



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 24, 2026 – 07:31 AM UTC

PDB ID : 8FJT / pdb_00008fjt
Title : Human mitochondrial serine hydroxymethyltransferase (SHMT2) in complex with PLP, glycine and AGF362 inhibitor
Authors : Katinas, J.M.; Dann III, C.E.
Deposited on : 2022-12-20
Resolution : 2.47 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 ⓘ 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

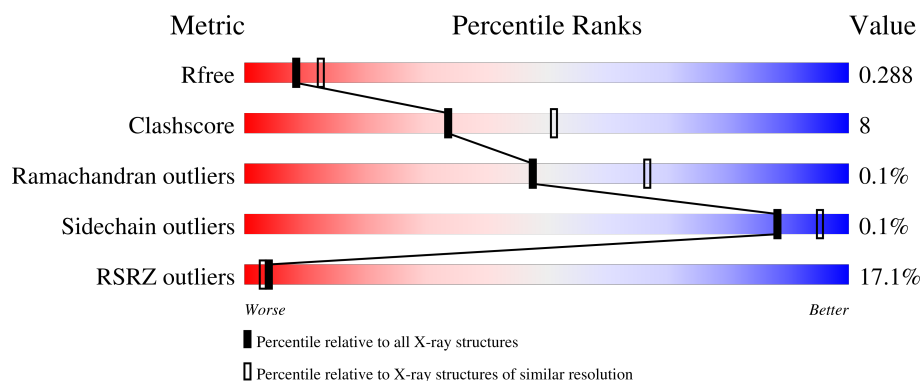
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.47 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	7589 (2.50-2.46)
Clashscore	190562	8295 (2.50-2.46)
Ramachandran outliers	187476	8164 (2.50-2.46)
Sidechain outliers	187428	8166 (2.50-2.46)
RSRZ outliers	180081	7593 (2.50-2.46)

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	493	3% 78% 14% 8%
1	B	493	28% 72% 19% 9%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7373 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
1	A	455	Total	C	N	O	S	0	1	0
			3553	2239	637	661	16			
1	B	451	Total	C	N	O	S	0	1	0
			3472	2184	624	648	16			

There are 34 discrepancies between the modelled and reference sequences:

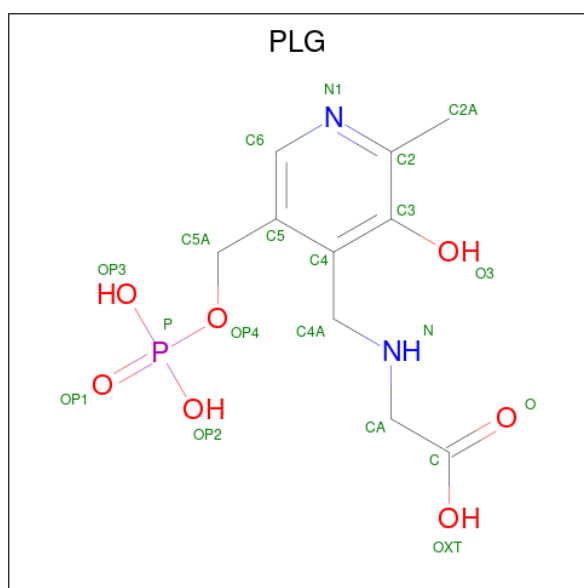
Chain	Residue	Modelled	Actual	Comment	Reference
A	12	MET	-	initiating methionine	UNP P34897
A	13	GLY	-	expression tag	UNP P34897
A	14	SER	-	expression tag	UNP P34897
A	15	SER	-	expression tag	UNP P34897
A	16	HIS	-	expression tag	UNP P34897
A	17	HIS	-	expression tag	UNP P34897
A	18	HIS	-	expression tag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

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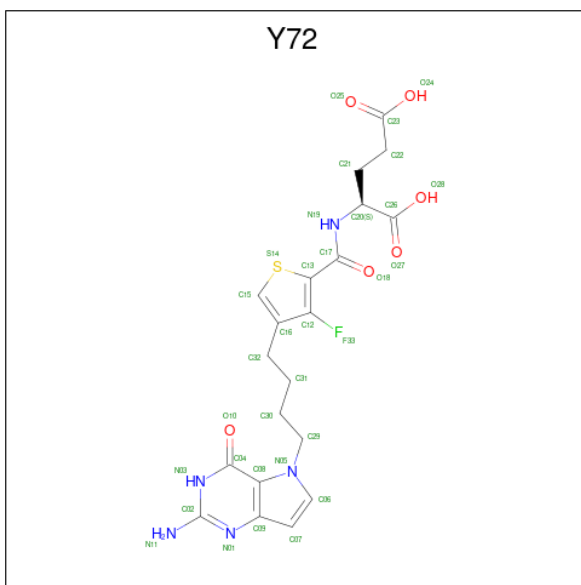
Chain	Residue	Modelled	Actual	Comment	Reference
B	20	HIS	-	expression tag	UNP P34897
B	21	HIS	-	expression tag	UNP P34897
B	22	SER	-	expression tag	UNP P34897
B	23	SER	-	expression tag	UNP P34897
B	24	GLY	-	expression tag	UNP P34897
B	25	LEU	-	expression tag	UNP P34897
B	26	VAL	-	expression tag	UNP P34897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

- Molecule 2 is N-GLYCINE-[3-HYDROXY-2-METHYL-5-PHOSPHONOOXYMETHYL-PYRIDIN-4-YL-METHANE] (CCD ID: PLG) (formula: C₁₀H₁₅N₂O₇P).



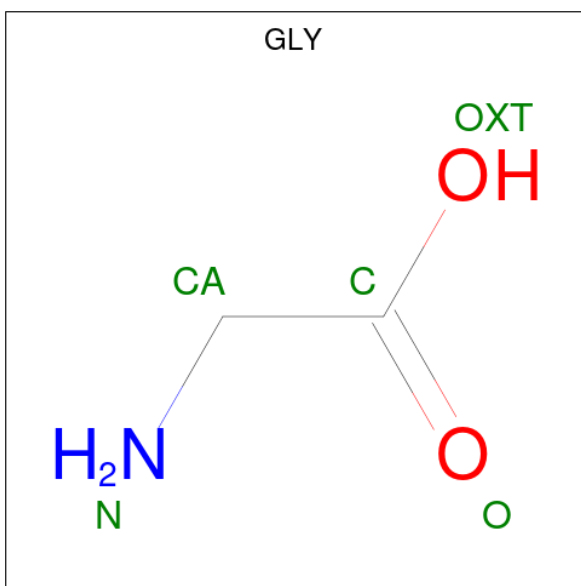
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			20	10	2	7	1		

- Molecule 3 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 (CCD ID: Y72) (formula: C₂₀H₂₂FN₅O₆S) (labeled as "Ligand of Interest" by depositor).



