

# Full wwPDB X-ray Structure Validation Report (i)

#### Apr 21, 2024 – 04:10 pm BST

PDB ID : 4D09

Title: PDE2a catalytic domain in complex with a brain penetrant inhibitor

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Υ.

Deposited on : 2014-04-24

Resolution : 2.50 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 (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 (i)) were used in the production of this report:

MolProbity: 4.02b-467

Mogul : 1.8.4, CSD as 541be (2020)

Xtriage (Phenix) : 1.13

EDS : 2.36.2

buster-report : 1.1.7 (2018)

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)

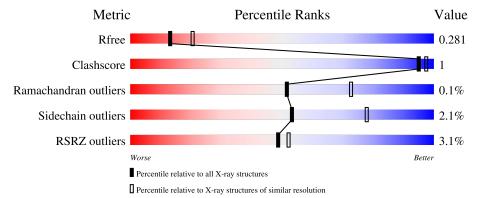
Validation Pipeline (wwPDB-VP) : 2.36.2

## 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 2.50 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	$(\# \mathrm{Entries})$	$(\#  ext{Entries},  ext{ resolution range}( ext{Å}))$
$R_{free}$	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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 <=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	353	92%	
1	В	353	90%	6% •
1	С	353	90%	• 7%
1	D	353	90%	• 8%



# 2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 11118 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-DEPENDENT 3', 5'-CYCLIC PHOSPHODIESTERASE.

Mol	Chain	Residues	${f Atoms}$			ZeroOcc	AltConf	Trace		
1	Λ	340	Total	С	N	О	S	0	0	0
1	A	340	2728	1739	463	503	23	U	0	
1	В	338	Total	С	N	О	S	0	0	0
1	Ъ	330	2721	1736	459	501	25	U	0	
1	С	329	Total	С	N	О	S	0	0	0
1		329	2643	1686	447	486	24	U	0	
1	D	326	Total	С	N	О	S	0	0	0
1	D	320	2633	1679	448	481	25	U	U	U

There are 36 discrepancies between the modelled and reference sequences:

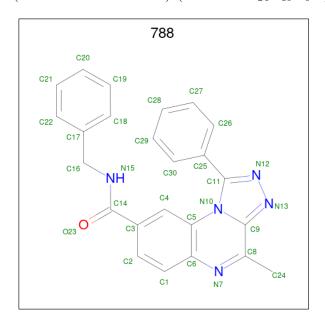
Chain	Residue	Modelled	Actual	Comment	Reference
A	576	MET	-	expression tag	UNP O00408
A	577	GLY	-	expression tag	UNP O00408
A	922	ARG	-	expression tag	UNP O00408
A	923	HIS	-	expression tag	UNP O00408
A	924	HIS	-	expression tag	UNP O00408
A	925	HIS	-	expression tag	UNP O00408
A	926	HIS	-	expression tag	UNP O00408
A	927	HIS	-	expression tag	UNP O00408
A	928	HIS	-	expression tag	UNP O00408
В	576	MET	-	expression tag	UNP O00408
В	577	GLY	-	expression tag	UNP O00408
В	922	ARG	-	expression tag	UNP O00408
В	923	HIS	-	expression tag	UNP O00408
В	924	HIS	-	expression tag	UNP O00408
В	925	HIS	-	expression tag	UNP O00408
В	926	HIS	-	expression tag	UNP O00408
В	927	HIS	-	expression tag	UNP O00408
В	928	HIS	-	expression tag	UNP O00408
С	576	MET	-	expression tag	UNP O00408
С	577	GLY	-	expression tag	UNP O00408
С	922	ARG	_	expression tag	UNP O00408



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Chain	Residue	Modelled	Actual	Comment	Reference
С	923	HIS	-	expression tag	UNP O00408
С	924	HIS	-	expression tag	UNP O00408
С	925	HIS	-	expression tag	UNP O00408
С	926	HIS	-	expression tag	UNP O00408
С	927	HIS	-	expression tag	UNP O00408
С	928	HIS	-	expression tag	UNP O00408
D	576	MET	-	expression tag	UNP O00408
D	577	GLY	-	expression tag	UNP O00408
D	922	ARG	-	expression tag	UNP O00408
D	923	HIS	-	expression tag	UNP O00408
D	924	HIS	-	expression tag	UNP O00408
D	925	HIS	-	expression tag	UNP O00408
D	926	HIS	-	expression tag	UNP O00408
D	927	HIS	-	expression tag	UNP O00408
D	928	HIS	-	expression tag	UNP O00408

