



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 14, 2026 – 08:32 PM UTC

PDB ID : 8ZTZ / pdb_00008ztz
Title : Structure of ATP-dependent diazotase CmaA6
Authors : Katsuyama, Y.; Kawai, S.; Ohnishi, Y.
Deposited on : 2024-06-07
Resolution : 2.93 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 ⓘ 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

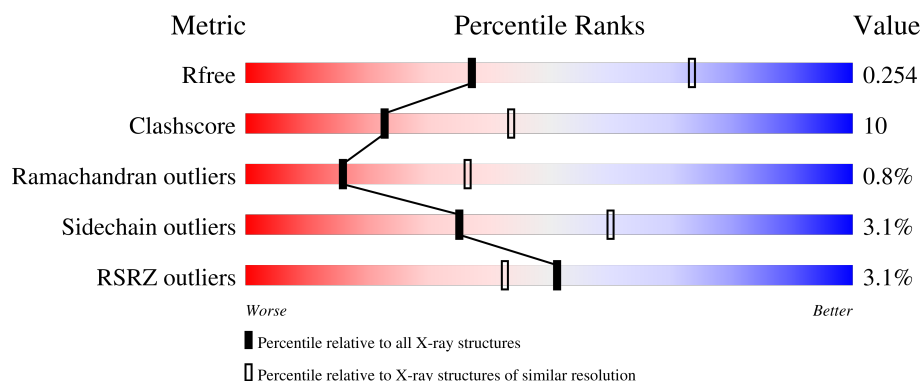
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.93 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}	180053	1159 (2.96-2.92)
Clashscore	190562	1184 (2.96-2.92)
Ramachandran outliers	187476	1131 (2.96-2.92)
Sidechain outliers	187428	1131 (2.96-2.92)
RSRZ outliers	180081	1159 (2.96-2.92)

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	569	% 73% 18% 8%
1	B	569	8% 64% 27% • 8%
1	C	569	% 71% 19% • 8%
1	D	569	% 73% 22% • •
1	E	569	• • 97%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 16715 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 Putative AMP-binding enzyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	524	Total	C	N	O	S	0	0	0
			4003	2518	707	765	13			
1	A	521	Total	C	N	O	S	0	0	0
			3982	2507	704	758	13			
1	C	521	Total	C	N	O	S	0	0	0
			3982	2507	704	758	13			
1	D	553	Total	C	N	O	S	0	0	0
			4225	2651	754	806	14			
1	E	16	Total	C	N	O	S	0	0	0
			135	79	32	23	1			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1	MET	-	initiating methionine	UNP W5W4E6
B	2	ASN	-	expression tag	UNP W5W4E6
B	3	HIS	-	expression tag	UNP W5W4E6
B	4	LYS	-	expression tag	UNP W5W4E6
B	5	VAL	-	expression tag	UNP W5W4E6
B	6	HIS	-	expression tag	UNP W5W4E6
B	7	HIS	-	expression tag	UNP W5W4E6
B	8	HIS	-	expression tag	UNP W5W4E6
B	9	HIS	-	expression tag	UNP W5W4E6
B	10	HIS	-	expression tag	UNP W5W4E6
B	11	HIS	-	expression tag	UNP W5W4E6
B	12	ILE	-	expression tag	UNP W5W4E6
B	13	GLU	-	expression tag	UNP W5W4E6
B	14	GLY	-	expression tag	UNP W5W4E6
B	15	ARG	-	expression tag	UNP W5W4E6
B	16	HIS	-	expression tag	UNP W5W4E6
A	1	MET	-	initiating methionine	UNP W5W4E6
A	2	ASN	-	expression tag	UNP W5W4E6
A	3	HIS	-	expression tag	UNP W5W4E6