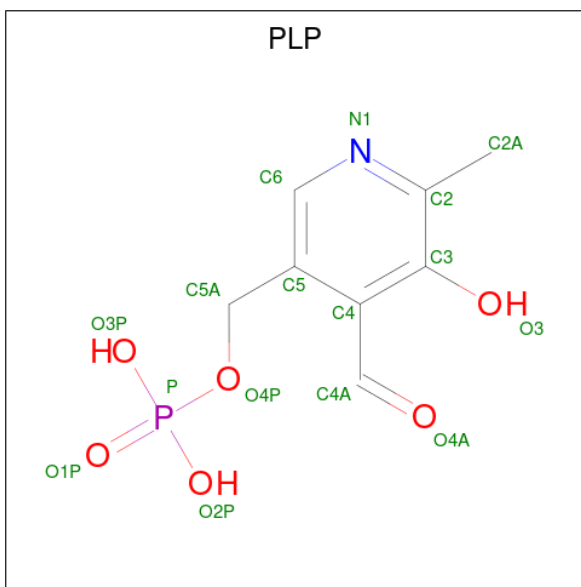
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total 33	C 20	F 1	N 5	O 6	S 1	0	0
3	B	1	Total 33	C 20	F 1	N 5	O 6	S 1	0	0

- Molecule 4 is GLYCINE (CCD ID: GLY) (formula: $\text{C}_2\text{H}_5\text{NO}_2$).



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

- Molecule 5 is PYRIDOXAL-5'-PHOSPHATE (CCD ID: PLP) (formula: $\text{C}_8\text{H}_{10}\text{NO}_6\text{P}$).



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

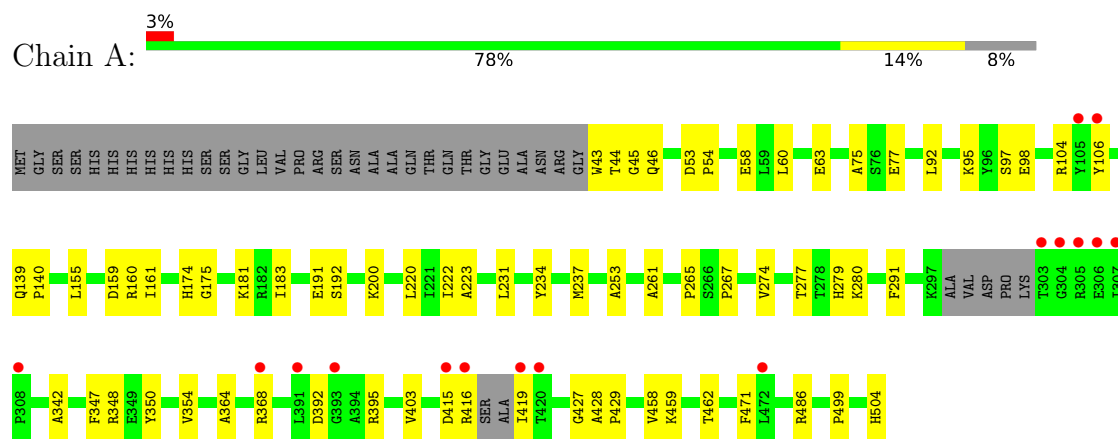
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	148	Total	O	0	0
			148	148		
6	B	94	Total	O	0	0
			94	94		

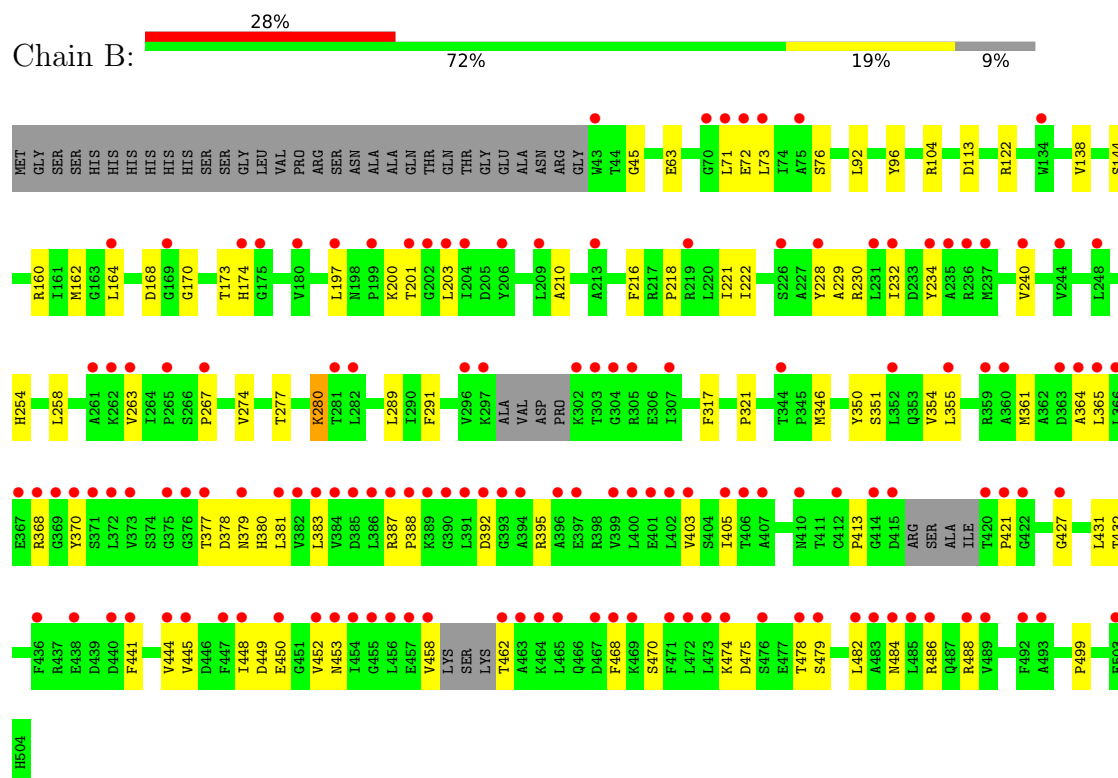
3 Residue-property plots [i](#)