 $\bullet$  Molecule 2 is N-benzyl-4-methyl-1-phenyl [1,2,4]triazolo<br/>[4,3-a]quinoxaline-8-carboxamide (three-letter code: 788) (formula:<br/>  $C_{24}H_{19}N_5O).$ 



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total (			0	0
2	В	1	Total (30 2	C N	О	0	0
2	С	1	Total (	0 N 4 5	O 1	0	0



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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	D	1	Total	С	N	О	0	0
2	D	1	30	24	5	1	U	0

• Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Zn 1 1	0	0
3	В	1	Total Zn 1 1	0	0
3	С	1	Total Zn 1 1	0	0
3	D	1	Total Zn 1 1	0	0

• Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Mg 1 1	0	0
4	В	1	Total Mg 1 1	0	0
4	С	1	Total Mg 1 1	0	0
4	D	1	Total Mg 1 1	0	0

• Molecule 5 is water.

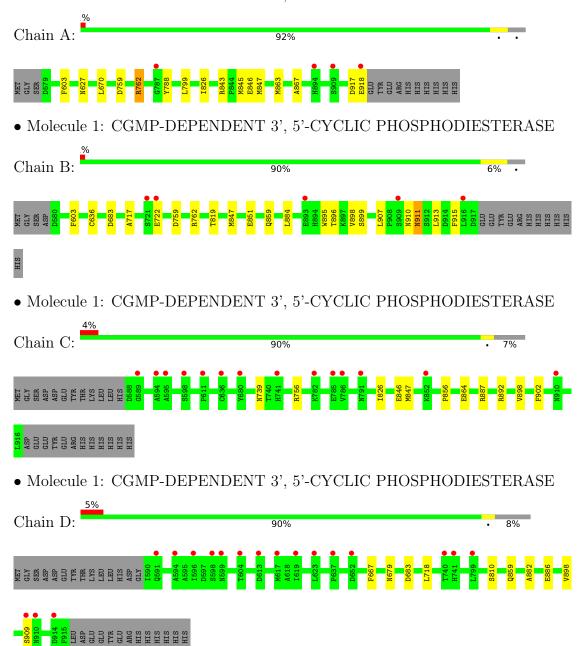
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	88	Total O 88 88	0	0
5	В	84	Total O 84 84	0	0
5	С	32	Total O 32 32	0	0
5	D	61	Total O 61 61	0	0



## 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 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: CGMP-DEPENDENT 3', 5'-CYCLIC PHOSPHODIESTERASE





# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants	56.14Å 73.43Å 91.62Å	Donogitor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$109.37^{\circ}$ $91.82^{\circ}$ $91.05^{\circ}$	Depositor
Resolution (Å)	19.77 - 2.50	Depositor
rtesolution (A)	19.77 - 2.50	EDS
% Data completeness	93.7 (19.77-2.50)	Depositor
(in resolution range)	93.9 (19.77-2.50)	EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	2.01 (at 2.50Å)	Xtriage
Refinement program	REFMAC 5.8.0071	Depositor
Ρ. Р.	0.206 , 0.277	Depositor
$R, R_{free}$	0.211 , $0.281$	DCC
$R_{free}$ test set	2266 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	29.2	Xtriage
Anisotropy	0.149	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.36 , 40.0	EDS
L-test for twinning <sup>2</sup>	$< L >=0.47, < L^2>=0.30$	Xtriage
Estimated twinning fraction	0.034 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	11118	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 7.20% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>Theoretical values of <|L|>,  $<L^2>$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

# 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: ZN, 788, MG

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	
MIOI		RMSZ	# Z  > 5	RMSZ	# Z  > 5
1	A	0.34	0/2795	0.52	0/3785
1	В	0.35	0/2788	0.53	0/3773
1	С	0.34	0/2708	0.49	0/3665
1	D	0.33	0/2698	0.52	0/3649
All	All	0.34	0/10989	0.52	0/14872

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	2728	0	2602	8	0
1	В	2721	0	2610	10	0
1	С	2643	0	2535	3	0
1	D	2633	0	2540	3	0
2	A	30	0	19	3	0
2	В	30	0	19	2	0
2	С	30	0	19	1	0
2	D	30	0	19	0	0
3	A	1	0	0	0	0



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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	В	1	0	0	0	0
3	С	1	0	0	0	0
3	D	1	0	0	0	0
4	A	1	0	0	0	0
4	В	1	0	0	0	0
4	С	1	0	0	0	0
4	D	1	0	0	0	0
5	A	88	0	0	0	0
5	В	84	0	0	0	0
5	С	32	0	0	0	0
5	D	61	0	0	1	0
All	All	11118	0	10363	25	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 1.

