



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 14, 2026 – 02:11 PM EDT

PDB ID : 9Y6B / pdb_00009y6b
Title : CRYSTAL STRUCTURE OF A149T VARIANT OF SERINE HYDROXY METHYLTRANSFERASE 8 FROM SOYBEAN CULTIVAR ESSEX IN COMPLEX WITH PLP-GLYCINE
Authors : Beamer, L.J.; Samarakoon, V.; Owuocha, L.F.
Deposited on : 2025-09-08
Resolution : 1.90 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

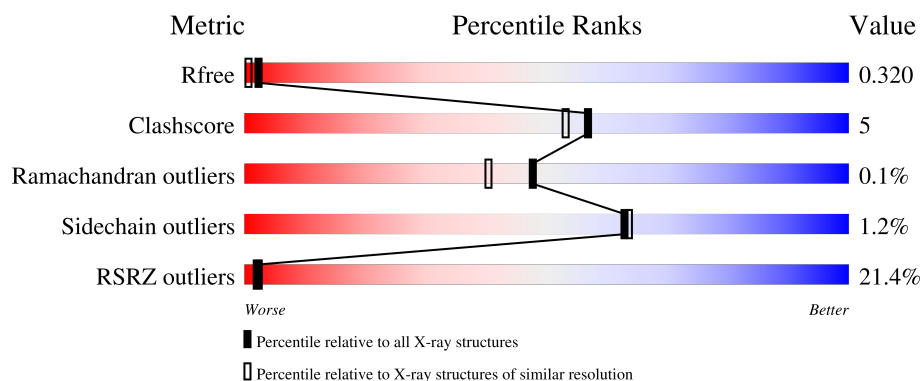
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	496	<div> <div>14%</div> <div> <div></div> <div>80%</div> <div>11%</div> <div>8%</div> </div> </div>
1	B	496	<div> <div>18%</div> <div> <div></div> <div>83%</div> <div>9%</div> <div>8%</div> </div> </div>
1	C	496	<div> <div>25%</div> <div> <div></div> <div>83%</div> <div>9%</div> <div>7%</div> </div> </div>
1	D	496	<div> <div>15%</div> <div> <div></div> <div>81%</div> <div>12%</div> <div>6%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	E	496	<div><div></div><div>28%</div><div>82%</div><div>11%</div><div>7%</div></div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 17910 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	457	Total	C	N	O	S	0	0	0
			3426	2177	587	645	17			
1	B	458	Total	C	N	O	S	0	0	0
			3448	2189	594	648	17			
1	C	460	Total	C	N	O	S	0	0	0
			3429	2176	588	648	17			
1	D	464	Total	C	N	O	S	0	0	0
			3481	2213	597	654	17			
1	E	460	Total	C	N	O	S	0	0	0
			3398	2155	582	644	17			

There are 130 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-24	MET	-	initiating methionine	UNP K4FZF8
A	-23	GLY	-	expression tag	UNP K4FZF8
A	-22	MET	-	expression tag	UNP K4FZF8
A	-21	HIS	-	expression tag	UNP K4FZF8
A	-20	HIS	-	expression tag	UNP K4FZF8
A	-19	HIS	-	expression tag	UNP K4FZF8
A	-18	HIS	-	expression tag	UNP K4FZF8
A	-17	HIS	-	expression tag	UNP K4FZF8
A	-16	HIS	-	expression tag	UNP K4FZF8
A	-15	SER	-	expression tag	UNP K4FZF8
A	-14	SER	-	expression tag	UNP K4FZF8
A	-13	GLY	-	expression tag	UNP K4FZF8
A	-12	VAL	-	expression tag	UNP K4FZF8
A	-11	ASP	-	expression tag	UNP K4FZF8
A	-10	LEU	-	expression tag	UNP K4FZF8
A	-9	GLY	-	expression tag	UNP K4FZF8
A	-8	THR	-	expression tag	UNP K4FZF8
A	-7	GLU	-	expression tag	UNP K4FZF8
A	-6	ASN	-	expression tag	UNP K4FZF8

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	LEU	-	expression tag	UNP K4FZF8
A	-4	TYR	-	expression tag	UNP K4FZF8
A	-3	PHE	-	expression tag	UNP K4FZF8
A	-2	GLN	-	expression tag	UNP K4FZF8
A	-1	SER	-	expression tag	UNP K4FZF8
A	0	ASN	-	expression tag	UNP K4FZF8
A	149	THR	ALA	engineered mutation	UNP K4FZF8
B	-24	MET	-	initiating methionine	UNP K4FZF8
B	-23	GLY	-	expression tag	UNP K4FZF8
B	-22	MET	-	expression tag	UNP K4FZF8
B	-21	HIS	-	expression tag	UNP K4FZF8
B	-20	HIS	-	expression tag	UNP K4FZF8
B	-19	HIS	-	expression tag	UNP K4FZF8
B	-18	HIS	-	expression tag	UNP K4FZF8
B	-17	HIS	-	expression tag	UNP K4FZF8
B	-16	HIS	-	expression tag	UNP K4FZF8
B	-15	SER	-	expression tag	UNP K4FZF8
B	-14	SER	-	expression tag	UNP K4FZF8
B	-13	GLY	-	expression tag	UNP K4FZF8
B	-12	VAL	-	expression tag	UNP K4FZF8
B	-11	ASP	-	expression tag	UNP K4FZF8
B	-10	LEU	-	expression tag	UNP K4FZF8
B	-9	GLY	-	expression tag	UNP K4FZF8
B	-8	THR	-	expression tag	UNP K4FZF8
B	-7	GLU	-	expression tag	UNP K4FZF8
B	-6	ASN	-	expression tag	UNP K4FZF8
B	-5	LEU	-	expression tag	UNP K4FZF8
B	-4	TYR	-	expression tag	UNP K4FZF8
B	-3	PHE	-	expression tag	UNP K4FZF8
B	-2	GLN	-	expression tag	UNP K4FZF8
B	-1	SER	-	expression tag	UNP K4FZF8
B	0	ASN	-	expression tag	UNP K4FZF8
B	149	THR	ALA	engineered mutation	UNP K4FZF8
C	-24	MET	-	initiating methionine	UNP K4FZF8
C	-23	GLY	-	expression tag	UNP K4FZF8
C	-22	MET	-	expression tag	UNP K4FZF8
C	-21	HIS	-	expression tag	UNP K4FZF8
C	-20	HIS	-	expression tag	UNP K4FZF8
C	-19	HIS	-	expression tag	UNP K4FZF8
C	-18	HIS	-	expression tag	UNP K4FZF8
C	-17	HIS	-	expression tag	UNP K4FZF8
C	-16	HIS	-	expression tag	UNP K4FZF8

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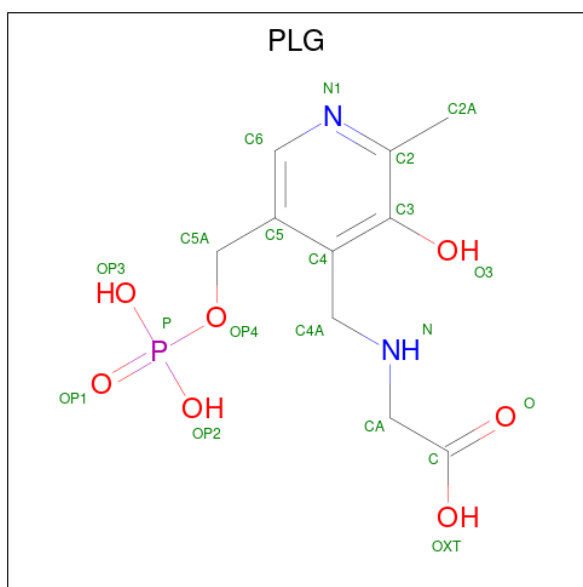
Chain	Residue	Modelled	Actual	Comment	Reference
C	-15	SER	-	expression tag	UNP K4FZF8
C	-14	SER	-	expression tag	UNP K4FZF8
C	-13	GLY	-	expression tag	UNP K4FZF8
C	-12	VAL	-	expression tag	UNP K4FZF8
C	-11	ASP	-	expression tag	UNP K4FZF8
C	-10	LEU	-	expression tag	UNP K4FZF8
C	-9	GLY	-	expression tag	UNP K4FZF8
C	-8	THR	-	expression tag	UNP K4FZF8
C	-7	GLU	-	expression tag	UNP K4FZF8
C	-6	ASN	-	expression tag	UNP K4FZF8
C	-5	LEU	-	expression tag	UNP K4FZF8
C	-4	TYR	-	expression tag	UNP K4FZF8
C	-3	PHE	-	expression tag	UNP K4FZF8
C	-2	GLN	-	expression tag	UNP K4FZF8
C	-1	SER	-	expression tag	UNP K4FZF8
C	0	ASN	-	expression tag	UNP K4FZF8
C	149	THR	ALA	engineered mutation	UNP K4FZF8
D	-24	MET	-	initiating methionine	UNP K4FZF8
D	-23	GLY	-	expression tag	UNP K4FZF8
D	-22	MET	-	expression tag	UNP K4FZF8
D	-21	HIS	-	expression tag	UNP K4FZF8
D	-20	HIS	-	expression tag	UNP K4FZF8
D	-19	HIS	-	expression tag	UNP K4FZF8
D	-18	HIS	-	expression tag	UNP K4FZF8
D	-17	HIS	-	expression tag	UNP K4FZF8
D	-16	HIS	-	expression tag	UNP K4FZF8
D	-15	SER	-	expression tag	UNP K4FZF8
D	-14	SER	-	expression tag	UNP K4FZF8
D	-13	GLY	-	expression tag	UNP K4FZF8
D	-12	VAL	-	expression tag	UNP K4FZF8
D	-11	ASP	-	expression tag	UNP K4FZF8
D	-10	LEU	-	expression tag	UNP K4FZF8
D	-9	GLY	-	expression tag	UNP K4FZF8
D	-8	THR	-	expression tag	UNP K4FZF8
D	-7	GLU	-	expression tag	UNP K4FZF8
D	-6	ASN	-	expression tag	UNP K4FZF8
D	-5	LEU	-	expression tag	UNP K4FZF8
D	-4	TYR	-	expression tag	UNP K4FZF8
D	-3	PHE	-	expression tag	UNP K4FZF8
D	-2	GLN	-	expression tag	UNP K4FZF8
D	-1	SER	-	expression tag	UNP K4FZF8
D	0	ASN	-	expression tag	UNP K4FZF8