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Chain	Residue	Modelled	Actual	Comment	Reference
A	4	LYS	-	expression tag	UNP W5W4E6
A	5	VAL	-	expression tag	UNP W5W4E6
A	6	HIS	-	expression tag	UNP W5W4E6
A	7	HIS	-	expression tag	UNP W5W4E6
A	8	HIS	-	expression tag	UNP W5W4E6
A	9	HIS	-	expression tag	UNP W5W4E6
A	10	HIS	-	expression tag	UNP W5W4E6
A	11	HIS	-	expression tag	UNP W5W4E6
A	12	ILE	-	expression tag	UNP W5W4E6
A	13	GLU	-	expression tag	UNP W5W4E6
A	14	GLY	-	expression tag	UNP W5W4E6
A	15	ARG	-	expression tag	UNP W5W4E6
A	16	HIS	-	expression tag	UNP W5W4E6
C	1	MET	-	initiating methionine	UNP W5W4E6
C	2	ASN	-	expression tag	UNP W5W4E6
C	3	HIS	-	expression tag	UNP W5W4E6
C	4	LYS	-	expression tag	UNP W5W4E6
C	5	VAL	-	expression tag	UNP W5W4E6
C	6	HIS	-	expression tag	UNP W5W4E6
C	7	HIS	-	expression tag	UNP W5W4E6
C	8	HIS	-	expression tag	UNP W5W4E6
C	9	HIS	-	expression tag	UNP W5W4E6
C	10	HIS	-	expression tag	UNP W5W4E6
C	11	HIS	-	expression tag	UNP W5W4E6
C	12	ILE	-	expression tag	UNP W5W4E6
C	13	GLU	-	expression tag	UNP W5W4E6
C	14	GLY	-	expression tag	UNP W5W4E6
C	15	ARG	-	expression tag	UNP W5W4E6
C	16	HIS	-	expression tag	UNP W5W4E6
D	1	MET	-	initiating methionine	UNP W5W4E6
D	2	ASN	-	expression tag	UNP W5W4E6
D	3	HIS	-	expression tag	UNP W5W4E6
D	4	LYS	-	expression tag	UNP W5W4E6
D	5	VAL	-	expression tag	UNP W5W4E6
D	6	HIS	-	expression tag	UNP W5W4E6
D	7	HIS	-	expression tag	UNP W5W4E6
D	8	HIS	-	expression tag	UNP W5W4E6
D	9	HIS	-	expression tag	UNP W5W4E6
D	10	HIS	-	expression tag	UNP W5W4E6
D	11	HIS	-	expression tag	UNP W5W4E6
D	12	ILE	-	expression tag	UNP W5W4E6
D	13	GLU	-	expression tag	UNP W5W4E6

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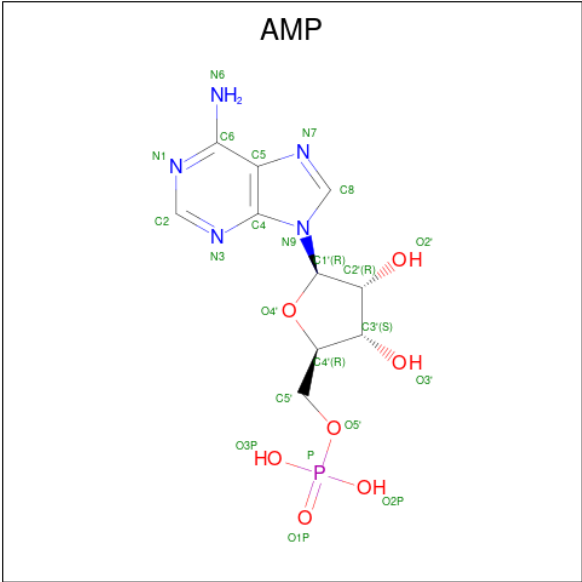
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Chain	Residue	Modelled	Actual	Comment	Reference
D	14	GLY	-	expression tag	UNP W5W4E6
D	15	ARG	-	expression tag	UNP W5W4E6
D	16	HIS	-	expression tag	UNP W5W4E6
E	1	MET	-	initiating methionine	UNP W5W4E6
E	2	ASN	-	expression tag	UNP W5W4E6
E	3	HIS	-	expression tag	UNP W5W4E6
E	4	LYS	-	expression tag	UNP W5W4E6
E	5	VAL	-	expression tag	UNP W5W4E6
E	6	HIS	-	expression tag	UNP W5W4E6
E	7	HIS	-	expression tag	UNP W5W4E6
E	8	HIS	-	expression tag	UNP W5W4E6
E	9	HIS	-	expression tag	UNP W5W4E6
E	10	HIS	-	expression tag	UNP W5W4E6
E	11	HIS	-	expression tag	UNP W5W4E6
E	12	ILE	-	expression tag	UNP W5W4E6
E	13	GLU	-	expression tag	UNP W5W4E6
E	14	GLY	-	expression tag	UNP W5W4E6
E	15	ARG	-	expression tag	UNP W5W4E6
E	16	HIS	-	expression tag	UNP W5W4E6

