



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:39 AM UTC

PDB ID : 8T4O / pdb_00008t4o
Title : Human mitochondrial serine hydroxymethyltransferase (SHMT2) in complex with PLP, glycine and AGF347 inhibitor with no glutamate
Authors : Katinas, J.M.; Dann III, C.E.
Deposited on : 2023-06-09
Resolution : 2.68 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

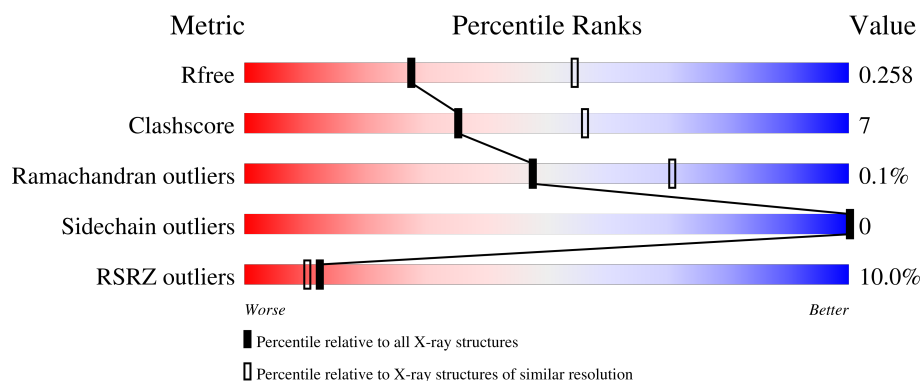
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.68 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	5070 (2.70-2.66)
Clashscore	190562	5409 (2.70-2.66)
Ramachandran outliers	187476	5324 (2.70-2.66)
Sidechain outliers	187428	5324 (2.70-2.66)
RSRZ outliers	180081	5070 (2.70-2.66)

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	4% 82% 10% 8%
1	B	493	15% 74% 19% 7%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7145 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	2237	640	660	16			
1	B	459	Total	C	N	O	S	0	1	0
			3504	2203	628	658	15			

There are 34 discrepancies between the modelled and reference sequences:

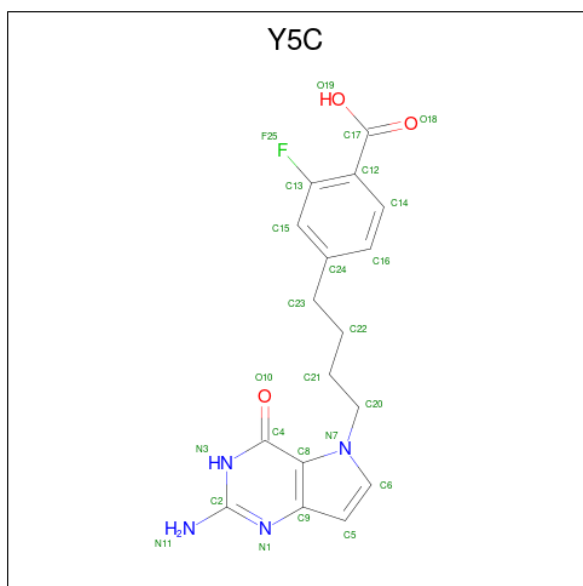
Chain	Residue	Modelled	Actual	Comment	Reference
A	12	MET	-	initiating methionine	UNP P34897
A	13	GLY	-	expression tag	UNP P34897
A	14	SER	-	expression tag	UNP P34897
A	15	SER	-	expression tag	UNP P34897
A	16	HIS	-	expression tag	UNP P34897
A	17	HIS	-	expression tag	UNP P34897
A	18	HIS	-	expression tag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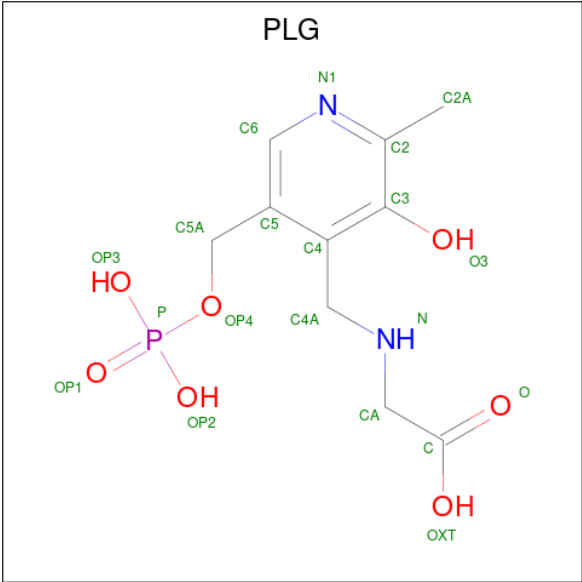
Chain	Residue	Modelled	Actual	Comment	Reference
B	20	HIS	-	expression tag	UNP P34897
B	21	HIS	-	expression tag	UNP P34897
B	22	SER	-	expression tag	UNP P34897
B	23	SER	-	expression tag	UNP P34897
B	24	GLY	-	expression tag	UNP P34897
B	25	LEU	-	expression tag	UNP P34897
B	26	VAL	-	expression tag	UNP P34897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

