



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 13, 2024 – 04:28 PM EDT

PDB ID : 8GKS  
Title : Human mitochondrial serine hydroxymethyltransferase (SHMT2) in complex with PLP, glycine and AGF291 inhibitor  
Authors : Katinas, J.M.; Dann III, C.E.  
Deposited on : 2023-03-20  
Resolution : 2.99 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>.

---

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

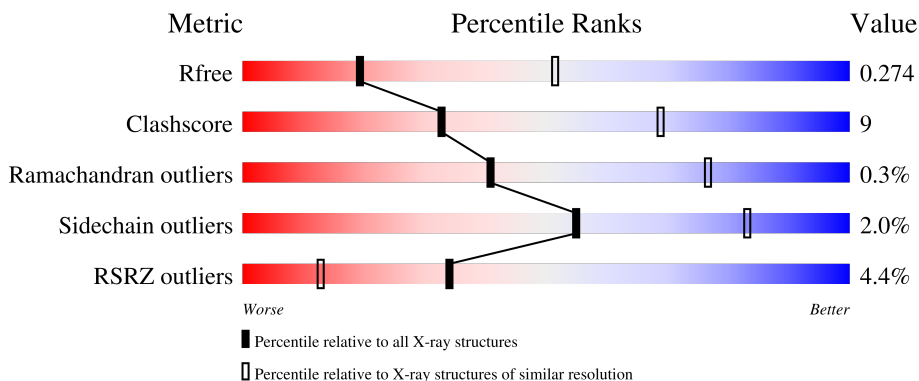
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.99 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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	
1	B	493	

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 7425 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	462	3613	2277	651	669	16	0	3	0
1	B	462	3585	2258	643	668	16	0	1	0

There are 34 discrepancies between the modelled and reference sequences:

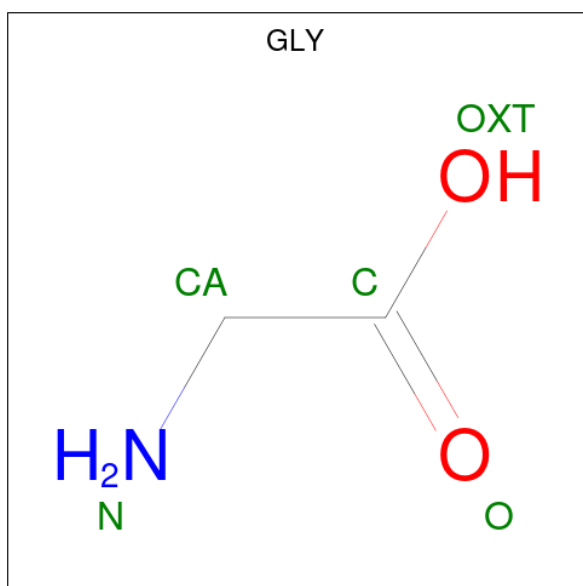
Chain	Residue	Modelled	Actual	Comment	Reference
A	12	MET	-	initiating methionine	UNP P34897
A	13	GLY	-	expression tag	UNP P34897
A	14	SER	-	expression tag	UNP P34897
A	15	SER	-	expression tag	UNP P34897
A	16	HIS	-	expression tag	UNP P34897
A	17	HIS	-	expression tag	UNP P34897
A	18	HIS	-	expression tag	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
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
B	19	HIS	-	expression tag	UNP P34897

*Continued on next page...*

Continued from previous page...

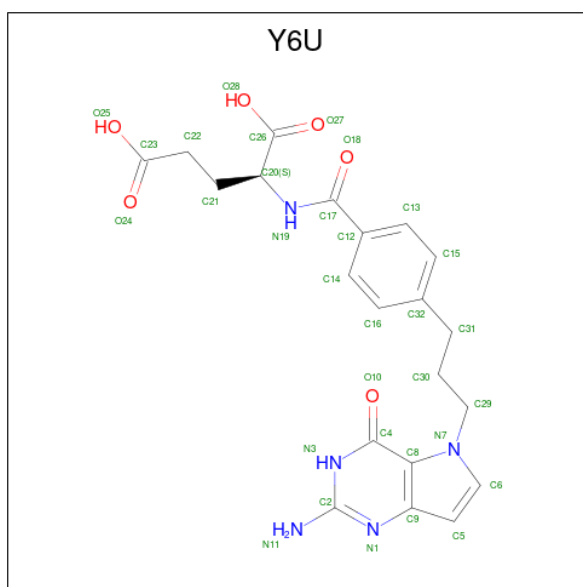
Chain	Residue	Modelled	Actual	Comment	Reference
B	20	HIS	-	expression tag	UNP P34897
B	21	HIS	-	expression tag	UNP P34897
B	22	SER	-	expression tag	UNP P34897
B	23	SER	-	expression tag	UNP P34897
B	24	GLY	-	expression tag	UNP P34897
B	25	LEU	-	expression tag	UNP P34897
B	26	VAL	-	expression tag	UNP P34897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

- Molecule 2 is GLYCINE (three-letter code: GLY) (formula:  $C_2H_5NO_2$ ).