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, α , β , γ	160.39Å 160.39Å 208.75Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.85 – 2.47 48.85 – 2.47	Depositor EDS
% Data completeness (in resolution range)	99.6 (48.85-2.47) 99.5 (48.85-2.47)	Depositor EDS
R_{merge}	0.29	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.21 (at 2.48Å)	Xtriage
Refinement program	PHENIX 1.13-2998	Depositor
R, R_{free}	0.241 , 0.285 0.246 , 0.288	Depositor DCC
R_{free} test set	2806 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	43.6	Xtriage
Anisotropy	0.403	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 33.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	7373	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.79% 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: Y72, PLP, PLG

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	0.10	0/3623	0.31	0/4897
1	B	0.13	0/3540	0.35	0/4789
All	All	0.12	0/7163	0.33	0/9686

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

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	3553	0	3528	42	0
1	B	3472	0	3402	74	0
2	A	20	0	11	1	0
3	A	33	0	0	0	0
3	B	33	0	0	0	0
4	B	5	0	2	2	0
5	B	15	0	6	0	0
6	A	148	0	0	1	0
6	B	94	0	0	0	0
All	All	7373	0	6949	108	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 8.

All (108) 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:361:MET:O	1:B:365:LEU:HD23	1.61	1.01
1:B:361:MET:O	1:B:365:LEU:CD2	2.37	0.72
1:B:450:GLU:OE2	1:B:488:ARG:NH2	2.23	0.71
1:A:44:THR:HG23	1:A:46:GLN:H	1.54	0.71
1:B:263:VAL:HG11	1:B:355:LEU:HD13	1.72	0.70
1:B:73:LEU:HD13	1:B:448:ILE:HD11	1.75	0.69
1:B:370:TYR:OH	1:B:452:VAL:HG21	1.93	0.68
1:B:484:ASN:OD1	1:B:488:ARG:NH1	2.28	0.66
1:A:97:SER:O	1:A:104:ARG:NH1	2.32	0.62
1:B:230:ARG:NH1	1:B:378:ASP:OD2	2.34	0.60
1:B:104:ARG:NE	1:B:113:ASP:OD1	2.31	0.59
1:B:361:MET:HG3	1:B:365:LEU:CD2	2.31	0.59
1:B:277:THR:HG21	1:B:280[B]:LYS:HE2	1.84	0.59
1:B:470:SER:HB3	1:B:474:LYS:HD2	1.86	0.58
1:B:73:LEU:O	1:B:427:GLY:N	2.38	0.56
1:B:392:ASP:OD1	1:B:392:ASP:N	2.37	0.55
1:B:160:ARG:HB2	1:B:218:PRO:HA	1.90	0.54
1:B:274:VAL:HB	1:B:291:PHE:HB2	1.90	0.54
1:B:162:MET:HB2	1:B:221:ILE:HG12	1.91	0.53
1:B:361:MET:HG3	1:B:365:LEU:HD21	1.91	0.53
1:B:387:ARG:HG2	1:B:388:PRO:HD3	1.92	0.52
1:A:92:LEU:HD23	1:B:63:GLU:HG2	1.93	0.51
1:B:403:VAL:HA	1:B:486:ARG:HB2	1.92	0.51
1:A:53:ASP:OD2	1:B:122:ARG:NH1	2.43	0.51
1:A:75:ALA:HA	1:A:427:GLY:HA3	1.93	0.51
1:B:403:VAL:HG23	1:B:405:ILE:HD12	1.93	0.51
1:B:458:VAL:O	1:B:462:THR:HG23	2.11	0.50
1:A:459:LYS:HA	1:A:462:THR:HG22	1.93	0.50
1:A:253:ALA:HB1	1:A:280:LYS:HZ2	1.75	0.50
1:A:45:GLY:HA3	1:B:499:PRO:HB3	1.94	0.50
1:B:368:ARG:HH22	1:B:453:ASN:ND2	2.10	0.50
1:B:395:ARG:HB3	1:B:468:PHE:CE2	2.46	0.50
1:B:479:SER:O	1:B:482:LEU:HB2	2.12	0.50
1:B:380:HIS:CE1	1:B:381:LEU:HD23	2.48	0.49
1:B:228:TYR:HA	1:B:383:LEU:HD11	1.95	0.48
1:A:155:LEU:HB3	1:A:159:ASP:HB2	1.96	0.48
1:A:175:GLY:O	1:A:192:SER:OG	2.19	0.48
1:A:60:LEU:HD23	1:A:504:HIS:HB2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:98:GLU:OE2	1:A:106:TYR:OH	2.27	0.48
1:B:228:TYR:O	1:B:379:ASN:ND2	2.44	0.48
1:B:361:MET:C	1:B:365:LEU:HD23	2.37	0.47
1:B:364:ALA:HB1	1:B:445:VAL:HG21	1.96	0.47
1:B:201:THR:HG23	1:B:203:LEU:H	1.79	0.47
1:A:160:ARG:HA	1:A:191:GLU:O	2.15	0.47
1:A:364:ALA:O	1:A:368[B]:ARG:HG2	2.15	0.47
1:B:441:PHE:O	1:B:445:VAL:HG13	2.15	0.47
1:A:416:ARG:H	1:A:419:ILE:HD12	1.79	0.46
1:B:449:ASP:HA	1:B:452:VAL:HG22	1.97	0.46
1:B:144:SER:HA	1:B:173:THR:HG21	1.96	0.46
1:A:231:LEU:HD13	1:A:265:PRO:HD2	1.97	0.46
1:B:475:ASP:HB3	1:B:478:THR:HB	1.98	0.46
1:A:63:GLU:HG2	1:B:92:LEU:HD23	1.97	0.46
1:B:71:LEU:HD13	1:B:444:VAL:HG22	1.98	0.46
1:A:415:ASP:OD1	1:A:415:ASP:N	2.41	0.45
1:B:351:SER:HA	1:B:354:VAL:HG23	1.98	0.45
1:B:254:HIS:HE1	4:B:802[B]:GLY:OXT	1.98	0.45
1:B:168:ASP:HB3	1:B:197:LEU:HG	1.99	0.45
1:B:232:ILE:HB	1:B:234:TYR:CZ	2.52	0.45
1:B:350:TYR:O	1:B:354:VAL:HG23	2.17	0.45
1:A:54:PRO:O	1:A:58:GLU:HG2	2.17	0.45
2:A:601:PLG:H5A1	2:A:601:PLG:H4A1	1.75	0.45
1:A:200:LYS:NZ	6:A:709:HOH:O	2.48	0.45
1:B:104:ARG:HH21	1:B:113:ASP:HA	1.82	0.44
1:A:234:TYR:CZ	1:A:267:PRO:HB3	2.53	0.44
1:A:261:ALA:HB1	1:A:348:ARG:HA	1.98	0.44
1:B:160:ARG:HB3	1:B:216:PHE:CE2	2.52	0.44
1:A:77:GLU:OE1	1:B:96:TYR:N	2.37	0.44
1:A:181:LYS:HE3	1:B:317:PHE:CZ	2.53	0.44
1:A:183:ILE:HG23	1:B:321:PRO:HG2	1.99	0.44
1:B:395:ARG:HB3	1:B:468:PHE:CZ	2.51	0.44
1:A:43:TRP:HB2	1:B:346:MET:HG3	1.99	0.44
1:A:223:ALA:HB2	1:A:237:MET:HE2	2.00	0.44
1:B:229:ALA:HB2	1:B:383:LEU:HG	2.00	0.44
1:B:361:MET:HG3	1:B:365:LEU:HD23	1.99	0.44
1:B:368:ARG:CZ	1:B:449:ASP:CB	2.96	0.43
1:A:342:ALA:HA	1:A:347:PHE:CG	2.54	0.43
1:B:76:SER:O	1:B:280[B]:LYS:HA	2.19	0.43
1:A:95:LYS:HA	1:A:95:LYS:HD2	1.89	0.43
1:A:428:ALA:H	1:A:429:PRO:HD3	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:138:VAL:HA	1:B:289:LEU:HD23	2.01	0.42
1:A:277:THR:HB	1:A:279:HIS:CE1	2.54	0.42
1:A:139:GLN:N	1:A:140:PRO:CD	2.83	0.42
1:A:458:VAL:HG13	1:A:471:PHE:CD2	2.53	0.42
1:B:72:GLU:H	1:B:431:LEU:HD21	1.85	0.42
1:A:106:TYR:OH	4:B:802[B]:GLY:HA3	2.19	0.42
1:B:230:ARG:HD3	1:B:230:ARG:HA	1.87	0.42
1:A:428:ALA:N	1:A:429:PRO:CD	2.82	0.42
1:B:162:MET:HG3	1:B:218:PRO:HB3	2.01	0.42
1:B:484:ASN:O	1:B:488:ARG:HG3	2.20	0.42
1:B:475:ASP:O	1:B:479:SER:N	2.47	0.42
1:B:200:LYS:HA	1:B:200:LYS:HD3	1.75	0.42
1:B:346:MET:HE3	1:B:346:MET:HB3	1.92	0.42
1:B:174:HIS:CD2	1:B:222:ILE:HG21	2.55	0.41
1:A:403:VAL:HA	1:A:486:ARG:HB2	2.01	0.41
1:B:164:LEU:HD23	1:B:170:GLY:N	2.34	0.41
1:A:350:TYR:O	1:A:354:VAL:HG23	2.21	0.41
1:B:229:ALA:HB1	1:B:377:THR:HA	2.03	0.41
1:A:161:ILE:HD13	1:A:220:LEU:HB3	2.02	0.41
1:A:274:VAL:HB	1:A:291:PHE:HB2	2.02	0.41
1:B:210:ALA:HB2	1:B:240:VAL:HG22	2.02	0.41
1:B:234:TYR:CZ	1:B:267:PRO:HB3	2.55	0.41
1:B:258:LEU:HD22	1:B:355:LEU:HD11	2.02	0.41
1:B:354:VAL:HG22	1:B:432:THR:HG21	2.02	0.41
1:B:392:ASP:HB2	1:B:421:PRO:O	2.21	0.41
1:A:174:HIS:CD2	1:A:222:ILE:HG21	2.56	0.40
1:A:392:ASP:OD1	1:A:395:ARG:HD2	2.22	0.40
1:B:368:ARG:HH22	1:B:453:ASN:CG	2.30	0.40
1:A:499:PRO:HB3	1:B:45:GLY:HA3	2.02	0.40