- Molecule 2 is 4-[4-(2-amino-4-oxo-3,4-dihydro-5H-pyrrolo[3,2-d]pyrimidin-5-yl)butyl]-2-fluorobenzoic acid (CCD ID: Y5C) (formula: C₁₇H₁₇FN₄O₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	0	0
			25	17	1	4	3		

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



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	19	Total	O	0	0
			19	19		
4	B	4	Total	O	0	0
			4	4		

4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	158.54Å 158.54Å 208.01Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.78 – 2.68 48.78 – 2.68	Depositor EDS
% Data completeness (in resolution range)	99.2 (48.78-2.68) 99.2 (48.78-2.68)	Depositor EDS
R_{merge}	0.47	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.62 (at 2.69Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.214 , 0.259 0.215 , 0.258	Depositor DCC
R_{free} test set	2190 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	44.6	Xtriage
Anisotropy	0.426	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 47.1	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	7145	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.76% 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: Y5C, 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	0.12	0/3622	0.32	0/4894
1	B	0.16	0/3573	0.36	0/4841
All	All	0.14	0/7195	0.34	0/9735

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	3527	32	0
1	B	3504	0	3387	76	0
2	A	25	0	0	0	0
3	A	20	0	11	3	0
3	B	20	0	11	2	0
4	A	19	0	0	0	0
4	B	4	0	0	0	0
All	All	7145	0	6936	104	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 7.