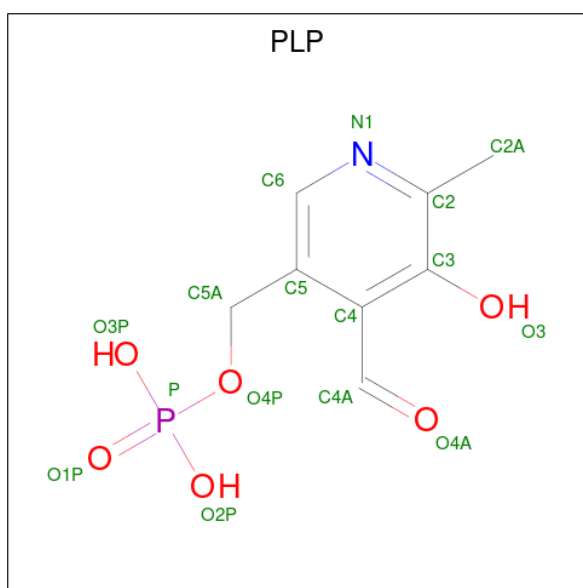
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	5	2	1	2	0	1
2	B	1	5	2	1	2	0	0

- Molecule 3 is N-{4-[3-(2-amino-4-oxo-3,4-dihydro-5H-pyrrolo[3,2-d]pyrimidin-5-yl)propyl]benzoyl}-L-glutamic acid (three-letter code: Y6U) (formula:  $C_{21}H_{23}N_5O_6$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			32	21	5	6		
3	A	1	Total	C	N	O	0	1
			32	21	5	6		

- Molecule 4 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
4	A	1	Total	C	N	O	P	0	1
			15	8	1	5	1		
4	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

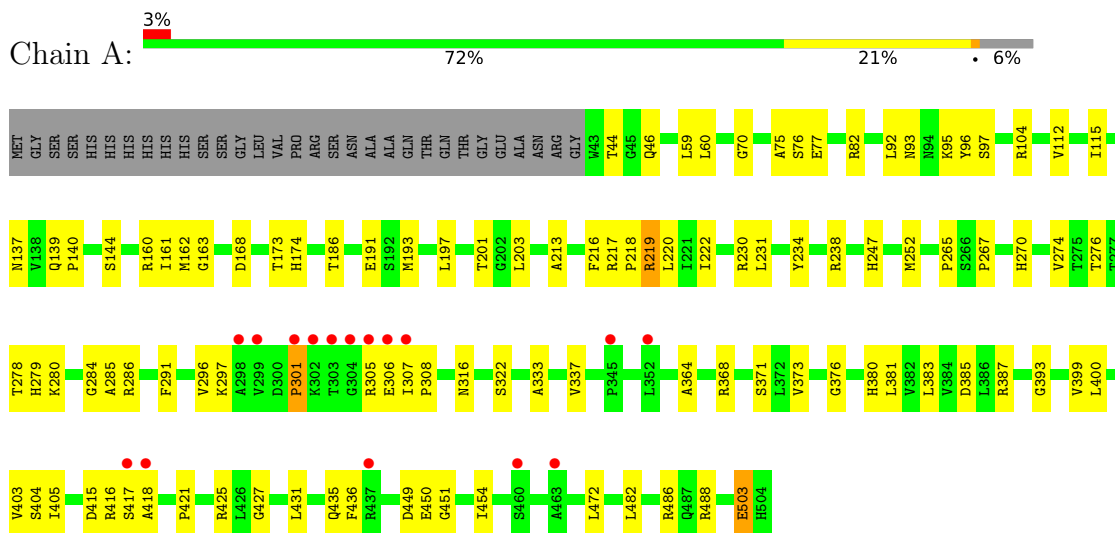
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	84	Total 84	O 84	0	0
5	B	39	Total 39	O 39	0	0

