



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 08:31 AM UTC

PDB ID : 8FJU / pdb_00008fju
Title : Human mitochondrial serine hydroxymethyltransferase (SHMT2) in complex with PLP, glycine and AGF347 inhibitor
Authors : Katinas, J.M.; Dann III, C.E.
Deposited on : 2022-12-20
Resolution : 2.51 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

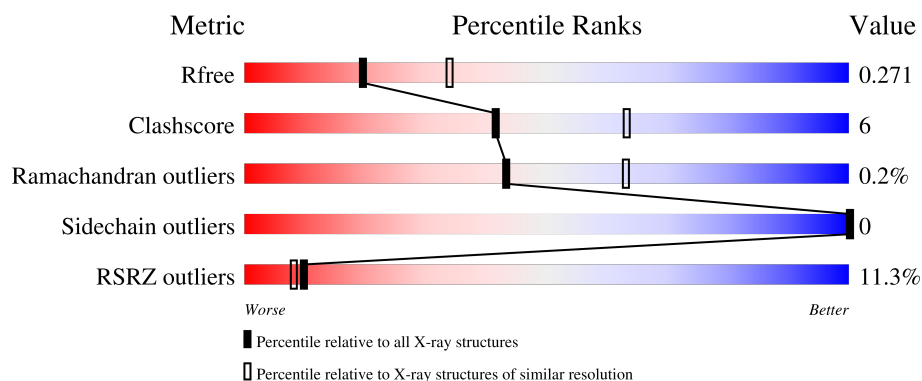
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.51 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	16% 74% 18% 8%
1	B	493	4% 81% 12% 7%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7406 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	456	Total	C	N	O	S	0	0	0
			3501	2204	621	660	16			
1	B	459	Total	C	N	O	S	0	0	0
			3559	2243	640	660	16			

There are 34 discrepancies between the modelled and reference sequences:

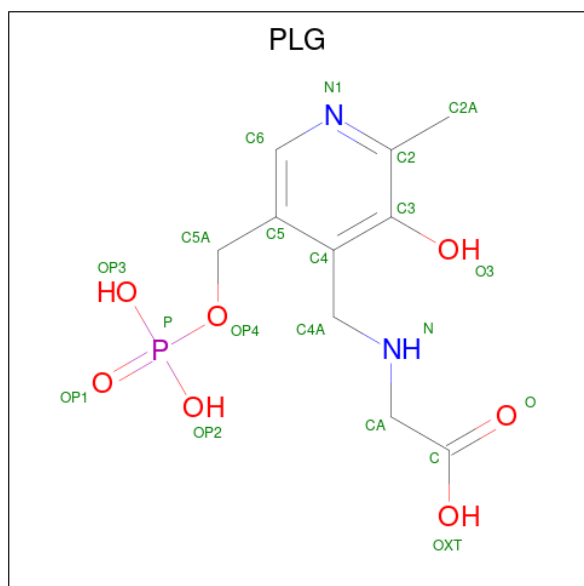
Chain	Residue	Modelled	Actual	Comment	Reference
A	12	MET	-	initiating methionine	UNP P34897
A	13	GLY	-	expression tag	UNP P34897
A	14	SER	-	expression tag	UNP P34897
A	15	SER	-	expression tag	UNP P34897
A	16	HIS	-	expression tag	UNP P34897
A	17	HIS	-	expression tag	UNP P34897
A	18	HIS	-	expression tag	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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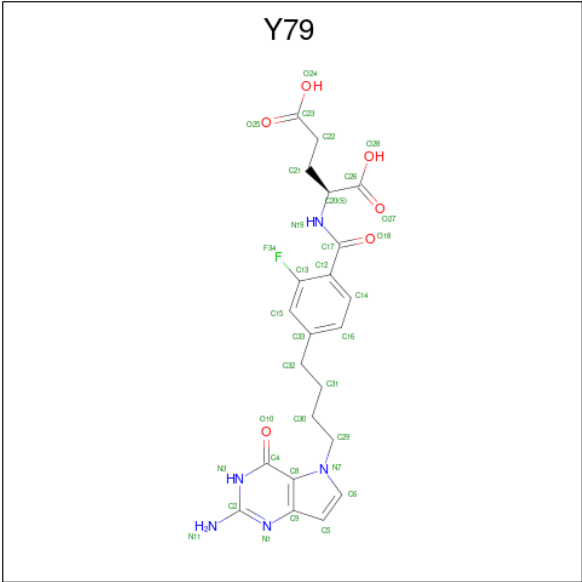
Chain	Residue	Modelled	Actual	Comment	Reference
B	20	HIS	-	expression tag	UNP P34897
B	21	HIS	-	expression tag	UNP P34897
B	22	SER	-	expression tag	UNP P34897
B	23	SER	-	expression tag	UNP P34897
B	24	GLY	-	expression tag	UNP P34897
B	25	LEU	-	expression tag	UNP P34897
B	26	VAL	-	expression tag	UNP P34897
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) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			20	10	2	7	1		
2	B	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]-2-fluorobenzoyl}-L-glutamic acid (CCD ID: Y79) (formula: C₂₂H₂₄FN₅O₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	F	N	O	0	0
			34	22	1	5	6		
3	B	1	Total	C	F	N	O	0	1
			68	44	2	10	12		

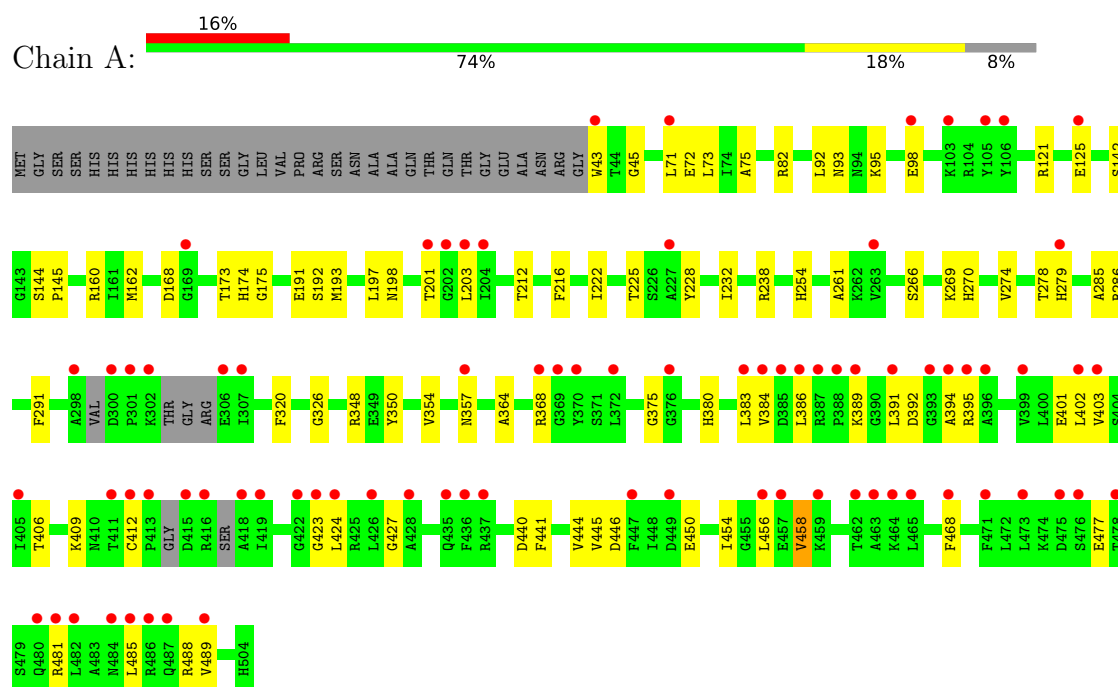
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	69	Total	O	0	0
			69	69		
4	B	135	Total	O	0	0
			135	135		

