



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 13, 2024 – 04:23 PM EDT

PDB ID : 8GKZ  
Title : Human mitochondrial serine hydroxymethyltransferase (SHMT2) Y105F in complex with PLP, glycine and AGF362 inhibitor  
Authors : Katinas, J.M.; Dann III, C.E.  
Deposited on : 2023-03-20  
Resolution : 2.75 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](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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
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

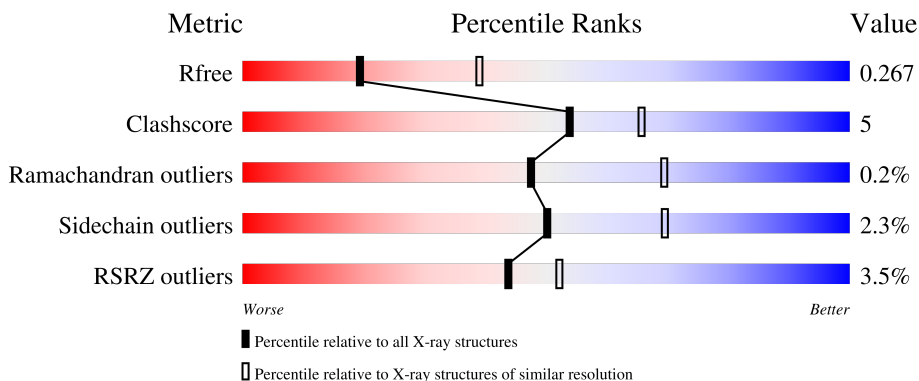
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.75 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))
$R_{free}$	130704	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

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  $\geq 3$ , 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	493	 83% 9% 8%
1	B	493	 5% 76% 17% 7%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GLY	A	601	-	X	-	-

## 2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 7205 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 Serine hydroxymethyltransferase, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	456	3563	2244	641	662	16	0	1	0
1	B	458	3549	2235	634	664	16	0	0	0

There are 36 discrepancies between the modelled and reference sequences:

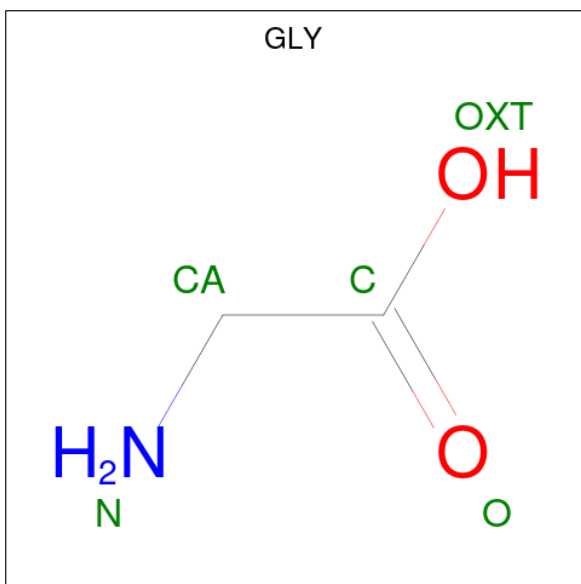
Chain	Residue	Modelled	Actual	Comment	Reference
A	12	MET	-	initiating methionine	UNP P34897
A	13	GLY	-	expression tag	UNP P34897
A	14	SER	-	expression tag	UNP P34897
A	15	SER	-	expression tag	UNP P34897
A	16	HIS	-	expression tag	UNP P34897
A	17	HIS	-	expression tag	UNP P34897
A	18	HIS	-	expression tag	UNP P34897
A	19	HIS	-	expression tag	UNP P34897
A	20	HIS	-	expression tag	UNP P34897
A	21	HIS	-	expression tag	UNP P34897
A	22	SER	-	expression tag	UNP P34897
A	23	SER	-	expression tag	UNP P34897
A	24	GLY	-	expression tag	UNP P34897
A	25	LEU	-	expression tag	UNP P34897
A	26	VAL	-	expression tag	UNP P34897
A	27	PRO	-	expression tag	UNP P34897
A	28	ARG	-	expression tag	UNP P34897
A	105	PHE	TYR	engineered mutation	UNP P34897
B	12	MET	-	initiating methionine	UNP P34897
B	13	GLY	-	expression tag	UNP P34897
B	14	SER	-	expression tag	UNP P34897
B	15	SER	-	expression tag	UNP P34897
B	16	HIS	-	expression tag	UNP P34897
B	17	HIS	-	expression tag	UNP P34897
B	18	HIS	-	expression tag	UNP P34897