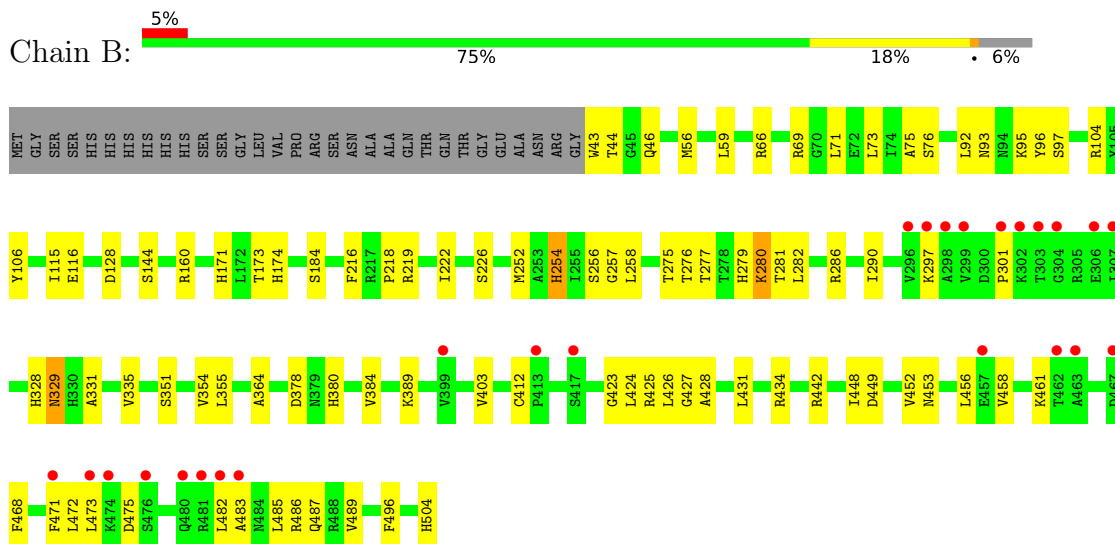
### 3 Residue-property plots i

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, $\alpha$ , $\beta$ , $\gamma$	157.93Å 157.93Å 206.67Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.54 – 2.99 48.53 – 2.99	Depositor EDS
% Data completeness (in resolution range)	99.5 (48.54-2.99) 99.5 (48.53-2.99)	Depositor EDS
$R_{merge}$	0.86	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.23 (at 3.01Å)	Xtrriage
Refinement program	PHENIX 1.13-2998	Depositor
R, $R_{free}$	0.223 , 0.274 0.223 , 0.274	Depositor DCC
$R_{free}$ test set	1575 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	45.7	Xtrriage
Anisotropy	0.304	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 50.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	7425	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	46.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.59% 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: Y6U, PLP

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	0.25	0/3686	0.42	1/4986 (0.0%)
1	B	0.25	0/3657	0.42	1/4948 (0.0%)
All	All	0.25	0/7343	0.42	2/9934 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	301	PRO	N-CA-CB	5.89	110.37	103.30
1	A	301	PRO	N-CA-CB	5.54	109.95	103.30

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	3613	0	3585	67	0
1	B	3585	0	3542	66	0
2	A	5	0	2	2	0
2	B	5	0	2	0	0
3	A	64	0	0	0	0
4	A	15	0	6	0	0
4	B	15	0	6	1	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	84	0	0	2	0
5	B	39	0	0	0	0
All	All	7425	0	7143	125	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 9.