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Mg 2 2	2	0
2	D	2	Total Mg 2 2	2	0

- Molecule 3 is ADENOSINE MONOPHOSPHATE (CCD ID: AMP) (formula: C₁₀H₁₄N₅O₇P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	D	1	Total	C	N	O	P	23	0
			23	10	5	7	1		

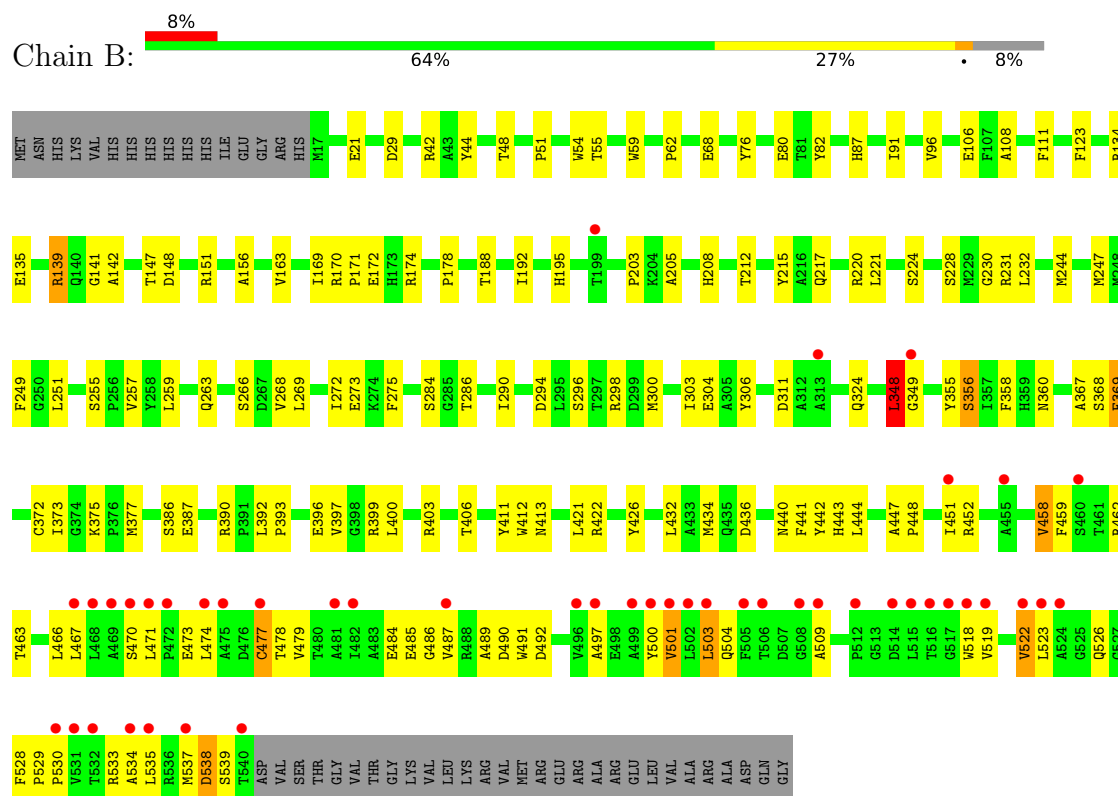
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	56	Total	O	0	0
			56	56		
4	A	134	Total	O	0	0
			134	134		
4	C	92	Total	O	0	0
			92	92		
4	D	78	Total	O	0	0
			78	78		
4	E	1	Total	O	0	0
			1	1		

3 Residue-property plots [i](#)

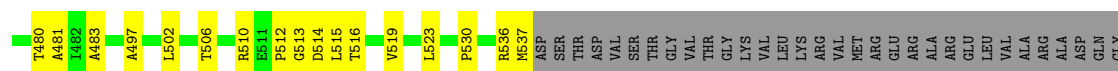
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Putative AMP-binding enzyme