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Chain	Residue	Modelled	Actual	Comment	Reference
D	149	THR	ALA	engineered mutation	UNP K4FZF8
E	-24	MET	-	initiating methionine	UNP K4FZF8
E	-23	GLY	-	expression tag	UNP K4FZF8
E	-22	MET	-	expression tag	UNP K4FZF8
E	-21	HIS	-	expression tag	UNP K4FZF8
E	-20	HIS	-	expression tag	UNP K4FZF8
E	-19	HIS	-	expression tag	UNP K4FZF8
E	-18	HIS	-	expression tag	UNP K4FZF8
E	-17	HIS	-	expression tag	UNP K4FZF8
E	-16	HIS	-	expression tag	UNP K4FZF8
E	-15	SER	-	expression tag	UNP K4FZF8
E	-14	SER	-	expression tag	UNP K4FZF8
E	-13	GLY	-	expression tag	UNP K4FZF8
E	-12	VAL	-	expression tag	UNP K4FZF8
E	-11	ASP	-	expression tag	UNP K4FZF8
E	-10	LEU	-	expression tag	UNP K4FZF8
E	-9	GLY	-	expression tag	UNP K4FZF8
E	-8	THR	-	expression tag	UNP K4FZF8
E	-7	GLU	-	expression tag	UNP K4FZF8
E	-6	ASN	-	expression tag	UNP K4FZF8
E	-5	LEU	-	expression tag	UNP K4FZF8
E	-4	TYR	-	expression tag	UNP K4FZF8
E	-3	PHE	-	expression tag	UNP K4FZF8
E	-2	GLN	-	expression tag	UNP K4FZF8
E	-1	SER	-	expression tag	UNP K4FZF8
E	0	ASN	-	expression tag	UNP K4FZF8
E	149	THR	ALA	engineered mutation	UNP K4FZF8

- Molecule 2 is N-GLYCINE-[3-HYDROXY-2-METHYL-5-PHOSPHONOXYMETHYL-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		
2	C	1	Total	C	N	O	P	0	0
			20	10	2	7	1		
2	D	1	Total	C	N	O	P	0	0
			20	10	2	7	1		
2	E	1	Total	C	N	O	P	0	0
			20	10	2	7	1		

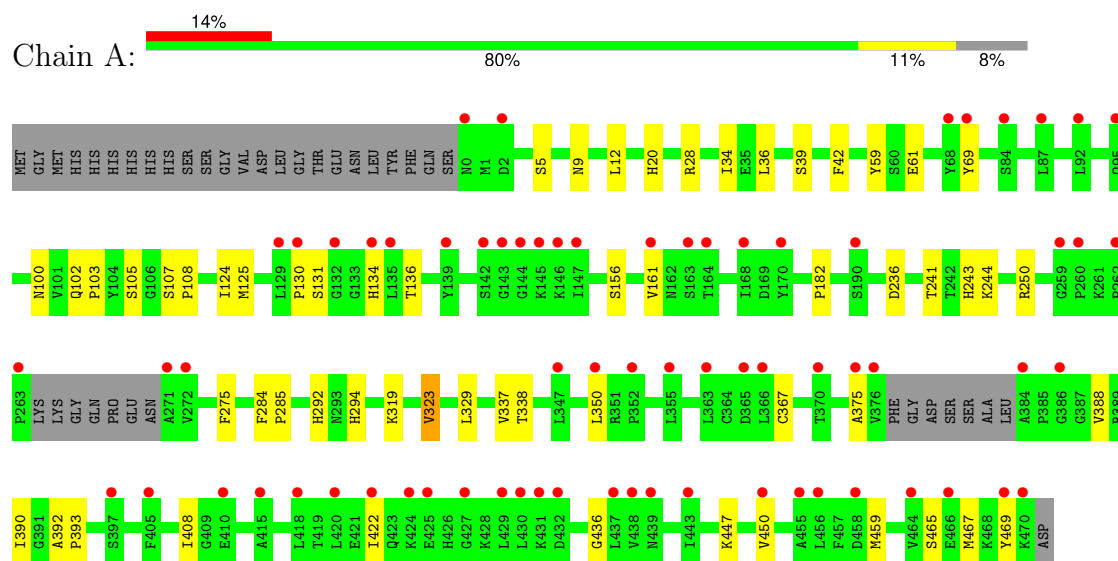
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	134	Total	O	0	0
			134	134		
3	B	135	Total	O	0	0
			135	135		
3	C	107	Total	O	0	0
			107	107		
3	D	164	Total	O	0	0
			164	164		
3	E	88	Total	O	0	0
			88	88		

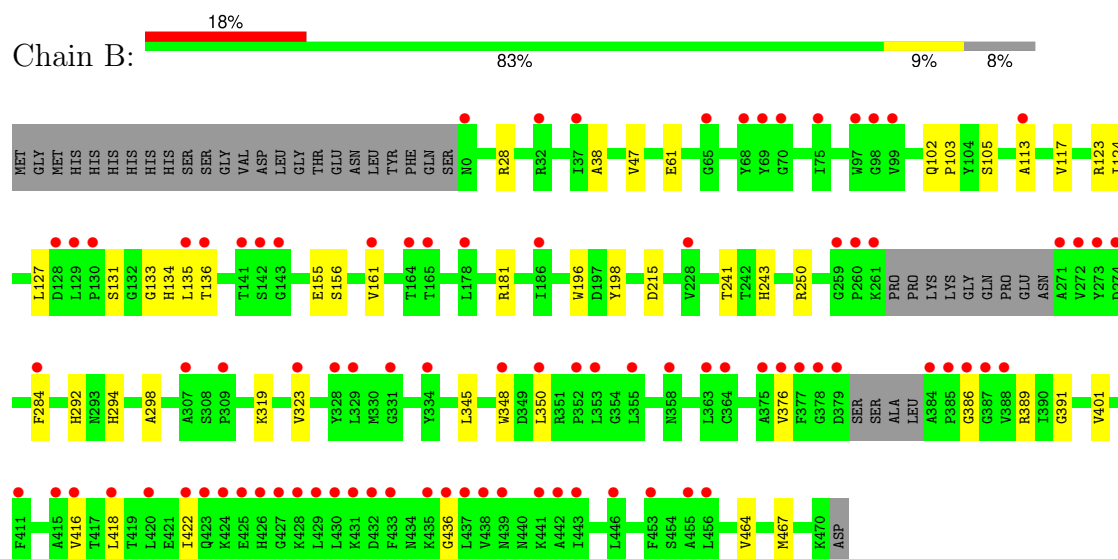
3 Residue-property plots [i](#)

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.