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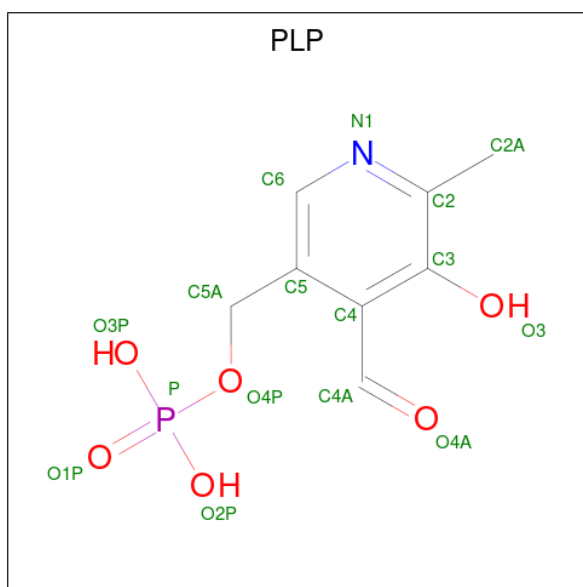
Chain	Residue	Modelled	Actual	Comment	Reference
B	19	HIS	-	expression tag	UNP P34897
B	20	HIS	-	expression tag	UNP P34897
B	21	HIS	-	expression tag	UNP P34897
B	22	SER	-	expression tag	UNP P34897
B	23	SER	-	expression tag	UNP P34897
B	24	GLY	-	expression tag	UNP P34897
B	25	LEU	-	expression tag	UNP P34897
B	26	VAL	-	expression tag	UNP P34897
B	27	PRO	-	expression tag	UNP P34897
B	28	ARG	-	expression tag	UNP P34897
B	105	PHE	TYR	engineered mutation	UNP P34897

- Molecule 2 is GLYCINE (three-letter code: GLY) (formula: C<sub>2</sub>H<sub>5</sub>NO<sub>2</sub>).



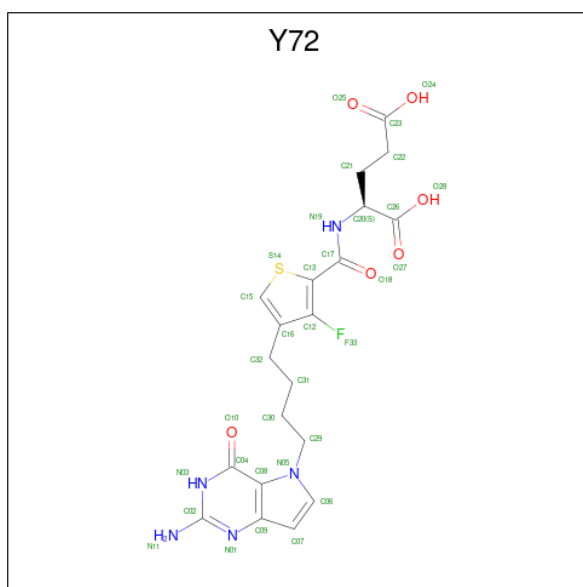
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	5	2	1	2	0	0
2	B	1	5	2	1	2	0	0

- Molecule 3 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: C<sub>8</sub>H<sub>10</sub>NO<sub>6</sub>P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	A	1	15	8	1	5	1	0	0
3	B	1	15	8	1	5	1	0	0

- Molecule 4 is N-{4-[4-(2-amino-4-oxo-3,4-dihydro-5H-pyrrolo[3,2-d]pyrimidin-5-yl)butyl]-3-fluorothiophene-2-carbonyl}-L-glutamic acid (three-letter code: Y72) (formula: C<sub>20</sub>H<sub>22</sub>FN<sub>5</sub>O<sub>6</sub>S) (labeled as "Ligand of Interest" by depositor).