There are no symmetry-related clashes.

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	450/493 (91%)	433 (96%)	17 (4%)	0	100	100
1	B	443/493 (90%)	410 (93%)	32 (7%)	1 (0%)	43	61
All	All	893/986 (91%)	843 (94%)	49 (6%)	1 (0%)	48	66

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	413	PRO

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	373/405 (92%)	373 (100%)	0	100	100
1	B	358/405 (88%)	357 (100%)	1 (0%)	86	93
All	All	731/810 (90%)	730 (100%)	1 (0%)	88	95

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	280[B]	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	329	ASN
1	A	466	GLN
1	B	46	GLN

5.3.3 RNA ⓘ

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](#)

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	PLG	A	601	-	20,20,20	2.46	3 (15%)	26,28,28	1.78	6 (23%)
3	Y72	A	602	-	33,35,35	2.98	13 (39%)	40,49,49	2.28	10 (25%)
4	GLY	B	802[B]	-	4,4,4	0.97	0	3,4,4	1.07	0
3	Y72	B	801	-	33,35,35	3.00	13 (39%)	40,49,49	2.33	12 (30%)
5	PLP	B	803[B]	1	15,15,16	0.77	1 (6%)	21,22,23	0.64	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	PLG	A	601	-	-	3/12/12/12	0/1/1/1
3	Y72	A	602	-	-	8/24/24/24	0/3/3/3
4	GLY	B	802[B]	-	-	2/2/2/2	-
3	Y72	B	801	-	-	5/24/24/24	0/3/3/3
5	PLP	B	803[B]	1	-	0/6/6/8	0/1/1/1