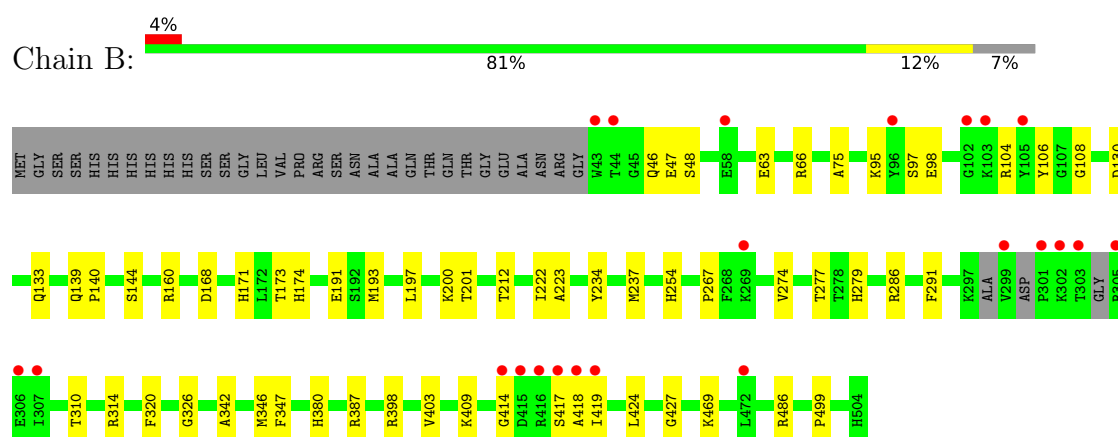
3 Residue-property plots [i](#)

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	157.34Å 157.34Å 207.55Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.55 – 2.51 48.55 – 2.51	Depositor EDS
% Data completeness (in resolution range)	99.4 (48.55-2.51) 99.4 (48.55-2.51)	Depositor EDS
R_{merge}	0.41	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.18 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.13-2998	Depositor
R, R_{free}	0.232 , 0.273 0.234 , 0.271	Depositor DCC
R_{free} test set	2768 reflections (4.81%)	wwPDB-VP
Wilson B-factor (Å ²)	43.0	Xtriage
Anisotropy	0.494	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 43.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7406	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.68% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PLG, Y79

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	0.17	0/3568	0.37	1/4831 (0.0%)
1	B	0.17	0/3629	0.35	0/4906
All	All	0.17	0/7197	0.36	1/9737 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	458	VAL	N-CA-C	-5.05	107.91	112.96

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	3501	0	3414	56	0
1	B	3559	0	3519	38	0
2	A	20	0	11	3	0
2	B	20	0	11	2	0
3	A	34	0	0	0	0
3	B	68	0	0	0	0
4	A	69	0	0	0	0
4	B	135	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	7406	0	6955	90	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 6.