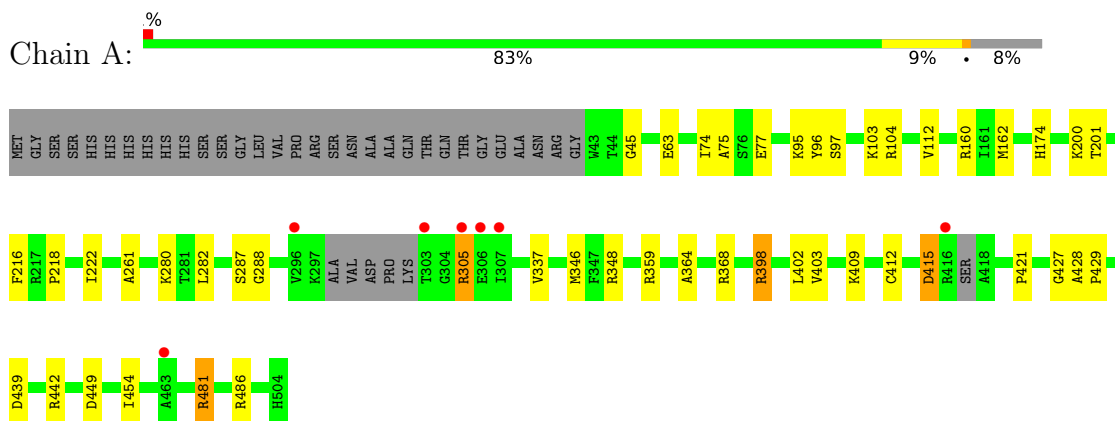
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	15	Total 15	O 15	0	0
5	B	5	Total 5	O 5	0	0

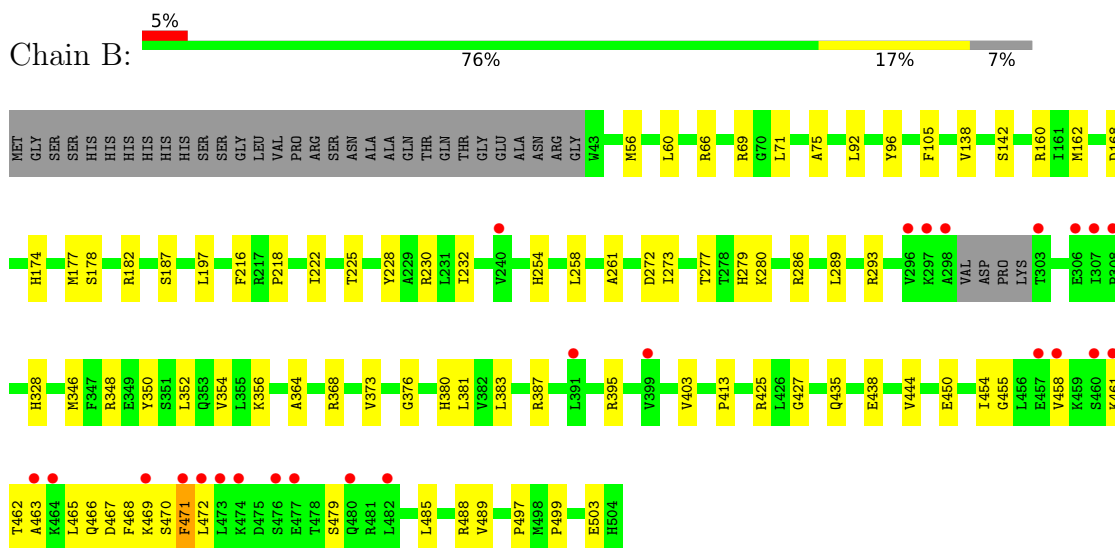
### 3 Residue-property plots [i](#)

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: Serine hydroxymethyltransferase, mitochondrial