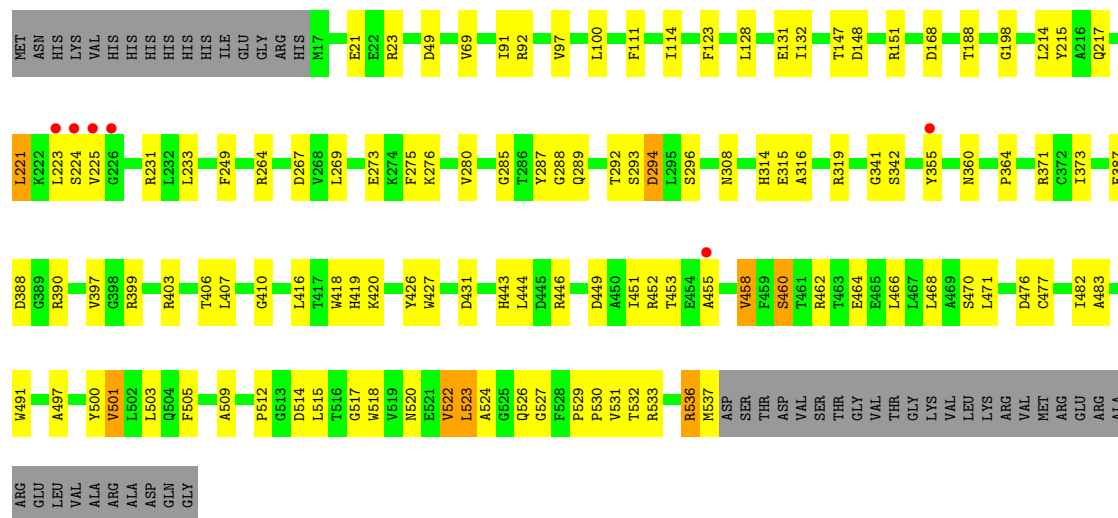


• Molecule 1: Putative AMP-binding enzyme

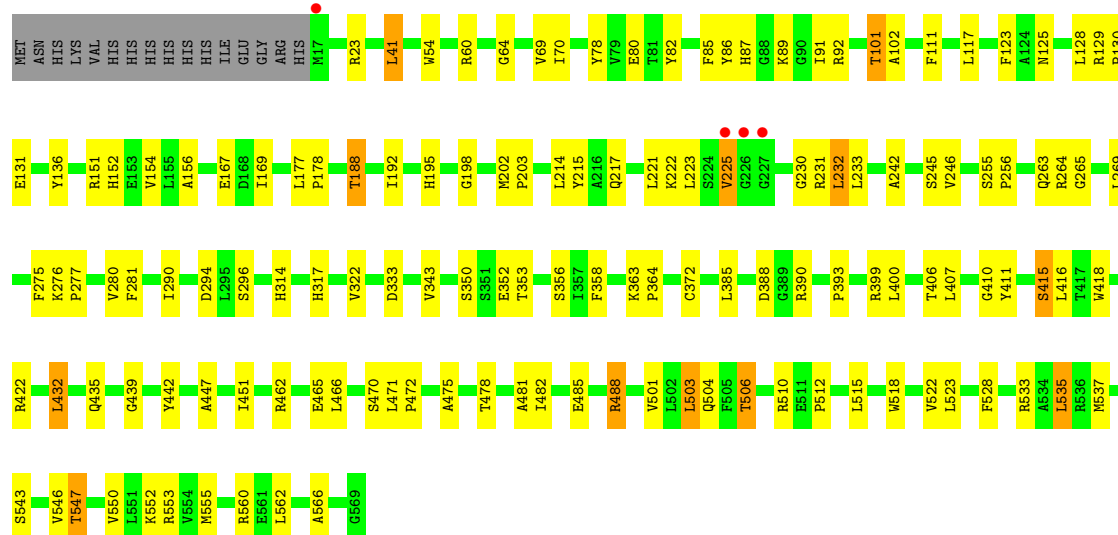
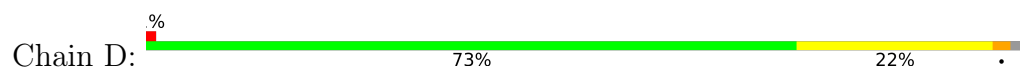