All (104) 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:230:ARG:NH2	1:B:374:SER:O	1.71	1.24
1:B:230:ARG:NH2	1:B:374:SER:C	2.06	1.14
1:B:230:ARG:HH22	1:B:374:SER:C	1.66	1.00
1:B:201:THR:HG22	1:B:203:LEU:H	1.41	0.85
1:B:230:ARG:HH21	1:B:374:SER:CB	1.97	0.77
1:B:160:ARG:HB2	1:B:218:PRO:HA	1.69	0.74
1:B:230:ARG:HH21	1:B:374:SER:C	1.97	0.73
1:B:485:LEU:O	1:B:489:VAL:HG23	1.90	0.72
1:B:198:ASN:HB3	1:B:201:THR:HB	1.71	0.71
1:B:66:ARG:HA	1:B:69:ARG:HB2	1.73	0.70
1:B:197:LEU:CB	1:B:204:ILE:HA	2.21	0.70
1:B:197:LEU:HA	1:B:205:ASP:HB2	1.80	0.64
1:B:197:LEU:HB2	1:B:204:ILE:HA	1.80	0.62
1:B:272:ASP:HA	1:B:293:ARG:HG3	1.80	0.62
1:B:225:THR:HG23	1:B:232:ILE:HD11	1.81	0.61
1:B:71:LEU:HD12	1:B:71:LEU:N	2.17	0.59
1:B:263:VAL:HG11	1:B:355:LEU:HD11	1.84	0.59
1:B:279:HIS:ND1	1:B:286:ARG:HA	2.17	0.59
1:B:230:ARG:NH2	1:B:374:SER:CB	2.65	0.58
1:B:476:SER:HA	1:B:479:SER:HB3	1.85	0.58
1:B:351:SER:O	1:B:354:VAL:HG22	2.04	0.58
1:B:197:LEU:HB3	1:B:204:ILE:HA	1.84	0.58
1:B:470:SER:C	1:B:474:LYS:HD3	2.30	0.57
1:A:223:ALA:HB2	1:A:237:MET:HE2	1.88	0.56
1:A:60:LEU:HD23	1:A:504:HIS:HB2	1.88	0.56
1:A:503:GLU:OE2	1:A:503:GLU:N	2.40	0.54
1:B:195:TYR:CG	1:B:209:LEU:HD12	2.43	0.53
1:B:57:TRP:HA	1:B:60:LEU:HD13	1.89	0.53
1:A:104:ARG:NH2	1:A:116:GLU:OE2	2.41	0.53
1:A:75:ALA:HA	1:A:427:GLY:HA3	1.90	0.52
1:B:357:ASN:HA	1:B:360:ALA:HB3	1.92	0.52
1:B:56:MET:HG3	1:B:60:LEU:HD11	1.91	0.51
1:B:466:GLN:O	1:B:470:SER:OG	2.18	0.51
1:B:405:ILE:HD11	1:B:489:VAL:HG11	1.94	0.50
1:B:277:THR:HG22	1:B:279:HIS:H	1.76	0.50
1:B:71:LEU:HB3	1:B:431:LEU:HD11	1.93	0.50
1:A:428:ALA:N	1:A:429:PRO:HD2	2.27	0.50
1:B:440:ASP:O	1:B:444:VAL:HG23	2.12	0.49
1:B:454:ILE:HG12	1:B:481:ARG:CZ	2.43	0.49
1:A:111:VAL:HG11	1:B:62:ARG:HB3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:193:MET:HE1	1:B:212:THR:HB	1.93	0.49
1:B:142:SER:HG	3:B:601:PLG:P	2.36	0.48
1:B:450:GLU:OE1	1:B:488:ARG:NH2	2.45	0.48
1:A:97:SER:O	1:A:104:ARG:NH1	2.47	0.48
1:A:403:VAL:HA	1:A:486:ARG:HB2	1.95	0.48
1:B:254:HIS:CE1	1:B:425:ARG:NH2	2.82	0.48
1:A:177:MET:HG2	1:A:187:SER:HB3	1.96	0.47
1:A:403:VAL:HG11	1:A:485:LEU:HD23	1.97	0.47
1:B:373:VAL:C	1:B:375:GLY:H	2.22	0.47
3:B:601:PLG:O3	3:B:601:PLG:N	2.46	0.47
1:A:160:ARG:HB3	1:A:216:PHE:CE2	2.49	0.47
1:B:475:ASP:O	1:B:479:SER:N	2.48	0.46
1:B:470:SER:HB3	1:B:474:LYS:CD	2.46	0.46
1:B:199:PRO:HG2	1:B:200:LYS:NZ	2.31	0.46
1:A:63:GLU:HG2	1:B:92:LEU:HD23	1.96	0.46
1:B:66:ARG:HB2	1:B:69:ARG:NH2	2.31	0.46
1:B:204:ILE:HD11	1:B:237:MET:HE2	1.96	0.46
1:B:80:CYS:HB3	1:B:85:LEU:HD21	1.97	0.45
1:B:272:ASP:HB2	1:B:273:ILE:HD12	1.99	0.45
1:A:279:HIS:ND1	1:A:286:ARG:HA	2.32	0.45
1:B:365:LEU:CD1	1:B:372:LEU:HD21	2.46	0.45
1:A:193:MET:HE1	1:A:212:THR:HB	1.99	0.45
1:B:250:ALA:HB3	1:B:274:VAL:HG22	1.99	0.44
1:A:380:HIS:HB2	1:A:429:PRO:HD3	2.00	0.44
1:B:428:ALA:H	1:B:429:PRO:HD3	1.81	0.44
1:B:205:ASP:OD1	1:B:207:ASN:HB2	2.17	0.44
1:B:365:LEU:HD13	1:B:372:LEU:HD21	2.00	0.44
1:A:272:ASP:HB3	1:A:311:PHE:CE2	2.53	0.44
1:B:199:PRO:HA	1:B:413:PRO:HB3	2.00	0.44
1:A:98:GLU:HB3	1:A:320:PHE:CZ	2.53	0.43
1:B:253:ALA:HB1	1:B:277:THR:OG1	2.18	0.43
3:A:602[B]:PLG:OXT	1:B:106:TYR:OH	2.31	0.43
1:B:227:ALA:HB1	1:B:383:LEU:HD21	2.00	0.43
1:A:280:LYS:HZ1	3:A:602[B]:PLG:C4	2.31	0.43
1:B:110:GLU:H	1:B:110:GLU:HG3	1.56	0.43
1:A:280:LYS:HZ1	3:A:602[B]:PLG:C3	2.32	0.43
1:B:296:VAL:HA	1:B:308:PRO:HA	2.01	0.43
1:A:368[B]:ARG:NH2	1:A:446:ASP:OD1	2.48	0.43
1:B:263:VAL:HG11	1:B:355:LEU:CD1	2.49	0.43
1:A:96:TYR:OH	1:B:279:HIS:NE2	2.50	0.42
1:A:231:LEU:HD13	1:A:265:PRO:HD2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:256:SER:HB3	1:B:276:THR:OG1	2.20	0.42
1:B:220:LEU:HD12	1:B:247:HIS:HB2	2.01	0.42
1:B:450:GLU:O	1:B:454:ILE:HG13	2.20	0.42
1:A:53:ASP:OD2	1:B:122:ARG:NH1	2.52	0.41
1:A:174:HIS:CD2	1:A:222:ILE:HG21	2.55	0.41
1:B:373:VAL:HG22	1:B:383:LEU:HB2	2.01	0.41
1:B:162:MET:HG3	1:B:218:PRO:HB3	2.02	0.41
1:A:279:HIS:HB2	1:A:280:LYS:H	1.74	0.41
1:B:274:VAL:HB	1:B:291:PHE:HB2	2.03	0.41
1:B:475:ASP:OD2	1:B:477:GLU:HB2	2.20	0.41
1:A:139:GLN:N	1:A:140:PRO:CD	2.84	0.41
1:B:56:MET:O	1:B:59:LEU:N	2.52	0.41
1:A:49:LEU:HD23	1:A:57:TRP:HE3	1.85	0.41
1:B:351:SER:O	1:B:355:LEU:HD12	2.21	0.40
1:B:387:ARG:HB2	1:B:388:PRO:HD3	2.02	0.40
1:A:155:LEU:HB3	1:A:159:ASP:HB2	2.03	0.40
1:A:261:ALA:HB1	1:A:348:ARG:HA	2.02	0.40
1:B:387:ARG:NH2	1:B:414:GLY:H	2.19	0.40
1:A:144:SER:HA	1:A:173:THR:HG21	2.04	0.40
1:A:92:LEU:HD23	1:B:63:GLU:HG2	2.04	0.40
1:B:138:VAL:HA	1:B:289:LEU:HD23	2.02	0.40
1:B:234:TYR:HB2	1:B:270:HIS:ND1	2.37	0.40
1:B:372:LEU:CD2	1:B:384:VAL:HA	2.50	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	448/493 (91%)	429 (96%)	19 (4%)	0	100	100
1	B	454/493 (92%)	417 (92%)	36 (8%)	1 (0%)	43	65