All (90) 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:198:ASN:HB3	1:A:201:THR:HB	1.66	0.76
1:A:201:THR:HG22	1:A:203:LEU:H	1.54	0.72
1:B:130:ASP:HB3	1:B:133:GLN:HG2	1.79	0.64
1:A:98:GLU:HG2	1:A:326:GLY:HA2	1.81	0.61
1:A:71:LEU:CD1	1:A:489:VAL:HG13	2.31	0.60
1:B:200:LYS:HG3	1:B:201:THR:HG23	1.83	0.60
1:B:387:ARG:NH1	1:B:414:GLY:O	2.35	0.60
1:A:403:VAL:HG21	1:A:485:LEU:HG	1.84	0.60
1:B:274:VAL:HB	1:B:291:PHE:HB2	1.85	0.58
1:A:368:ARG:NH1	1:A:446:ASP:OD1	2.39	0.56
1:B:398:ARG:HG2	1:B:469:LYS:HD3	1.86	0.56
1:A:477:GLU:O	1:A:481:ARG:HG3	2.05	0.56
1:B:417:SER:O	1:B:419:ILE:N	2.39	0.55
1:A:394:ALA:HA	1:A:409:LYS:HE3	1.89	0.55
1:A:75:ALA:HA	1:A:427:GLY:HA3	1.89	0.55
1:A:389:LYS:HG3	1:A:456:LEU:HD11	1.89	0.55
1:A:73:LEU:O	1:A:427:GLY:N	2.33	0.54
1:B:46:GLN:N	1:B:47:GLU:OE1	2.42	0.53
1:A:278:THR:OG1	1:A:285:ALA:O	2.24	0.52
1:A:225:THR:HG23	1:A:232:ILE:HD11	1.92	0.51
1:A:350:TYR:O	1:A:354:VAL:HG23	2.11	0.51
1:B:174:HIS:CD2	1:B:222:ILE:HG21	2.46	0.51
1:A:142:SER:OG	2:A:601:PLG:OP1	2.28	0.51
1:A:95:LYS:HD3	1:B:66:ARG:NH2	2.27	0.50
1:B:98:GLU:OE2	1:B:106:TYR:OH	2.27	0.50
1:A:238:ARG:NH1	1:A:270:HIS:O	2.41	0.49
1:A:43:TRP:HB2	1:B:346:MET:HG3	1.94	0.49
1:B:144:SER:HA	1:B:173:THR:HG21	1.95	0.49
1:A:72:GLU:HA	1:A:406:THR:OG1	2.13	0.49
1:B:98:GLU:HB3	1:B:320:PHE:CZ	2.49	0.48
1:B:409:LYS:HA	1:B:424:LEU:HD12	1.95	0.48
1:B:75:ALA:HA	1:B:427:GLY:HA3	1.94	0.48
1:A:71:LEU:CD2	1:A:444:VAL:HG22	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:277:THR:HB	1:B:279:HIS:CE1	2.49	0.48
1:B:168:ASP:HB3	1:B:197:LEU:HG	1.95	0.48
1:B:193:MET:HE1	1:B:212:THR:HB	1.95	0.48
1:A:254:HIS:HB3	1:A:380:HIS:CE1	2.49	0.48
1:A:274:VAL:HB	1:A:291:PHE:HB2	1.96	0.48
1:B:310:THR:HG23	1:B:314:ARG:HH21	1.79	0.47
1:A:82:ARG:NH2	1:B:48:SER:OG	2.47	0.47
1:A:121:ARG:O	1:A:125:GLU:HG2	2.14	0.47
1:A:254:HIS:HB3	1:A:380:HIS:HE1	1.79	0.47
1:B:403:VAL:HA	1:B:486:ARG:HB2	1.97	0.47
1:A:357:ASN:HB3	1:A:441:PHE:CD1	2.48	0.47
1:A:144:SER:HA	1:A:173:THR:HG21	1.95	0.47
1:B:47:GLU:OE1	1:B:47:GLU:N	2.45	0.46
1:A:92:LEU:HD23	1:B:63:GLU:HG2	1.98	0.46
1:A:45:GLY:HA3	1:B:499:PRO:HB3	1.97	0.46
1:A:228:TYR:HA	1:A:383:LEU:HD11	1.96	0.46
1:A:395:ARG:HD2	1:A:468:PHE:CD2	2.50	0.46
1:A:454:ILE:O	1:A:458:VAL:HG23	2.16	0.46
1:A:175:GLY:O	1:A:192:SER:OG	2.23	0.45
1:B:160:ARG:HA	1:B:191:GLU:O	2.17	0.45
1:A:279:HIS:ND1	1:A:286:ARG:HA	2.31	0.45
1:B:98:GLU:HG2	1:B:326:GLY:HA2	1.99	0.45
1:A:364:ALA:HB3	1:A:445:VAL:HG21	1.99	0.45
1:A:261:ALA:HB1	1:A:348:ARG:HA	1.99	0.44
1:A:412:CYS:SG	1:A:423:GLY:N	2.91	0.44
1:B:223:ALA:HB2	1:B:237:MET:HE2	1.99	0.44
1:A:144:SER:HB2	1:A:145:PRO:HD3	1.99	0.44
1:A:450:GLU:CD	1:A:488:ARG:HH22	2.26	0.44
1:A:98:GLU:HB3	1:A:320:PHE:CZ	2.53	0.44
1:A:168:ASP:HB3	1:A:197:LEU:HG	2.00	0.43
1:B:234:TYR:CZ	1:B:267:PRO:HB3	2.53	0.43
1:A:386:LEU:HB3	1:A:391:LEU:O	2.18	0.43
1:B:254:HIS:HB3	1:B:380:HIS:CE1	2.54	0.43
1:A:160:ARG:HA	1:A:191:GLU:O	2.18	0.43
1:A:193:MET:HE1	1:A:212:THR:HB	2.01	0.43
2:A:601:PLG:H4A1	4:B:702:HOH:O	2.19	0.42
1:B:97:SER:O	1:B:104:ARG:NE	2.51	0.42
1:A:395:ARG:HB2	1:A:468:PHE:CE1	2.54	0.42
1:B:95:LYS:HA	1:B:95:LYS:HD2	1.87	0.42
1:A:160:ARG:HB3	1:A:216:PHE:CE2	2.53	0.42
1:A:392:ASP:OD2	1:A:395:ARG:HG2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:266:SER:H	1:A:269:LYS:HZ2	1.67	0.42
2:B:601:PLG:H4A1	2:B:601:PLG:H5A1	1.89	0.42
1:A:174:HIS:CD2	1:A:222:ILE:HG21	2.55	0.42
1:A:401:GLU:HG3	1:B:108:GLY:H	1.85	0.42
1:B:139:GLN:N	1:B:140:PRO:CD	2.83	0.41
1:B:346:MET:HE3	1:B:346:MET:HB3	1.95	0.41
1:A:266:SER:HB3	1:A:269:LYS:NZ	2.35	0.41
1:A:93:ASN:OD1	1:B:286:ARG:HG3	2.20	0.41
2:A:601:PLG:O3	2:A:601:PLG:N	2.50	0.41
1:B:342:ALA:HA	1:B:347:PHE:CG	2.55	0.41
1:A:384:VAL:HG22	1:A:424:LEU:O	2.21	0.41
1:A:402:LEU:HD23	1:A:402:LEU:HA	1.90	0.41
1:B:171:HIS:CD2	2:B:601:PLG:H	2.39	0.40
1:A:162:MET:HE2	1:A:162:MET:HB3	1.97	0.40
1:B:310:THR:HG23	1:B:314:ARG:NH2	2.36	0.40
1:A:440:ASP:O	1:A:444:VAL:HG23	2.21	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	446/493 (90%)	418 (94%)	27 (6%)	1 (0%)	43	63
1	B	452/493 (92%)	437 (97%)	14 (3%)	1 (0%)	43	63
All	All	898/986 (91%)	855 (95%)	41 (5%)	2 (0%)	43	63

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	418	ALA
1	A	375	GLY

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	361/405 (89%)	361 (100%)	0	100	100
1	B	370/405 (91%)	370 (100%)	0	100	100
All	All	731/810 (90%)	731 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	480	GLN
1	B	46	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 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
3	Y79	A	602	-	35,36,36	2.23	6 (17%)	46,50,50	2.10	15 (32%)
3	Y79	B	602[B]	-	35,36,36	2.19	5 (14%)	46,50,50	1.88	10 (21%)
2	PLG	A	601	-	20,20,20	2.51	3 (15%)	26,28,28	1.71	5 (19%)
2	PLG	B	601	-	20,20,20	2.44	3 (15%)	26,28,28	1.74	6 (23%)
3	Y79	B	602[A]	-	35,36,36	2.20	5 (14%)	46,50,50	1.88	10 (21%)

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	Y79	A	602	-	-	9/24/24/24	0/3/3/3
3	Y79	B	602[B]	-	-	4/24/24/24	0/3/3/3
2	PLG	A	601	-	-	2/12/12/12	0/1/1/1
2	PLG	B	601	-	-	4/12/12/12	0/1/1/1
3	Y79	B	602[A]	-	-	1/24/24/24	0/3/3/3