All (125) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:403:VAL:HG21	1:B:485:LEU:HG	1.61	0.82
1:B:486:ARG:HA	1:B:489:VAL:HB	1.69	0.73
1:B:277:THR:HG21	1:B:280[A]:LYS:HE2	1.74	0.69
1:A:162:MET:HG2	1:A:193:MET:O	1.91	0.69
1:B:171:HIS:HB2	4:B:602:PLP:H2A3	1.81	0.63
1:A:220:LEU:HD13	1:A:247:HIS:HB2	1.81	0.63
1:B:160:ARG:HB2	1:B:218:PRO:HA	1.80	0.63
1:A:219:ARG:NH2	5:A:801:HOH:O	2.27	0.62
1:A:286:ARG:NH1	1:B:93:ASN:O	2.33	0.61
1:A:161:ILE:HG22	1:A:220:LEU:HB3	1.84	0.60
1:B:258:LEU:HD11	1:B:380:HIS:HB3	1.84	0.59
1:A:75:ALA:HA	1:A:427:GLY:HA3	1.84	0.59
1:B:257:GLY:H	1:B:281:THR:HB	1.68	0.58
1:A:230:ARG:HH21	1:A:376:GLY:H	1.52	0.58
1:B:160:ARG:NH1	1:B:216:PHE:O	2.37	0.57
1:B:449:ASP:O	1:B:453:ASN:ND2	2.34	0.57
1:B:384:VAL:HG23	1:B:424:LEU:H	1.71	0.56
1:A:162:MET:HE1	1:A:213:ALA:HA	1.88	0.56
1:B:92:LEU:O	1:B:329:ASN:ND2	2.39	0.56
1:A:278:THR:OG1	1:A:285:ALA:O	2.22	0.56
1:A:416:ARG:O	1:A:418:ALA:N	2.39	0.56
1:A:503:GLU:OE2	1:A:503:GLU:N	2.35	0.56
1:B:472:LEU:HD23	1:B:482:LEU:HD11	1.88	0.56
1:A:162:MET:CE	1:A:213:ALA:HA	2.36	0.55
1:B:73:LEU:O	1:B:427:GLY:N	2.35	0.55
1:B:258:LEU:HG	1:B:281:THR:HG21	1.86	0.55
1:B:104:ARG:NH2	1:B:116:GLU:OE1	2.39	0.55
1:A:44:THR:HG23	1:A:46:GLN:H	1.72	0.55
1:B:403:VAL:HA	1:B:486:ARG:HB3	1.90	0.54
1:A:279:HIS:HA	1:A:284:GLY:H	1.73	0.54
1:A:201:THR:HG23	1:A:203:LEU:H	1.72	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:368[A]:ARG:NH1	1:A:449:ASP:OD2	2.41	0.54
1:B:144:SER:HA	1:B:173:THR:HG21	1.89	0.54
1:B:256:SER:OG	1:B:282:LEU:HD12	2.07	0.54
1:A:59:LEU:HD13	1:B:115:ILE:HG12	1.89	0.53
2:A:601[B]:GLY:OXT	1:B:106:TYR:OH	2.23	0.53
1:B:73:LEU:HD13	1:B:426:LEU:HD22	1.89	0.53
1:A:97:SER:O	1:A:104:ARG:NH1	2.41	0.53
1:B:254:HIS:O	1:B:281:THR:OG1	2.26	0.52
1:B:403:VAL:HG23	1:B:486:ARG:HB3	1.92	0.52
1:B:256:SER:OG	1:B:282:LEU:CD1	2.58	0.52
1:A:174:HIS:CD2	1:A:222:ILE:HG21	2.45	0.52
1:A:95:LYS:HG2	1:A:112:VAL:HG11	1.93	0.51
1:B:448:ILE:O	1:B:452:VAL:HG23	2.11	0.51
1:A:137:ASN:ND2	1:A:316:ASN:OD1	2.36	0.51
1:B:75:ALA:HA	1:B:427:GLY:HA3	1.93	0.50
1:A:274:VAL:HB	1:A:291:PHE:HB2	1.94	0.50
1:A:162:MET:CE	1:A:218:PRO:HG3	2.40	0.50
1:B:471:PHE:CE2	1:B:475:ASP:HB2	2.46	0.50
1:A:333:ALA:O	1:A:337:VAL:HG23	2.11	0.50
1:A:431:LEU:HB3	1:A:436:PHE:CG	2.46	0.50
1:B:403:VAL:HG22	1:B:403:VAL:O	2.11	0.50
1:B:226:SER:O	1:B:425:ARG:NH1	2.44	0.49
1:A:403:VAL:HA	1:A:486:ARG:HB2	1.95	0.49
1:A:400:LEU:HB3	1:A:405:ILE:HB	1.94	0.49
1:B:354:VAL:HG13	1:B:428:ALA:HB3	1.95	0.48
1:A:450:GLU:O	1:A:454:ILE:HG13	2.13	0.48
1:A:92:LEU:HD21	1:A:115:ILE:HD12	1.96	0.48
1:B:277:THR:HG1	1:B:279:HIS:CE1	2.32	0.48
1:A:77:GLU:OE2	1:B:96:TYR:N	2.47	0.48
1:B:252:MET:HG3	1:B:276:THR:OG1	2.14	0.48
1:B:458:VAL:HA	1:B:461:LYS:HB2	1.97	0.47
1:A:144:SER:HA	1:A:173:THR:HG21	1.96	0.47
1:A:296:VAL:HA	1:A:308:PRO:HA	1.96	0.47
1:A:160:ARG:HA	1:A:191:GLU:O	2.14	0.47
1:B:331:ALA:O	1:B:335:VAL:HG13	2.15	0.46
1:B:434:ARG:NH2	1:B:496:PHE:O	2.44	0.46
1:A:160:ARG:HB3	1:A:216:PHE:CE2	2.51	0.46
1:A:399:VAL:HG11	1:A:451:GLY:O	2.16	0.46
1:A:82:ARG:NH1	5:A:808:HOH:O	2.47	0.46
1:A:435:GLN:NE2	1:B:43:TRP:O	2.49	0.46
1:B:403:VAL:CG2	1:B:485:LEU:HG	2.38	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:483:ALA:O	1:B:487:GLN:HG2	2.15	0.46
1:A:93:ASN:O	1:B:286:ARG:NH1	2.42	0.46
1:A:322:SER:HA	1:B:184:SER:HA	1.96	0.46
1:A:230:ARG:HH21	1:A:376:GLY:N	2.15	0.45
1:A:393:GLY:N	1:A:421:PRO:O	2.47	0.45
1:B:66:ARG:HA	1:B:69:ARG:HG2	1.97	0.45
1:B:275:THR:HG22	1:B:290:ILE:HG12	1.98	0.45
1:A:70:GLY:HA2	1:A:404:SER:HB3	1.98	0.45
1:B:389:LYS:HG3	1:B:456:LEU:HD11	1.99	0.45
1:B:364:ALA:HB2	1:B:442:ARG:HG3	1.99	0.45
1:A:162:MET:HE3	1:A:218:PRO:HG3	1.99	0.44
1:B:97:SER:HB2	1:B:104:ARG:NH1	2.32	0.44
1:A:380:HIS:CE1	1:A:381:LEU:HD23	2.53	0.44
1:B:71:LEU:HB3	1:B:431:LEU:HD11	1.99	0.44
1:B:71:LEU:CD2	1:B:489:VAL:HG13	2.47	0.44
1:B:44:THR:HG22	1:B:46:GLN:HG3	2.00	0.44
1:B:226:SER:HA	1:B:254:HIS:ND1	2.33	0.44
1:A:252:MET:HG3	1:A:276:THR:HB	1.99	0.43
1:A:364:ALA:O	1:A:368[B]:ARG:HG2	2.18	0.43
1:A:238:ARG:HD3	1:A:270:HIS:O	2.18	0.43
1:B:95:LYS:HA	1:B:95:LYS:HD2	1.75	0.43
1:A:387:ARG:NH1	1:A:415:ASP:OD2	2.52	0.43
1:B:160:ARG:HB3	1:B:216:PHE:CE2	2.53	0.43
1:A:472:LEU:HD22	1:A:482:LEU:HD11	2.01	0.43
1:A:163:GLY:HA3	1:A:174:HIS:HB3	2.01	0.43
1:B:277:THR:CG2	1:B:280[A]:LYS:HE2	2.46	0.43
1:A:115:ILE:HG12	1:B:59:LEU:HD13	2.00	0.43
1:A:297:LYS:N	1:A:307:ILE:O	2.48	0.43
1:B:403:VAL:O	1:B:489:VAL:HG11	2.19	0.43
1:B:468:PHE:CE1	1:B:472:LEU:HD11	2.53	0.42
1:A:373:VAL:HB	1:A:383:LEU:HB2	2.01	0.42
1:A:60:LEU:HA	1:A:60:LEU:HD23	1.76	0.42
1:A:231:LEU:HD22	1:A:265:PRO:HD2	2.02	0.42
1:A:337:VAL:HG22	1:B:56:MET:HG2	2.02	0.42
1:A:425:ARG:NH1	2:A:601[B]:GLY:O	2.52	0.42
1:B:174:HIS:CD2	1:B:222:ILE:HG21	2.54	0.42
1:A:139:GLN:N	1:A:140:PRO:CD	2.83	0.42
1:B:92:LEU:HD21	1:B:115:ILE:HD12	2.01	0.42
1:A:161:ILE:HD11	1:A:186:THR:HG22	2.01	0.41
1:B:412:CYS:SG	1:B:423:GLY:HA3	2.60	0.41
1:A:76:SER:O	1:A:280[B]:LYS:HG2	2.20	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:458:VAL:HG13	1:B:468:PHE:CE2	2.56	0.41
1:A:174:HIS:CG	1:A:222:ILE:HG21	2.56	0.41
1:A:371:SER:OG	1:A:385:ASP:HB3	2.20	0.41
1:A:234:TYR:CZ	1:A:267:PRO:HB3	2.56	0.41
1:B:351:SER:O	1:B:355:LEU:HD12	2.21	0.41
1:A:168:ASP:HB3	1:A:197:LEU:HG	2.02	0.40
1:A:296:VAL:HG21	1:A:306:GLU:HB3	2.03	0.40
1:A:162:MET:HE2	1:A:218:PRO:HG3	2.02	0.40
1:A:279:HIS:HD1	1:A:286:ARG:HA	1.85	0.40
1:B:226:SER:HA	1:B:254:HIS:HD1	1.86	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	Percentiles	
1	A	462/493 (94%)	438 (95%)	22 (5%)	2 (0%)	34	72
1	B	460/493 (93%)	417 (91%)	42 (9%)	1 (0%)	47	82
All	All	922/986 (94%)	855 (93%)	64 (7%)	3 (0%)	41	76