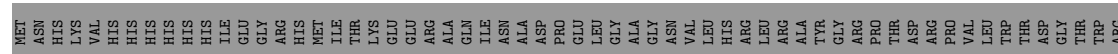
● Molecule 1: Putative AMP-binding enzyme



● Molecule 1: Putative AMP-binding enzyme



● Molecule 1: Putative AMP-binding enzyme



ASP	ASP	ALA	LEU	GLY	SER	ASN	TRP	PRO	ALA
VAL	ASP	ILE	ARG	ILE	ILE	ALA	PRO	PRO	ASP
SER	SER	ALA	LEU	LYS	SER	ALA	TYR	PHE	SER
GLY	GLY	GLU	GLY	GLY	ALA	SER	HIS	ALA	SER
VAL	VAL	GLY	TRP	SER	TYR	VAL	ASP	ALA	HIS
GLY	VAL	GLY	TRP	ALA	TYR	VAL	ASP	LEU	PRO
ARG	GLY	ARG	LEU	SER	ASN	MET	THR	GLU	GLY
ALA	VAL	ALA	THR	PHE	THR	PHE	ASP	ARG	VAL
ASP	VAL	ASP	GLY	GLY	GLY	GLY	PRO	PRO	ILE
TRP	ASP	TRP	ASP	ARG	ASP	LEU	ILE	GLU	THR
ASP	LYS	ASP	LEU	CYS	ALA	LEU	ILE	ILE	LEU
R553	R553	GLY	ALA	ILE	ALA	LEU	ILE	ALA	GLY
V554	V554	ASP	MET	GLY	HIS	ASP	SER	ARG	LEU
M555	M555	GLY	GLN	LYS	GLY	SER	HIS	GLU	GLY
R556	R556	VAL	ASP	PRO	ALA	PRO	SER	TYR	TYR
R557	R557	ALA	ALA	MET	HIS	VAL	SER	ILE	GLY
A558	A558	GLU	GLU	SER	ILE	TYR	GLY	ARG	TYR
L562	L562	ALA	GLY	PHE	ARG	GLN	THR	ARG	VAL
V563	V563	TYR	ASN	ALA	VAL	GLN	THR	ARG	GLN
A564	A564	VAL	PHE	GLN	LEU	SER	MET	GLY	TYR
R565	R565	LEU	TYR	ALA	VAL	SER	PRO	ALA	THR
R566	R566	LEU	HIS	ALA	ALA	GLN	LYS	SER	ALA
Q568	Q568	PHE	LEU	VAL	GLN	ARG	LYS	GLY	GLY
GLY	GLY	THR	ASP	ARG	SER	GLY	THR	ALA	PHE
		GLN	ASP	ALA	GLY	GLY	HIS	GLY	GLY
		ARG	LEU	ALA	ILE	ASP	THR	GLY	ILE
		GLN	ASP	VAL	GLY	GLY	THR	GLY	GLY
		THR	GLY	GLY	ILE	GLY	THR	GLY	GLY
		ASP	GLY	GLY	GLY	GLY	THR	GLY	GLY
		VAL	ARG	VAL	SER	GLY	LYS	PHE	ALA
		LEU	THR	ARG	VAL	PHE	LEU	VAL	SER
		ALA	GLU	SER	PHE	SER	VAL	SER	THR
		GLN	LEU	THR	THR	GLY	VAL	ALA	PHE
		GLY	LEU	THR	ASP	TYR	GLY	GLY	THR
		PHE	LEU	THR	LEU	GLY	SER	ASP	ALA
		PRO	ALA	PRO	GLY	GLN	MET	ILE	ILE
		THR	SER	GLY	SER	ILE	GLY	ARG	ALA
		VAL	LEU	TYR	SER	ALA	ARG	PRO	PHE
		THR	PRO	TRP	GLU	THR	LEU	GLU	MET
		ARG	GLU	ASN	THR	SER	VAL	HIS	ALA
		ALA	LEU	ASP	GLY	ASP	VAL	ARG	ILE
		LEU	ALA	SER	TYR	LEU	ALA	ASN	ASN
		ARG	ASP	LEU	SER	SER	LEU	GLN	SER
		MET	CYS	THR	ILE	THR	PRO	LEU	GLY
		ASP	THR	PHE	PHE	ARG	GLY	PRO	GLY
		SER	VAL	HIS	ASN	MET	HIS	GLN	TYR

