



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 03:37 AM UTC

PDB ID : 8T4P / pdb_00008t4p
Title : Human mitochondrial serine hydroxymethyltransferase (SHMT2) in complex with PLP, glycine and di-glutamate AGF347 inhibitor
Authors : Katinas, J.M.; Dann III, C.E.
Deposited on : 2023-06-09
Resolution : 2.80 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

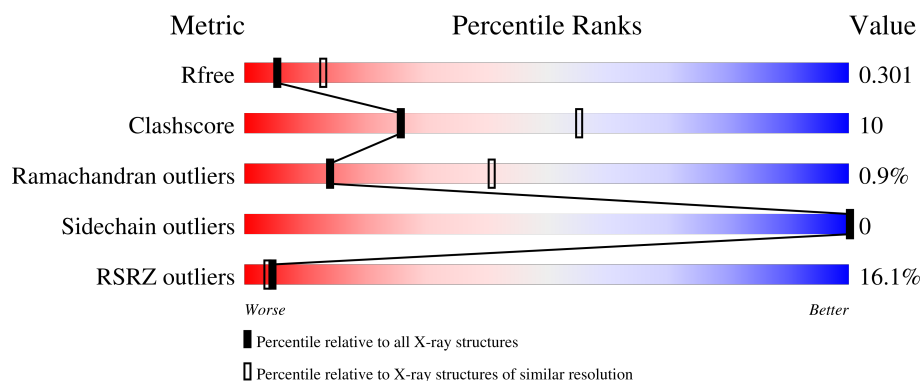
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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% 73% 19% 8%
1	B	493	26% 70% 22% 8%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6980 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	454	Total	C	N	O	S	0	1	0
			3521	2217	628	660	16			
1	B	454	Total	C	N	O	S	0	0	0
			3351	2098	609	631	13			

There are 36 discrepancies between the modelled and reference sequences:

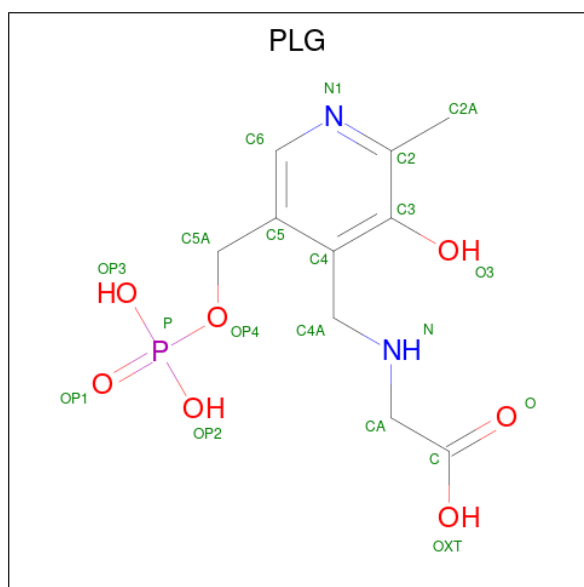
Chain	Residue	Modelled	Actual	Comment	Reference
A	12	MET	-	initiating methionine	UNP P34897
A	13	GLY	-	expression tag	UNP P34897
A	14	SER	-	expression tag	UNP P34897
A	15	SER	-	expression tag	UNP P34897
A	16	HIS	-	expression tag	UNP P34897
A	17	HIS	-	expression tag	UNP P34897
A	18	HIS	-	expression tag	UNP P34897
A	19	HIS	-	expression tag	UNP P34897
A	20	HIS	-	expression tag	UNP P34897
A	21	HIS	-	expression tag	UNP P34897
A	22	SER	-	expression tag	UNP P34897
A	23	SER	-	expression tag	UNP P34897
A	24	GLY	-	expression tag	UNP P34897
A	25	LEU	-	expression tag	UNP P34897
A	26	VAL	-	expression tag	UNP P34897
A	27	PRO	-	expression tag	UNP P34897
A	28	ARG	-	expression tag	UNP P34897
A	418	THR	ALA	conflict	UNP P34897
B	12	MET	-	initiating methionine	UNP P34897
B	13	GLY	-	expression tag	UNP P34897
B	14	SER	-	expression tag	UNP P34897
B	15	SER	-	expression tag	UNP P34897
B	16	HIS	-	expression tag	UNP P34897
B	17	HIS	-	expression tag	UNP P34897
B	18	HIS	-	expression tag	UNP P34897

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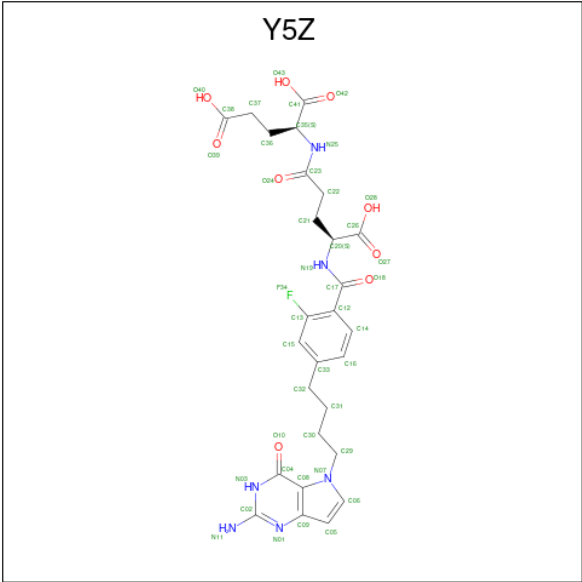
Chain	Residue	Modelled	Actual	Comment	Reference
B	19	HIS	-	expression tag	UNP P34897
B	20	HIS	-	expression tag	UNP P34897
B	21	HIS	-	expression tag	UNP P34897
B	22	SER	-	expression tag	UNP P34897
B	23	SER	-	expression tag	UNP P34897
B	24	GLY	-	expression tag	UNP P34897
B	25	LEU	-	expression tag	UNP P34897
B	26	VAL	-	expression tag	UNP P34897
B	27	PRO	-	expression tag	UNP P34897
B	28	ARG	-	expression tag	UNP P34897
B	418	THR	ALA	conflict	UNP P34897

- Molecule 2 is N-GLYCINE-[3-HYDROXY-2-METHYL-5-PHOSPHONOXYMETHYL-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		
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-gamma-glutamyl-L-glutamic acid (CCD ID: Y5Z) (formula: C₂₇H₃₁FN₆O₉) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	F	N	O	5	0
			43	27	1	6	9		