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	902/986 (92%)	846 (94%)	55 (6%)	1 (0%)	48 71

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	178	SER

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	372/405 (92%)	372 (100%)	0	100 100
1	B	354/405 (87%)	354 (100%)	0	100 100
All	All	726/810 (90%)	726 (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 (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	GLN
1	A	270	HIS
1	A	410	ASN
1	B	198	ASN
1	B	487	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

3 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	PLG	B	601	-	20,20,20	2.55	3 (15%)	26,28,28	1.82	3 (11%)
2	Y5C	A	601	-	26,27,27	2.51	5 (19%)	34,38,38	2.08	11 (32%)
3	PLG	A	602[B]	-	20,20,20	2.48	3 (15%)	26,28,28	1.91	5 (19%)

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	PLG	B	601	-	-	2/12/12/12	0/1/1/1
2	Y5C	A	601	-	-	6/11/11/11	0/3/3/3
3	PLG	A	602[B]	-	-	5/12/12/12	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	Y5C	O10-C4	8.92	1.40	1.23
3	B	601	PLG	C3-C2	7.46	1.48	1.41
3	A	602[B]	PLG	C3-C2	6.94	1.48	1.41
3	A	602[B]	PLG	C3-C4	5.90	1.48	1.40
3	B	601	PLG	C5-C4	5.84	1.48	1.40
3	A	602[B]	PLG	C5-C4	5.66	1.48	1.40
3	B	601	PLG	C3-C4	5.59	1.48	1.40
2	A	601	Y5C	O19-C17	5.27	1.46	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	Y5C	C2-N11	4.85	1.45	1.34
2	A	601	Y5C	C4-N3	-3.13	1.33	1.38
2	A	601	Y5C	C6-N7	-2.39	1.32	1.38

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	602[B]	PLG	C4A-N-CA	6.67	120.49	112.72
3	B	601	PLG	C4A-N-CA	6.55	120.35	112.72
2	A	601	Y5C	C8-C9-N1	-5.49	119.56	124.81
2	A	601	Y5C	C8-C4-N3	4.58	118.99	110.94
2	A	601	Y5C	C9-C8-C4	-4.36	117.88	121.36
2	A	601	Y5C	C5-C9-N1	3.25	134.07	123.36
2	A	601	Y5C	C15-C13-C12	-3.19	119.95	123.48
2	A	601	Y5C	C20-N7-C8	-3.07	123.83	128.85
2	A	601	Y5C	C14-C12-C13	2.93	119.95	116.70
3	A	602[B]	PLG	C4A-C4-C3	2.60	123.43	119.98
2	A	601	Y5C	O10-C4-C8	-2.58	121.29	127.62
2	A	601	Y5C	C9-N1-C2	2.57	120.66	116.63
3	A	602[B]	PLG	C6-N1-C2	2.33	123.42	119.20
3	B	601	PLG	C6-N1-C2	2.30	123.37	119.20
3	A	602[B]	PLG	C3-C4-C5	-2.14	116.79	118.73
2	A	601	Y5C	C13-C12-C17	-2.12	119.79	123.13
2	A	601	Y5C	C2-N3-C4	-2.07	121.36	125.11
3	A	602[B]	PLG	C6-C5-C4	2.03	119.60	118.06
3	B	601	PLG	C4A-C4-C5	2.02	121.94	119.75

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	602[B]	PLG	C5-C4-C4A-N
3	B	601	PLG	C5-C4-C4A-N
3	A	602[B]	PLG	O-C-CA-N
3	A	602[B]	PLG	OXT-C-CA-N
3	A	602[B]	PLG	C4-C4A-N-CA
3	B	601	PLG	C3-C4-C4A-N
2	A	601	Y5C	C20-C21-C22-C23
3	A	602[B]	PLG	C3-C4-C4A-N
2	A	601	Y5C	C21-C20-N7-C6
2	A	601	Y5C	C21-C20-N7-C8
2	A	601	Y5C	N7-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
2	A	601	Y5C	C22-C23-C24-C16
2	A	601	Y5C	C22-C23-C24-C15