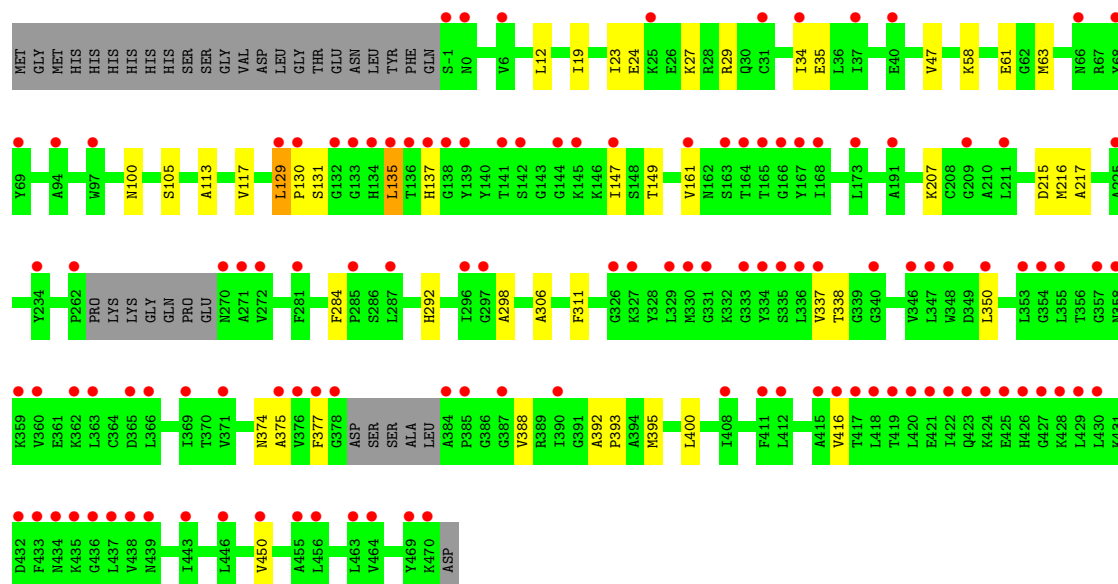
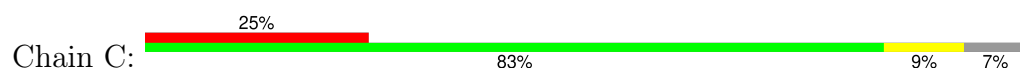
• Molecule 1: Serine hydroxymethyltransferase



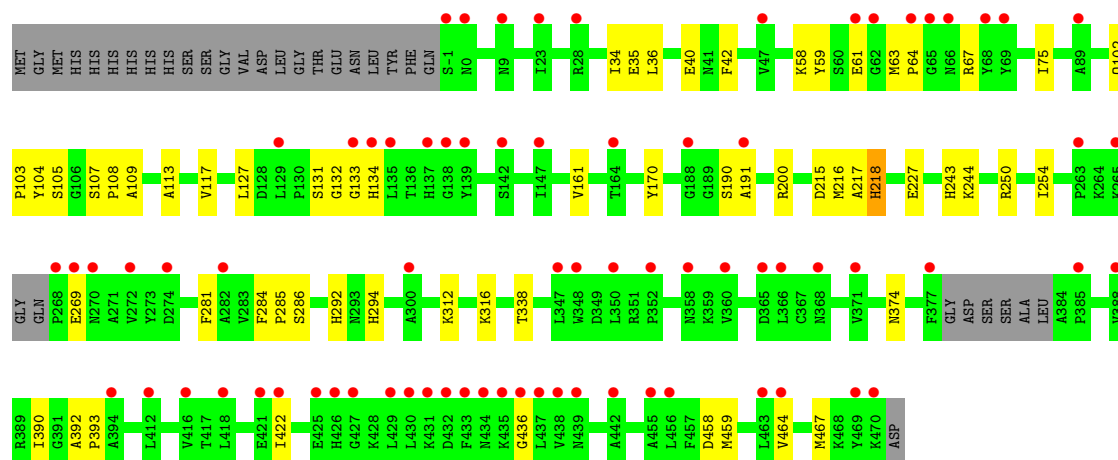
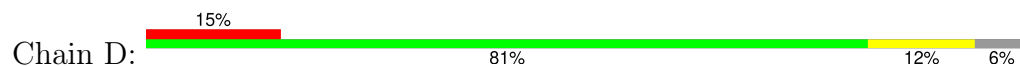
• Molecule 1: Serine hydroxymethyltransferase



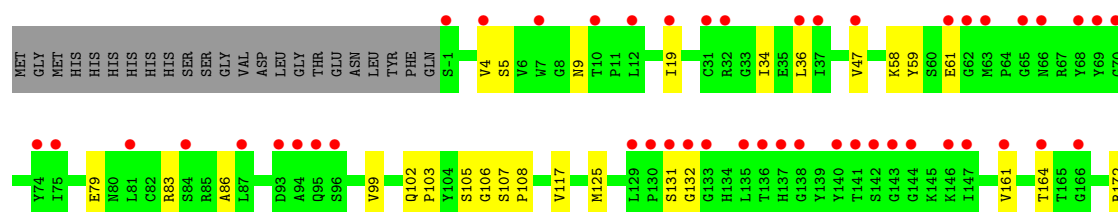
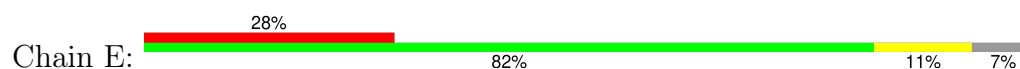
• Molecule 1: Serine hydroxymethyltransferase

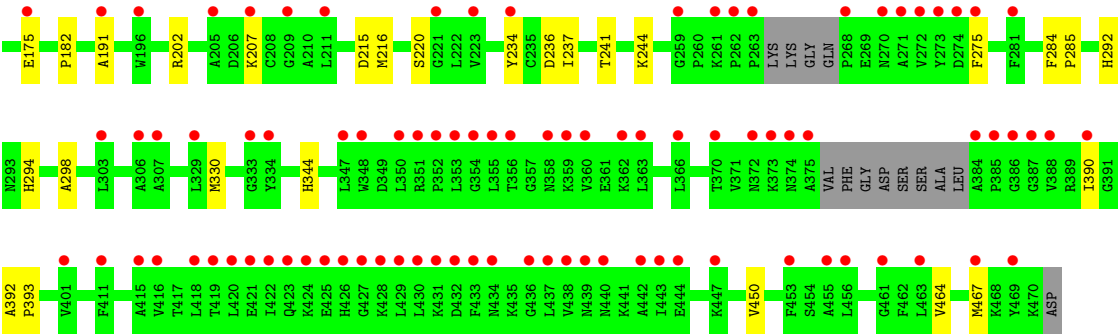


• Molecule 1: Serine hydroxymethyltransferase



• Molecule 1: Serine hydroxymethyltransferase





4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	174.35Å 174.35Å 183.63Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.54 – 1.90 48.54 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.4 (48.54-1.90) 99.4 (48.54-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.20 (at 1.90Å)	Xtriage
Refinement program	PHENIX 1.21.2_5419	Depositor
R, R_{free}	0.282 , 0.319 0.284 , 0.320	Depositor DCC
R_{free} test set	12724 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	29.2	Xtriage
Anisotropy	0.474	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 39.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.024 for -h,-k,l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	17910	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 29.74 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.4728e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

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	0.30	0/3505	0.48	0/4763
1	B	0.28	0/3526	0.47	0/4785
1	C	0.30	0/3506	0.49	0/4762
1	D	0.31	0/3563	0.51	0/4842
1	E	0.31	0/3477	0.50	0/4730
All	All	0.30	0/17577	0.49	0/23882

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 [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	3426	0	3249	33	0
1	B	3448	0	3278	28	0
1	C	3429	0	3242	28	0
1	D	3481	0	3303	41	0
1	E	3398	0	3171	33	0
2	A	20	0	12	1	0
2	B	20	0	12	1	0
2	C	20	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	20	0	12	4	0
2	E	20	0	12	3	0
3	A	134	0	0	1	0
3	B	135	0	0	0	0
3	C	107	0	0	0	0
3	D	164	0	0	3	0
3	E	88	0	0	0	0
All	All	17910	0	16303	154	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 5.