All (25) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

A 4 a see 1	A4 a 2	Interatomic	Clash	
Atom-1	Atom-2	${\rm distance}(\mathring{\rm A})$	overlap (Å)	
1:A:847:MET:HE1	2:A:1:788:H2	1.84	0.59	
1:A:762:ARG:HG3	1:B:717:ALA:HB1	1.89	0.54	
1:B:895:TRP:O	1:B:899:SER:N	2.41	0.53	
1:C:864:GLU:HG3	1:C:892:ARG:HD2	1.93	0.51	
1:B:847:MET:HE1	2:B:1:788:H2	1.93	0.51	
2:A:1:788:C30	2:A:1:788:H4	2.42	0.50	
1:B:910:ASN:O	1:B:911:ASN:HB2	2.12	0.49	
1:B:907:LEU:HD23	1:B:913:LEU:HD21	1.95	0.48	
1:C:864:GLU:CG	1:C:892:ARG:HD2	2.44	0.47	
1:D:882:ALA:O	1:D:886:GLU:HG2	2.15	0.47	
1:D:859:GLN:NE2	5:D:2049:HOH:O	2.40	0.46	
1:A:845:MET:O	1:A:846:GLU:C	2.54	0.45	
1:B:603:PHE:CD1	1:B:884:LEU:HD21	2.51	0.45	
1:A:847:MET:CE	2:A:1:788:H2	2.46	0.44	
1:A:603:PHE:HA	1:A:670:LEU:HD13	1.99	0.43	
1:B:895:TRP:HA	1:B:898:VAL:HG12	2.01	0.43	
1:B:907:LEU:CD2	1:B:913:LEU:HD21	2.48	0.43	
1:C:856:PRO:HG3	1:C:902:PHE:CD1	2.55	0.42	
2:C:1:788:H4	2:C:1:788:C30	2.49	0.42	
1:A:788:TYR:CE1	1:A:799:LEU:HD22	2.55	0.41	
1:A:863:MET:HA	1:A:867:ALA:HB3	2.02	0.41	
1:B:759:ASP:OD1	1:B:762:ARG:NH2	2.53	0.41	



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Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	$\begin{array}{c} \text{Clash} \\ \text{overlap } (\text{\AA}) \end{array}$
1:B:859:GLN:OE1	2:B:1:788:H241	2.20	0.41
1:D:667:PHE:CD1	1:D:810:SER:HB2	2.56	0.40
1:A:917:ASP:O	1:A:918:GLU:CG	2.70	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	Perce	$\mathbf{ntiles}$
1	A	338/353~(96%)	328 (97%)	10 (3%)	0	100	100
1	В	336/353~(95%)	320 (95%)	15 (4%)	1 (0%)	41	61
1	C	327/353~(93%)	317 (97%)	10 (3%)	0	100	100
1	D	324/353~(92%)	313 (97%)	11 (3%)	0	100	100
All	All	$1325/1412 \ (94\%)$	1278 (96%)	46 (4%)	1 (0%)	51	73

#### All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	В	915	PHE

#### 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	292/319~(92%)	287 (98%)	5 (2%)	60 82		
1	В	294/319 (92%)	287 (98%)	7 (2%)	49 74		
1	С	285/319 (89%)	278 (98%)	7 (2%)	47 73		
1	D	286/319 (90%)	281 (98%)	5 (2%)	60 82		
All	All	1157/1276 (91%)	1133 (98%)	24 (2%)	53 78		