- Molecule 1: Serine hydroxymethyltransferase, mitochondrial





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	158.25Å 158.25Å 207.99Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.74 – 2.75 48.74 – 2.75	Depositor EDS
% Data completeness (in resolution range)	99.1 (48.74-2.75) 99.1 (48.74-2.75)	Depositor EDS
$R_{merge}$	0.18	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.59 (at 2.77Å)	Xtrriage
Refinement program	PHENIX 1.13-2998	Depositor
R, $R_{free}$	0.215 , 0.267 0.215 , 0.267	Depositor DCC
$R_{free}$ test set	2045 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	45.4	Xtrriage
Anisotropy	0.414	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 42.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	7205	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	50.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.70% 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: PLP, Y72

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	0.27	0/3633	0.46	0/4910
1	B	0.28	0/3620	0.46	0/4899
All	All	0.27	0/7253	0.46	0/9809

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	3563	0	3540	25	0
1	B	3549	0	3506	53	0
2	A	5	0	2	0	0
2	B	5	0	2	2	0
3	A	15	0	7	1	0
3	B	15	0	7	3	0
4	B	33	0	0	1	0
5	A	15	0	0	0	0
5	B	5	0	0	0	0
All	All	7205	0	7064	76	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 5.

All (76) 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:439:ASP:OD1	1:A:442:ARG:NH1	2.28	0.67
1:B:461:LYS:HE3	1:B:471:PHE:CZ	2.29	0.67
1:B:455:GLY:HA2	1:B:458:VAL:HG12	1.79	0.65
1:B:177:MET:HG2	1:B:187:SER:HB3	1.79	0.64
1:B:425:ARG:HH12	2:B:602:GLY:HA3	1.63	0.64
1:B:395:ARG:HB3	1:B:468:PHE:CZ	2.35	0.62
1:B:403:VAL:O	1:B:489:VAL:HG21	1.98	0.62
1:B:280:LYS:NZ	3:B:603:PLP:O3	2.33	0.60
1:B:279:HIS:ND1	1:B:286:ARG:HA	2.18	0.59
1:A:368[A]:ARG:NH1	1:A:449:ASP:OD2	2.36	0.59
1:B:465:LEU:O	1:B:468:PHE:HB3	2.04	0.58
1:B:461:LYS:HE3	1:B:471:PHE:HZ	1.68	0.58
1:B:225:THR:HG23	1:B:232:ILE:HD11	1.84	0.57
1:B:352:LEU:O	1:B:356:LYS:HG3	2.04	0.57
1:B:66:ARG:HA	1:B:69:ARG:HG2	1.87	0.56
1:B:485:LEU:O	1:B:489:VAL:HG13	2.07	0.55
1:B:168:ASP:HB3	1:B:197:LEU:HG	1.89	0.55
1:B:138:VAL:HG12	1:B:289:LEU:HD22	1.89	0.54
1:B:450:GLU:O	1:B:454:ILE:HG13	2.07	0.54
1:A:403:VAL:HA	1:A:486:ARG:HB2	1.89	0.53
1:A:97:SER:O	1:A:104:ARG:NH1	2.42	0.52
1:A:412:CYS:O	1:A:415:ASP:HB3	2.09	0.52
1:B:462:THR:OG1	1:B:463:ALA:N	2.42	0.52
1:B:468:PHE:O	1:B:472:LEU:HD12	2.09	0.52
1:A:75:ALA:HA	1:A:427:GLY:HA3	1.92	0.51
1:A:398:ARG:NH2	1:A:402:LEU:HD21	2.26	0.51
1:B:277:THR:HG21	1:B:280:LYS:HE3	1.93	0.50
1:A:63:GLU:HG2	1:B:92:LEU:HD23	1.95	0.48
1:B:160:ARG:HB2	1:B:218:PRO:HA	1.95	0.48
1:A:280:LYS:NZ	3:A:602:PLP:O3	2.39	0.48
1:B:56:MET:HG3	1:B:60:LEU:HD11	1.96	0.48
1:B:160:ARG:HB3	1:B:216:PHE:CE2	2.49	0.48
1:B:468:PHE:CE1	1:B:472:LEU:HD11	2.48	0.48