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	801	Y72	O10-C04	8.91	1.40	1.23
3	A	602	Y72	O10-C04	8.82	1.40	1.23
2	A	601	PLG	C3-C2	7.30	1.48	1.41
3	A	602	Y72	O27-C26	6.17	1.40	1.22
3	B	801	Y72	O27-C26	6.16	1.40	1.22
3	B	801	Y72	C17-N19	5.74	1.46	1.34
3	A	602	Y72	O25-C23	5.66	1.40	1.22
3	A	602	Y72	C17-N19	5.65	1.46	1.34
3	B	801	Y72	O25-C23	5.63	1.40	1.22
2	A	601	PLG	C3-C4	5.39	1.48	1.40
2	A	601	PLG	C5-C4	5.38	1.48	1.40
3	B	801	Y72	C02-N11	4.90	1.45	1.34
3	A	602	Y72	C02-N11	4.89	1.45	1.34
3	B	801	Y72	C15-C16	4.65	1.40	1.36
3	A	602	Y72	C15-C16	4.62	1.40	1.36
3	A	602	Y72	O28-C26	3.18	1.40	1.30
3	B	801	Y72	O28-C26	3.16	1.40	1.30
3	B	801	Y72	C04-N03	-3.13	1.33	1.38
3	A	602	Y72	C04-N03	-3.10	1.33	1.38
3	A	602	Y72	O24-C23	2.87	1.40	1.30
3	B	801	Y72	O24-C23	2.86	1.40	1.30
3	B	801	Y72	C16-C12	2.60	1.43	1.39
3	B	801	Y72	O18-C17	-2.55	1.18	1.23
3	A	602	Y72	C16-C12	2.50	1.43	1.39
3	A	602	Y72	C06-N05	-2.45	1.32	1.38
5	B	803[B]	PLP	C4A-C4	-2.44	1.46	1.51
3	A	602	Y72	O18-C17	-2.38	1.19	1.23
3	B	801	Y72	C06-N05	-2.36	1.32	1.38
3	B	801	Y72	C13-S14	-2.10	1.69	1.72
3	A	602	Y72	C13-S14	-2.04	1.69	1.72

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	801	Y72	C16-C15-S14	-6.18	106.50	113.46
3	B	801	Y72	C15-S14-C13	6.06	99.09	91.78
3	A	602	Y72	C16-C15-S14	-6.02	106.69	113.46
3	A	602	Y72	C15-S14-C13	5.93	98.92	91.78
3	B	801	Y72	C08-C09-N01	-5.34	119.69	124.81
3	A	602	Y72	C08-C09-N01	-5.17	119.85	124.81
3	A	602	Y72	C09-C08-C04	-4.84	117.50	121.36
3	A	602	Y72	C08-C04-N03	4.79	119.38	110.94
3	B	801	Y72	C08-C04-N03	4.74	119.29	110.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	801	Y72	C09-C08-C04	-4.58	117.71	121.36
2	A	601	PLG	C4A-N-CA	4.25	117.67	112.72
3	B	801	Y72	C07-C09-N01	3.26	134.09	123.36
3	A	602	Y72	C07-C09-N01	3.24	134.02	123.36
2	A	601	PLG	C5A-C5-C4	-2.90	116.55	122.67
2	A	601	PLG	C5A-C5-C6	2.72	123.80	119.36
3	A	602	Y72	O10-C04-C08	-2.68	121.05	127.62
2	A	601	PLG	OP4-C5A-C5	2.64	114.30	109.36
3	B	801	Y72	C13-C17-N19	2.63	119.41	115.99
3	B	801	Y72	C29-N05-C08	-2.61	124.58	128.85
3	B	801	Y72	O10-C04-C08	-2.49	121.51	127.62
3	B	801	Y72	O28-C26-O27	-2.41	118.60	124.08
3	A	602	Y72	C09-N01-C02	2.37	120.35	116.63
3	B	801	Y72	C02-N03-C04	-2.36	120.83	125.11
3	B	801	Y72	C09-N01-C02	2.33	120.28	116.63
3	A	602	Y72	C29-N05-C08	-2.32	125.05	128.85
3	A	602	Y72	C02-N03-C04	-2.31	120.92	125.11
2	A	601	PLG	C6-N1-C2	2.22	123.23	119.20
2	A	601	PLG	C6-C5-C4	2.07	119.62	118.06

There are no chirality outliers.

All (18) torsion outliers are listed below:

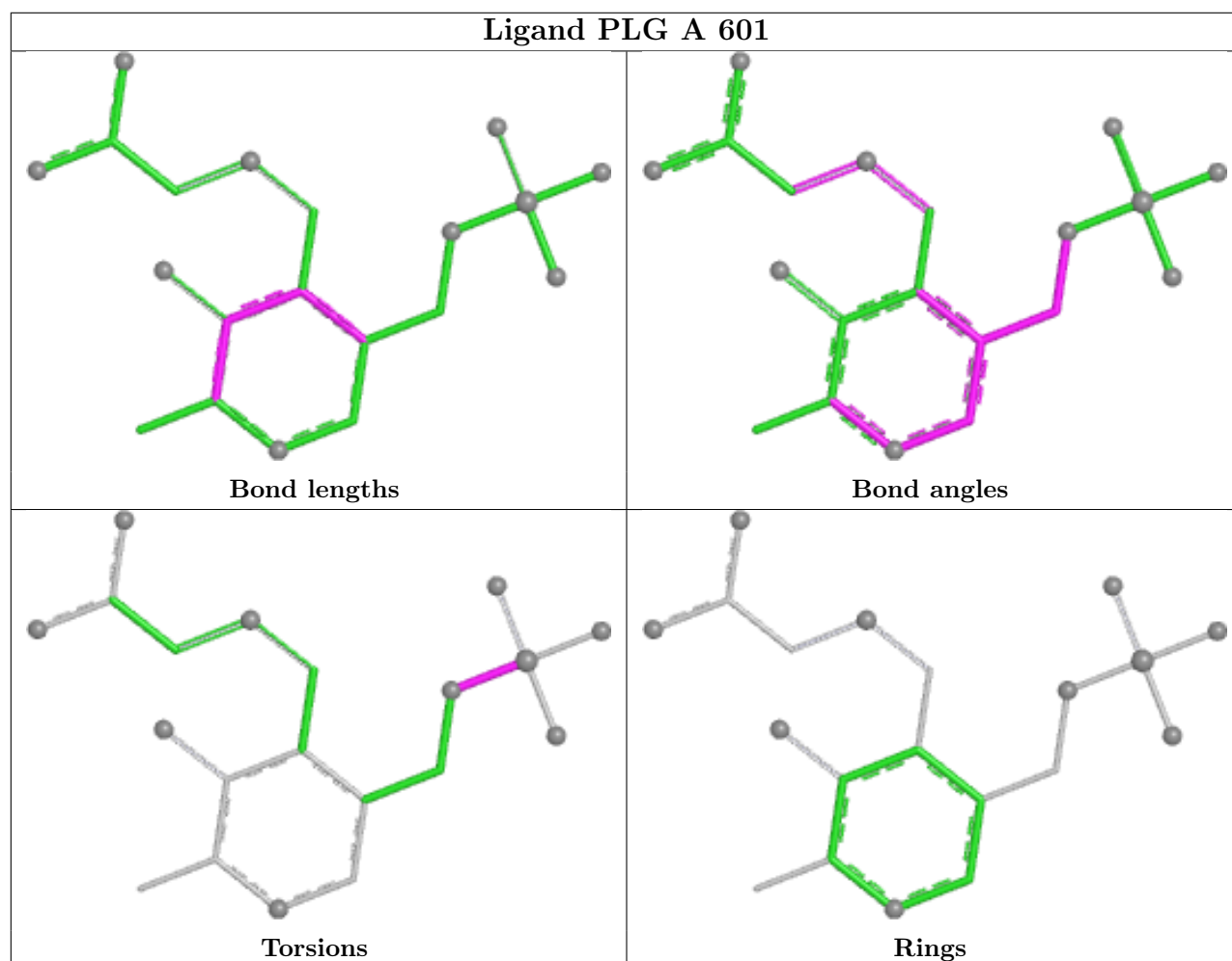
Mol	Chain	Res	Type	Atoms
2	A	601	PLG	C5A-OP4-P-OP1
2	A	601	PLG	C5A-OP4-P-OP2
2	A	601	PLG	C5A-OP4-P-OP3
3	A	602	Y72	N19-C20-C21-C22
4	B	802[B]	GLY	O-C-CA-N
4	B	802[B]	GLY	OXT-C-CA-N
3	B	801	Y72	N19-C20-C21-C22
3	A	602	Y72	C26-C20-C21-C22
3	B	801	Y72	N19-C20-C26-O27
3	B	801	Y72	C26-C20-C21-C22
3	A	602	Y72	N19-C20-C26-O28
3	A	602	Y72	N19-C20-C26-O27
3	B	801	Y72	N19-C20-C26-O28
3	A	602	Y72	C21-C20-C26-O28
3	B	801	Y72	C21-C20-C26-O27
3	A	602	Y72	C21-C20-N19-C17
3	A	602	Y72	C21-C20-C26-O27
3	A	602	Y72	C12-C13-C17-O18