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	627	ASN
1	A	759	ASP
1	A	762	ARG
1	A	826	ILE
1	A	843	ARG
1	В	636	CYS
1	В	683	ASP
1	В	722	GLU
1	В	819	THR
1	В	851	GLU
1	В	896	THR
1	В	911	ASN
1	C C C C C	739	ASN
1	С	756	ARG
1	С	826	ILE
1	С	846	GLU
1	С	847	MET
1	С	887	ARG
1		898	VAL
1	D	679	ASN
1	D	683	ASP
1	D	718	LEU
1	D	898	VAL
1	D	909	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	$\operatorname{Res}$	$\mathbf{Type}$
1	A	591	GLN
1	A	624	GLN
1	В	587	HIS



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Mol	Chain	Res	Type
1	В	708	GLN
1	В	910	ASN
1	В	911	ASN
1	D	859	GLN

#### 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 12 ligands modelled in this entry, 8 are monoatomic - leaving 4 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	Mol   Type   Chain		Chain Res L		Bond lengths			Bond angles		
MIOI					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	788	В	1	-	30,34,34	0.83	1 (3%)	37,48,48	0.72	2 (5%)
2	788	A	1	-	30,34,34	0.91	2 (6%)	37,48,48	0.67	1 (2%)
2	788	D	1	-	30,34,34	0.85	1 (3%)	37,48,48	0.70	2 (5%)
2	788	С	1	-	30,34,34	0.85	2 (6%)	37,48,48	0.70	2 (5%)

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
2	788	В	1	-	-	2/13/13/13	0/5/5/5
2	788	A	1	-	-	2/13/13/13	0/5/5/5
2	788	D	1	-	-	2/13/13/13	0/5/5/5
2	788	С	1	-	-	2/13/13/13	0/5/5/5

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$\operatorname{Observed}(\text{\AA})$	Ideal(A)
2	A	1	788	C8-N7	-3.10	1.29	1.32
2	D	1	788	C8-N7	-3.03	1.29	1.32
2	В	1	788	C8-N7	-2.72	1.29	1.32
2	С	1	788	C8-N7	-2.69	1.29	1.32
2	С	1	788	C11-N12	-2.09	1.31	1.33
2	A	1	788	C11-N12	-2.04	1.31	1.33

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$\mathbf{Observed}(^o)$	$Ideal(^{o})$
2	В	1	788	C24-C8-N7	2.75	119.81	116.00
2	С	1	788	C24-C8-N7	2.58	119.58	116.00
2	В	1	788	C24-C8-C9	-2.57	117.44	121.74
2	A	1	788	C24-C8-N7	2.56	119.55	116.00
2	D	1	788	C24-C8-N7	2.56	119.54	116.00
2	С	1	788	C24-C8-C9	-2.21	118.05	121.74
2	D	1	788	C24-C8-C9	-2.16	118.14	121.74

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1	788	N12-C11-C25-C30
2	В	1	788	N12-C11-C25-C30
2	В	1	788	N12-C11-C25-C26
2	С	1	788	N12-C11-C25-C30
2	D	1	788	N12-C11-C25-C30
2	С	1	788	N12-C11-C25-C26
2	D	1	788	N12-C11-C25-C26
2	A	1	788	N12-C11-C25-C26

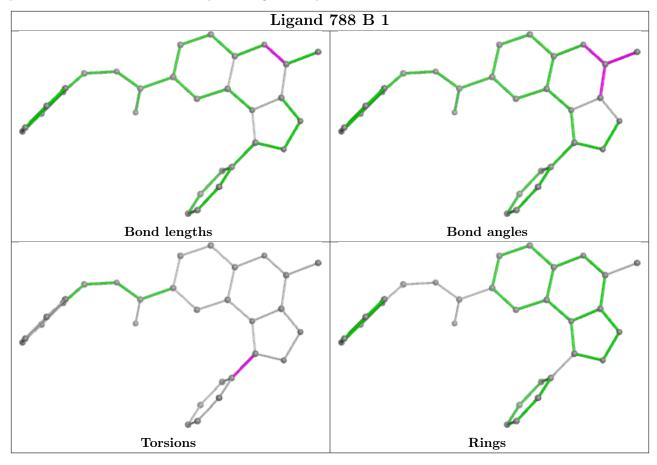
There are no ring outliers.