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	93.04Å 164.02Å 171.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.75 – 2.93 48.75 – 2.93	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.75-2.93) 100.0 (48.75-2.93)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.03 (at 2.91Å)	Xtriage
Refinement program	PHENIX 1.21.1_5286	Depositor
R, R_{free}	0.186 , 0.255 0.186 , 0.254	Depositor DCC
R_{free} test set	1935 reflections (3.38%)	wwPDB-VP
Wilson B-factor (Å ²)	51.5	Xtriage
Anisotropy	0.295	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 48.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	16715	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.50% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: AMP, 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	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.38	0/4082	0.56	2/5555 (0.0%)
1	B	0.35	0/4103	0.56	0/5584
1	C	0.39	0/4082	0.54	0/5555
1	D	0.36	0/4325	0.57	0/5880
1	E	0.46	0/134	0.56	0/176
All	All	0.37	0/16726	0.56	2/22750 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	52	VAL	CA-C-N	-5.56	113.72	122.73
1	A	52	VAL	C-N-CA	-5.56	113.72	122.73

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	369	PHE	Peptide

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	3982	0	3866	67	1
1	B	4003	0	3882	107	0
1	C	3982	0	3866	77	1
1	D	4225	0	4120	90	0
1	E	135	0	141	4	0
2	A	2	0	0	0	0
2	D	2	0	0	0	0
3	D	23	0	12	0	0
4	A	134	0	0	5	0
4	B	56	0	0	1	0
4	C	92	0	0	2	0
4	D	78	0	0	2	0
4	E	1	0	0	0	0
All	All	16715	0	15887	335	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 10.

The worst 5 of 335 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:D:471:LEU:HD21	1:D:522:VAL:HG21	1.45	0.99
1:B:434:MET:HE1	1:A:334:PHE:HB3	1.59	0.84
1:B:231:ARG:NH1	1:B:275:PHE:O	2.14	0.80
1:B:501:VAL:HG11	1:B:519:VAL:HG11	1.65	0.78
1:B:387:GLU:OE1	1:B:399:ARG:NH2	2.18	0.77

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:170:ARG:NH2	1:C:168:ASP:OD1[4_545]	2.02	0.18

5.3 Torsion angles

5.3.1 Protein backbone

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	519/569 (91%)	494 (95%)	20 (4%)	5 (1%)	12	31
1	B	522/569 (92%)	464 (89%)	52 (10%)	6 (1%)	11	29
1	C	519/569 (91%)	487 (94%)	29 (6%)	3 (1%)	21	45
1	D	551/569 (97%)	515 (94%)	33 (6%)	3 (0%)	24	49
1	E	14/569 (2%)	14 (100%)	0	0	100	100
All	All	2125/2845 (75%)	1974 (93%)	134 (6%)	17 (1%)	16	36

5 of 17 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	348	LEU
1	B	538	ASP
1	A	229	MET
1	A	513	GLY
1	C	294	ASP

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	414/455 (91%)	409 (99%)	5 (1%)	63	78
1	B	417/455 (92%)	404 (97%)	13 (3%)	35	60
1	C	414/455 (91%)	400 (97%)	14 (3%)	32	58
1	D	440/455 (97%)	422 (96%)	18 (4%)	27	52

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	13/455 (3%)	11 (85%)	2 (15%)	2	8
All	All	1698/2275 (75%)	1646 (97%)	52 (3%)	35	60

5 of 52 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	522	VAL
1	D	221	LEU
1	D	550	VAL
1	C	523	LEU
1	D	41	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	308	ASN
1	D	435	GLN
1	C	308	ASN
1	C	314	HIS
1	C	359	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 4 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$
3	AMP	D	601	2	25,25,25	1.36	4 (16%)	37,38,38	1.80	11 (29%)

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	AMP	D	601	2	-	4/10/26/26	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	601	AMP	C5-C4	4.39	1.46	1.39
3	D	601	AMP	C5-C6	2.59	1.48	1.41
3	D	601	AMP	C4-N9	-2.27	1.33	1.37
3	D	601	AMP	C5-N7	-2.15	1.35	1.39

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	601	AMP	C5-C4-N3	-4.30	120.80	126.72
3	D	601	AMP	N3-C4-N9	3.70	133.46	127.17
3	D	601	AMP	C4-C5-N7	-3.35	106.75	110.58
3	D	601	AMP	C4-N9-C8	3.32	109.23	105.74
3	D	601	AMP	C2-N3-C4	2.98	119.12	111.83

There are no chirality outliers.

