R847  
E851  
H852  
H853  
H854  
S857  
L861  
Y862  
N869  
L872  
H873  
R881  
F882  
R883  
F884  
L885  
Y886  
L887  
L891  
D900  
F905  
N910  
D911  
Y912  
N913  
S914  
N915  
R925  
Q930  
Y931  
C932  
Y933  
K934  
L935  
A936  
D937  
I938  
Y939  
G940  
P941  
R945  
D946  
L947  
Y952  
V956  
N957  
E958  
F959  
Q962  
G963  
D964  
E965  
E966  
L969  
I973  
S974  
P975  
F976  
N977  
R979  
S980  
S981  
P982  
Q983  
L984  
A985  
K986  
L987  
Q988  
F991  
V996  
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E1015  
A1016  
E1017  
F1018  
S1019

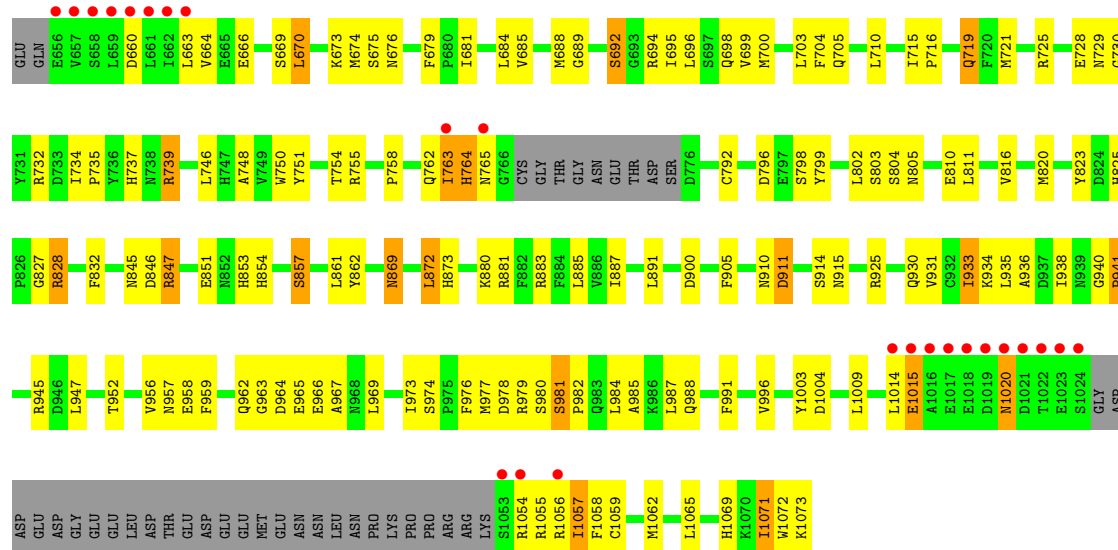




- Molecule 1: cGMP-inhibited 3',5'-cyclic phosphodiesterase B

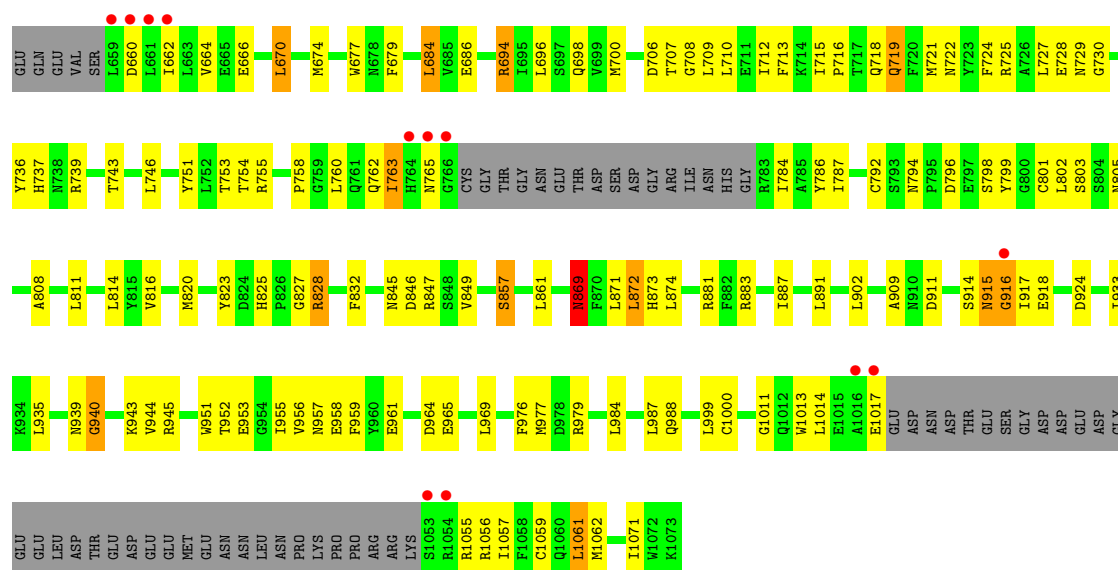


- Molecule 1: cGMP-inhibited 3',5'-cyclic phosphodiesterase B



- Molecule 1: cGMP-inhibited 3',5'-cyclic phosphodiesterase B





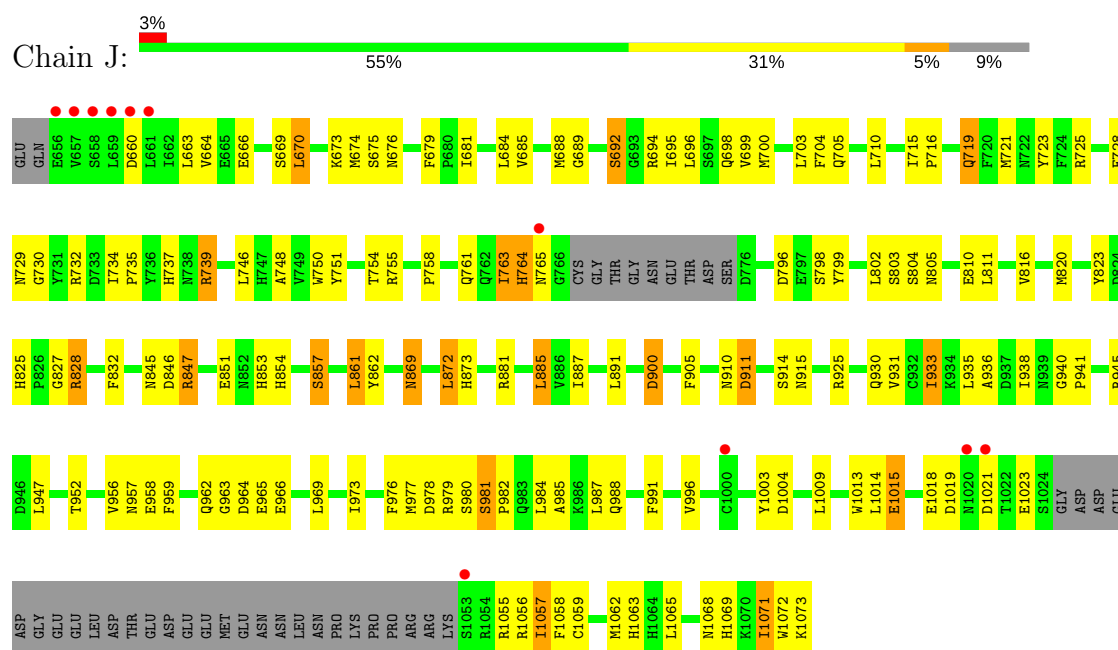
• Molecule 1: cGMP-inhibited 3',5'-cyclic phosphodiesterase B