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	417	SER
1	B	297	LYS
1	A	301	PRO

### 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	377/405 (93%)	371 (98%)	6 (2%)	62	86
1	B	374/405 (92%)	365 (98%)	9 (2%)	49	79
All	All	751/810 (93%)	736 (98%)	15 (2%)	55	83

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	96	TYR
1	A	217	ARG
1	A	219	ARG
1	A	305	ARG
1	A	488	ARG
1	A	503	GLU
1	B	128	ASP
1	B	219	ARG
1	B	254	HIS
1	B	280[A]	LYS
1	B	328	HIS
1	B	329	ASN
1	B	378	ASP
1	B	473	LEU
1	B	504	HIS

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

Mol	Chain	Res	Type
1	A	93	ASN

### 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](#)

6 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	B	601	-	4,4,4	1.13	1 (25%)	3,4,4	1.63	1 (33%)
3	Y6U	A	701	-	31,34,34	2.43	9 (29%)	38,47,47	1.03	2 (5%)
4	PLP	A	602[B]	1	15,15,16	0.80	1 (6%)	20,22,23	0.96	1 (5%)
3	Y6U	A	702[A]	-	31,34,34	2.48	9 (29%)	38,47,47	1.25	5 (13%)
4	PLP	B	602	1	15,15,16	0.77	1 (6%)	20,22,23	0.75	0
2	GLY	A	601[B]	-	4,4,4	1.14	1 (25%)	3,4,4	1.67	1 (33%)

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	B	601	-	-	0/2/2/2	-
3	Y6U	A	701	-	-	7/23/23/23	0/3/3/3
4	PLP	A	602[B]	1	-	0/6/6/8	0/1/1/1
3	Y6U	A	702[A]	-	-	10/23/23/23	0/3/3/3
4	PLP	B	602	1	-	0/6/6/8	0/1/1/1
2	GLY	A	601[B]	-	-	0/2/2/2	-

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	702[A]	Y6U	O10-C4	8.26	1.40	1.23
3	A	701	Y6U	O10-C4	8.11	1.39	1.23
3	A	702[A]	Y6U	C17-N19	6.19	1.47	1.34
3	A	701	Y6U	C17-N19	5.80	1.46	1.34
3	A	701	Y6U	C2-N11	4.32	1.44	1.34
3	A	702[A]	Y6U	C2-N11	4.31	1.44	1.34
3	A	701	Y6U	C6-N7	-4.04	1.32	1.38
3	A	702[A]	Y6U	C6-N7	-3.85	1.32	1.38
3	A	702[A]	Y6U	C4-N3	-3.52	1.32	1.37
3	A	701	Y6U	C4-N3	-3.51	1.32	1.37
3	A	701	Y6U	C9-N1	-2.66	1.34	1.39
3	A	702[A]	Y6U	C9-N1	-2.64	1.34	1.39
4	A	602[B]	PLP	C4A-C4	-2.59	1.46	1.51
4	B	602	PLP	C4A-C4	-2.43	1.46	1.51
3	A	702[A]	Y6U	O18-C17	-2.39	1.18	1.23
3	A	701	Y6U	O18-C17	-2.39	1.18	1.23
2	A	601[B]	GLY	OXT-C	-2.15	1.23	1.30
2	B	601	GLY	OXT-C	-2.12	1.23	1.30
3	A	702[A]	Y6U	C2-N3	-2.10	1.32	1.37
3	A	701	Y6U	C2-N3	-2.06	1.32	1.37
3	A	702[A]	Y6U	C12-C17	2.04	1.54	1.50
3	A	701	Y6U	C12-C17	2.01	1.54	1.50