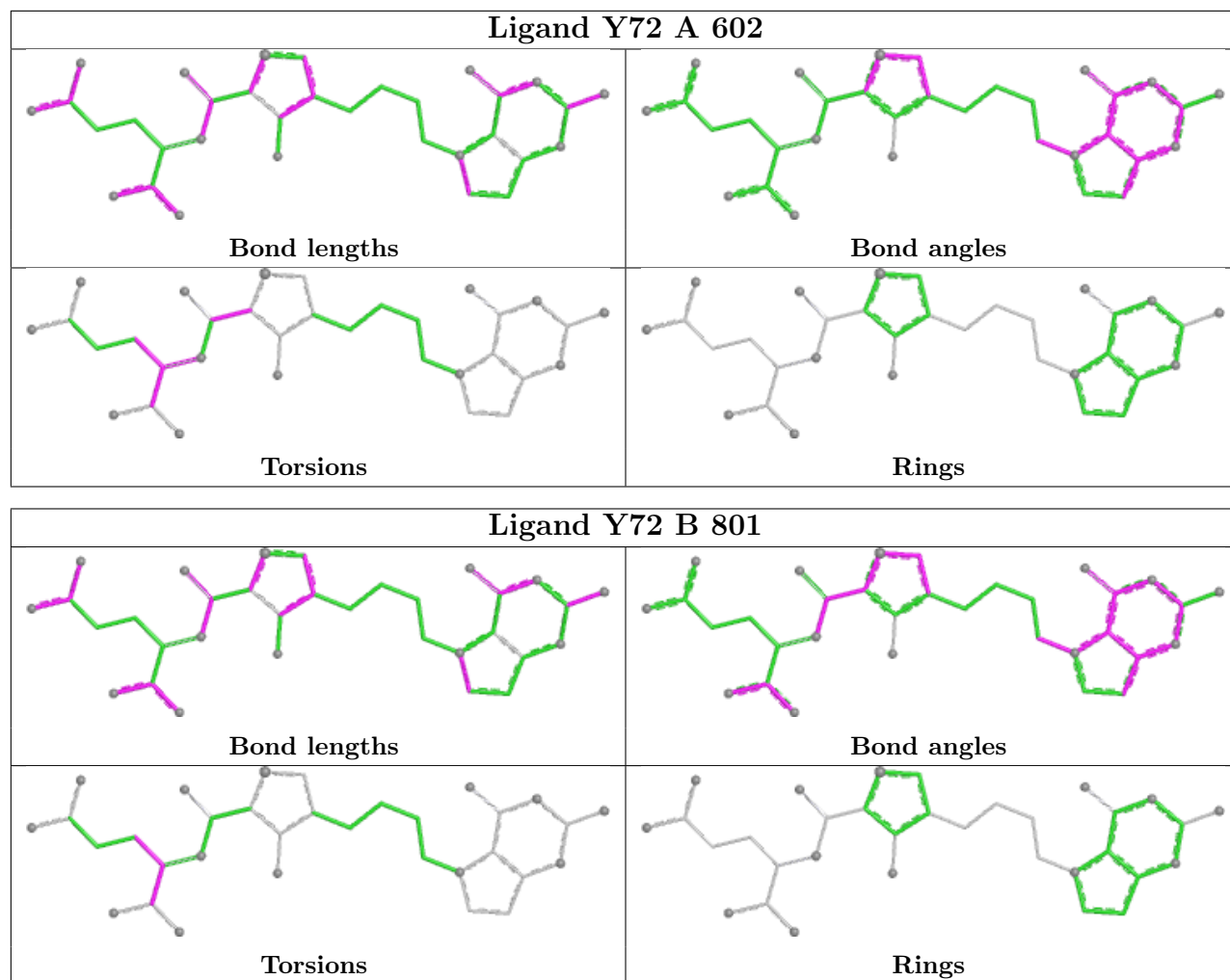
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	PLG	1	0
4	B	802[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, 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	455/493 (92%)	0.28	16 (3%)	47 43	25, 39, 70, 108	1 (0%)
1	B	451/493 (91%)	1.45	139 (30%)	1 1	31, 59, 91, 120	0
All	All	906/986 (91%)	0.86	155 (17%)	4 3	25, 47, 80, 120	1 (0%)