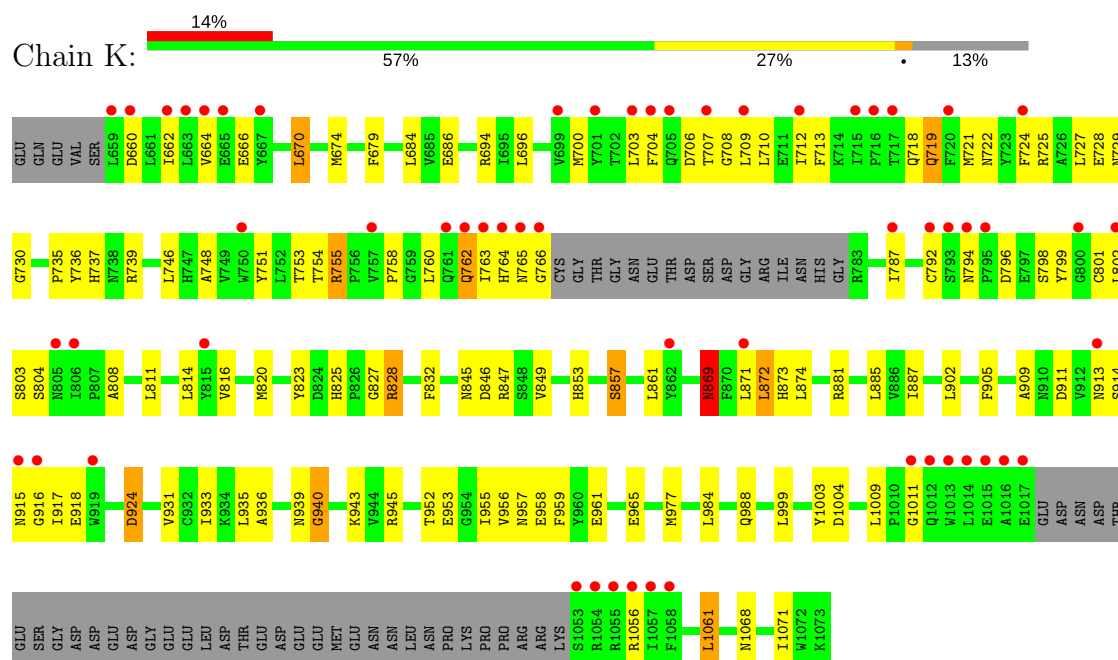
• Molecule 1: cGMP-inhibited 3',5'-cyclic phosphodiesterase B



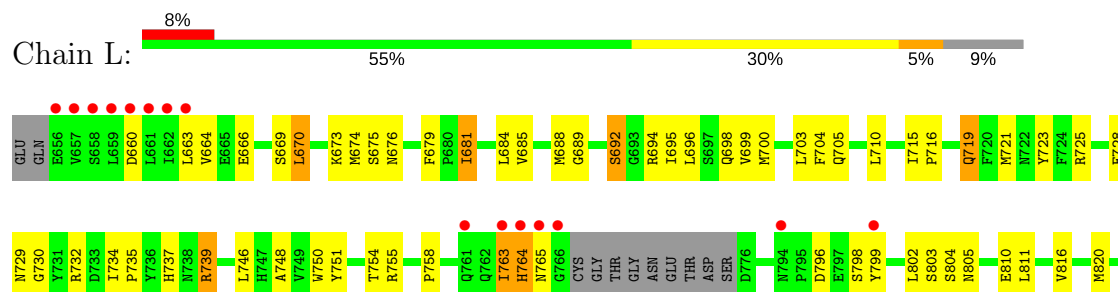


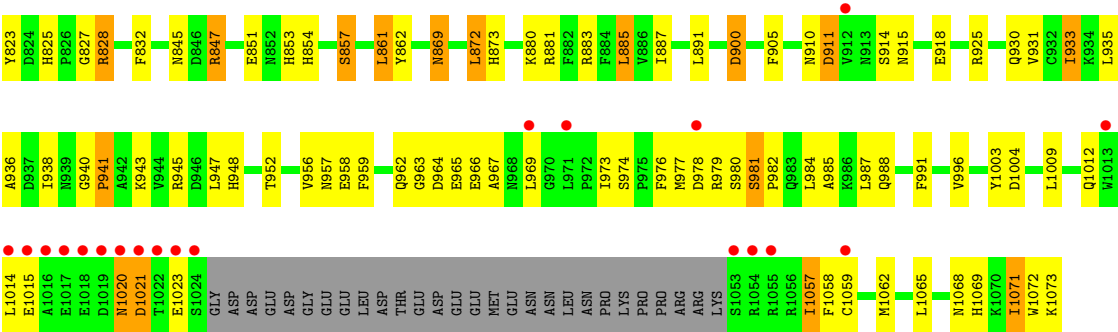


• Molecule 1: cGMP-inhibited 3',5'-cyclic phosphodiesterase B



• Molecule 1: cGMP-inhibited 3',5'-cyclic phosphodiesterase B





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	275.05Å 147.08Å 253.49Å 90.00° 109.84° 90.00°	Depositor
Resolution (Å)	30.00 – 2.90 49.61 – 2.90	Depositor EDS
% Data completeness (in resolution range)	97.7 (30.00-2.90) 96.6 (49.61-2.90)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.14 (at 2.91Å)	Xtriage
Refinement program	CNX	Depositor
R, $R_{free}$	0.231 , 0.249 0.228 , 0.242	Depositor DCC
$R_{free}$ test set	10128 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	49.3	Xtriage
Anisotropy	0.691	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 59.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	36048	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.30% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: MG, IBM