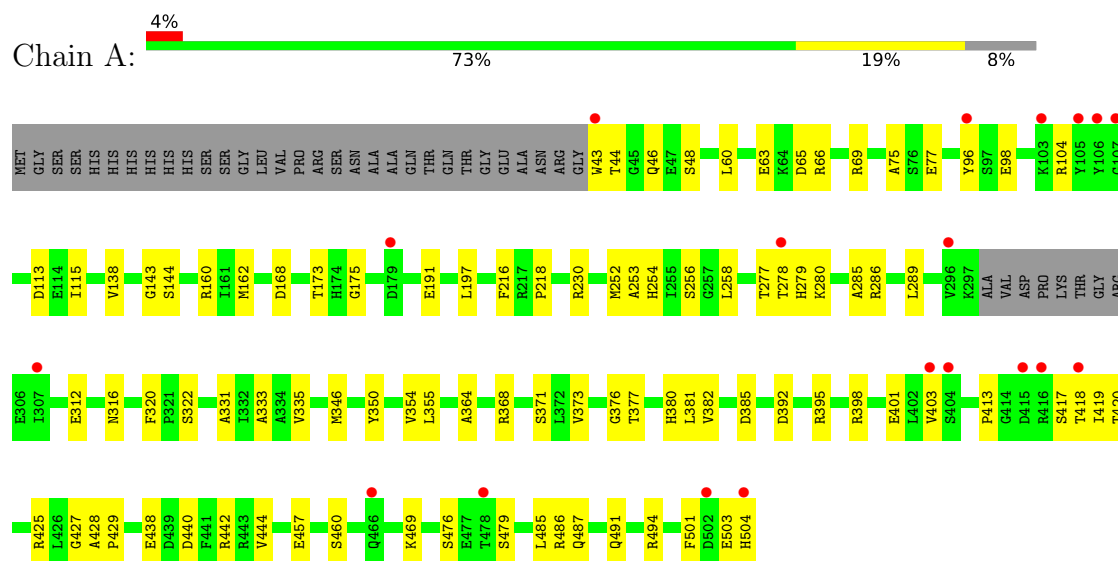
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	17	Total	O	0	0
			17	17		
4	B	8	Total	O	0	0
			8	8		

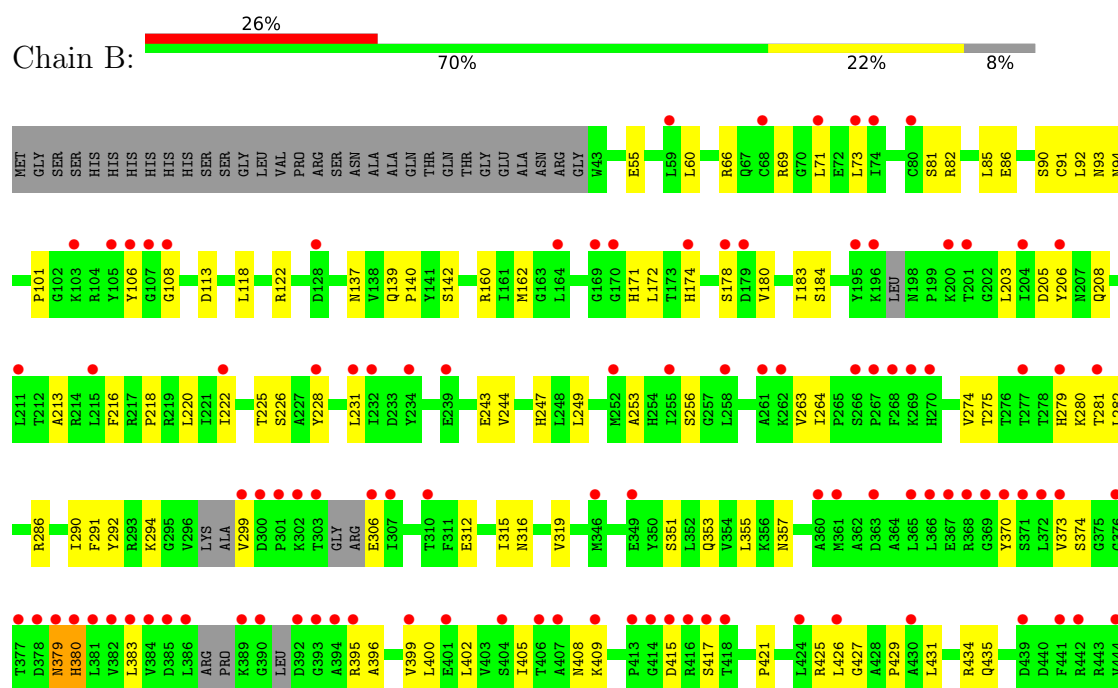
3 Residue-property plots

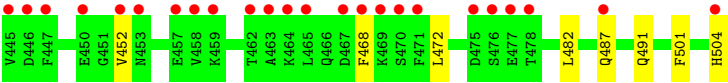
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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	159.29Å 159.29Å 208.65Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.79 – 2.80 48.79 – 2.80	Depositor EDS
% Data completeness (in resolution range)	91.8 (48.79-2.80) 91.7 (48.79-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.88 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.258 , 0.300 0.260 , 0.301	Depositor DCC
R_{free} test set	1760 reflections (4.51%)	wwPDB-VP
Wilson B-factor (Å ²)	49.6	Xtriage
Anisotropy	0.370	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 45.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	6980	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.67% 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: PLG, Y5Z

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	0/3592	0.33	0/4864
1	B	0.13	0/3414	0.34	0/4631
All	All	0.13	0/7006	0.34	0/9495

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	3521	0	3461	61	0
1	B	3351	0	3108	76	0
2	A	20	0	11	1	0
2	B	20	0	11	2	0
3	A	43	0	0	0	0
4	A	17	0	0	0	0
4	B	8	0	0	0	0
All	All	6980	0	6591	129	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 10.