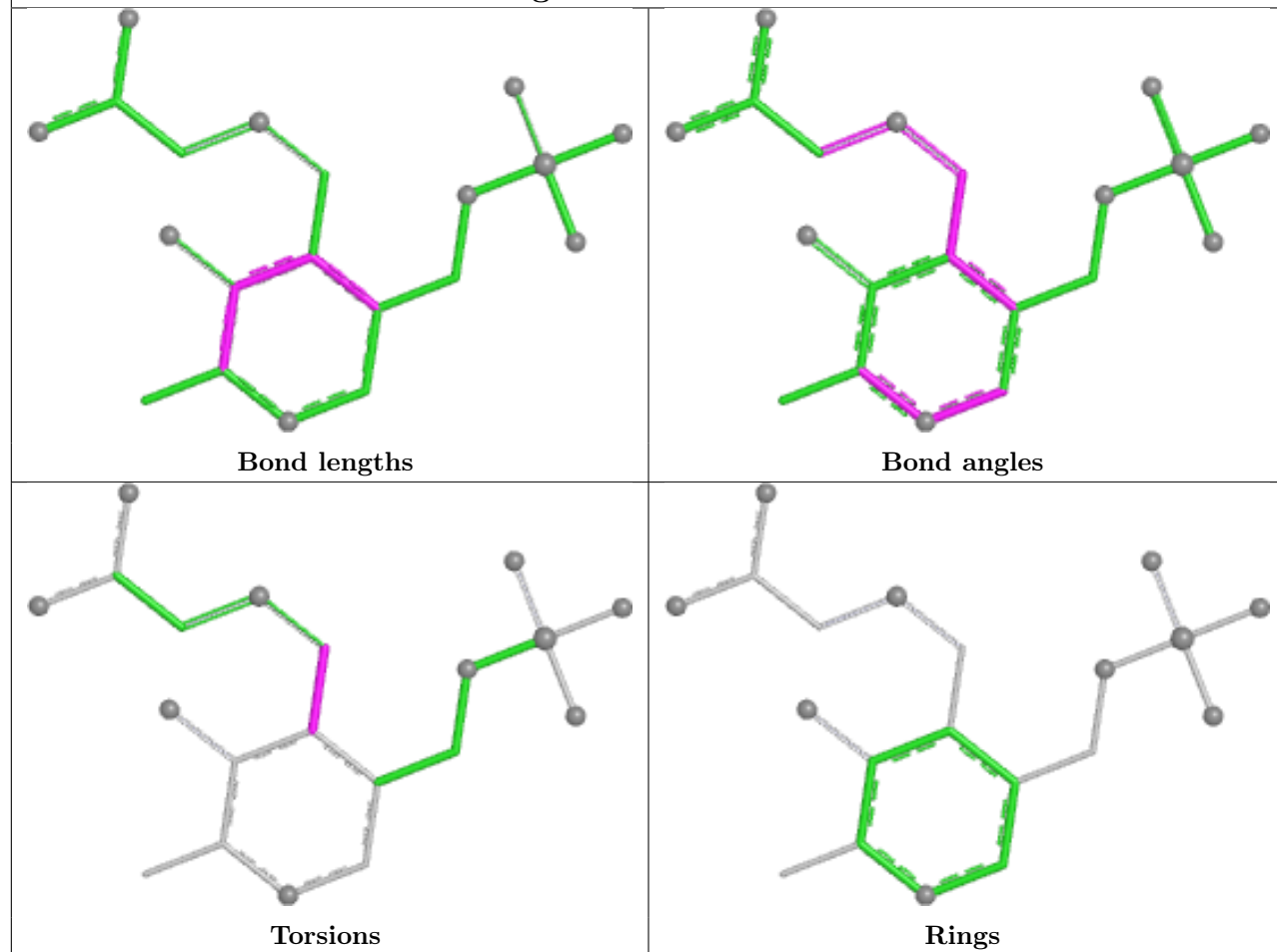
There are no ring outliers.

2 monomers are involved in 5 short contacts:

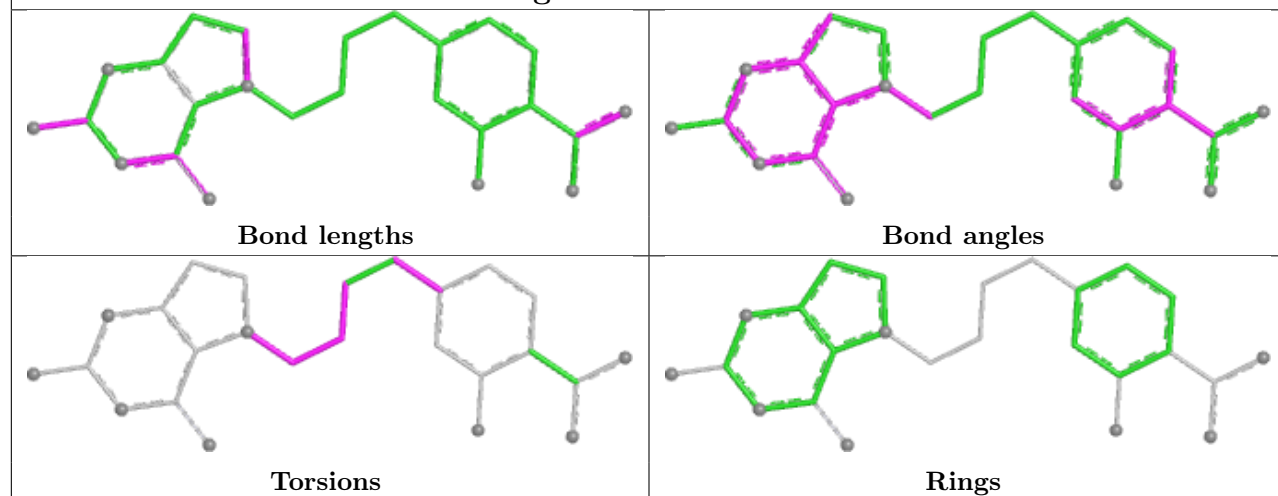
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	601	PLG	2	0
3	A	602[B]	PLG	3	0