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	0.45	0/2982	0.59	0/4053
1	B	0.44	0/3092	0.59	0/4203
1	C	0.45	0/2982	0.59	0/4053
1	D	0.47	0/3092	0.60	0/4203
1	E	0.47	1/2982 (0.0%)	0.59	0/4053
1	F	0.46	0/3092	0.59	0/4203
1	G	0.45	0/2982	0.59	0/4053
1	H	0.45	0/3092	0.59	1/4203 (0.0%)
1	I	0.45	0/2982	0.58	0/4053
1	J	0.46	0/3092	0.59	0/4203
1	K	0.47	0/2982	0.59	0/4053
1	L	0.47	0/3092	0.60	0/4203
All	All	0.46	1/36444 (0.0%)	0.59	1/49536 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	1000	CYS	CB-SG	-5.15	1.73	1.81

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	795	PRO	N-CA-CB	5.03	109.34	103.30

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	2907	0	2772	110	0
1	B	3017	0	2834	132	0
1	C	2907	0	2772	124	0
1	D	3017	0	2834	134	0
1	E	2907	0	2772	114	0
1	F	3017	0	2834	119	0
1	G	2907	0	2772	109	0
1	H	3017	0	2834	126	0
1	I	2907	0	2772	108	0
1	J	3017	0	2834	143	0
1	K	2907	0	2772	108	0
1	L	3017	0	2834	125	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
2	G	2	0	0	0	0
2	H	2	0	0	0	0
2	I	2	0	0	0	0
2	J	2	0	0	0	0
2	K	2	0	0	0	0
2	L	2	0	0	0	0
3	A	16	0	14	0	0
3	B	16	0	14	0	0
3	C	16	0	14	0	0
3	D	16	0	14	0	0
3	E	16	0	14	0	0
3	F	16	0	14	0	0
3	G	16	0	14	0	0
3	H	16	0	14	0	0
3	I	16	0	14	0	0
3	J	16	0	14	0	0
3	K	16	0	14	0	0
3	L	16	0	14	0	0
4	A	24	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	24	0	0	3	0
4	C	24	0	0	1	0
4	D	24	0	0	1	0
4	E	23	0	0	2	0
4	F	25	0	0	1	0
4	G	23	0	0	1	0
4	H	25	0	0	0	0
4	I	24	0	0	1	0
4	J	24	0	0	0	0
4	K	24	0	0	1	0
4	L	24	0	0	1	0
All	All	36048	0	33804	1360	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 20.

The worst 5 of 1360 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:719:GLN:H	1:A:719:GLN:HE21	1.04	1.00
1:E:825:HIS:HD2	1:E:827:GLY:H	1.10	1.00
1:I:719:GLN:H	1:I:719:GLN:HE21	1.06	0.98
1:K:762:GLN:HE22	1:K:804:SER:HB2	1.28	0.98
1:K:719:GLN:H	1:K:719:GLN:HE21	1.06	0.98

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	358/420 (85%)	332 (93%)	21 (6%)	5 (1%)	12 39

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	375/420 (89%)	337 (90%)	28 (8%)	10 (3%)	5	22
1	C	358/420 (85%)	330 (92%)	22 (6%)	6 (2%)	10	34
1	D	375/420 (89%)	334 (89%)	31 (8%)	10 (3%)	5	22
1	E	358/420 (85%)	334 (93%)	18 (5%)	6 (2%)	10	34
1	F	375/420 (89%)	335 (89%)	31 (8%)	9 (2%)	6	25
1	G	358/420 (85%)	333 (93%)	22 (6%)	3 (1%)	21	54
1	H	375/420 (89%)	339 (90%)	28 (8%)	8 (2%)	8	29
1	I	358/420 (85%)	332 (93%)	20 (6%)	6 (2%)	10	34
1	J	375/420 (89%)	338 (90%)	28 (8%)	9 (2%)	6	25
1	K	358/420 (85%)	327 (91%)	25 (7%)	6 (2%)	10	34
1	L	375/420 (89%)	334 (89%)	30 (8%)	11 (3%)	5	20
All	All	4398/5040 (87%)	4005 (91%)	304 (7%)	89 (2%)	8	30

5 of 89 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	869	ASN
1	C	765	ASN
1	C	869	ASN
1	D	764	HIS
1	E	763	ILE