All (129) 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:73:LEU:HD12	1:B:426:LEU:HB3	1.26	1.07
1:A:403:VAL:HG11	1:A:485:LEU:HD23	1.33	1.04
1:B:174:HIS:HD2	1:B:222:ILE:HG21	1.46	0.80
1:A:60:LEU:HD21	1:A:504:HIS:HB2	1.65	0.79
1:A:403:VAL:HG11	1:A:485:LEU:CD2	2.15	0.75
1:B:137:ASN:HB2	1:B:316:ASN:HD21	1.50	0.74
1:B:160:ARG:HB3	1:B:216:PHE:CE2	2.26	0.71
1:A:96:TYR:OH	1:B:280:LYS:NZ	2.23	0.70
1:B:66:ARG:HA	1:B:69:ARG:HG2	1.76	0.68
1:A:322:SER:HA	1:B:184:SER:HA	1.79	0.65
1:B:274:VAL:HB	1:B:291:PHE:HB2	1.79	0.64
1:B:249:LEU:HD21	1:B:275:THR:HG23	1.78	0.63
1:A:403:VAL:HG13	1:A:486:ARG:HA	1.81	0.63
1:B:396:ALA:O	1:B:400:LEU:HG	2.00	0.61
1:B:137:ASN:HB2	1:B:316:ASN:ND2	2.16	0.60
1:A:503:GLU:N	1:A:503:GLU:OE1	2.34	0.60
1:B:162:MET:HE2	1:B:218:PRO:HG3	1.84	0.60
1:A:65:ASP:OD1	1:A:494:ARG:NH1	2.23	0.59
1:A:253:ALA:HB1	1:A:280:LYS:HE2	1.86	0.57
1:B:73:LEU:HD12	1:B:426:LEU:CB	2.19	0.57
1:B:73:LEU:HD21	1:B:405:ILE:CG2	2.35	0.57
1:B:226:SER:O	1:B:425:ARG:NH1	2.36	0.57
1:B:370:TYR:OH	1:B:452:VAL:HG11	2.05	0.57
1:B:228:TYR:O	1:B:379:ASN:ND2	2.38	0.57
1:B:290:ILE:HG21	1:B:315:ILE:HG21	1.87	0.56
1:A:104:ARG:NE	1:A:113:ASP:OD1	2.40	0.54
1:A:44:THR:HG23	1:A:46:GLN:H	1.72	0.54
1:A:43:TRP:O	1:B:435:GLN:NE2	2.40	0.53
1:B:279:HIS:CD2	1:B:286:ARG:HG2	2.43	0.53
1:B:222:ILE:HG23	1:B:249:LEU:HD12	1.89	0.53
1:B:299:VAL:O	1:B:306:GLU:N	2.40	0.53
1:B:431:LEU:HD23	1:B:434:ARG:HD3	1.89	0.53
1:A:48:SER:HA	1:B:82:ARG:HH11	1.74	0.53
1:A:476:SER:HA	1:A:479:SER:HB3	1.90	0.53
1:B:178:SER:C	1:B:180:VAL:H	2.18	0.51
1:B:171:HIS:HB3	1:B:174:HIS:CE1	2.46	0.50
1:A:373:VAL:HG11	1:A:413:PRO:HD2	1.92	0.50
1:A:428:ALA:H	1:A:429:PRO:HD2	1.76	0.50
1:B:73:LEU:HB2	1:B:427:GLY:H	1.76	0.50
1:A:77:GLU:HG2	1:B:94:ASN:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:137:ASN:ND2	1:B:140:PRO:HD3	2.27	0.50
1:B:205:ASP:HB3	1:B:208:GLN:HB3	1.93	0.49
1:A:75:ALA:HB3	1:A:425:ARG:HH11	1.77	0.49
1:B:468:PHE:O	1:B:472:LEU:HG	2.12	0.49
2:B:601:PLG:N	2:B:601:PLG:O3	2.46	0.49
1:A:230:ARG:HH21	1:A:376:GLY:H	1.60	0.49
1:B:71:LEU:HA	1:B:431:LEU:HD21	1.95	0.49
1:A:417:SER:O	1:A:419:ILE:N	2.46	0.48
1:B:263:VAL:HG21	1:B:355:LEU:HD11	1.95	0.48
1:B:90:SER:OG	1:B:91:CYS:N	2.44	0.48
1:B:501:PHE:HB2	1:B:504:HIS:OXT	2.14	0.48
1:A:403:VAL:CG1	1:A:485:LEU:HD23	2.23	0.47
1:B:353:GLN:NE2	1:B:357:ASN:OD1	2.45	0.47
1:A:75:ALA:HA	1:A:427:GLY:HA3	1.96	0.47
1:A:364:ALA:O	1:A:368[B]:ARG:HG2	2.14	0.47
1:B:487:GLN:O	1:B:491:GLN:HG3	2.14	0.47
1:A:428:ALA:N	1:A:429:PRO:HD2	2.29	0.47
1:A:63:GLU:HG2	1:B:92:LEU:HD23	1.96	0.47
1:B:60:LEU:C	1:B:60:LEU:HD23	2.40	0.47
1:A:286:ARG:HG3	1:B:93:ASN:OD1	2.15	0.46
1:A:380:HIS:NE2	1:A:381:LEU:HD23	2.30	0.46
1:A:144:SER:HA	1:A:173:THR:HG21	1.97	0.46
1:B:415:ASP:OD2	1:B:417:SER:N	2.35	0.46
1:B:174:HIS:CD2	1:B:222:ILE:HG21	2.36	0.46
1:B:373:VAL:HG23	1:B:383:LEU:O	2.16	0.46
1:A:380:HIS:HB2	1:A:429:PRO:HD3	1.96	0.45
1:A:160:ARG:HB3	1:A:216:PHE:CE1	2.51	0.45
1:A:417:SER:OG	1:A:420:THR:HB	2.16	0.45
1:B:203:LEU:HB3	1:B:206:TYR:HE2	1.82	0.45
1:B:395:ARG:HH11	1:B:468:PHE:HD2	1.64	0.45
1:B:220:LEU:HD12	1:B:247:HIS:HB2	1.97	0.45
1:A:487:GLN:HE21	1:A:491:GLN:HE21	1.64	0.45
1:B:213:ALA:HB1	1:B:244:VAL:HG11	1.98	0.45
1:B:253:ALA:HB1	1:B:280:LYS:HE2	1.99	0.45
1:A:371:SER:HB2	1:A:385:ASP:HB3	1.98	0.45
1:B:178:SER:O	1:B:178:SER:OG	2.27	0.45
1:A:168:ASP:HB3	1:A:197:LEU:HG	1.99	0.45
1:B:118:LEU:HD11	1:B:122:ARG:CZ	2.46	0.45
1:A:60:LEU:HD11	1:B:90:SER:HB2	1.99	0.45
1:A:401:GLU:HG3	1:B:108:GLY:H	1.81	0.45
1:A:457:GLU:O	1:A:460:SER:OG	2.34	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:399:VAL:HG12	1:B:472:LEU:HD11	1.99	0.45
1:B:415:ASP:OD1	1:B:421:PRO:HA	2.18	0.45
1:A:162:MET:HG3	1:A:218:PRO:HB3	1.98	0.44
1:A:258:LEU:HD13	1:A:355:LEU:HD21	1.98	0.44
1:A:160:ARG:HA	1:A:191:GLU:O	2.18	0.44
1:B:137:ASN:ND2	1:B:319:VAL:HG21	2.31	0.44
1:B:280:LYS:C	1:B:282:LEU:H	2.24	0.44
1:A:312:GLU:O	1:A:316:ASN:ND2	2.51	0.44
1:B:292:TYR:CE1	1:B:312:GLU:HB2	2.52	0.44
1:A:350:TYR:O	1:A:354:VAL:HG23	2.17	0.44
2:A:601:PLG:OXT	1:B:106:TYR:OH	2.33	0.44
1:B:142:SER:OG	2:B:601:PLG:OP2	2.35	0.43
1:B:225:THR:OG1	1:B:228:TYR:HB3	2.18	0.43
1:A:331:ALA:O	1:A:335:VAL:HG23	2.18	0.43
1:B:243:GLU:HG3	1:B:244:VAL:HG13	2.00	0.43
1:A:98:GLU:HB3	1:A:320:PHE:CZ	2.54	0.43
1:B:81:SER:O	1:B:85:LEU:HG	2.18	0.43
1:B:402:LEU:HD13	1:B:482:LEU:HD13	2.00	0.43
1:A:392:ASP:OD1	1:A:395:ARG:HG2	2.19	0.43
1:B:380:HIS:HB2	1:B:429:PRO:HD3	2.01	0.43
1:A:346:MET:HE3	1:A:346:MET:HB3	1.92	0.43
1:B:274:VAL:O	1:B:291:PHE:N	2.41	0.42
1:B:351:SER:O	1:B:355:LEU:HD12	2.20	0.42
1:B:86:GLU:HG3	1:B:501:PHE:HZ	1.84	0.42
1:B:101:PRO:HA	1:B:113:ASP:OD2	2.18	0.42
1:A:143:GLY:HA3	1:A:277:THR:HG22	2.01	0.42
1:A:254:HIS:HB3	1:A:380:HIS:CE1	2.54	0.42
1:B:139:GLN:N	1:B:140:PRO:CD	2.83	0.42
1:B:231:LEU:HD21	1:B:264:ILE:HD12	2.02	0.42
1:A:403:VAL:HG13	1:A:486:ARG:CA	2.48	0.42
1:B:279:HIS:HD1	1:B:279:HIS:C	2.26	0.42
1:A:440:ASP:O	1:A:444:VAL:HG23	2.19	0.42
1:A:377:THR:OG1	1:A:382:VAL:HG12	2.20	0.41
1:A:438:GLU:HB3	1:A:442:ARG:NH2	2.35	0.41
1:B:256:SER:OG	1:B:282:LEU:HD13	2.20	0.41
1:A:66:ARG:HA	1:A:69:ARG:HG2	2.03	0.41
1:B:355:LEU:HD12	1:B:355:LEU:H	1.84	0.41
1:A:115:ILE:HD12	1:A:333:ALA:HB2	2.02	0.41
1:B:408:ASN:ND2	1:B:409:LYS:O	2.54	0.41
1:A:278:THR:HG23	1:A:285:ALA:O	2.21	0.41
1:B:171:HIS:CD2	1:B:172:LEU:H	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:398:ARG:HG2	1:A:469:LYS:HG2	2.02	0.41
1:A:279:HIS:HD1	1:A:286:ARG:HA	1.85	0.41
1:B:294:LYS:HE2	1:B:312:GLU:OE1	2.21	0.41
1:A:138:VAL:HG12	1:A:289:LEU:HD22	2.03	0.41
1:A:252:MET:HE3	1:A:256:SER:HB3	2.02	0.41
1:A:403:VAL:O	1:A:403:VAL:HG12	2.20	0.40
1:A:501:PHE:HB2	1:A:504:HIS:OXT	2.21	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	451/493 (92%)	418 (93%)	31 (7%)	2 (0%)	30	60
1	B	442/493 (90%)	400 (90%)	36 (8%)	6 (1%)	9	30
All	All	893/986 (91%)	818 (92%)	67 (8%)	8 (1%)	14	41