3 monomers are involved in 6 short contacts:

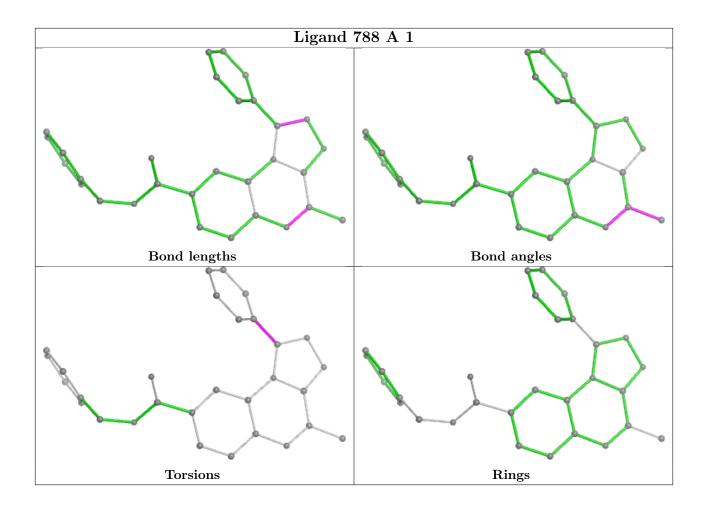


Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	В	1	788	2	0
2	A	1	788	3	0
2	С	1	788	1	0

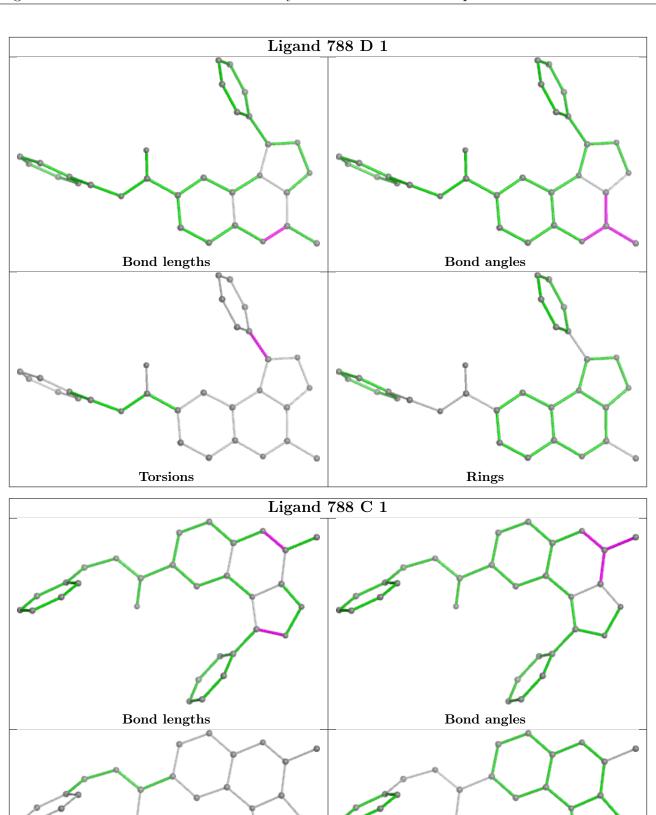
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.













Torsions

Rings

# 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,  $95^{th}$  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>	$\# \mathrm{RSRZ}{>}2$	$OWAB(A^2)$	Q<0.9
1	A	340/353 (96%)	-0.06	4 (1%) 79 80	15, 26, 40, 63	0
1	В	338/353 (95%)	0.00	5 (1%) 73 75	16, 28, 41, 58	0
1	С	329/353~(93%)	0.21	14 (4%) 35 38	20, 35, 54, 65	0
1	D	326/353~(92%)	0.12	18 (5%) 25 26	21, 32, 51, 78	0
All	All	1333/1412 (94%)	0.07	41 (3%) 49 52	15, 29, 50, 78	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	С	598	SER	3.5
1	D	591	GLN	3.2
1	D	637	PRO	3.1
1	С	595	ALA	3.1
1	A	918	GLU	3.0
1	С	594	ALA	3.0
1	D	598	SER	2.9
1	С	786	VAL	2.8
1	D	741	HIS	2.8
1	D	604	THR	2.8
1	D	909	SER	2.8
1	В	722	GLU	2.6
1	С	785	GLU	2.6
1	A	894	HIS	2.6
1	С	680	TYR	2.5
1	В	916	LEU	2.5
1	В	893	GLU	2.5
1	С	782	LYS	2.5
1	D	617	MET	2.5
1	С	589	GLY	2.5
1	A	909	SER	2.4