All (155) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	303	THR	7.0
1	B	456	LEU	6.0
1	B	448	ILE	5.7
1	B	302	LYS	5.1
1	B	396	ALA	5.0
1	B	462	THR	4.9
1	B	403	VAL	4.8
1	B	458	VAL	4.8
1	A	305	ARG	4.7
1	A	416	ARG	4.7
1	B	482	LEU	4.5
1	B	452	VAL	4.5
1	B	472	LEU	4.5
1	B	307	ILE	4.4
1	A	420	THR	4.3
1	B	305	ARG	4.3
1	A	304	GLY	4.3
1	B	415	ASP	4.2
1	B	201	THR	4.2
1	B	391	LEU	4.2
1	B	399	VAL	4.2
1	B	303	THR	4.1
1	B	468	PHE	4.0
1	B	412	CYS	4.0

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Mol	Chain	Res	Type	RSRZ
1	B	369	GLY	4.0
1	B	366	LEU	3.9
1	B	471	PHE	3.9
1	B	263	VAL	3.9
1	B	204	ILE	3.8
1	B	383	LEU	3.8
1	B	420	THR	3.8
1	A	415	ASP	3.8
1	B	370	TYR	3.7
1	B	384	VAL	3.5
1	B	465	LEU	3.4
1	B	371	SER	3.4
1	B	261	ALA	3.4
1	B	463	ALA	3.3
1	B	485	LEU	3.3
1	A	419	ILE	3.3
1	B	441	PHE	3.3
1	A	106	TYR	3.2
1	B	372	LEU	3.2
1	B	231	LEU	3.2
1	B	469	LYS	3.2
1	B	397	GLU	3.1
1	B	368	ARG	3.1
1	B	447	PHE	3.0
1	B	202	GLY	3.0
1	A	307	ILE	3.0
1	B	244	VAL	3.0
1	B	382	VAL	3.0
1	B	385	ASP	3.0
1	B	71	LEU	3.0
1	B	197	LEU	3.0
1	B	503	GLU	3.0
1	B	213	ALA	3.0
1	B	464	LYS	3.0
1	B	381	LEU	2.9
1	B	394	ALA	2.9
1	B	199	PRO	2.9
1	B	421	PRO	2.9
1	B	206	TYR	2.9
1	B	393	GLY	2.9
1	B	467	ASP	2.9
1	B	234	TYR	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	376	GLY	2.9
1	B	453	ASN	2.8
1	B	454	ILE	2.8
1	B	386	LEU	2.8
1	B	445	VAL	2.8
1	B	355	LEU	2.8
1	B	226	SER	2.7
1	B	389	LYS	2.7
1	B	367	GLU	2.7
1	B	457	GLU	2.7
1	B	388	PRO	2.7
1	B	444	VAL	2.7
1	B	364	ALA	2.7
1	B	377	THR	2.7
1	A	105	TYR	2.7
1	B	344	THR	2.7
1	B	455	GLY	2.7
1	B	175	GLY	2.6
1	B	414	GLY	2.6
1	B	489	VAL	2.6
1	B	304	GLY	2.6
1	B	401	GLU	2.6
1	A	368[A]	ARG	2.5
1	B	392	ASP	2.5
1	B	203	LEU	2.5
1	B	483	ALA	2.5
1	B	407	ALA	2.5
1	B	237	MET	2.5
1	B	474	LYS	2.5
1	B	486	ARG	2.5
1	B	476	SER	2.5
1	B	400	LEU	2.5
1	B	228	TYR	2.4
1	B	359	ARG	2.4
1	B	387	ARG	2.4
1	A	306	GLU	2.4
1	B	473	LEU	2.4
1	B	373	VAL	2.4
1	A	308	PRO	2.4
1	B	390	GLY	2.4
1	B	164	LEU	2.4
1	B	209	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	488	ARG	2.4
1	A	393	GLY	2.3
1	B	436	PHE	2.3
1	B	410	ASN	2.3
1	B	484	ASN	2.3
1	B	70	GLY	2.3
1	B	232	ILE	2.3
1	B	365	LEU	2.3
1	B	262	LYS	2.3
1	B	236	ARG	2.3
1	B	478	THR	2.3
1	B	375	GLY	2.3
1	B	479	SER	2.3
1	B	282	LEU	2.3
1	B	72	GLU	2.3
1	B	267	PRO	2.3
1	B	240	VAL	2.2
1	B	297	LYS	2.2
1	B	73	LEU	2.2
1	B	438	GLU	2.2
1	B	219	ARG	2.2
1	B	169	GLY	2.2
1	B	440	ASP	2.2
1	B	265	PRO	2.2
1	B	281	THR	2.2
1	B	450	GLU	2.2
1	B	75	ALA	2.1
1	A	472	LEU	2.1
1	B	235	ALA	2.1
1	B	427	GLY	2.1
1	B	405	ILE	2.1
1	B	492	PHE	2.1
1	B	180	VAL	2.1
1	B	296	VAL	2.1
1	A	391	LEU	2.1
1	B	134	TRP	2.1
1	B	402	LEU	2.1
1	B	406	THR	2.1
1	B	360	ALA	2.0
1	B	493	ALA	2.0
1	B	352	LEU	2.0
1	B	422	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	248	LEU	2.0
1	B	379	ASN	2.0
1	B	43	TRP	2.0
1	B	363	ASP	2.0
1	B	174	HIS	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