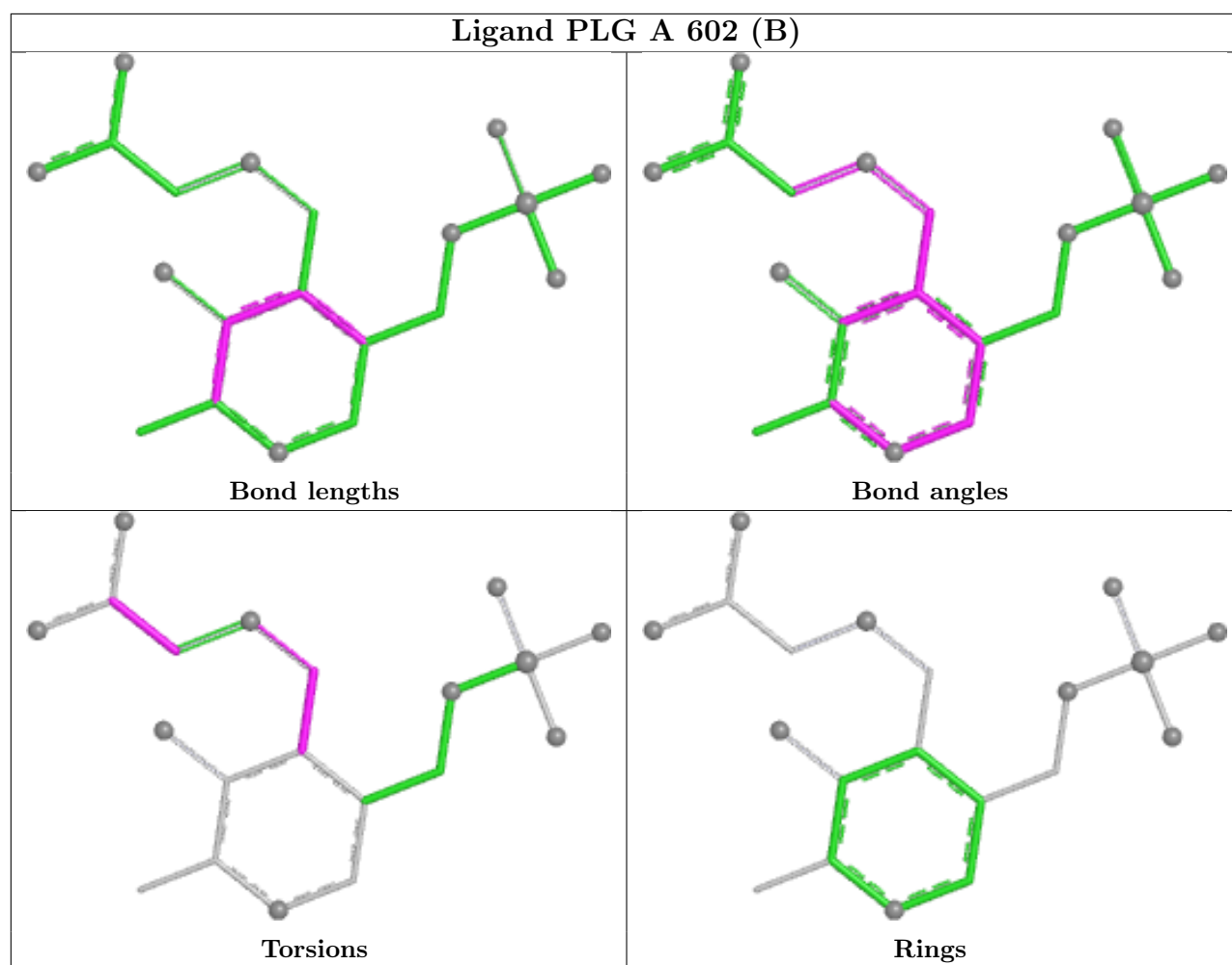
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 PLG B 601



Ligand Y5C A 601





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%)	-0.08	18 (3%) 42 37	23, 39, 76, 111	1 (0%)
1	B	459/493 (93%)	0.93	73 (15%) 5 4	30, 70, 116, 159	1 (0%)
All	All	914/986 (92%)	0.43	91 (9%) 12 10	23, 52, 109, 159	2 (0%)