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	702[A]	Y6U	C20-N19-C17	3.06	129.09	121.60
3	A	702[A]	Y6U	C21-C20-N19	2.52	115.96	110.88
3	A	701	Y6U	C2-N3-C4	-2.42	120.64	125.10
3	A	702[A]	Y6U	C2-N3-C4	-2.36	120.75	125.10
4	A	602[B]	PLP	O4P-C5A-C5	2.34	113.81	109.35
3	A	702[A]	Y6U	O18-C17-C12	-2.23	116.96	120.94
3	A	701	Y6U	C9-N1-C2	2.16	120.03	117.93
3	A	702[A]	Y6U	C9-N1-C2	2.13	120.01	117.93
2	A	601[B]	GLY	OXT-C-O	-2.12	118.01	123.30
2	B	601	GLY	OXT-C-O	-2.06	118.16	123.30

There are no chirality outliers.

All (17) torsion outliers are listed below:



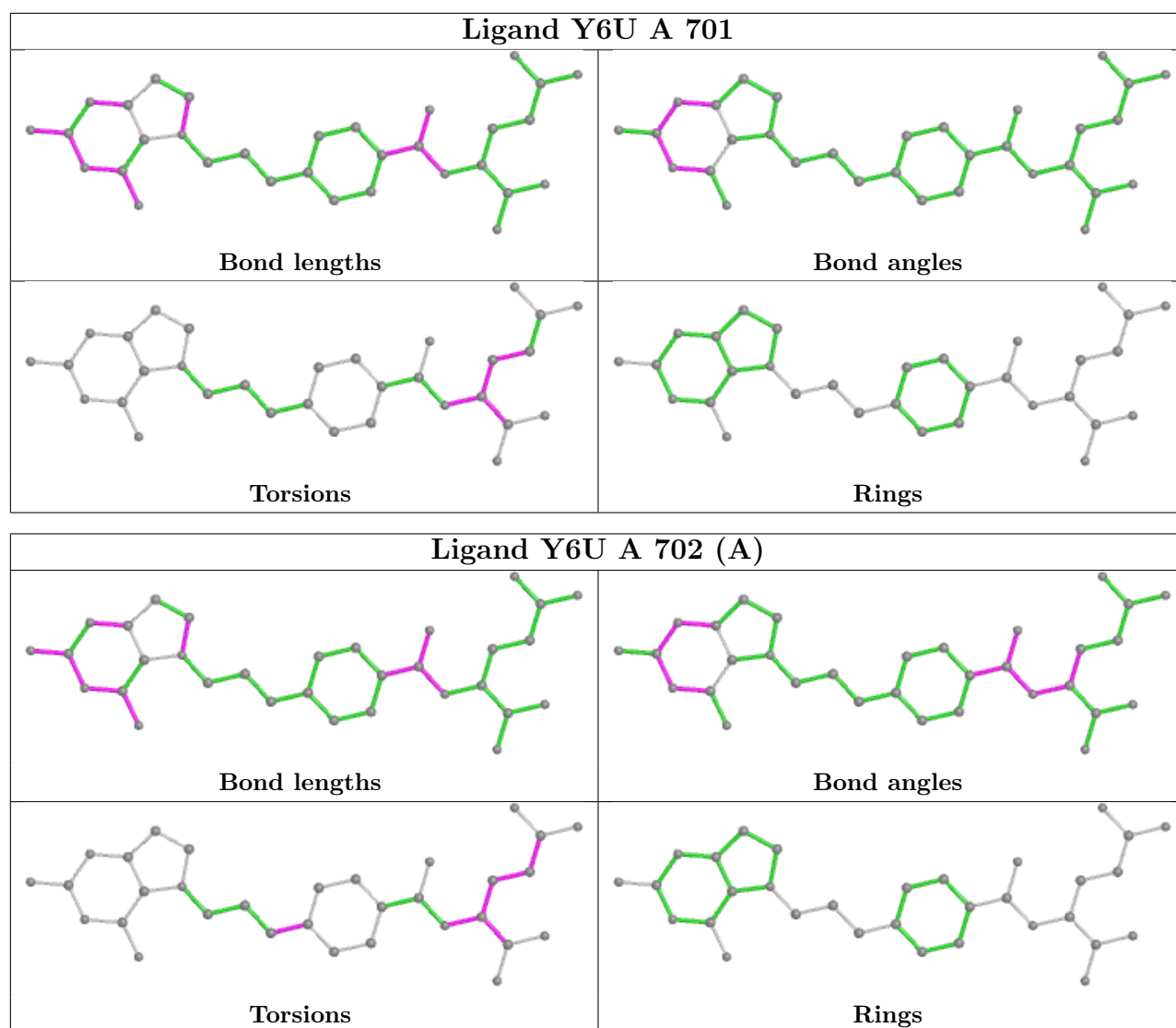
Mol	Chain	Res	Type	Atoms
3	A	702[A]	Y6U	C21-C20-N19-C17
3	A	701	Y6U	C26-C20-C21-C22
3	A	701	Y6U	N19-C20-C21-C22
3	A	701	Y6U	C21-C20-N19-C17
3	A	702[A]	Y6U	C26-C20-C21-C22
3	A	702[A]	Y6U	C20-C21-C22-C23
3	A	702[A]	Y6U	N19-C20-C21-C22
3	A	701	Y6U	C26-C20-N19-C17
3	A	701	Y6U	C21-C20-C26-O27
3	A	701	Y6U	C21-C20-C26-O28
3	A	701	Y6U	C20-C21-C22-C23
3	A	702[A]	Y6U	C21-C20-C26-O28
3	A	702[A]	Y6U	C21-C22-C23-O25
3	A	702[A]	Y6U	C21-C22-C23-O24
3	A	702[A]	Y6U	C30-C31-C32-C16
3	A	702[A]	Y6U	C30-C31-C32-C15
3	A	702[A]	Y6U	C21-C20-C26-O27