All (154) 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:5:SER:HA	1:A:9:ASN:HD22	1.56	0.69
1:D:61:GLU:HB3	1:D:284:PHE:CZ	2.33	0.63
1:E:131:SER:HB3	1:E:161:VAL:HG13	1.81	0.61
1:B:131:SER:HB3	1:B:161:VAL:HG13	1.81	0.61
1:D:170:TYR:CD1	1:D:200:ARG:HG2	2.36	0.60
1:C:63:MET:HE1	1:C:100:ASN:HD21	1.66	0.59
1:C:135:LEU:CD1	1:D:285:PRO:HB2	2.33	0.58
1:A:319:LYS:O	1:A:323:VAL:HG12	2.03	0.58
1:A:131:SER:HB3	1:A:161:VAL:HG13	1.85	0.58
1:A:5:SER:HB2	1:E:330:MET:HE3	1.87	0.57
1:E:132:GLY:HA2	1:E:191:ALA:HB3	1.86	0.57
1:C:34:ILE:HG13	1:C:450:VAL:HG13	1.86	0.57
1:E:244:LYS:NZ	2:E:501:PLG:H4A2	2.21	0.56
1:B:319:LYS:O	1:B:323:VAL:HG12	2.06	0.55
1:E:244:LYS:HZ1	2:E:501:PLG:H4A2	1.71	0.55
1:C:337:VAL:HG12	1:C:338:THR:HG23	1.89	0.54
1:A:422:ILE:HG23	1:A:436:GLY:HA3	1.90	0.54
1:C:131:SER:HB3	1:C:161:VAL:HG13	1.90	0.54
1:C:137:HIS:HE1	1:C:215:ASP:OD2	1.90	0.54
1:D:42:PHE:CD1	1:D:459:MET:HE1	2.43	0.53
1:A:34:ILE:HG13	1:A:450:VAL:HG13	1.91	0.53
1:C:113:ALA:O	1:C:117:VAL:HG22	2.08	0.53
1:B:464:VAL:O	1:B:467:MET:HG2	2.09	0.53
1:C:58:LYS:HD2	1:D:40:GLU:OE2	2.09	0.53
1:A:42:PHE:CD1	1:A:459:MET:HE1	2.45	0.52
1:B:61:GLU:HB3	1:B:284:PHE:CZ	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:125:MET:HG3	1:E:182:PRO:HB3	1.92	0.52
1:C:135:LEU:HD11	1:D:285:PRO:HB2	1.92	0.52
1:D:131:SER:HB3	1:D:161:VAL:HG13	1.90	0.51
1:A:241:THR:HB	1:A:243:HIS:CE1	2.45	0.51
1:B:241:THR:HB	1:B:243:HIS:CE1	2.45	0.51
1:A:243:HIS:ND1	1:A:250:ARG:HA	2.26	0.51
1:A:61:GLU:HB3	1:A:284:PHE:CZ	2.47	0.50
1:B:401:VAL:HG22	1:E:164:THR:HG21	1.94	0.50
1:C:61:GLU:HB3	1:C:284:PHE:CZ	2.47	0.50
1:B:134:HIS:CE1	1:B:136:THR:HG23	2.47	0.50
1:D:464:VAL:HA	1:D:467:MET:HG3	1.94	0.50
1:E:34:ILE:HG13	1:E:450:VAL:HG13	1.93	0.50
1:E:47:VAL:HG13	1:E:298:ALA:HB1	1.94	0.49
1:E:86:ALA:HB3	1:E:99:VAL:HG11	1.94	0.49
1:A:36:LEU:HB3	1:A:390:ILE:HG23	1.95	0.48
1:A:28:ARG:HD2	1:A:469:TYR:HB3	1.95	0.48
1:E:292:HIS:HB3	1:E:294:HIS:CE1	2.48	0.48
1:A:292:HIS:HB3	1:A:294:HIS:CE1	2.50	0.47
1:E:202:ARG:HB2	1:E:234:TYR:HB3	1.97	0.47
1:D:458:ASP:HB3	3:D:729:HOH:O	2.14	0.47
1:C:306:ALA:HA	1:C:311:PHE:CG	2.50	0.47
1:D:292:HIS:HB3	1:D:294:HIS:CE1	2.50	0.47
1:E:36:LEU:HB3	1:E:390:ILE:HG23	1.96	0.47
1:A:236:ASP:HB3	1:A:275:PHE:CE2	2.50	0.46
1:D:312:LYS:HE3	1:D:316:LYS:HE2	1.97	0.46
1:A:124:ILE:O	1:A:156:SER:HA	2.16	0.46
1:D:58:LYS:HG2	1:D:75:ILE:HG13	1.96	0.46
1:C:147:ILE:HD12	1:D:281:PHE:HZ	1.79	0.46
1:A:350:LEU:HD11	1:A:388:VAL:HG13	1.98	0.46
1:E:61:GLU:HB3	1:E:284:PHE:CZ	2.51	0.45
1:B:47:VAL:HG13	1:B:298:ALA:HB1	1.97	0.45
1:D:227:GLU:CD	1:D:316:LYS:HG2	2.42	0.45
1:E:34:ILE:HG22	1:E:36:LEU:HG	1.98	0.45
1:A:125:MET:HG3	1:A:182:PRO:HB3	1.98	0.45
1:B:127:LEU:O	1:B:133:GLY:HA3	2.17	0.45
1:C:395:MET:HB3	1:C:400:LEU:HD22	1.98	0.45
1:D:392:ALA:N	1:D:393:PRO:HD3	2.31	0.45
1:D:63:MET:HE3	1:D:64:PRO:HD2	1.99	0.45
1:B:422:ILE:HG23	1:B:436:GLY:HA3	1.98	0.45
1:C:149:THR:HG23	1:D:286:SER:O	2.17	0.45
1:A:42:PHE:CE1	1:A:459:MET:HE1	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:337:VAL:HG12	1:A:338:THR:HG23	1.99	0.44
1:A:130:PRO:HA	1:A:375:ALA:HB3	1.99	0.44
1:C:392:ALA:N	1:C:393:PRO:CD	2.80	0.44
1:D:67:ARG:HB3	3:D:655:HOH:O	2.18	0.44
1:D:284:PHE:CD1	1:D:285:PRO:HA	2.53	0.44
1:D:132:GLY:HA2	1:D:191:ALA:HB3	2.00	0.44
1:C:129:LEU:HD21	1:C:135:LEU:HD23	1.98	0.44
1:D:34:ILE:HG22	1:D:36:LEU:HG	2.00	0.43
1:A:34:ILE:HD13	1:A:408:ILE:HG12	2.00	0.43
1:A:102:GLN:N	1:A:103:PRO:CD	2.82	0.43
1:E:464:VAL:HA	1:E:467:MET:HG3	2.00	0.43
1:A:392:ALA:N	1:A:393:PRO:CD	2.82	0.43
1:B:28:ARG:HA	1:B:467:MET:HE1	2.00	0.43
1:B:113:ALA:O	1:B:117:VAL:HG22	2.18	0.43
1:B:292:HIS:HB3	1:B:294:HIS:CE1	2.53	0.43
1:B:38:ALA:HA	1:B:391:GLY:HA3	2.01	0.43
1:C:19:ILE:O	1:C:23:ILE:HG13	2.19	0.43
1:B:350:LEU:HB2	1:B:386:GLY:O	2.19	0.43
1:B:418:LEU:HD23	1:B:418:LEU:HA	1.77	0.43
1:E:236:ASP:HB3	1:E:275:PHE:CE2	2.54	0.43
1:E:172:ARG:HD2	1:E:175:GLU:OE1	2.19	0.43
1:C:63:MET:HE1	1:C:100:ASN:ND2	2.33	0.42
1:E:107:SER:HB2	1:E:108:PRO:HD3	2.00	0.42
1:A:12:LEU:HG	1:A:20:HIS:HB2	2.02	0.42
1:B:102:GLN:N	1:B:103:PRO:CD	2.83	0.42
1:A:100:ASN:OD1	1:A:103:PRO:HD3	2.20	0.42
1:C:47:VAL:HG13	1:C:298:ALA:HB1	2.01	0.42
1:C:350:LEU:HD11	1:C:388:VAL:HG22	2.00	0.42
1:A:329:LEU:HD23	1:A:329:LEU:HA	1.89	0.42
1:B:345:LEU:HD22	1:B:389:ARG:HD2	2.00	0.42
1:D:134:HIS:HE2	2:D:501:PLG:H4A1	1.84	0.42
1:B:215:ASP:OD2	2:B:501:PLG:N1	2.52	0.42
1:D:107:SER:HB2	1:D:108:PRO:HD3	2.01	0.42
1:A:323:VAL:HG13	3:A:632:HOH:O	2.19	0.42
1:C:24:GLU:HA	1:C:27:LYS:HD3	2.01	0.42
1:D:113:ALA:O	1:D:117:VAL:HG22	2.20	0.42
1:A:107:SER:HB2	1:A:108:PRO:HD3	2.02	0.42
1:D:243:HIS:ND1	1:D:250:ARG:HA	2.35	0.42
2:D:501:PLG:N	2:D:501:PLG:O3	2.53	0.42
2:A:501:PLG:H5A1	2:A:501:PLG:H4A1	1.88	0.42
1:E:5:SER:HA	1:E:9:ASN:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:392:ALA:N	1:E:393:PRO:CD	2.83	0.42
1:B:348:TRP:CH2	1:B:416:VAL:HG21	2.55	0.42
1:C:135:LEU:HD12	1:D:285:PRO:HB2	1.98	0.42
1:E:216:MET:HG3	1:E:220:SER:HB3	2.02	0.42
1:D:127:LEU:O	1:D:133:GLY:HA3	2.20	0.41
1:D:244:LYS:HZ1	2:D:501:PLG:C4A	2.32	0.41
1:A:467:MET:HB3	1:A:467:MET:HE2	1.78	0.41
1:D:58:LYS:HA	1:D:58:LYS:HD2	1.91	0.41
1:D:190:SER:HA	1:D:218:HIS:CD2	2.55	0.41
1:B:345:LEU:HD12	1:B:345:LEU:C	2.45	0.41
1:E:102:GLN:N	1:E:103:PRO:CD	2.84	0.41
1:B:123:ARG:HA	1:B:155:GLU:O	2.21	0.41
1:B:196:TRP:HB2	1:B:198:TYR:CZ	2.55	0.41
1:B:418:LEU:O	1:B:422:ILE:HG13	2.21	0.41
1:D:35:GLU:CD	1:D:40:GLU:OE1	2.63	0.41
1:D:215:ASP:OD2	2:D:501:PLG:N1	2.54	0.41
1:A:39:SER:HB2	1:A:244:LYS:HE3	2.03	0.41
1:C:216:MET:O	1:C:217:ALA:C	2.64	0.41
1:B:243:HIS:ND1	1:B:250:ARG:HA	2.35	0.41
1:C:207:LYS:HB2	1:C:207:LYS:HE2	1.71	0.41
1:E:58:LYS:HD2	1:E:58:LYS:HA	1.85	0.41
1:E:207:LYS:HA	1:E:207:LYS:HD3	1.78	0.41
1:A:134:HIS:CE1	1:A:136:THR:HG23	2.56	0.41
1:D:36:LEU:HB3	1:D:390:ILE:HG23	2.02	0.41
1:D:338:THR:HA	3:D:634:HOH:O	2.21	0.41
1:E:19:ILE:HD13	1:E:19:ILE:HA	1.87	0.41
1:E:344:HIS:HD1	1:E:344:HIS:H	1.67	0.41
1:A:367:CYS:HA	1:A:447:LYS:HB2	2.01	0.41
1:B:181:ARG:HA	1:B:181:ARG:HD3	1.91	0.40
1:C:131:SER:OG	1:C:161:VAL:HG22	2.20	0.40
1:D:109:ALA:O	1:D:254:ILE:HD11	2.21	0.40
1:E:117:VAL:HG11	1:E:237:ILE:HD11	2.02	0.40
1:E:79:GLU:O	1:E:83:ARG:HG3	2.20	0.40
1:E:284:PHE:CD1	1:E:285:PRO:HA	2.55	0.40
1:C:29:ARG:NH2	1:D:58:LYS:HD3	2.36	0.40
1:C:292:HIS:HE1	1:D:104:TYR:O	2.04	0.40
1:D:102:GLN:N	1:D:103:PRO:CD	2.84	0.40
1:D:392:ALA:N	1:D:393:PRO:CD	2.84	0.40
1:D:422:ILE:HG23	1:D:436:GLY:HA3	2.03	0.40
1:A:285:PRO:HB2	1:B:135:LEU:HD13	2.02	0.40
1:B:124:ILE:O	1:B:156:SER:HA	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:130:PRO:HA	1:C:375:ALA:HB3	2.03	0.40
1:E:106:GLY:HA3	1:E:241:THR:HG22	2.04	0.40
1:E:125:MET:HE2	1:E:125:MET:HB3	1.99	0.40
1:D:216:MET:O	1:D:217:ALA:C	2.65	0.40
1:E:215:ASP:OD2	2:E:501:PLG:N1	2.55	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	451/496 (91%)	438 (97%)	13 (3%)	0	100	100
1	B	452/496 (91%)	437 (97%)	15 (3%)	0	100	100
1	C	454/496 (92%)	437 (96%)	16 (4%)	1 (0%)	43	36
1	D	458/496 (92%)	445 (97%)	12 (3%)	1 (0%)	43	36
1	E	454/496 (92%)	437 (96%)	17 (4%)	0	100	100
All	All	2269/2480 (92%)	2194 (97%)	73 (3%)	2 (0%)	48	40