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	374	SER
1	B	55	GLU
1	A	418	THR
1	B	379	ASN
1	B	380	HIS
1	B	281	THR
1	B	183	ILE
1	A	175	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	367/406 (90%)	367 (100%)	0	100	100
1	B	316/406 (78%)	316 (100%)	0	100	100
All	All	683/812 (84%)	683 (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 (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	270	HIS
1	A	410	ASN
1	A	491	GLN
1	B	316	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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
2	PLG	B	601	-	20,20,20	2.54	3 (15%)	26,28,28	1.74	3 (11%)
3	Y5Z	A	602	-	44,45,45	2.24	13 (29%)	58,62,62	1.63	9 (15%)
2	PLG	A	601	-	20,20,20	2.51	3 (15%)	26,28,28	1.80	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
2	PLG	B	601	-	-	6/12/12/12	0/1/1/1
3	Y5Z	A	602	-	-	14/37/37/37	0/3/3/3
2	PLG	A	601	-	-	3/12/12/12	0/1/1/1

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	PLG	C3-C2	7.59	1.48	1.41
2	B	601	PLG	C3-C2	7.19	1.48	1.41
2	B	601	PLG	C5-C4	6.12	1.49	1.40
3	A	602	Y5Z	C23-N25	5.70	1.46	1.34
2	B	601	PLG	C3-C4	5.62	1.48	1.40
3	A	602	Y5Z	C02-N01	5.62	1.46	1.33
2	A	601	PLG	C5-C4	5.41	1.48	1.40
2	A	601	PLG	C3-C4	5.40	1.48	1.40
3	A	602	Y5Z	C17-N19	5.12	1.46	1.34
3	A	602	Y5Z	C02-N11	4.95	1.45	1.34
3	A	602	Y5Z	C09-N01	4.48	1.48	1.38
3	A	602	Y5Z	C08-C04	4.07	1.53	1.43
3	A	602	Y5Z	C02-N03	3.13	1.45	1.37
3	A	602	Y5Z	C04-N03	2.69	1.43	1.38
3	A	602	Y5Z	C06-N07	-2.47	1.32	1.38
3	A	602	Y5Z	O10-C04	-2.45	1.18	1.23
3	A	602	Y5Z	C08-N07	-2.43	1.34	1.39
3	A	602	Y5Z	O24-C23	-2.17	1.19	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	602	Y5Z	C05-C09	-2.08	1.40	1.45