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	602[A]	Y79	O10-C4	8.85	1.40	1.23
3	B	602[B]	Y79	O10-C4	8.83	1.40	1.23
3	A	602	Y79	O10-C4	8.83	1.40	1.23
2	A	601	PLG	C3-C2	7.43	1.48	1.41
2	B	601	PLG	C3-C2	7.01	1.48	1.41
2	B	601	PLG	C5-C4	5.69	1.48	1.40
2	A	601	PLG	C5-C4	5.65	1.48	1.40
2	A	601	PLG	C3-C4	5.51	1.48	1.40
3	A	602	Y79	C17-N19	5.47	1.46	1.34
2	B	601	PLG	C3-C4	5.25	1.47	1.40
3	B	602[B]	Y79	C17-N19	5.24	1.46	1.34
3	B	602[A]	Y79	C17-N19	5.22	1.46	1.34
3	B	602[A]	Y79	C2-N11	4.82	1.45	1.34
3	A	602	Y79	C2-N11	4.81	1.45	1.34
3	B	602[B]	Y79	C2-N11	4.78	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	602	Y79	C4-N3	-3.09	1.33	1.38
3	B	602[A]	Y79	C4-N3	-3.02	1.33	1.38
3	B	602[B]	Y79	C4-N3	-3.01	1.33	1.38
3	B	602[B]	Y79	C6-N7	-2.46	1.32	1.38
3	B	602[A]	Y79	C6-N7	-2.44	1.32	1.38
3	A	602	Y79	C6-N7	-2.36	1.32	1.38
3	A	602	Y79	C12-C17	2.12	1.54	1.50

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	PLG	C4A-N-CA	5.92	119.61	112.72
3	B	602[A]	Y79	C8-C9-N1	-5.86	119.19	124.81
3	B	602[B]	Y79	C8-C9-N1	-5.85	119.21	124.81
3	A	602	Y79	C8-C9-N1	-5.76	119.29	124.81
3	A	602	Y79	C12-C17-N19	4.91	127.32	116.67
2	B	601	PLG	C4A-N-CA	4.82	118.34	112.72
3	B	602[A]	Y79	C8-C4-N3	4.74	119.28	110.94
3	B	602[B]	Y79	C8-C4-N3	4.69	119.19	110.94
3	A	602	Y79	C8-C4-N3	4.65	119.13	110.94
3	B	602[A]	Y79	C9-C8-C4	-4.28	117.95	121.36
3	B	602[B]	Y79	C9-C8-C4	-4.24	117.98	121.36
3	A	602	Y79	C9-C8-C4	-4.24	117.98	121.36
3	B	602[B]	Y79	C14-C12-C13	3.40	120.47	116.70
3	A	602	Y79	C5-C9-N1	3.35	134.37	123.36
3	B	602[A]	Y79	C5-C9-N1	3.33	134.33	123.36
3	B	602[B]	Y79	C5-C9-N1	3.33	134.32	123.36
3	B	602[A]	Y79	C14-C12-C13	3.30	120.37	116.70
3	A	602	Y79	O18-C17-N19	-3.29	116.21	122.47
3	B	602[B]	Y79	C15-C13-C12	-3.23	119.91	123.48
3	B	602[A]	Y79	C15-C13-C12	-3.22	119.92	123.48
3	A	602	Y79	C20-N19-C17	2.91	128.55	121.56
3	B	602[A]	Y79	C9-N1-C2	2.83	121.07	116.63
3	B	602[B]	Y79	C9-N1-C2	2.81	121.04	116.63
3	A	602	Y79	C13-C12-C17	-2.73	116.90	124.32
3	A	602	Y79	C9-N1-C2	2.64	120.76	116.63
2	B	601	PLG	C6-C5-C4	2.62	120.05	118.06
3	B	602[B]	Y79	O10-C4-C8	-2.60	121.23	127.62
3	B	602[A]	Y79	O10-C4-C8	-2.59	121.27	127.62
3	A	602	Y79	O18-C17-C12	-2.49	116.47	121.03
3	A	602	Y79	C15-C13-C12	-2.42	120.81	123.48
3	A	602	Y79	O10-C4-C8	-2.37	121.80	127.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	602	Y79	C14-C12-C13	2.31	119.27	116.70
3	B	602[A]	Y79	C2-N3-C4	-2.28	120.98	125.11
2	B	601	PLG	C3-C4-C5	-2.25	116.69	118.73
3	B	602[B]	Y79	C2-N3-C4	-2.24	121.04	125.11
2	B	601	PLG	C5A-C5-C4	-2.23	117.97	122.67
2	A	601	PLG	C6-C5-C4	2.20	119.73	118.06
2	A	601	PLG	C3-C4-C5	-2.18	116.75	118.73
2	B	601	PLG	C6-N1-C2	2.17	123.14	119.20
3	A	602	Y79	C2-N3-C4	-2.14	121.23	125.11
2	A	601	PLG	C6-N1-C2	2.13	123.07	119.20
3	B	602[A]	Y79	C29-N7-C8	-2.13	125.36	128.85
2	B	601	PLG	OP4-C5A-C5	2.13	113.34	109.36
3	B	602[B]	Y79	C13-C12-C17	-2.10	118.61	124.32
3	A	602	Y79	C29-N7-C8	-2.06	125.48	128.85
2	A	601	PLG	O3-C3-C2	2.05	121.82	117.58

There are no chirality outliers.

All (20) torsion outliers are listed below:

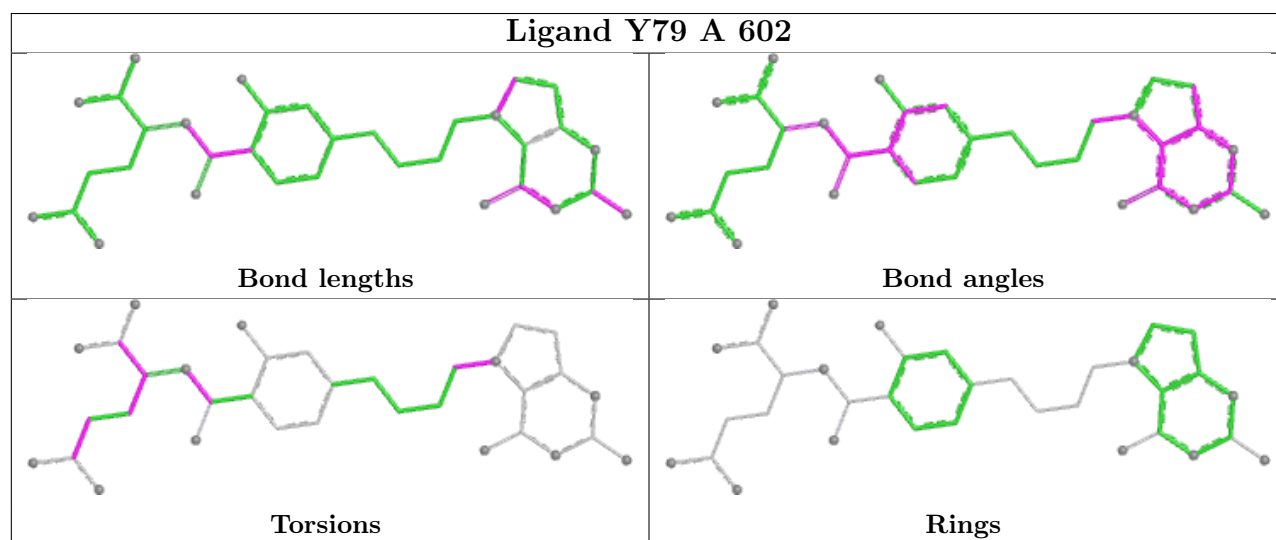
Mol	Chain	Res	Type	Atoms
2	A	601	PLG	C3-C4-C4A-N
2	A	601	PLG	C5-C4-C4A-N
2	B	601	PLG	C5A-OP4-P-OP2
2	B	601	PLG	C5A-OP4-P-OP3
3	A	602	Y79	C12-C17-N19-C20
3	A	602	Y79	O18-C17-N19-C20
3	A	602	Y79	N19-C20-C21-C22
3	A	602	Y79	C26-C20-C21-C22
3	A	602	Y79	N19-C20-C26-O28
3	B	602[A]	Y79	C30-C31-C32-C33
2	B	601	PLG	C5A-OP4-P-OP1
3	A	602	Y79	N19-C20-C26-O27
3	A	602	Y79	C30-C29-N7-C8
3	B	602[B]	Y79	C21-C22-C23-O24
3	A	602	Y79	C21-C22-C23-O25
3	A	602	Y79	C21-C22-C23-O24
3	B	602[B]	Y79	C21-C22-C23-O25
3	B	602[B]	Y79	C31-C32-C33-C16
3	B	602[B]	Y79	C31-C32-C33-C15
2	B	601	PLG	C4-C5-C5A-OP4

There are no ring outliers.

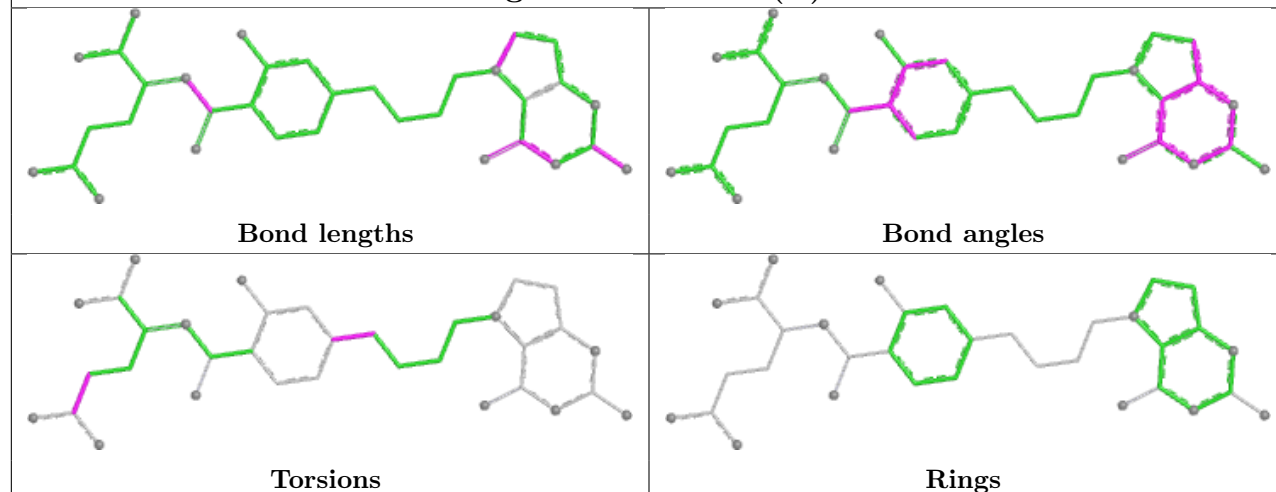
2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	PLG	3	0
2	B	601	PLG	2	0