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	377	PHE
1	D	269	GLU

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	342/408 (84%)	337 (98%)	5 (2%)	57	56
1	B	344/408 (84%)	342 (99%)	2 (1%)	78	81
1	C	340/408 (83%)	333 (98%)	7 (2%)	47	44
1	D	348/408 (85%)	344 (99%)	4 (1%)	65	67
1	E	331/408 (81%)	328 (99%)	3 (1%)	70	73
All	All	1705/2040 (84%)	1684 (99%)	21 (1%)	63	63

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	59	TYR
1	A	69	TYR
1	A	105	SER
1	A	323	VAL
1	A	465	SER
1	B	105	SER
1	B	376	VAL
1	C	12	LEU
1	C	35	GLU
1	C	105	SER
1	C	129	LEU
1	C	135	LEU
1	C	374	ASN
1	C	416	VAL
1	D	59	TYR
1	D	105	SER
1	D	218	HIS
1	D	374	ASN
1	E	4	VAL
1	E	59	TYR
1	E	105	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	ASN
1	A	293	ASN

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Mol	Chain	Res	Type
1	A	295	GLN
1	B	407	GLN
1	C	137	HIS
1	D	20	HIS
1	D	293	ASN
1	D	305	GLN
1	D	407	GLN
1	E	0	ASN
1	E	20	HIS
1	E	293	ASN
1	E	295	GLN
1	E	407	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
2	PLG	C	501	-	20,20,20	1.26	2 (10%)	26,28,28	1.16	2 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PLG	E	501	-	20,20,20	1.32	4 (20%)	26,28,28	1.27	3 (11%)
2	PLG	D	501	-	20,20,20	1.37	2 (10%)	26,28,28	1.25	4 (15%)
2	PLG	A	501	-	20,20,20	1.33	3 (15%)	26,28,28	1.84	7 (26%)
2	PLG	B	501	-	20,20,20	1.33	3 (15%)	26,28,28	1.73	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	C	501	-	-	7/12/12/12	0/1/1/1
2	PLG	E	501	-	-	4/12/12/12	0/1/1/1
2	PLG	D	501	-	-	8/12/12/12	0/1/1/1
2	PLG	A	501	-	-	5/12/12/12	0/1/1/1
2	PLG	B	501	-	-	6/12/12/12	0/1/1/1

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	PLG	C5-C4	-3.03	1.36	1.40
2	A	501	PLG	C5-C4	-2.81	1.36	1.40
2	B	501	PLG	C5-C4	-2.73	1.36	1.40
2	E	501	PLG	C5-C4	-2.61	1.36	1.40
2	D	501	PLG	C2A-C2	2.41	1.54	1.50
2	A	501	PLG	C3-C2	-2.30	1.38	1.41
2	B	501	PLG	C3-C4	-2.24	1.36	1.40
2	A	501	PLG	C3-C4	-2.20	1.36	1.40
2	E	501	PLG	C3-C4	-2.11	1.36	1.40
2	C	501	PLG	C3-C2	-2.09	1.38	1.41
2	C	501	PLG	C5-C4	-2.09	1.37	1.40
2	E	501	PLG	C2A-C2	2.09	1.53	1.50
2	E	501	PLG	C3-C2	-2.06	1.38	1.41
2	B	501	PLG	C2A-C2	2.01	1.53	1.50

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	PLG	C4A-N-CA	-4.90	107.02	112.72
2	B	501	PLG	C4A-N-CA	-4.53	107.45	112.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	PLG	C6-C5-C4	3.60	120.78	118.06
2	A	501	PLG	C6-C5-C4	3.42	120.65	118.06
2	E	501	PLG	C6-C5-C4	3.41	120.64	118.06
2	B	501	PLG	C5-C6-N1	-3.10	118.78	123.83
2	A	501	PLG	C5-C6-N1	-2.76	119.34	123.83
2	E	501	PLG	C5-C6-N1	-2.68	119.47	123.83
2	A	501	PLG	C4A-C4-C3	2.66	123.51	119.98
2	A	501	PLG	C4A-C4-C5	-2.60	116.92	119.75
2	D	501	PLG	C6-C5-C4	2.42	119.89	118.06
2	D	501	PLG	C4A-C4-C3	2.36	123.12	119.98
2	B	501	PLG	C4A-C4-C3	2.34	123.09	119.98
2	A	501	PLG	OP4-P-OP1	2.32	112.71	106.44
2	C	501	PLG	C6-C5-C4	2.29	119.79	118.06
2	D	501	PLG	OXT-C-CA	2.25	121.37	112.81
2	A	501	PLG	OP4-C5A-C5	2.23	113.54	109.36
2	E	501	PLG	OXT-C-CA	2.18	121.09	112.81
2	C	501	PLG	C5-C6-N1	-2.16	120.31	123.83
2	D	501	PLG	C5-C6-N1	-2.11	120.40	123.83
2	B	501	PLG	C4A-C4-C5	-2.08	117.48	119.75

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	PLG	C5A-OP4-P-OP3
2	B	501	PLG	C5A-OP4-P-OP1
2	B	501	PLG	C5A-OP4-P-OP3
2	D	501	PLG	C5-C4-C4A-N
2	D	501	PLG	C5A-OP4-P-OP1
2	D	501	PLG	C5A-OP4-P-OP3
2	E	501	PLG	C5A-OP4-P-OP3
2	A	501	PLG	C5-C4-C4A-N
2	B	501	PLG	C5-C4-C4A-N
2	C	501	PLG	C5-C4-C4A-N
2	E	501	PLG	C5-C4-C4A-N
2	A	501	PLG	C3-C4-C4A-N
2	C	501	PLG	C4-C4A-N-CA
2	D	501	PLG	C4-C4A-N-CA
2	A	501	PLG	C5A-OP4-P-OP1
2	C	501	PLG	C5A-OP4-P-OP1
2	E	501	PLG	C5A-OP4-P-OP1
2	B	501	PLG	C3-C4-C4A-N