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	PLG	C4A-N-CA	5.82	119.50	112.72
2	A	601	PLG	C4A-N-CA	5.51	119.13	112.72
3	A	602	Y5Z	C08-C04-N03	5.13	119.97	110.94
3	A	602	Y5Z	C08-C09-N01	-4.53	120.47	124.81
3	A	602	Y5Z	C15-C13-C12	-3.10	120.06	123.48
3	A	602	Y5Z	C05-C09-N01	2.91	132.93	123.36
3	A	602	Y5Z	C14-C12-C13	2.87	119.88	116.70
3	A	602	Y5Z	C02-N03-C04	-2.86	119.92	125.11
3	A	602	Y5Z	O10-C04-C08	-2.76	120.85	127.62
2	B	601	PLG	C6-N1-C2	2.70	124.10	119.20
2	A	601	PLG	C5A-C5-C4	-2.45	117.50	122.67
3	A	602	Y5Z	C09-C08-C04	-2.31	119.52	121.36
2	B	601	PLG	C4A-C4-C5	2.29	122.24	119.75
3	A	602	Y5Z	C09-N01-C02	2.26	120.17	116.63
2	A	601	PLG	C6-C5-C4	2.24	119.75	118.06
2	A	601	PLG	C6-N1-C2	2.10	123.01	119.20
2	A	601	PLG	C5A-C5-C6	2.08	122.75	119.36

There are no chirality outliers.

All (23) 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	B	601	PLG	C5-C4-C4A-N
3	A	602	Y5Z	N25-C35-C36-C37
3	A	602	Y5Z	C13-C12-C17-N19
2	B	601	PLG	C3-C4-C4A-N
3	A	602	Y5Z	C41-C35-C36-C37
3	A	602	Y5Z	C21-C22-C23-N25
3	A	602	Y5Z	C21-C22-C23-O24
2	B	601	PLG	C4-C4A-N-CA
3	A	602	Y5Z	N25-C35-C41-O42
3	A	602	Y5Z	C13-C12-C17-O18
3	A	602	Y5Z	N25-C35-C41-O43
2	B	601	PLG	OXT-C-CA-N
3	A	602	Y5Z	C36-C35-C41-O43

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Mol	Chain	Res	Type	Atoms
2	B	601	PLG	O-C-CA-N
2	B	601	PLG	C5A-OP4-P-OP1
3	A	602	Y5Z	C36-C35-C41-O42
3	A	602	Y5Z	C30-C29-N07-C08
3	A	602	Y5Z	C36-C37-C38-O40
3	A	602	Y5Z	C36-C37-C38-O39
2	A	601	PLG	C5A-OP4-P-OP3
3	A	602	Y5Z	N19-C20-C21-C22

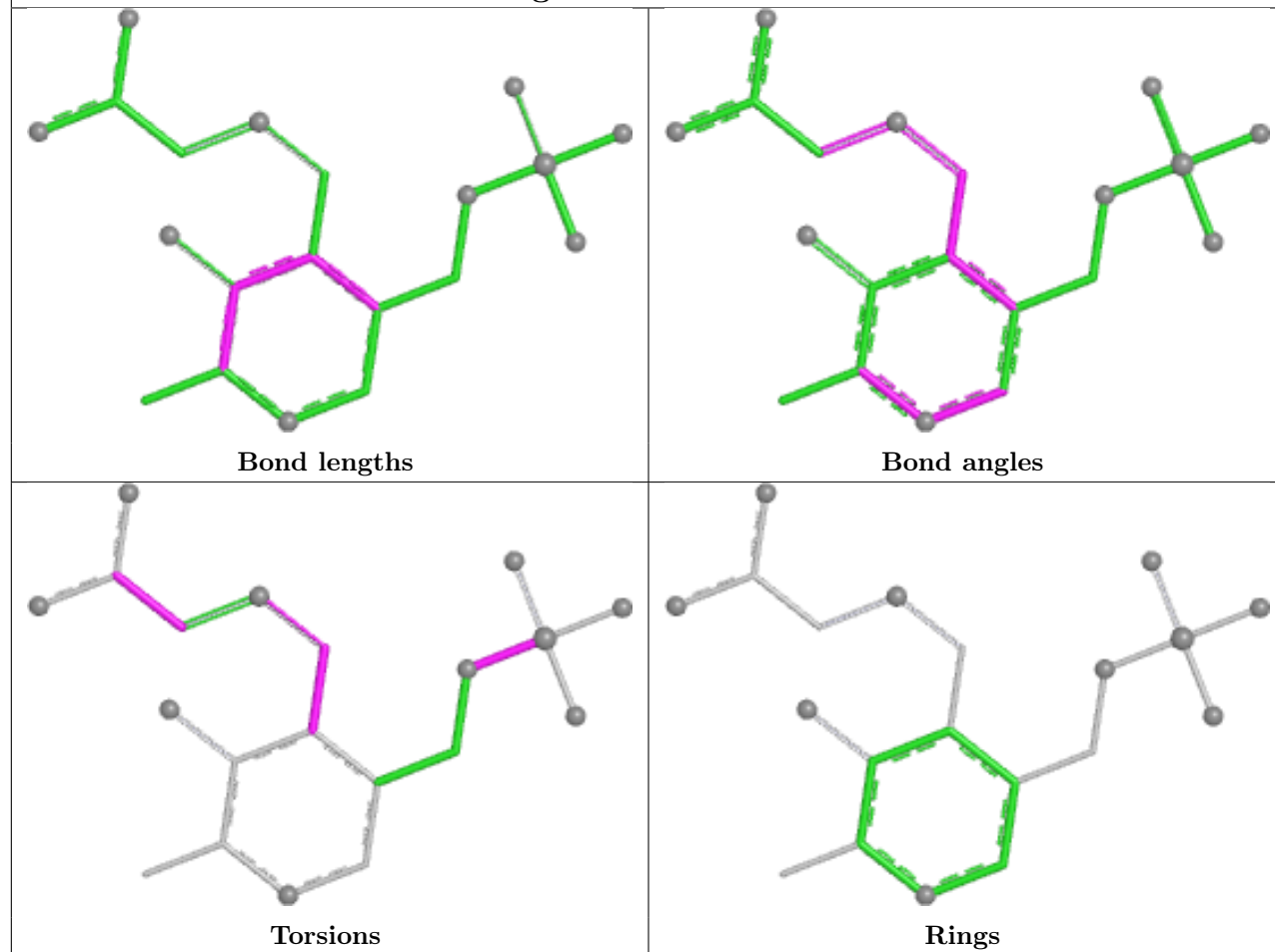
There are no ring outliers.