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	602	PLP	1	0
2	A	601[B]	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	462/493 (93%)	-0.15	16 (3%) 44 18	18, 36, 73, 109	0
1	B	462/493 (93%)	0.14	25 (5%) 25 9	22, 51, 90, 128	0
All	All	924/986 (93%)	-0.01	41 (4%) 34 13	18, 42, 85, 128	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	298	ALA	5.1
1	A	299	VAL	4.5
1	B	307	ILE	4.2
1	A	303	THR	4.2
1	B	304	GLY	4.1
1	A	306	GLU	3.9
1	B	296	VAL	3.7
1	A	305	ARG	3.6
1	B	473	LEU	3.6
1	A	307	ILE	3.5
1	B	299	VAL	3.3
1	B	474	LYS	3.1
1	A	304	GLY	3.1
1	B	298	ALA	3.0
1	B	471	PHE	3.0
1	B	301	PRO	2.8
1	B	303	THR	2.8
1	A	301	PRO	2.8
1	B	417	SER	2.7
1	B	399	VAL	2.7
1	B	483	ALA	2.7
1	A	302	LYS	2.6
1	B	302	LYS	2.6
1	B	306	GLU	2.6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	467	ASP	2.6
1	B	297	LYS	2.5
1	B	413	PRO	2.5
1	B	462	THR	2.5
1	B	463	ALA	2.4
1	A	460	SER	2.3
1	A	417	SER	2.3
1	A	463	ALA	2.3
1	B	482	LEU	2.2
1	A	418	ALA	2.2
1	A	352	LEU	2.2
1	A	437	ARG	2.2
1	B	481	ARG	2.1
1	B	476	SER	2.1
1	B	480	GLN	2.1
1	A	345	PRO	2.1
1	B	457	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](#)

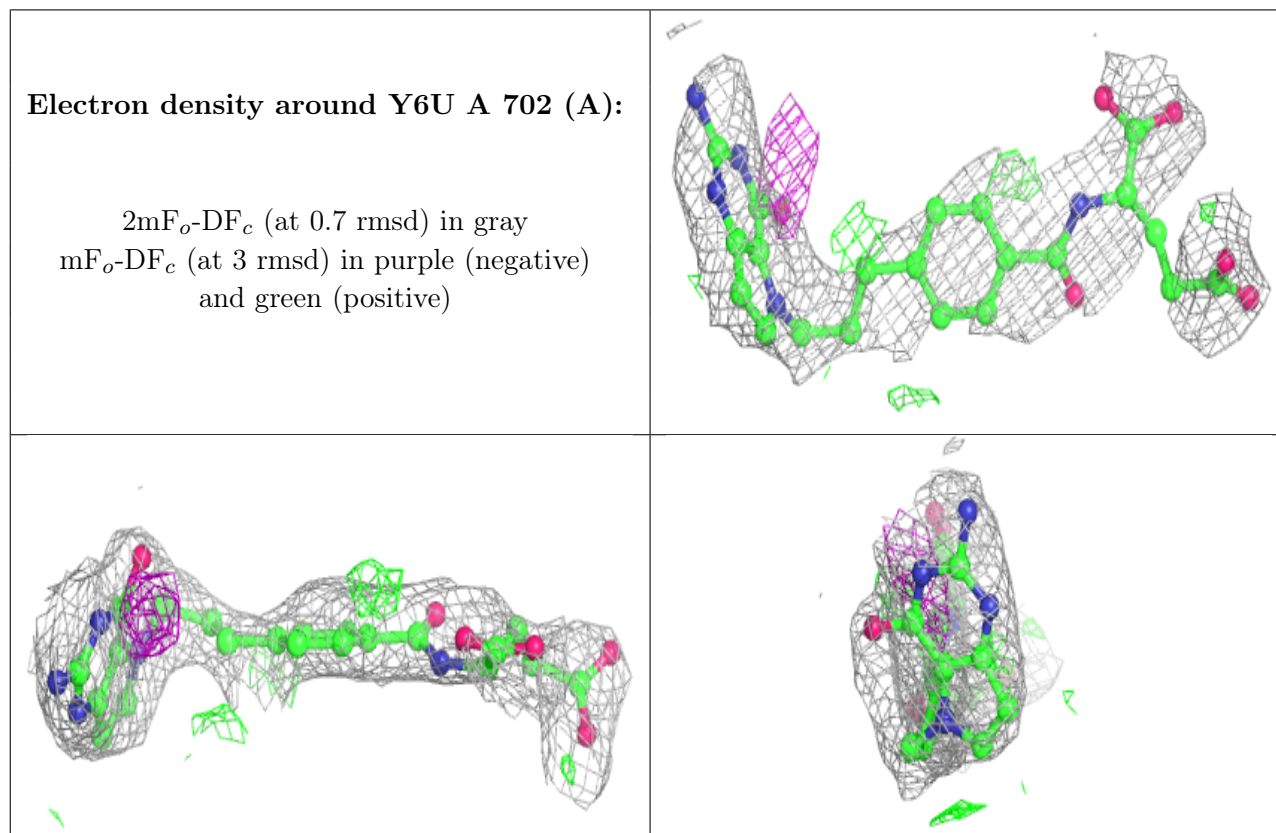
There are no monosaccharides in this entry.