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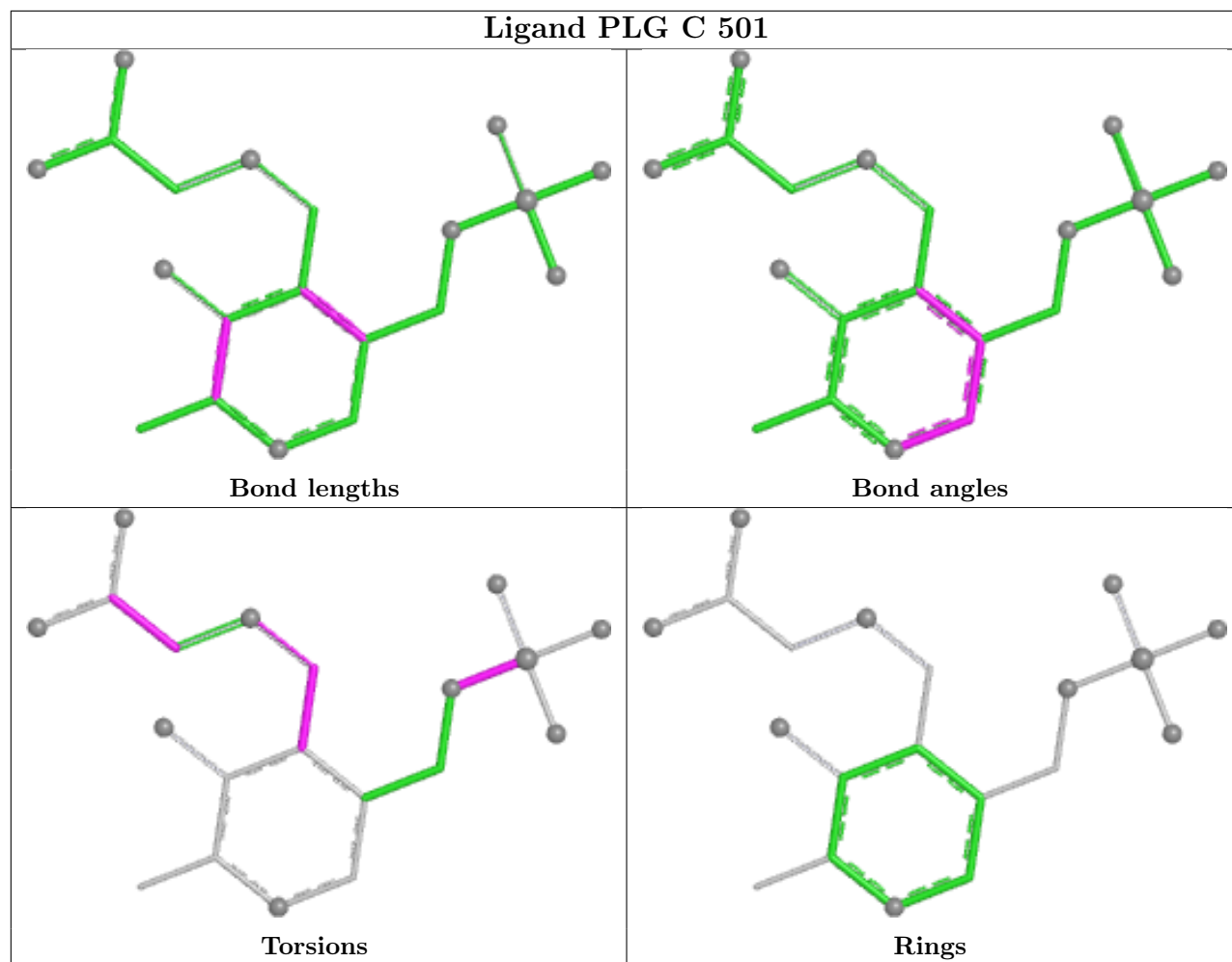
Mol	Chain	Res	Type	Atoms
2	C	501	PLG	C3-C4-C4A-N
2	E	501	PLG	C3-C4-C4A-N
2	C	501	PLG	OXT-C-CA-N
2	D	501	PLG	C3-C4-C4A-N
2	D	501	PLG	OXT-C-CA-N
2	A	501	PLG	C-CA-N-C4A
2	C	501	PLG	O-C-CA-N
2	D	501	PLG	O-C-CA-N
2	B	501	PLG	C5A-OP4-P-OP2
2	C	501	PLG	C5A-OP4-P-OP3
2	D	501	PLG	C5A-OP4-P-OP2
2	B	501	PLG	C4-C4A-N-CA

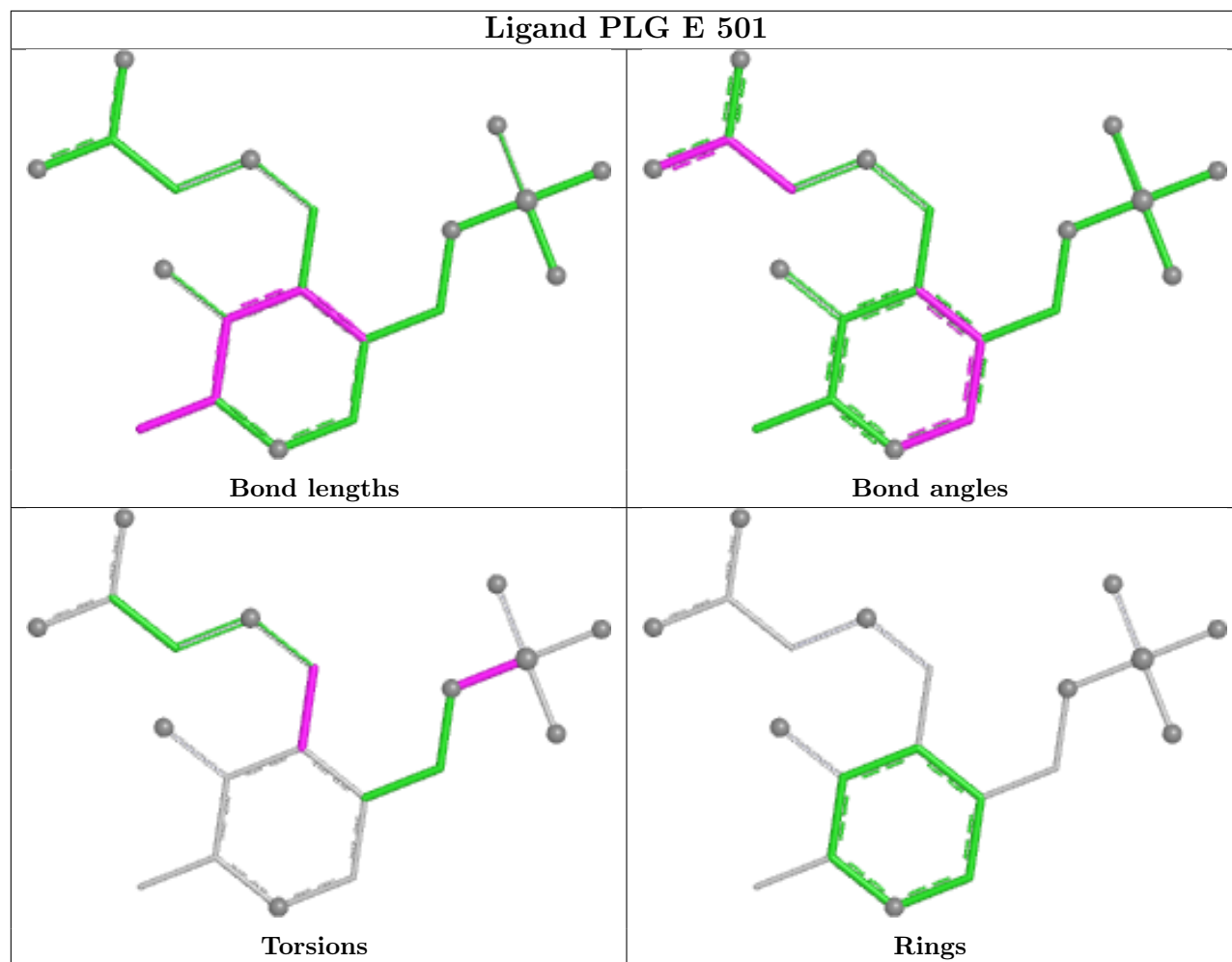
There are no ring outliers.