1:B:56:MET:O	1:B:60:LEU:HD12	2.13	0.47
1:B:364:ALA:O	1:B:368:ARG:HG3	2.14	0.47
1:B:469:LYS:HA	1:B:472:LEU:HD13	1.96	0.47
1:A:409:LYS:HD2	1:A:421:PRO:HG2	1.96	0.47
1:B:177:MET:HE3	1:B:182:ARG:HG2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:75:ALA:HA	1:B:427:GLY:HA3	1.97	0.47
1:A:364:ALA:O	1:A:368[B]:ARG:HG2	2.14	0.47
1:B:350:TYR:O	1:B:354:VAL:HG23	2.14	0.46
1:A:305:ARG:HD3	1:A:305:ARG:H	1.80	0.46
1:B:174:HIS:CD2	1:B:222:ILE:HG21	2.50	0.46
1:B:261:ALA:HB1	1:B:348:ARG:HA	1.97	0.46
1:B:142:SER:OG	3:B:603:PLP:O2P	2.26	0.46
1:A:74:ILE:HB	1:A:77:GLU:HG3	1.98	0.45
1:A:95:LYS:HG2	1:A:112:VAL:HG11	1.98	0.45
1:B:462:THR:OG1	1:B:467:ASP:HB2	2.17	0.45
1:B:258:LEU:HD11	1:B:380:HIS:HB3	2.00	0.44
1:A:287:SER:OG	1:A:288:GLY:N	2.50	0.44
1:B:272:ASP:HB2	1:B:273:ILE:HD12	1.98	0.44
1:B:356:LYS:HE3	1:B:438:GLU:OE2	2.17	0.43
1:A:261:ALA:HB1	1:A:348:ARG:HA	1.99	0.43
1:B:395:ARG:HD3	1:B:468:PHE:CE2	2.53	0.43
1:B:435:GLN:OE1	1:B:497:PRO:HG3	2.19	0.43
1:A:160:ARG:HG2	1:A:216:PHE:CZ	2.54	0.43
1:B:105:PHE:HZ	4:B:601:Y72:N19	2.17	0.43
1:B:228:TYR:HA	1:B:383:LEU:HD11	2.00	0.43
1:B:230:ARG:HH22	1:B:376:GLY:H	1.66	0.43
1:B:458:VAL:O	1:B:462:THR:HG22	2.19	0.43
2:B:602:GLY:N	3:B:603:PLP:HO3	2.16	0.43
1:A:162:MET:SD	1:A:218:PRO:HG3	2.59	0.42
1:A:428:ALA:N	1:A:429:PRO:CD	2.82	0.42
1:B:272:ASP:HA	1:B:293:ARG:NH1	2.34	0.42
1:B:450:GLU:OE1	1:B:488:ARG:NH2	2.51	0.42
1:B:380:HIS:NE2	1:B:381:LEU:HD23	2.34	0.42
1:A:454:ILE:HD11	1:A:481:ARG:HG2	2.01	0.42
1:B:71:LEU:HD22	1:B:444:VAL:HG22	2.02	0.42
1:B:279:HIS:HB2	1:B:280:LYS:H	1.67	0.42
1:A:337:VAL:HG22	1:B:56:MET:HG2	2.02	0.41
1:B:373:VAL:HG11	1:B:413:PRO:HD2	2.02	0.41
1:A:174:HIS:CD2	1:A:222:ILE:HG21	2.55	0.41
1:B:162:MET:HG3	1:B:218:PRO:HB3	2.02	0.41
1:A:45:GLY:HA3	1:B:499:PRO:HB3	2.01	0.41
1:A:282:LEU:HD23	1:A:282:LEU:HA	1.86	0.41
1:A:200:LYS:HG2	1:A:201:THR:HG23	2.03	0.41

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	451/493 (92%)	435 (96%)	15 (3%)	1 (0%)	47	69
1	B	454/493 (92%)	426 (94%)	27 (6%)	1 (0%)	47	69
All	All	905/986 (92%)	861 (95%)	42 (5%)	2 (0%)	47	69

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	415	ASP
1	B	178	SER

### 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	374/405 (92%)	367 (98%)	7 (2%)	57	73
1	B	371/405 (92%)	361 (97%)	10 (3%)	44	65
All	All	745/810 (92%)	728 (98%)	17 (2%)	50	69

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

Mol	Chain	Res	Type
1	A	96	TYR
1	A	103	LYS
1	A	305	ARG
1	A	346	MET

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Mol	Chain	Res	Type
1	A	359	ARG
1	A	398	ARG
1	A	481	ARG
1	B	96	TYR
1	B	254	HIS
1	B	328	HIS
1	B	346	MET
1	B	387	ARG
1	B	466	GLN
1	B	470	SER
1	B	471	PHE
1	B	479	SER
1	B	503	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	466	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](#)

5 ligands are modelled in this entry.