All (91) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	301	PRO	6.8
1	B	303	THR	6.0
1	A	106	TYR	5.5
1	B	298	ALA	5.4
1	B	419	ILE	5.2
1	B	415	ASP	5.2
1	A	420	THR	5.1
1	B	305	ARG	4.7
1	B	416	ARG	4.7
1	B	471	PHE	4.7
1	A	304	GLY	4.6
1	B	456	LEU	4.6
1	B	420	THR	4.5
1	B	369	GLY	4.5
1	B	304	GLY	4.4
1	A	415	ASP	4.3
1	A	298	ALA	4.3
1	B	417	SER	4.2
1	B	469	LYS	4.0
1	A	416	ARG	4.0
1	A	105	TYR	3.9
1	B	366	LEU	3.8
1	B	203	LEU	3.7
1	B	230	ARG	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	357	ASN	3.5
1	B	302	LYS	3.4
1	B	364	ALA	3.4
1	B	365	LEU	3.4
1	B	106	TYR	3.4
1	B	392	ASP	3.4
1	B	410	ASN	3.4
1	B	374	SER	3.3
1	A	503	GLU	3.3
1	A	303	THR	3.2
1	B	349[A]	GLU	3.1
1	B	478	THR	3.1
1	B	463	ALA	3.1
1	B	197	LEU	3.1
1	B	414	GLY	3.1
1	A	419	ILE	3.1
1	B	457	GLU	3.1
1	B	307	ILE	3.1
1	A	180	VAL	3.1
1	B	460	SER	3.0
1	B	399	VAL	3.0
1	B	412	CYS	2.9
1	B	211	LEU	2.9
1	B	368	ARG	2.9
1	B	453	ASN	2.9
1	B	472	LEU	2.9
1	B	383	LEU	2.9
1	B	105	TYR	2.8
1	B	391	LEU	2.8
1	B	465	LEU	2.8
1	B	387	ARG	2.7
1	B	356	LYS	2.7
1	B	270	HIS	2.5
1	B	201	THR	2.5
1	A	476	SER	2.5
1	B	449	ASP	2.5
1	A	96	TYR	2.5
1	B	467	ASP	2.4
1	A	58	GLU	2.4
1	A	414	GLY	2.4
1	B	388	PRO	2.4
1	B	200	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	466	GLN	2.4
1	B	376	GLY	2.4
1	B	413	PRO	2.3
1	B	202	GLY	2.3
1	B	474	LYS	2.2
1	B	378	ASP	2.2
1	B	367	GLU	2.2
1	B	473	LEU	2.2
1	B	445	VAL	2.2
1	A	272	ASP	2.2
1	B	435	GLN	2.1
1	B	375	GLY	2.1
1	B	204	ILE	2.1
1	A	306	GLU	2.1
1	B	306	GLU	2.1
1	B	231	LEU	2.1
1	A	107	GLY	2.1
1	B	477	GLU	2.1
1	B	263	VAL	2.1
1	B	452	VAL	2.1
1	B	464	LYS	2.0
1	B	421	PRO	2.0
1	B	422	GLY	2.0
1	B	262	LYS	2.0
1	B	403	VAL	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 ⓘ

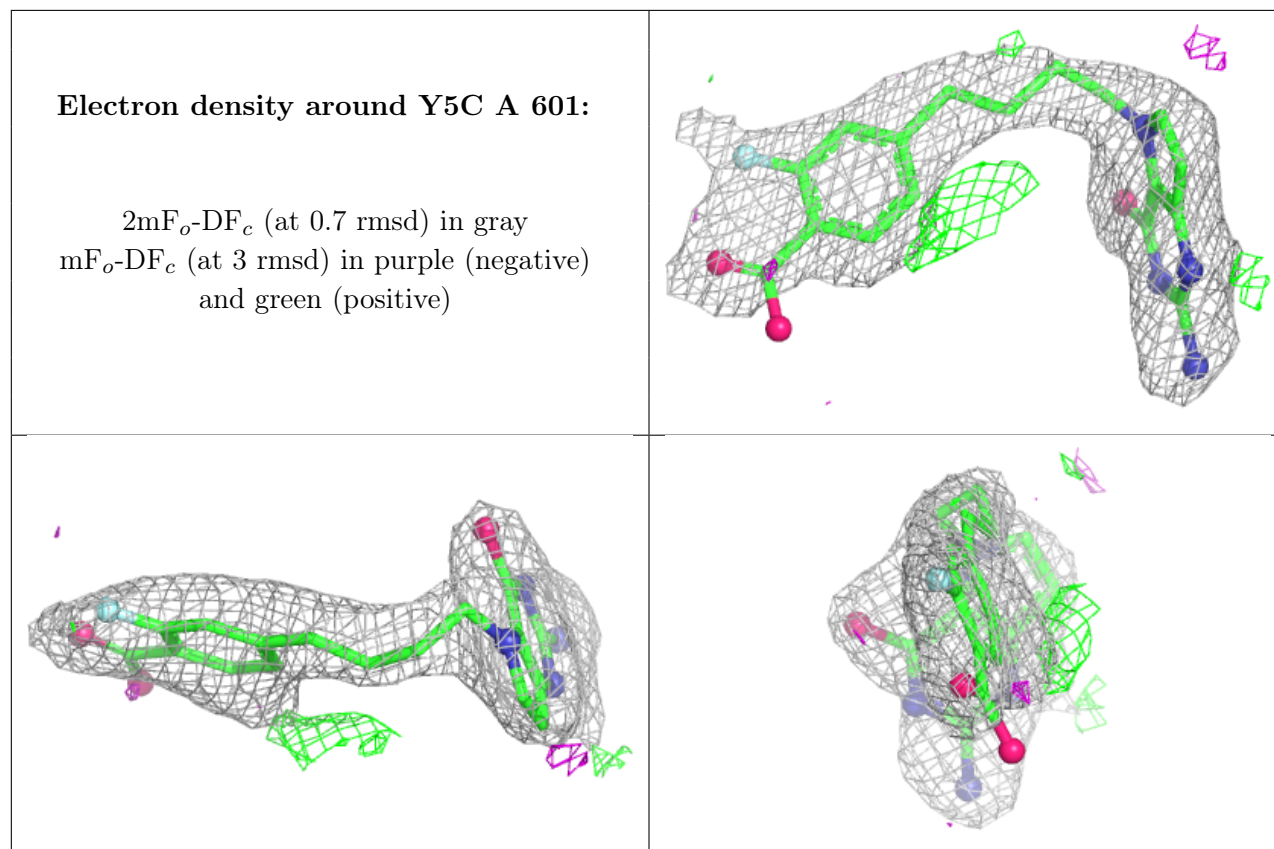
There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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.