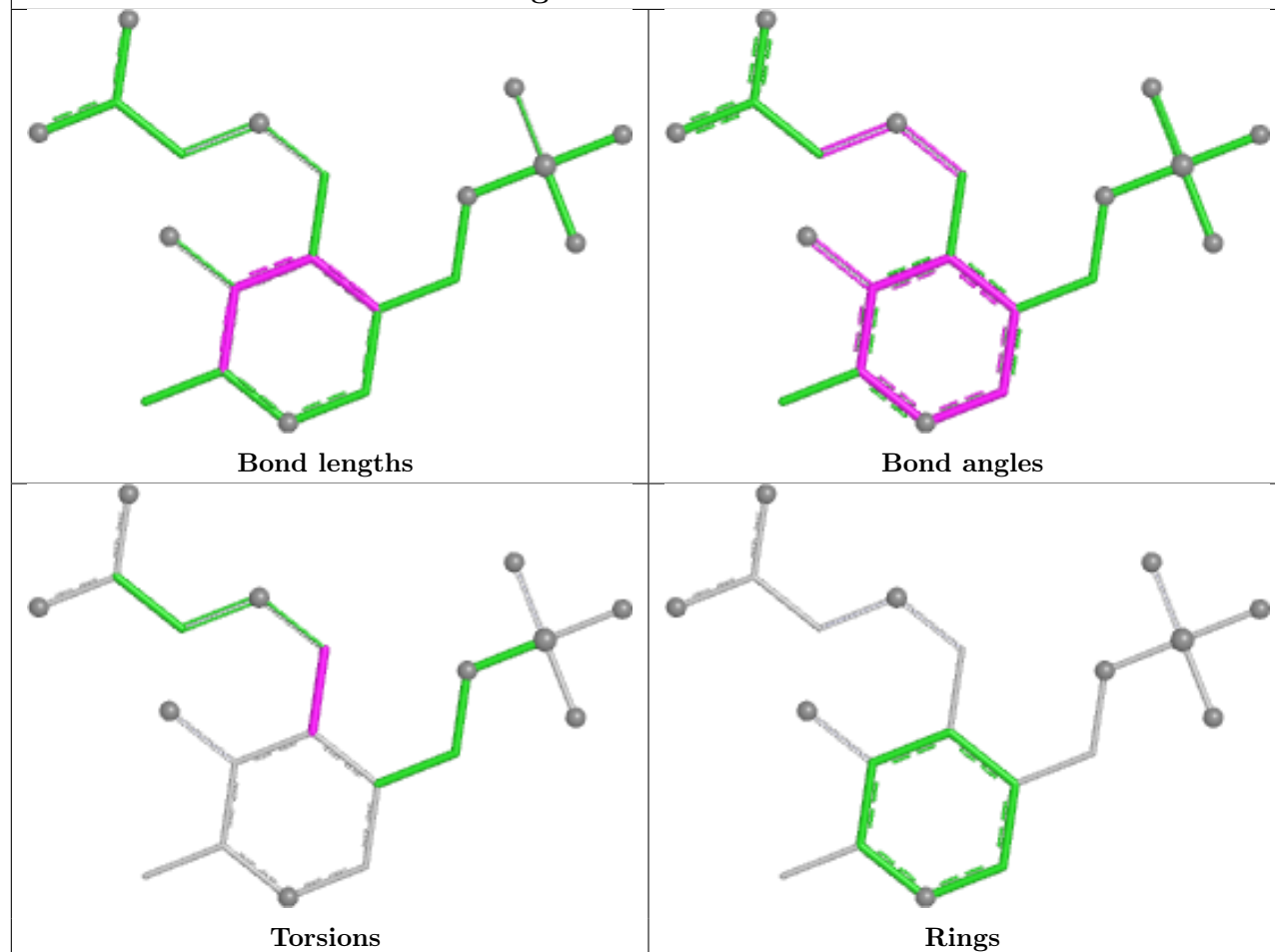
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

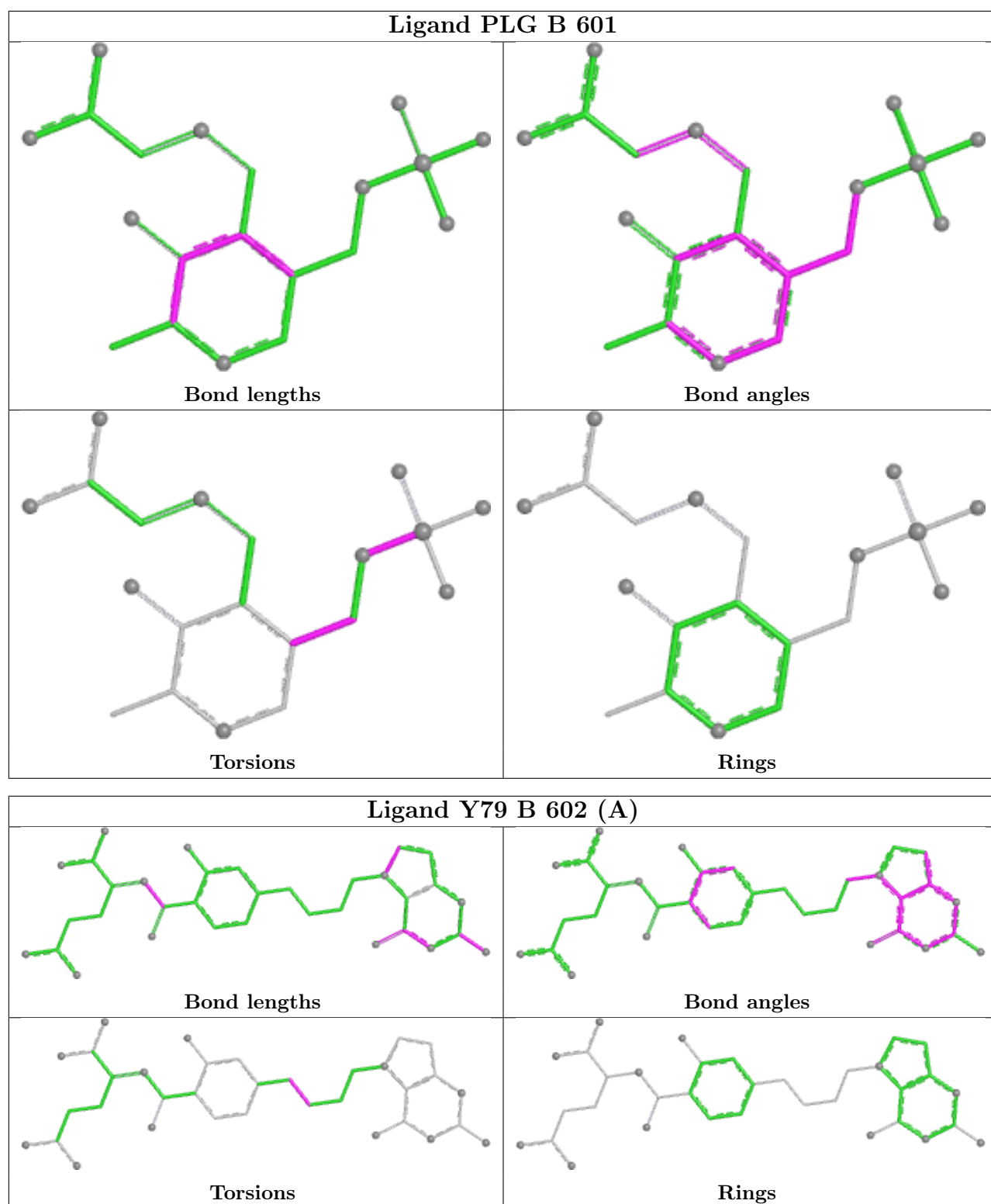


Ligand Y79 B 602 (B)



Ligand PLG A 601





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	456/493 (92%)	1.08	81 (17%) 4 3	28, 53, 82, 96	0
1	B	459/493 (93%)	0.26	22 (4%) 35 31	24, 38, 64, 96	0
All	All	915/986 (92%)	0.67	103 (11%) 10 8	24, 45, 79, 96	0