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
2	GLY	A	601	-	4,4,4	1.13	1 (25%)	3,4,4	1.66	1 (33%)
3	PLP	A	602	1	15,15,16	2.22	5 (33%)	20,22,23	1.46	4 (20%)
4	Y72	B	601	-	29,35,35	3.24	11 (37%)	31,49,49	1.53	7 (22%)
3	PLP	B	603	1	15,15,16	2.19	5 (33%)	20,22,23	1.25	1 (5%)
2	GLY	B	602	-	4,4,4	1.13	1 (25%)	3,4,4	1.50	0

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	GLY	A	601	-	-	2/2/2/2	-
3	PLP	A	602	1	-	2/6/6/8	0/1/1/1
4	Y72	B	601	-	-	9/20/24/24	0/3/3/3
3	PLP	B	603	1	-	0/6/6/8	0/1/1/1
2	GLY	B	602	-	-	0/2/2/2	-

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	601	Y72	O10-C04	8.54	1.40	1.23
4	B	601	Y72	C15-C16	6.41	1.41	1.37
4	B	601	Y72	O27-C26	6.02	1.40	1.22
4	B	601	Y72	C17-N19	5.65	1.46	1.34
4	B	601	Y72	O25-C23	5.53	1.40	1.22
3	A	602	PLP	C4A-C4	5.15	1.62	1.51
3	B	603	PLP	C4A-C4	5.02	1.62	1.51
4	B	601	Y72	C02-N11	4.84	1.45	1.34
4	B	601	Y72	C06-N05	-3.68	1.32	1.38
3	A	602	PLP	C2A-C2	3.56	1.56	1.50
3	B	603	PLP	C2A-C2	3.40	1.56	1.50
4	B	601	Y72	C04-N03	-3.18	1.33	1.37
4	B	601	Y72	O28-C26	3.14	1.40	1.30
3	B	603	PLP	C5-C4	-2.86	1.37	1.40
4	B	601	Y72	O24-C23	2.85	1.40	1.30
3	B	603	PLP	C6-N1	2.81	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	602	PLP	C6-N1	2.75	1.40	1.34
3	A	602	PLP	C5-C4	-2.40	1.37	1.40
3	A	602	PLP	C5A-C5	2.19	1.56	1.50
3	B	603	PLP	C5A-C5	2.15	1.56	1.50
2	A	601	GLY	OXT-C	-2.14	1.23	1.30
2	B	602	GLY	OXT-C	-2.10	1.23	1.30
4	B	601	Y72	O18-C17	-2.03	1.19	1.23

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	601	Y72	C16-C15-S14	-4.52	107.44	112.26
3	A	602	PLP	C4A-C4-C5	3.18	124.21	120.94
3	A	602	PLP	O4P-C5A-C5	3.02	115.10	109.35
3	B	603	PLP	O4P-C5A-C5	2.92	114.92	109.35
4	B	601	Y72	C20-N19-C17	2.46	127.63	121.60
4	B	601	Y72	C32-C16-C15	-2.29	121.53	126.81
3	A	602	PLP	C4A-C4-C3	-2.29	116.62	120.50
3	A	602	PLP	C5A-C5-C6	-2.26	115.66	119.37
4	B	601	Y72	C02-N03-C04	-2.25	120.96	125.10
4	B	601	Y72	C09-N01-C02	2.24	120.11	117.93
4	B	601	Y72	C06-N05-C08	2.21	111.04	108.58
4	B	601	Y72	C30-C29-N05	-2.20	108.21	112.31
2	A	601	GLY	OXT-C-O	-2.12	118.01	123.30