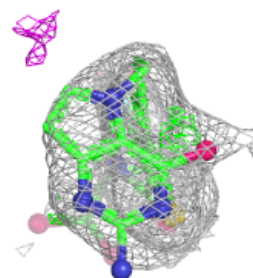
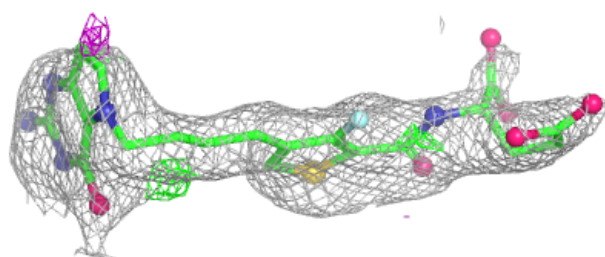
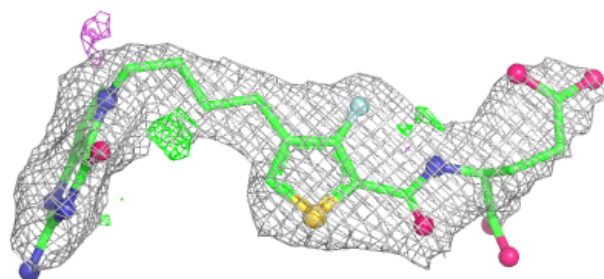
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	GLY	B	802[B]	5/5	0.76	0.19	59,60,66,70	0
3	Y72	A	602	33/33	0.80	0.20	55,64,78,80	33
3	Y72	B	801	33/33	0.89	0.14	35,49,74,75	0
5	PLP	B	803[B]	15/16	0.92	0.15	37,56,63,68	0
2	PLG	A	601	20/20	0.94	0.13	23,35,47,49	0

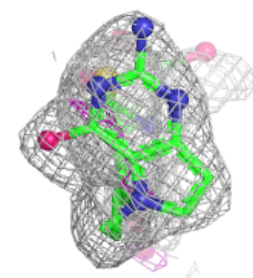
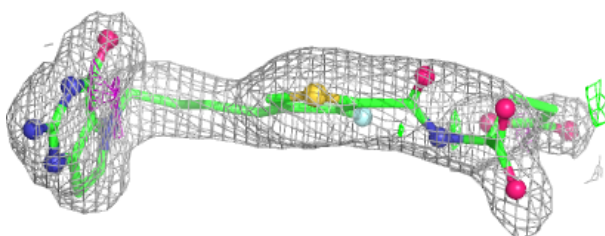
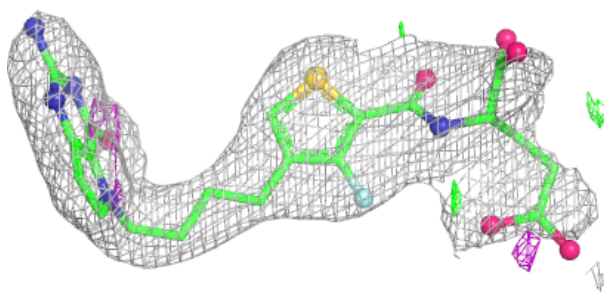
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

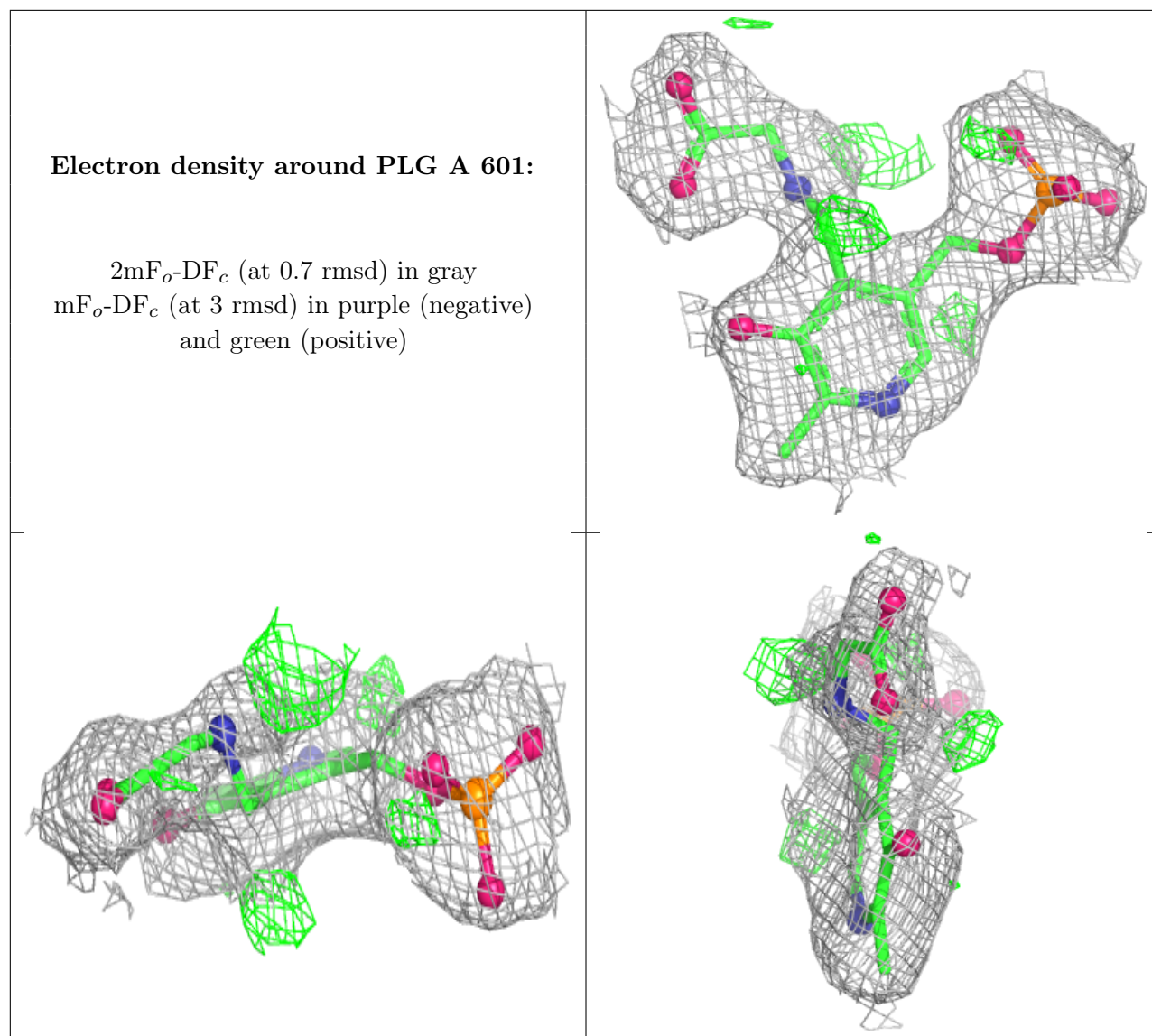
Electron density around Y72 A 602:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around Y72 B 801:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers [i](#)

There are no such residues in this entry.