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Mol	Chain	Res	Type	RSRZ
1	В	721	SER	2.4
1	D	613	ASP	2.4
1	D	914	ASP	2.3
1	С	852	LYS	2.3
1	В	909	SER	2.3
1	A	787	GLY	2.2
1	D	623	LEU	2.2
1	D	619	ILE	2.2
1	С	741	HIS	2.2
1	С	611	PRO	2.2
1	С	910	ASN	2.2
1	D	910	ASN	2.1
1	D	652	ASP	2.1
1	D	594	ALA	2.1
1	D	740	THR	2.1
1	D	799	LEU	2.1
1	С	636	CYS	2.1
1	D	599	ASN	2.0
1	С	791	ASN	2.0
1	D	596	ILE	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 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,  $95^{th}$  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.

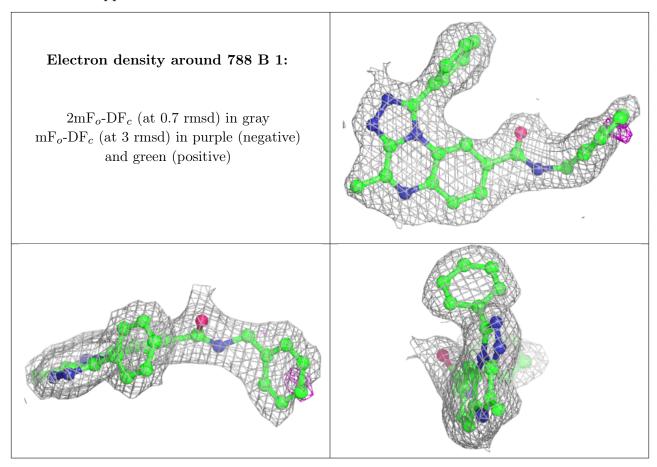
Mol	Type	Chain	Res	Atoms	RSCC	RSR	${f B-factors}({f \AA}^2)$	Q<0.9
2	788	В	1	30/30	0.89	0.16	24,26,35,36	0
2	788	A	1	30/30	0.91	0.16	21,22,29,29	0
4	MG	С	1002	1/1	0.93	0.09	28,28,28,28	0



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Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q<0.9
2	788	D	1	30/30	0.94	0.14	25,29,53,54	0
4	MG	D	1002	1/1	0.94	0.14	21,21,21,21	0
2	788	С	1	30/30	0.95	0.14	25,26,35,36	0
4	MG	В	1002	1/1	0.95	0.13	14,14,14,14	0
4	MG	A	1002	1/1	0.99	0.06	11,11,11,11	0
3	ZN	В	1001	1/1	0.99	0.04	24,24,24,24	0
3	ZN	С	1001	1/1	1.00	0.02	26,26,26,26	0
3	ZN	D	1001	1/1	1.00	0.03	27,27,27,27	0
3	ZN	A	1001	1/1	1.00	0.02	26,26,26,26	0

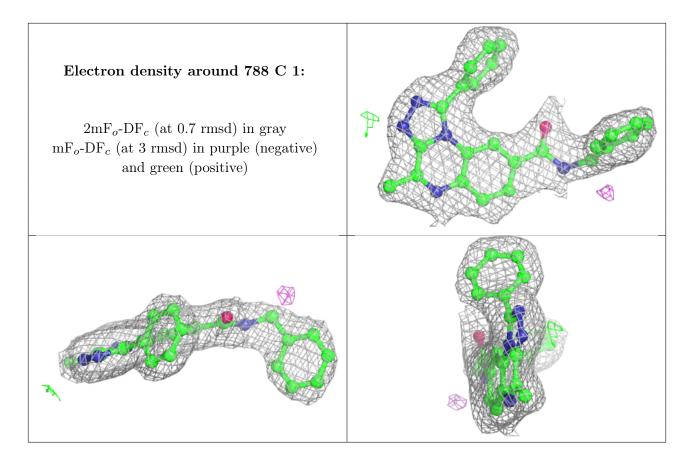
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.





# Electron density around 788 A 1: $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 0.7 rmsd) in gray ${ m mF}_o{ m -DF}_c$ (at 3 rmsd) in purple (negative) and green (positive) Electron density around 788 D 1: $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 0.7 rmsd) in gray $mF_o$ -DF<sub>c</sub> (at 3 rmsd) in purple (negative) and green (positive)





# 6.5 Other polymers (i)

There are no such residues in this entry.