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	GLY	O-C-CA-N
2	A	601	GLY	OXT-C-CA-N
3	A	602	PLP	C4-C5-C5A-O4P
3	A	602	PLP	C6-C5-C5A-O4P
4	B	601	Y72	N19-C20-C21-C22
4	B	601	Y72	C12-C16-C32-C31
4	B	601	Y72	N05-C29-C30-C31
4	B	601	Y72	C30-C31-C32-C16
4	B	601	Y72	C26-C20-C21-C22
4	B	601	Y72	N19-C20-C26-O27
4	B	601	Y72	N19-C20-C26-O28
4	B	601	Y72	C21-C20-N19-C17
4	B	601	Y72	C15-C16-C32-C31

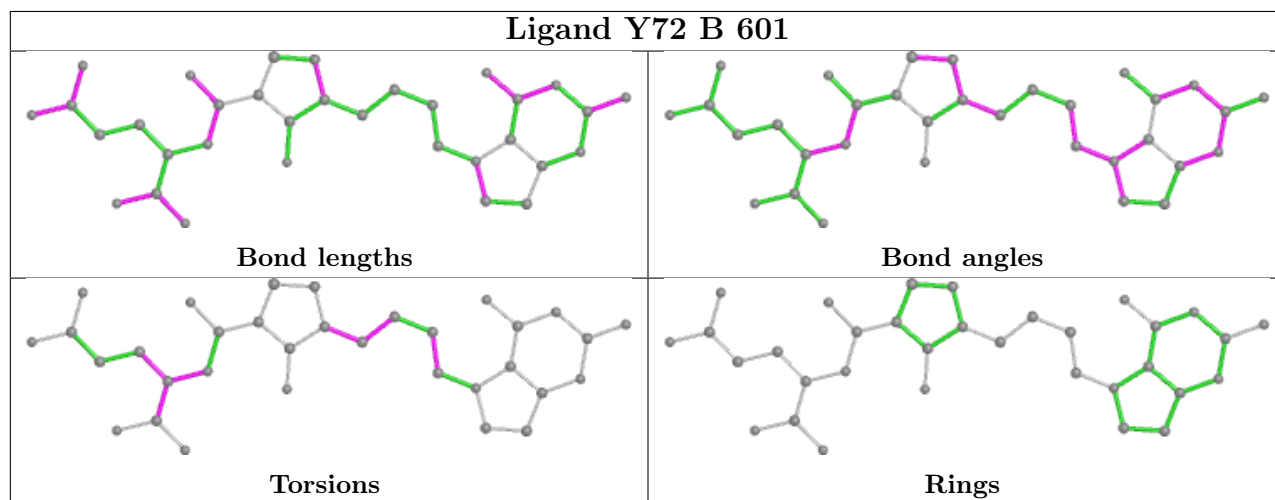


There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	602	PLP	1	0
4	B	601	Y72	1	0
3	B	603	PLP	3	0
2	B	602	GLY	2	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 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

### 6.1 Protein, DNA and RNA chains

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	456/493 (92%)	-0.16	7 (1%) 73 81	22, 38, 72, 120	0
1	B	458/493 (92%)	0.21	25 (5%) 25 30	25, 54, 99, 128	0
All	All	914/986 (92%)	0.03	32 (3%) 44 52	22, 45, 88, 128	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	306	GLU	4.5
1	B	471	PHE	4.0
1	B	399	VAL	3.9
1	B	306	GLU	3.6
1	B	298	ALA	3.5
1	B	460	SER	3.5
1	A	307	ILE	3.4
1	A	305	ARG	3.4
1	A	303	THR	3.2
1	B	480	GLN	3.1
1	B	391	LEU	3.0
1	B	303	THR	3.0
1	B	474	LYS	2.8
1	B	473	LEU	2.7
1	B	482	LEU	2.7
1	B	296	VAL	2.6
1	B	469	LYS	2.5
1	B	461	LYS	2.5
1	B	297	LYS	2.4
1	B	307	ILE	2.4
1	B	457	GLU	2.4
1	A	463	ALA	2.3
1	B	240	VAL	2.3
1	A	416	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	296	VAL	2.3
1	B	464	LYS	2.2
1	B	472	LEU	2.1
1	B	476	SER	2.1
1	B	458	VAL	2.1
1	B	308	PRO	2.0
1	B	463	ALA	2.0
1	B	477	GLU	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](#)