All (103) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	299	VAL	6.0
1	A	376	GLY	5.8
1	B	301	PRO	5.7
1	B	303	THR	5.2
1	A	298	ALA	4.9
1	B	305	ARG	4.9
1	A	418	ALA	4.8
1	A	369	GLY	4.6
1	A	419	ILE	4.5
1	B	302	LYS	4.5
1	A	302	LYS	4.5
1	B	418	ALA	4.3
1	A	416	ARG	4.3
1	B	105	TYR	4.2
1	A	301	PRO	4.1
1	A	306	GLU	4.0
1	A	105	TYR	4.0
1	A	415	ASP	3.9
1	B	417	SER	3.7
1	A	468	PHE	3.6
1	A	395	ARG	3.6
1	B	307	ILE	3.6
1	A	486	ARG	3.5
1	A	169	GLY	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	103	LYS	3.4
1	B	102	GLY	3.3
1	A	435	GLN	3.2
1	B	415	ASP	3.2
1	A	125	GLU	3.2
1	A	412	CYS	3.0
1	B	416	ARG	3.0
1	A	471	PHE	3.0
1	A	307	ILE	2.9
1	A	98	GLU	2.9
1	A	388	PRO	2.9
1	A	424	LEU	2.9
1	A	389	LYS	2.9
1	A	403	VAL	2.8
1	A	370	TYR	2.8
1	B	96	TYR	2.8
1	A	384	VAL	2.8
1	A	300	ASP	2.8
1	A	447	PHE	2.8
1	A	394	ALA	2.8
1	A	43	TRP	2.7
1	A	423	GLY	2.7
1	B	414	GLY	2.7
1	A	387	ARG	2.7
1	B	419	ILE	2.7
1	A	368	ARG	2.7
1	A	462	THR	2.6
1	B	44	THR	2.6
1	A	464	LYS	2.6
1	A	436	PHE	2.6
1	A	372	LEU	2.6
1	A	463	ALA	2.6
1	A	475	ASP	2.6
1	A	484	ASN	2.6
1	A	202	GLY	2.5
1	A	71	LEU	2.5
1	A	465	LEU	2.5
1	A	480	GLN	2.5
1	A	203	LEU	2.4
1	A	456	LEU	2.4
1	A	201	THR	2.4
1	A	391	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	481	ARG	2.4
1	A	473	LEU	2.3
1	A	478	THR	2.3
1	A	437	ARG	2.3
1	A	385	ASP	2.3
1	B	306	GLU	2.3
1	B	43	TRP	2.3
1	B	472	LEU	2.3
1	A	413	PRO	2.3
1	A	487	GLN	2.2
1	A	386	LEU	2.2
1	A	399	VAL	2.2
1	A	227	ALA	2.2
1	A	489	VAL	2.2
1	A	428	ALA	2.2
1	A	422	GLY	2.2
1	A	263	VAL	2.2
1	A	402	LEU	2.2
1	A	357	ASN	2.1
1	A	482	LEU	2.1
1	B	269	LYS	2.1
1	A	279	HIS	2.1
1	A	393	GLY	2.1
1	A	411	THR	2.1
1	A	426	LEU	2.1
1	A	103	LYS	2.1
1	A	485	LEU	2.1
1	A	204	ILE	2.1
1	A	457	GLU	2.1
1	A	459	LYS	2.1
1	A	106	TYR	2.0
1	A	383	LEU	2.0
1	A	396	ALA	2.0
1	B	58	GLU	2.0
1	A	405	ILE	2.0
1	A	449	ASP	2.0
1	A	476	SER	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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](#)

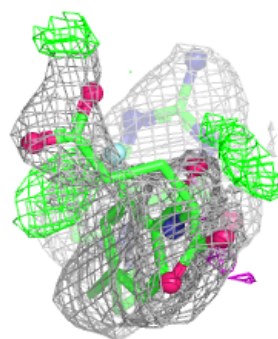
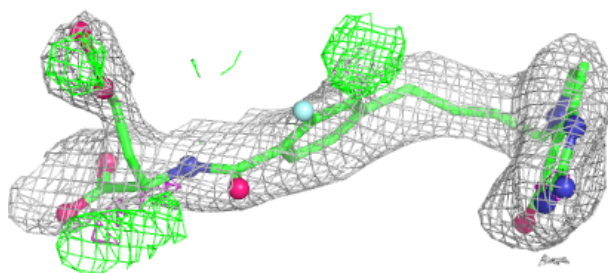
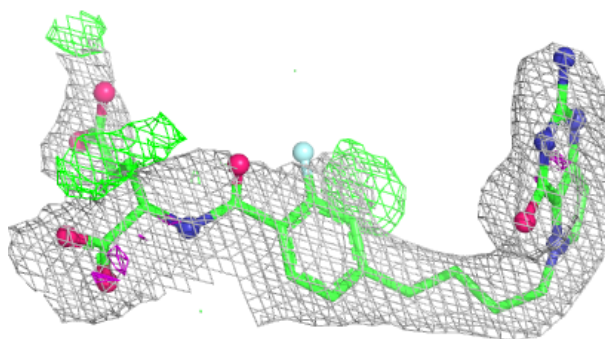
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
3	Y79	B	602[A]	34/34	0.73	0.19	36,47,57,59	34
3	Y79	B	602[B]	34/34	0.73	0.19	36,47,58,61	34
3	Y79	A	602	34/34	0.78	0.20	46,64,82,90	0
2	PLG	A	601	20/20	0.92	0.10	36,44,48,51	0
2	PLG	B	601	20/20	0.94	0.10	30,38,43,44	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.

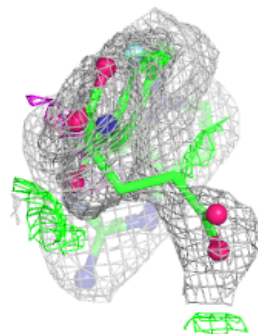
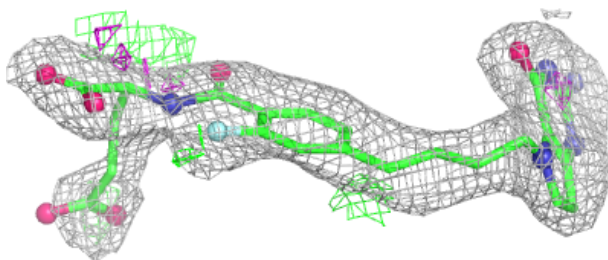
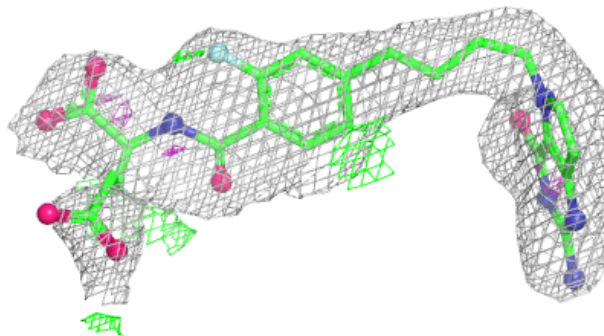
Electron density around Y79 B 602 (A):