2 monomers are involved in 3 short contacts:

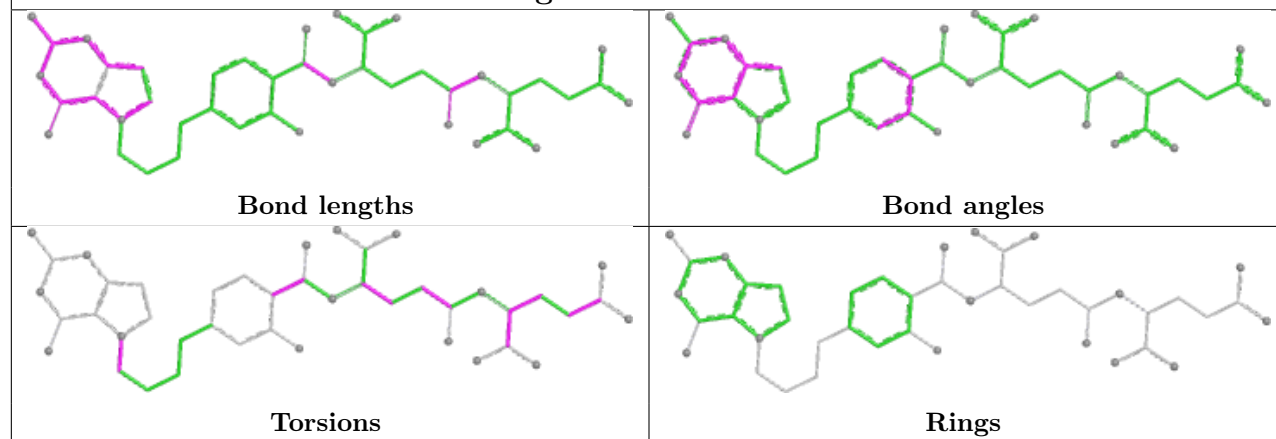
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	601	PLG	2	0
2	A	601	PLG	1	0

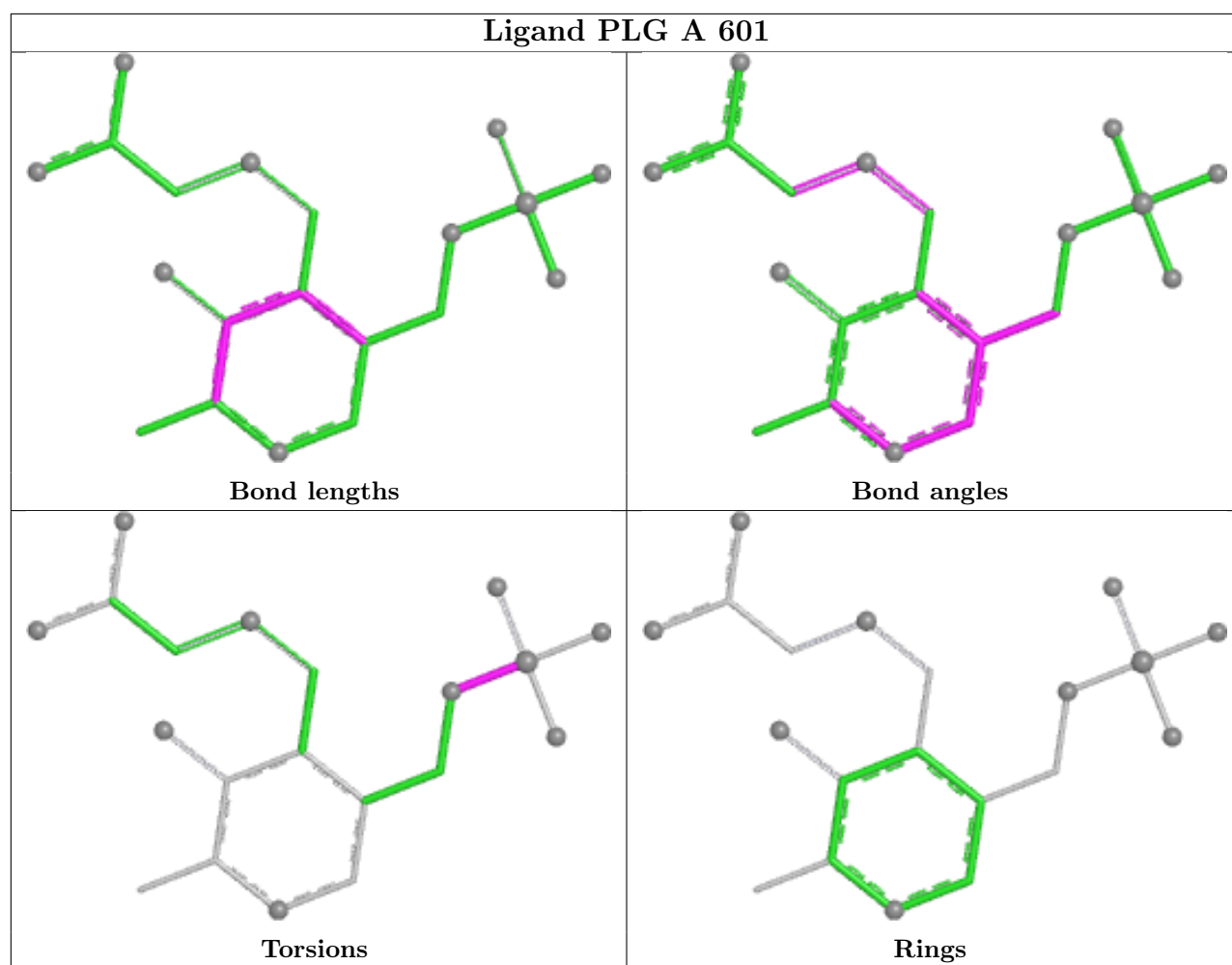
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 Y5Z A 602





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	454/493 (92%)	0.46	19 (4%)	40 32	22, 44, 77, 132	1 (0%)
1	B	454/493 (92%)	1.45	127 (27%)	1 1	33, 73, 113, 131	0
All	All	908/986 (92%)	0.96	146 (16%)	4 4	22, 56, 106, 132	1 (0%)