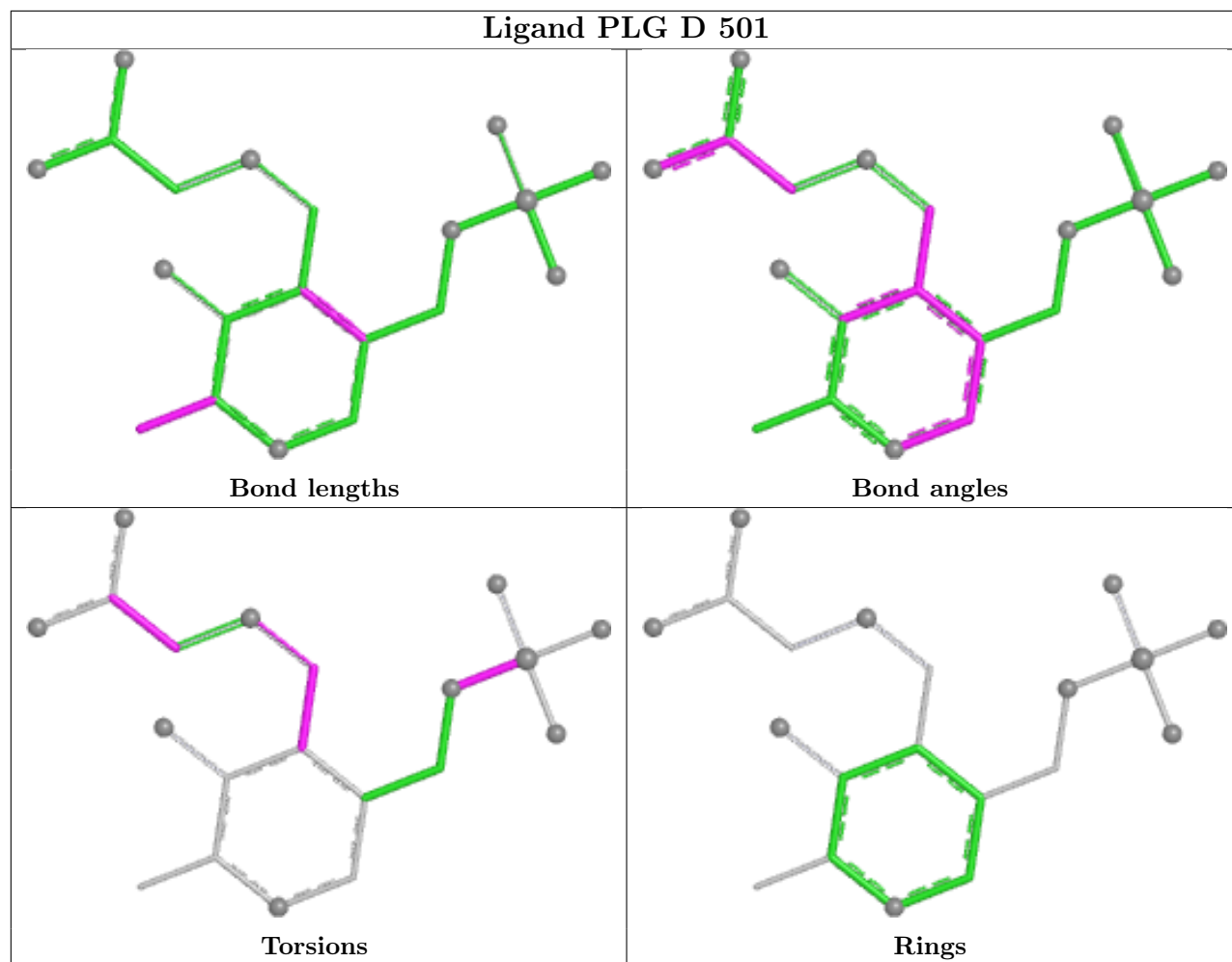
4 monomers are involved in 9 short contacts:

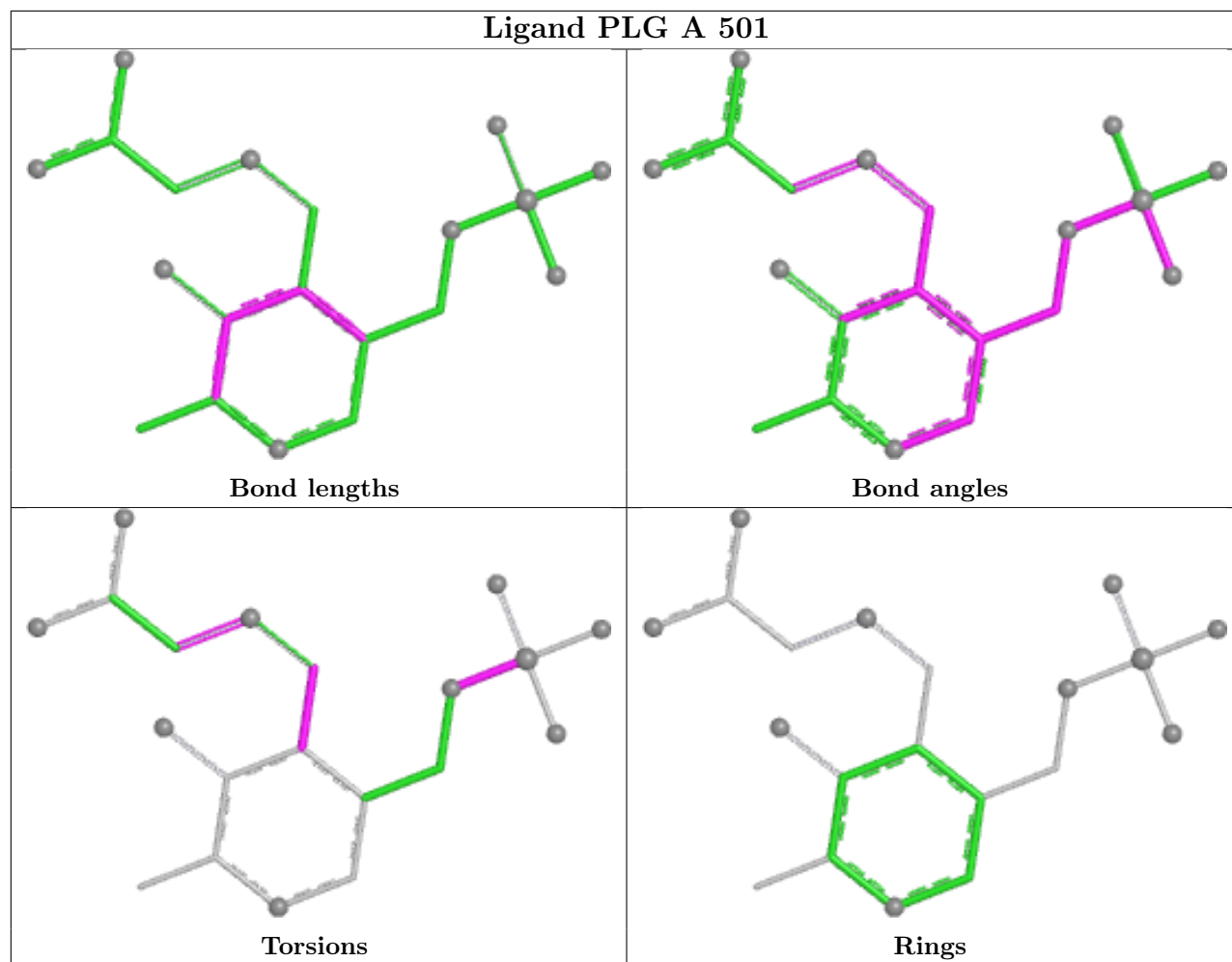
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	501	PLG	3	0
2	D	501	PLG	4	0
2	A	501	PLG	1	0
2	B	501	PLG	1	0