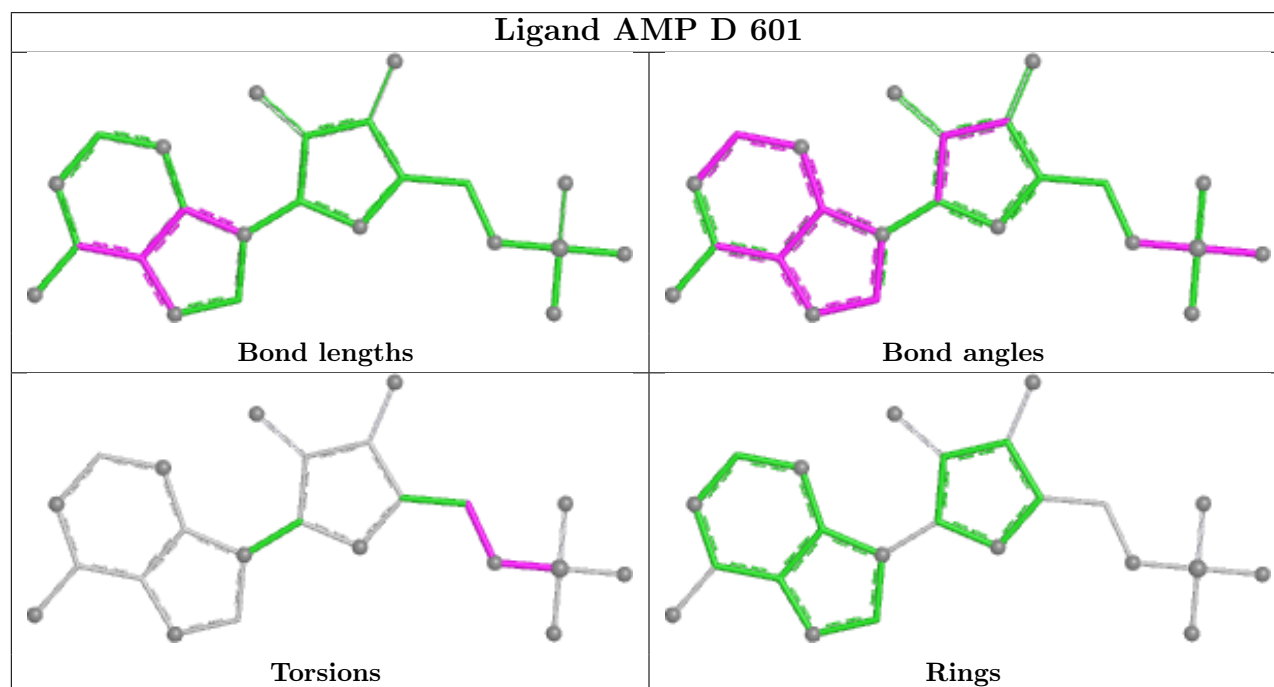
All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	601	AMP	C5'-O5'-P-O1P
3	D	601	AMP	C5'-O5'-P-O2P
3	D	601	AMP	C5'-O5'-P-O3P
3	D	601	AMP	C4'-C5'-O5'-P

There are no ring outliers.

No monomer is involved in short contacts.

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 than 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](#)

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	521/569 (91%)	-0.59	4 (0%) 82 77	18, 36, 64, 93	0
1	B	524/569 (92%)	0.20	46 (8%) 15 14	27, 55, 129, 145	0
1	C	521/569 (91%)	-0.37	6 (1%) 76 70	17, 40, 91, 116	0
1	D	553/569 (97%)	-0.40	4 (0%) 84 79	25, 44, 65, 95	0
1	E	16/569 (2%)	1.29	6 (37%) 1 1	66, 79, 85, 91	0
All	All	2135/2845 (75%)	-0.28	66 (3%) 51 43	17, 44, 94, 145	0

The worst 5 of 66 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	519	VAL	4.6
1	B	469	ALA	4.6
1	B	482	ILE	4.1
1	B	503	LEU	4.1
1	B	515	LEU	4.1

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 oligosaccharides in this entry.