All (146) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	279	HIS	7.2
1	A	106	TYR	7.1
1	B	399	VAL	5.8
1	B	390	GLY	5.6
1	A	105	TYR	5.6
1	B	385	ASP	5.3
1	B	376	GLY	4.9
1	B	389	LYS	4.7
1	B	303	THR	4.5
1	A	418	THR	4.5
1	B	414	GLY	4.3
1	A	43	TRP	4.1
1	B	106	TYR	4.1
1	A	416	ARG	4.0
1	B	406	THR	4.0
1	B	307	ILE	3.9
1	B	368	ARG	3.9
1	B	169	GLY	3.9
1	B	195	TYR	3.8
1	B	478	THR	3.8
1	B	418	THR	3.8
1	B	409	LYS	3.7
1	B	371	SER	3.7
1	B	204	ILE	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	502	ASP	3.6
1	B	373	VAL	3.5
1	B	450	GLU	3.5
1	B	378	ASP	3.5
1	B	270	HIS	3.5
1	A	404	SER	3.5
1	B	384	VAL	3.4
1	B	196	LYS	3.4
1	B	211	LEU	3.3
1	B	465	LEU	3.3
1	B	453	ASN	3.3
1	B	108	GLY	3.2
1	B	382	VAL	3.2
1	A	415	ASP	3.2
1	B	164	LEU	3.2
1	B	407	ALA	3.2
1	B	471	PHE	3.2
1	B	262	LYS	3.2
1	B	463	ALA	3.1
1	B	457	GLU	3.1
1	B	268	PHE	3.1
1	B	467	ASP	3.1
1	B	372	LEU	3.1
1	B	377	THR	3.1
1	B	370	TYR	3.1
1	B	475	ASP	3.1
1	A	504	HIS	3.0
1	B	234	TYR	3.0
1	B	252	MET	3.0
1	B	59	LEU	3.0
1	B	392	ASP	3.0
1	B	277	THR	3.0
1	B	255	ILE	2.9
1	B	369	GLY	2.9
1	B	299	VAL	2.9
1	B	261	ALA	2.9
1	B	379	ASN	2.8
1	B	71	LEU	2.8
1	B	201	THR	2.8
1	B	367	GLU	2.8
1	B	258	LEU	2.8
1	B	363	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	462	THR	2.8
1	A	107	GLY	2.8
1	B	360	ALA	2.7
1	B	468	PHE	2.7
1	B	179	ASP	2.7
1	B	128	ASP	2.7
1	B	266	SER	2.7
1	B	458	VAL	2.7
1	B	310	THR	2.7
1	B	477	GLU	2.7
1	B	231	LEU	2.7
1	B	413	PRO	2.7
1	A	403	VAL	2.7
1	B	232	ILE	2.6
1	B	269	LYS	2.6
1	B	469	LYS	2.6
1	B	417	SER	2.6
1	A	96	TYR	2.6
1	B	107	GLY	2.6
1	B	445	VAL	2.6
1	B	404	SER	2.6
1	B	301	PRO	2.6
1	B	74	ILE	2.6
1	B	452	VAL	2.5
1	B	300	ASP	2.5
1	B	415	ASP	2.5
1	B	441	PHE	2.5
1	B	365	LEU	2.5
1	A	307	ILE	2.4
1	B	470	SER	2.4
1	B	228	TYR	2.4
1	B	281	THR	2.4
1	B	302	LYS	2.4
1	B	459	LYS	2.4
1	B	239	GLU	2.4
1	B	366	LEU	2.4
1	B	424	LEU	2.4
1	B	306	GLU	2.3
1	A	278	THR	2.3
1	B	206	TYR	2.3
1	B	170	GLY	2.3
1	B	439	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	73	LEU	2.3
1	B	381	LEU	2.3
1	B	349	GLU	2.3
1	A	179	ASP	2.3
1	B	215	LEU	2.3
1	B	416	ARG	2.3
1	B	222	ILE	2.3
1	B	361	MET	2.2
1	B	430	ALA	2.2
1	A	103	LYS	2.2
1	B	174	HIS	2.2
1	B	267	PRO	2.2
1	B	178	SER	2.2
1	B	346	MET	2.2
1	B	447	PHE	2.2
1	B	401	GLU	2.2
1	B	446	ASP	2.2
1	B	80	CYS	2.2
1	B	200	LYS	2.2
1	B	464	LYS	2.2
1	A	478	THR	2.2
1	B	103	LYS	2.2
1	B	487	GLN	2.1
1	A	296	VAL	2.1
1	B	476	SER	2.1
1	B	504	HIS	2.1
1	A	466	GLN	2.1
1	B	393	GLY	2.1
1	B	426	LEU	2.1
1	B	442	ARG	2.1
1	B	395	ARG	2.1
1	B	394	ALA	2.1
1	B	105	TYR	2.1
1	B	380	HIS	2.0
1	B	444	VAL	2.0
1	B	68	CYS	2.0
1	B	383	LEU	2.0
1	B	386	LEU	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](#)

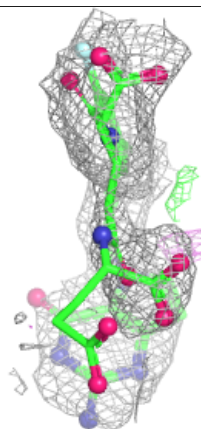
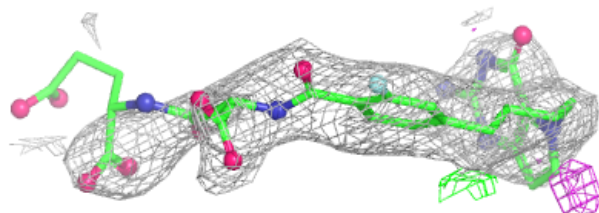
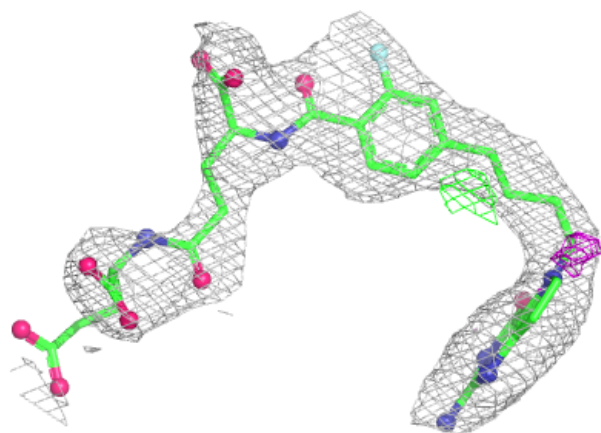
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists 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	Y5Z	A	602	43/43	0.88	0.16	31,64,95,98	5
2	PLG	B	601	20/20	0.92	0.12	51,65,75,77	0
2	PLG	A	601	20/20	0.95	0.10	23,42,57,63	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.