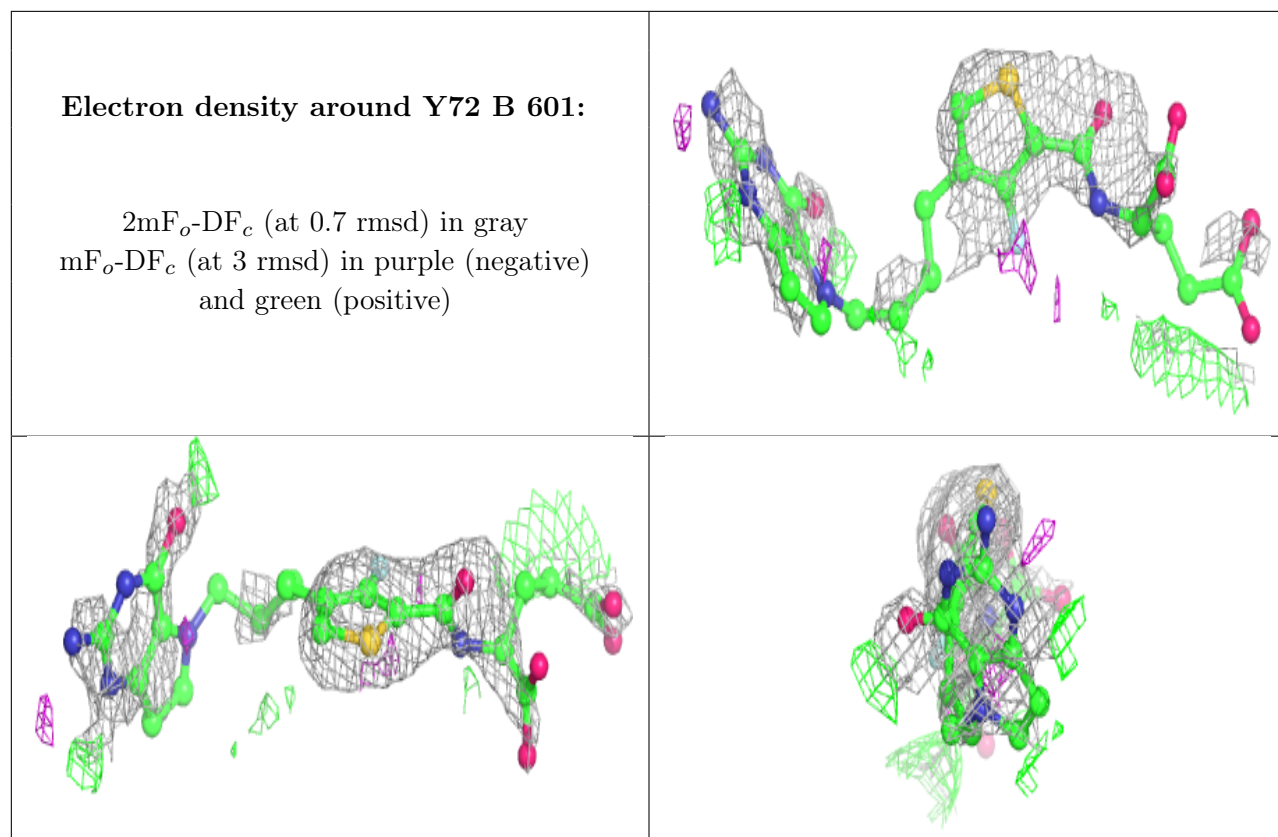
There are no monosaccharides in this entry.

## 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<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(Å <sup>2</sup> )	Q<0.9
4	Y72	B	601	33/33	0.76	0.39	68,87,97,98	0
2	GLY	B	602	5/5	0.85	0.29	66,70,76,81	0
2	GLY	A	601	5/5	0.93	0.28	74,80,83,89	0
3	PLP	B	603	15/16	0.97	0.20	31,41,51,61	0
3	PLP	A	602	15/16	0.98	0.19	21,27,39,39	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.



## 6.5 Other polymers [i](#)

There are no such residues in this entry.