### 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	306/370 (83%)	288 (94%)	18 (6%)	21	53
1	B	313/370 (85%)	291 (93%)	22 (7%)	16	44
1	C	306/370 (83%)	290 (95%)	16 (5%)	25	59
1	D	313/370 (85%)	291 (93%)	22 (7%)	16	44
1	E	306/370 (83%)	291 (95%)	15 (5%)	27	61

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	313/370 (85%)	292 (93%)	21 (7%)	18	46
1	G	306/370 (83%)	287 (94%)	19 (6%)	20	51
1	H	313/370 (85%)	291 (93%)	22 (7%)	16	44
1	I	306/370 (83%)	288 (94%)	18 (6%)	21	53
1	J	313/370 (85%)	292 (93%)	21 (7%)	18	46
1	K	306/370 (83%)	288 (94%)	18 (6%)	21	53
1	L	313/370 (85%)	292 (93%)	21 (7%)	18	46
All	All	3714/4440 (84%)	3481 (94%)	233 (6%)	20	50

5 of 233 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	900	ASP
1	G	965	GLU
1	L	719	GLN
1	F	933	ILE
1	G	706	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 131 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	737	HIS
1	G	913	ASN
1	K	957	ASN
1	F	825	HIS
1	G	719	GLN

### 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 [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 36 ligands modelled in this entry, 24 are monoatomic - leaving 12 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	IBM	A	2111	-	13,17,17	1.75	3 (23%)	19,25,25	2.63	6 (31%)
3	IBM	B	2112	-	13,17,17	1.66	3 (23%)	19,25,25	2.67	6 (31%)
3	IBM	C	2113	-	13,17,17	1.53	3 (23%)	19,25,25	2.59	6 (31%)
3	IBM	D	2114	-	13,17,17	1.65	3 (23%)	19,25,25	2.69	7 (36%)
3	IBM	E	2115	-	13,17,17	1.52	2 (15%)	19,25,25	2.57	6 (31%)
3	IBM	F	2116	-	13,17,17	1.49	2 (15%)	19,25,25	2.67	7 (36%)
3	IBM	G	2117	-	13,17,17	1.48	3 (23%)	19,25,25	2.64	6 (31%)
3	IBM	H	2118	-	13,17,17	1.51	3 (23%)	19,25,25	2.58	6 (31%)
3	IBM	I	2119	-	13,17,17	1.43	3 (23%)	19,25,25	2.61	7 (36%)
3	IBM	J	2120	-	13,17,17	1.46	3 (23%)	19,25,25	2.60	6 (31%)
3	IBM	K	2121	-	13,17,17	1.66	3 (23%)	19,25,25	2.59	6 (31%)
3	IBM	L	2122	-	13,17,17	1.66	3 (23%)	19,25,25	2.65	7 (36%)

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	IBM	A	2111	-	-	0/4/4/4	0/2/2/2
3	IBM	B	2112	-	-	0/4/4/4	0/2/2/2
3	IBM	C	2113	-	-	0/4/4/4	0/2/2/2
3	IBM	D	2114	-	-	0/4/4/4	0/2/2/2
3	IBM	E	2115	-	-	0/4/4/4	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	IBM	F	2116	-	-	0/4/4/4	0/2/2/2
3	IBM	G	2117	-	-	0/4/4/4	0/2/2/2
3	IBM	H	2118	-	-	0/4/4/4	0/2/2/2
3	IBM	I	2119	-	-	0/4/4/4	0/2/2/2
3	IBM	J	2120	-	-	0/4/4/4	0/2/2/2
3	IBM	K	2121	-	-	0/4/4/4	0/2/2/2
3	IBM	L	2122	-	-	0/4/4/4	0/2/2/2

The worst 5 of 34 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	2113	IBM	C5-C4	-3.07	1.33	1.52
3	A	2111	IBM	C5-C4	-3.07	1.33	1.52
3	J	2120	IBM	C5-C4	-3.03	1.33	1.52
3	B	2112	IBM	C5-C4	-3.02	1.33	1.52
3	I	2119	IBM	C5-C4	-3.01	1.33	1.52

The worst 5 of 76 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	2116	IBM	O6-C6-C5	-2.64	115.66	121.37
3	B	2112	IBM	O6-C6-C5	-2.62	115.69	121.37
3	A	2111	IBM	O6-C6-C5	-2.53	115.88	121.37
3	D	2114	IBM	O6-C6-C5	-2.44	116.08	121.37
3	K	2121	IBM	O6-C6-C5	-2.41	116.16	121.37