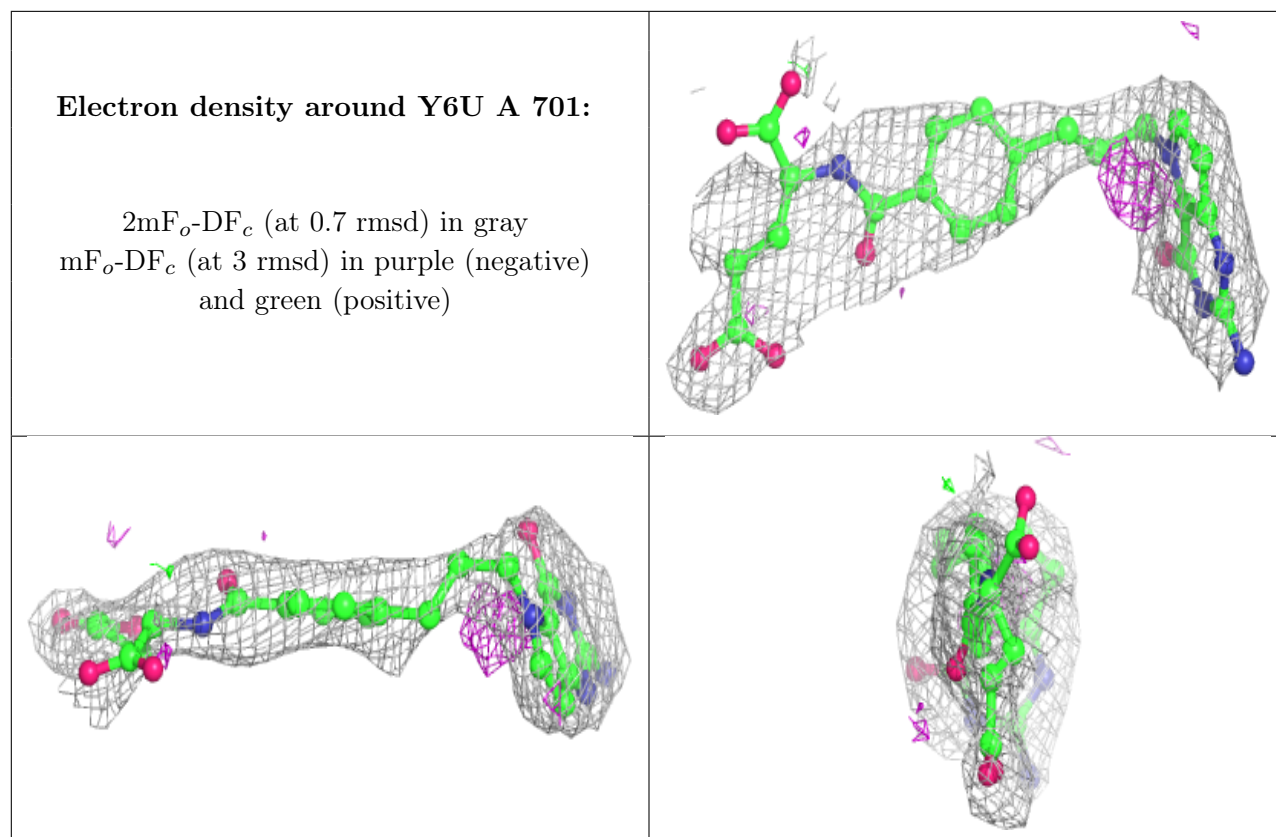
## 6.4 Ligands [i](#)

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
3	Y6U	A	702[A]	32/32	0.83	0.25	55,70,102,106	0
3	Y6U	A	701	32/32	0.90	0.23	42,57,112,117	0
2	GLY	B	601	5/5	0.92	0.26	51,56,62,70	0
2	GLY	A	601[B]	5/5	0.96	0.25	38,42,65,67	5
4	PLP	A	602[B]	15/16	0.96	0.23	17,46,59,60	0
4	PLP	B	602	15/16	0.96	0.20	29,40,50,56	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.