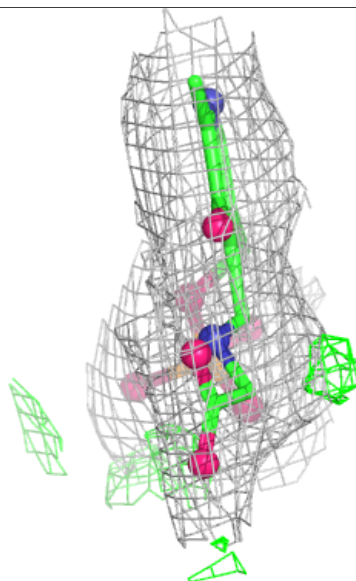
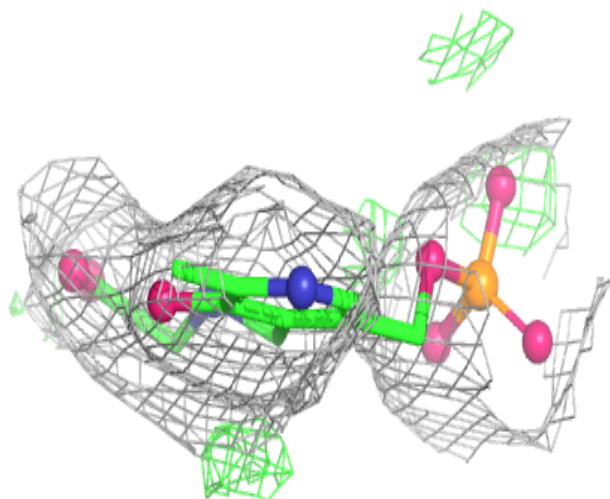
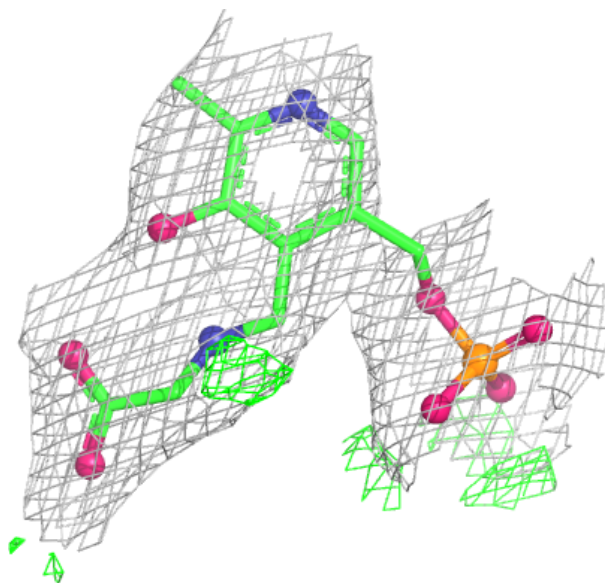
Electron density around Y5Z A 602:

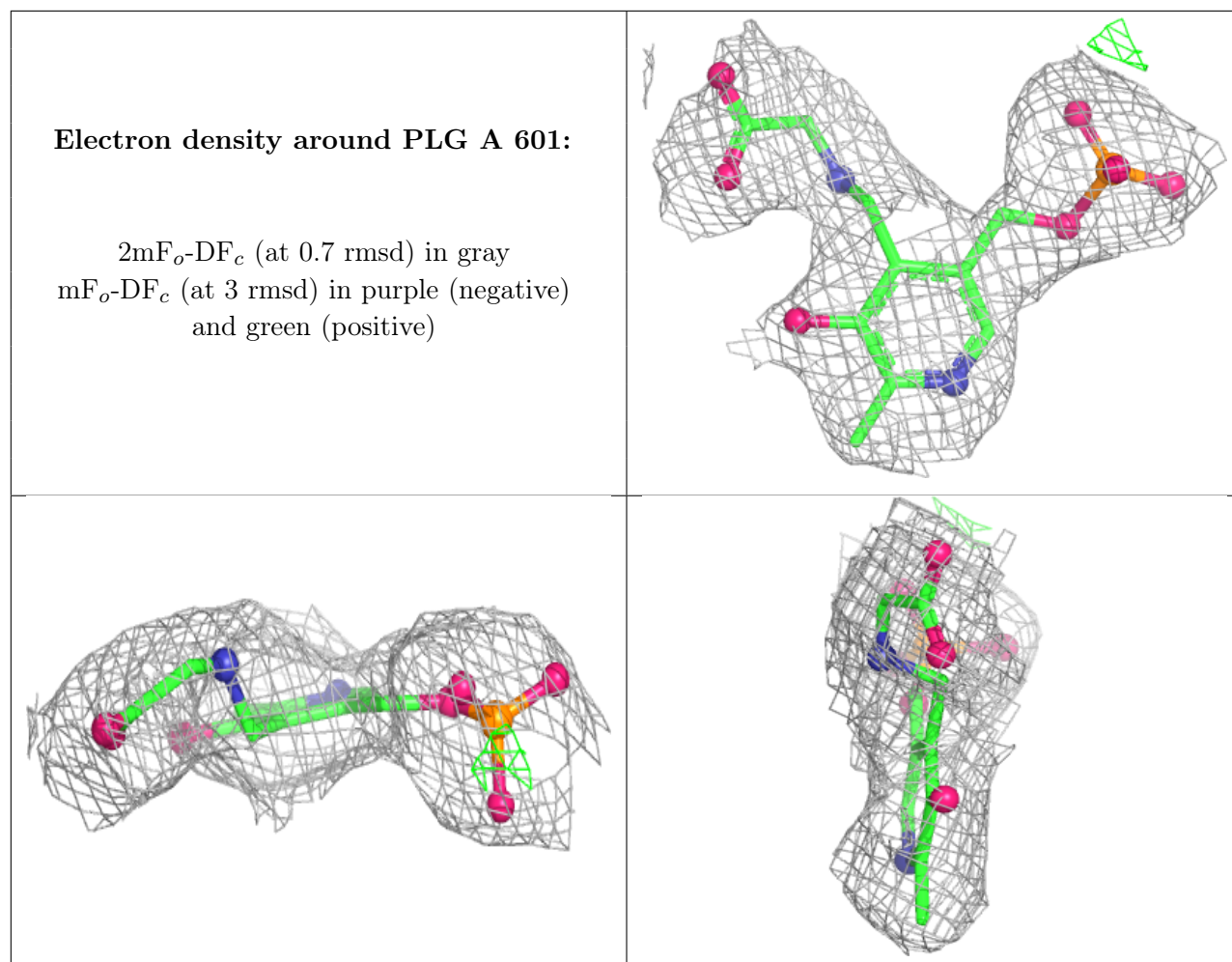
2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around PLG 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 [i](#)

There are no such residues in this entry.