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 [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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	364/420 (86%)	-0.00	9 (2%) 57 54	24, 42, 80, 100	0
1	B	381/420 (90%)	0.33	29 (7%) 14 10	25, 50, 92, 100	0
1	C	364/420 (86%)	0.09	14 (3%) 40 35	26, 43, 81, 100	0
1	D	381/420 (90%)	0.34	24 (6%) 20 15	22, 47, 89, 100	0
1	E	364/420 (86%)	0.07	12 (3%) 46 40	23, 42, 81, 100	0
1	F	381/420 (90%)	0.15	14 (3%) 41 36	21, 45, 79, 100	0
1	G	364/420 (86%)	-0.02	14 (3%) 40 35	24, 44, 83, 100	0
1	H	381/420 (90%)	0.28	23 (6%) 22 17	29, 52, 92, 100	0
1	I	364/420 (86%)	0.07	14 (3%) 40 35	23, 42, 81, 100	0
1	J	381/420 (90%)	0.11	11 (2%) 51 46	22, 46, 77, 100	0
1	K	364/420 (86%)	0.64	57 (15%) 2 1	28, 51, 87, 100	0
1	L	381/420 (90%)	0.55	35 (9%) 9 6	29, 54, 91, 100	0
All	All	4470/5040 (88%)	0.22	256 (5%) 24 19	21, 46, 85, 100	0

The worst 5 of 256 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	659	LEU	11.8
1	H	1022	THR	11.4
1	B	1024	SER	11.3
1	D	1021	ASP	10.7
1	H	1020	ASN	10.4

### 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 ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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<sup>th</sup> 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
2	MG	B	2126	1/1	0.93	0.11	56,56,56,56	0
3	IBM	H	2118	16/16	0.93	0.25	72,78,79,80	0
3	IBM	L	2122	16/16	0.94	0.22	68,77,78,79	0
2	MG	I	2140	1/1	0.95	0.12	27,27,27,27	0
3	IBM	B	2112	16/16	0.95	0.24	54,56,59,59	0
3	IBM	D	2114	16/16	0.96	0.20	35,53,56,57	0
3	IBM	G	2117	16/16	0.96	0.21	44,49,50,51	0
2	MG	L	2146	1/1	0.97	0.07	30,30,30,30	0
3	IBM	A	2111	16/16	0.97	0.18	36,38,42,42	0
2	MG	H	2138	1/1	0.97	0.06	32,32,32,32	0
2	MG	H	2137	1/1	0.97	0.13	12,12,12,12	0
3	IBM	E	2115	16/16	0.97	0.19	28,32,35,37	0
3	IBM	K	2121	16/16	0.97	0.19	54,59,60,61	0
2	MG	B	2125	1/1	0.98	0.10	4,4,4,4	0
3	IBM	C	2113	16/16	0.98	0.19	36,42,48,48	0
2	MG	L	2145	1/1	0.98	0.12	23,23,23,23	0
3	IBM	J	2120	16/16	0.98	0.23	31,35,40,41	0
2	MG	F	2134	1/1	0.98	0.07	19,19,19,19	0
3	IBM	I	2119	16/16	0.98	0.19	35,38,39,39	0
3	IBM	F	2116	16/16	0.98	0.17	28,37,40,40	0
2	MG	K	2143	1/1	0.98	0.12	20,20,20,20	0
2	MG	J	2142	1/1	0.99	0.11	39,39,39,39	0
2	MG	A	2124	1/1	0.99	0.11	41,41,41,41	0
2	MG	K	2144	1/1	0.99	0.12	40,40,40,40	0
2	MG	I	2139	1/1	0.99	0.15	5,5,5,5	0
2	MG	C	2128	1/1	0.99	0.10	29,29,29,29	0
2	MG	E	2132	1/1	0.99	0.14	29,29,29,29	0
2	MG	A	2123	1/1	0.99	0.13	2,2,2,2	0
2	MG	E	2131	1/1	0.99	0.15	1,1,1,1	0
2	MG	D	2129	1/1	0.99	0.16	9,9,9,9	0
2	MG	J	2141	1/1	0.99	0.14	6,6,6,6	0
2	MG	F	2133	1/1	0.99	0.16	1,1,1,1	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	MG	G	2136	1/1	0.99	0.10	28,28,28,28	0
2	MG	G	2135	1/1	0.99	0.12	1,1,1,1	0
2	MG	D	2130	1/1	0.99	0.11	22,22,22,22	0
2	MG	C	2127	1/1	1.00	0.14	5,5,5,5	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.