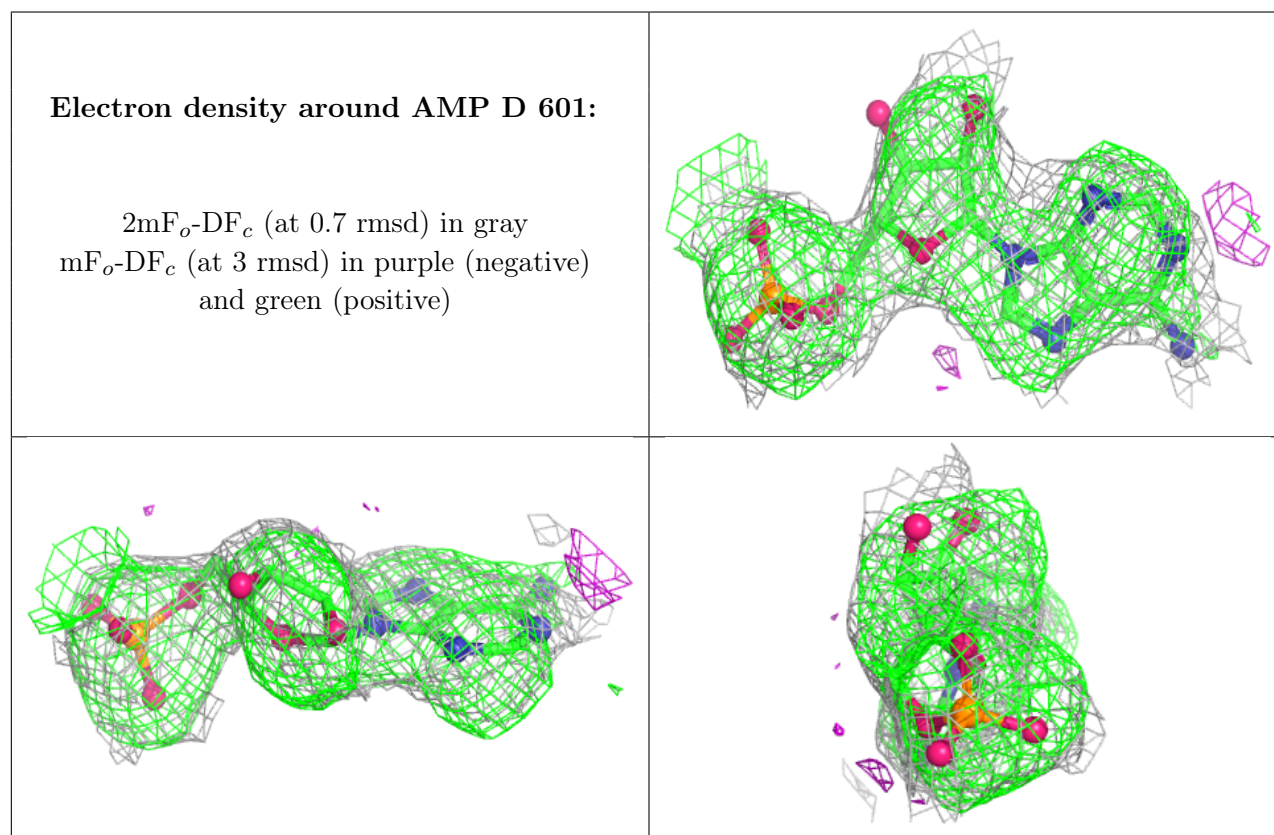
6.4 Ligands [i](#)

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
2	MG	A	601	1/1	-	-	37,37,37,37	1
2	MG	A	602	1/1	-	-	30,30,30,30	1
2	MG	D	602	1/1	-	-	36,36,36,36	1
2	MG	D	603	1/1	-	-	54,54,54,54	1
3	AMP	D	601	23/23	-	-	37,38,39,39	23

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.



6.5 Other polymers ⓘ

There are no such residues in this entry.