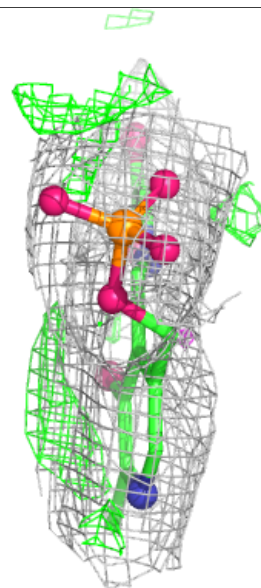
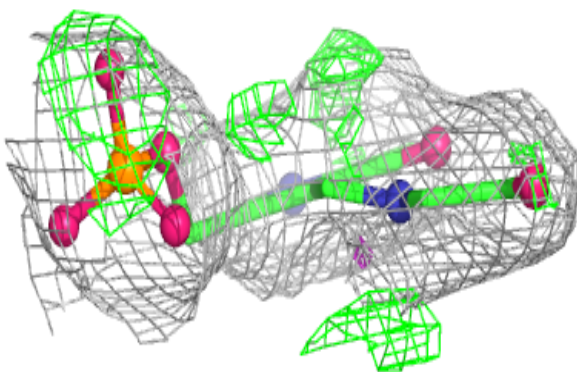
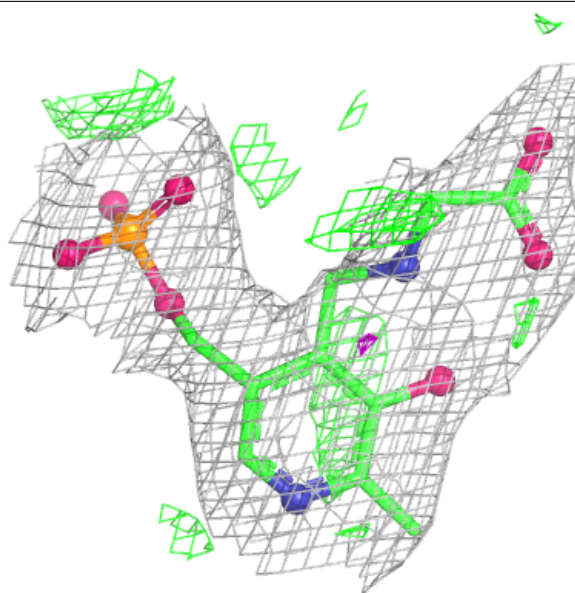
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	Y5C	A	601	25/25	0.87	0.15	26,59,75,84	0
3	PLG	B	601	20/20	0.94	0.14	40,61,90,93	0
3	PLG	A	602[B]	20/20	0.96	0.11	22,39,71,72	0

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.



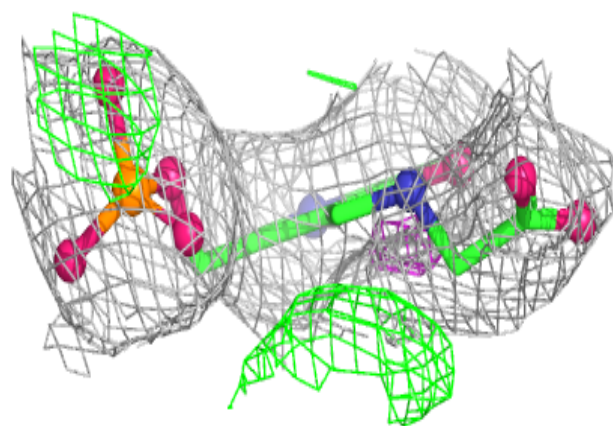
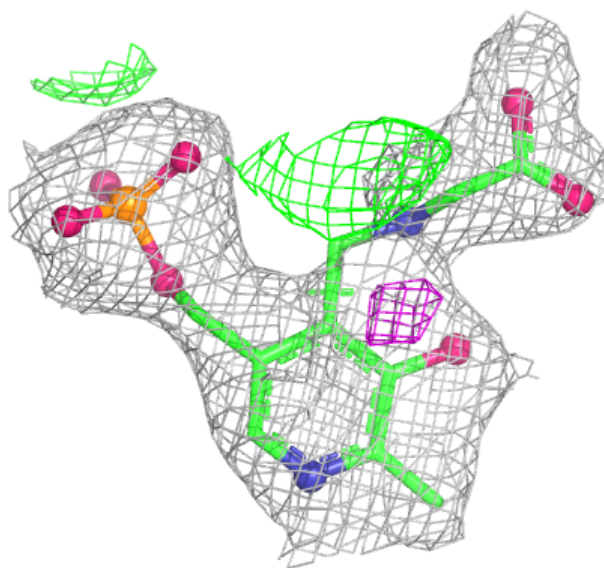
Electron density around PLG B 601:

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



Electron density around PLG A 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)



6.5 Other polymers ⓘ

There are no such residues in this entry.