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

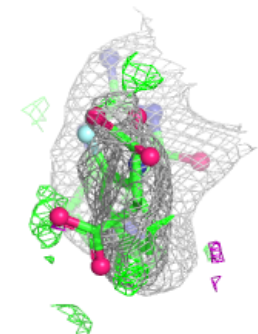
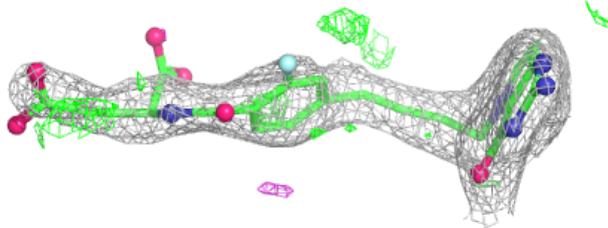
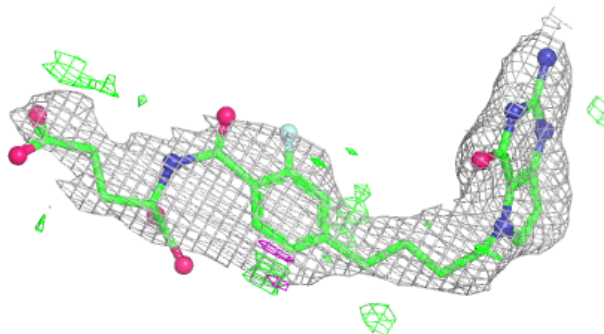


Electron density around Y79 B 602 (B):

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

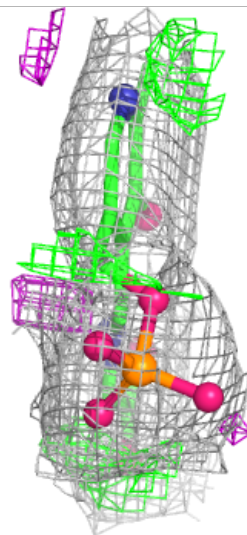
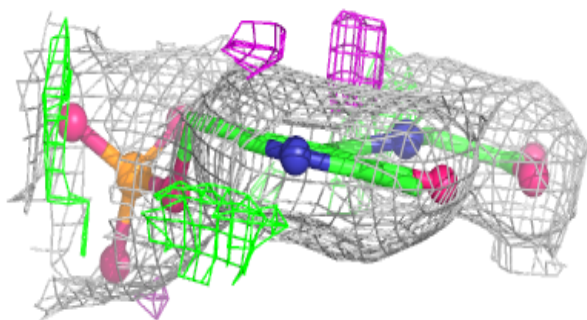
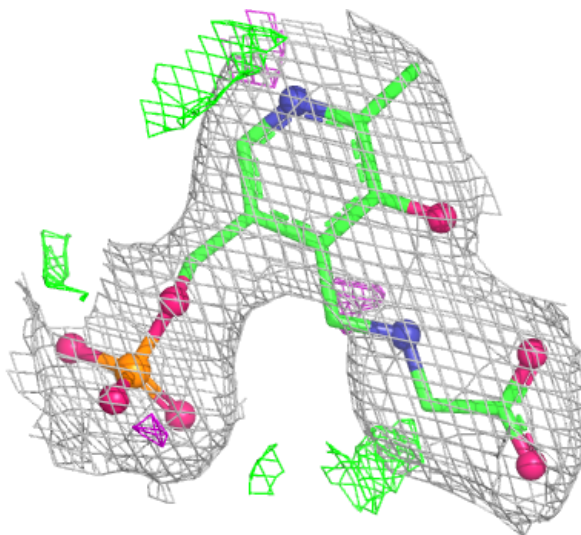
**Electron density around Y79 A 602:**

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



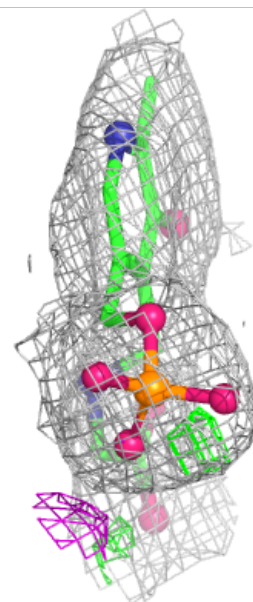
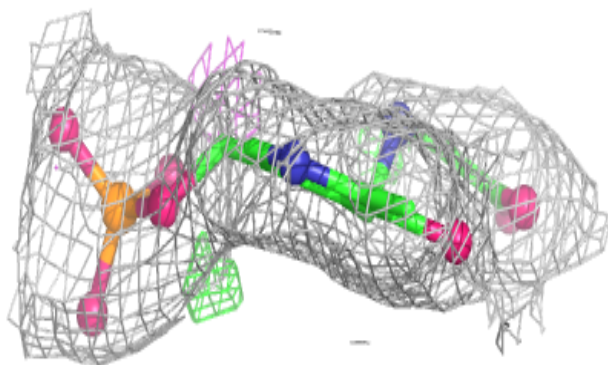
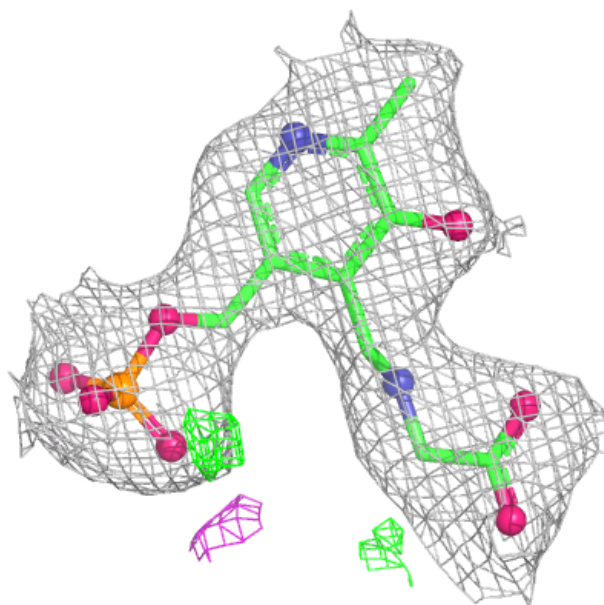
Electron density around PLG A 601:

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



Electron density around PLG B 601:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.