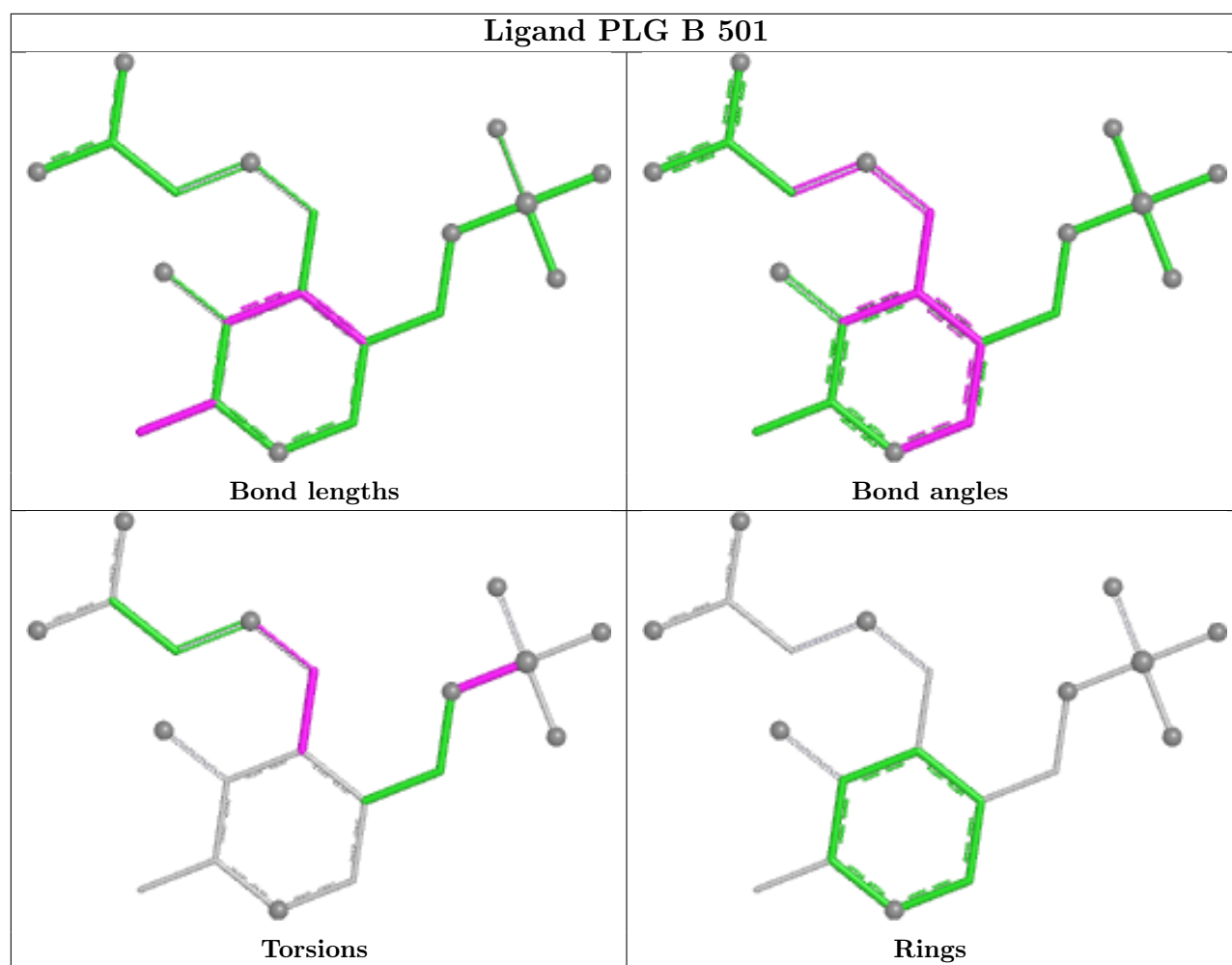
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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











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	457/496 (92%)	1.23	70 (15%) 5 5	23, 37, 64, 95	0
1	B	458/496 (92%)	1.23	88 (19%) 3 3	24, 35, 67, 90	0
1	C	460/496 (92%)	1.53	122 (26%) 1 1	26, 40, 75, 100	0
1	D	464/496 (93%)	1.22	75 (16%) 4 4	22, 33, 61, 82	0
1	E	460/496 (92%)	1.61	138 (30%) 1 1	30, 42, 78, 99	0
All	All	2299/2480 (92%)	1.36	493 (21%) 2 2	22, 38, 69, 100	0

All (493) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	375	ALA	7.4
1	A	142	SER	7.0
1	D	437	LEU	6.4
1	B	377	PHE	6.2
1	C	378	GLY	6.2
1	E	142	SER	6.1
1	C	418	LEU	5.7
1	C	437	LEU	5.7
1	D	129	LEU	5.7
1	E	437	LEU	5.7
1	C	384	ALA	5.5
1	A	376	VAL	5.5
1	E	384	ALA	5.4
1	E	263	PRO	5.4
1	E	427	GLY	5.4
1	A	0	ASN	5.3
1	E	422	ILE	5.3
1	E	433	PHE	5.3
1	A	375	ALA	5.2
1	A	430	LEU	5.1

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Mol	Chain	Res	Type	RSRZ
1	E	353	LEU	5.1
1	E	355	LEU	5.1
1	D	268	PRO	5.1
1	E	425	GLU	5.1
1	C	439	ASN	5.1
1	E	68	TYR	5.0
1	D	69	TYR	5.0
1	C	455	ALA	4.9
1	C	419	THR	4.9
1	C	137	HIS	4.8
1	C	138	GLY	4.8
1	E	94	ALA	4.8
1	A	263	PRO	4.7
1	B	430	LEU	4.7
1	C	262	PRO	4.7
1	A	384	ALA	4.6
1	B	437	LEU	4.6
1	C	433	PHE	4.6
1	B	355	LEU	4.6
1	E	69	TYR	4.5
1	D	456	LEU	4.5
1	E	420	LEU	4.5
1	E	137	HIS	4.5
1	E	455	ALA	4.5
1	C	430	LEU	4.5
1	E	418	LEU	4.5
1	C	387	GLY	4.5
1	A	271	ALA	4.5
1	B	384	ALA	4.4
1	B	378	GLY	4.4
1	C	135	LEU	4.4
1	C	438	VAL	4.4
1	D	438	VAL	4.4
1	E	363	LEU	4.4
1	E	95	GLN	4.4
1	D	455	ALA	4.4
1	A	143	GLY	4.3
1	E	66	ASN	4.3
1	C	164	THR	4.3
1	C	422	ILE	4.2
1	C	432	ASP	4.2
1	E	423	GLN	4.2

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Mol	Chain	Res	Type	RSRZ
1	E	443	ILE	4.2
1	C	333	GLY	4.2
1	D	436	GLY	4.2
1	E	358	ASN	4.2
1	B	363	LEU	4.2
1	C	429	LEU	4.2
1	C	132	GLY	4.1
1	E	268	PRO	4.1
1	E	426	HIS	4.1
1	C	281	PHE	4.1
1	C	331	GLY	4.0
1	E	143	GLY	4.0
1	A	455	ALA	4.0
1	A	130	PRO	4.0
1	C	335	SER	4.0
1	D	68	TYR	4.0
1	B	429	LEU	4.0
1	C	358	ASN	4.0
1	D	435	LYS	4.0
1	D	0	ASN	4.0
1	C	376	VAL	4.0
1	C	348	TRP	3.9
1	E	428	LYS	3.9
1	D	352	PRO	3.9
1	A	135	LEU	3.9
1	D	429	LEU	3.9
1	B	379	ASP	3.9
1	A	68	TYR	3.9
1	C	420	LEU	3.9
1	A	405	PHE	3.9
1	B	425	GLU	3.8
1	A	262	PRO	3.8
1	C	191	ALA	3.8
1	B	433	PHE	3.8
1	E	270	ASN	3.8
1	A	163	SER	3.8
1	C	129	LEU	3.8
1	C	412	LEU	3.8
1	B	426	HIS	3.8
1	E	348	TRP	3.8
1	B	142	SER	3.8
1	C	142	SER	3.8

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Mol	Chain	Res	Type	RSRZ
1	D	-1	SER	3.8
1	E	356	THR	3.8
1	D	439	ASN	3.8
1	A	129	LEU	3.7
1	E	439	ASN	3.7
1	B	68	TYR	3.7
1	D	270	ASN	3.7
1	C	385	PRO	3.7
1	D	135	LEU	3.7
1	D	147	ILE	3.7
1	C	139	TYR	3.6
1	E	362	LYS	3.6
1	E	436	GLY	3.6
1	D	426	HIS	3.6
1	A	132	GLY	3.6
1	B	438	VAL	3.6
1	C	377	PHE	3.6
1	C	456	LEU	3.6
1	B	261	LYS	3.6
1	C	436	GLY	3.6
1	C	147	ILE	3.6
1	C	443	ILE	3.6
1	C	360	VAL	3.6
1	C	167	TYR	3.5
1	C	-1	SER	3.5
1	E	385	PRO	3.5
1	D	269	GLU	3.5
1	E	87	LEU	3.5
1	D	134	HIS	3.5
1	B	431	LYS	3.5
1	A	429	LEU	3.5
1	B	442	ALA	3.5
1	E	347	LEU	3.5
1	E	274	ASP	3.5
1	D	142	SER	3.5
1	C	425	GLU	3.5
1	C	329	LEU	3.5
1	C	415	ALA	3.5
1	C	354	GLY	3.5
1	C	426	HIS	3.5
1	B	364	CYS	3.4
1	D	265	LYS	3.4

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Mol	Chain	Res	Type	RSRZ
1	E	62	GLY	3.4
1	E	138	GLY	3.4
1	B	135	LEU	3.4
1	B	350	LEU	3.4
1	B	432	ASP	3.4
1	C	353	LEU	3.4
1	C	165	THR	3.4
1	A	69	TYR	3.4
1	C	428	LYS	3.4
1	A	418	LEU	3.4
1	A	352	PRO	3.4
1	E	259	GLY	3.3
1	B	0	ASN	3.3
1	B	388	VAL	3.3
1	E	366	LEU	3.3
1	E	359	LYS	3.3
1	E	419	THR	3.3
1	B	65	GLY	3.3
1	D	188	GLY	3.3
1	E	333	GLY	3.3
1	E	-1	SER	3.3
1	E	140	TYR	3.3
1	E	438	VAL	3.3
1	B	420	LEU	3.3
1	C	347	LEU	3.3
1	E	135	LEU	3.3
1	C	423	GLN	3.2
1	B	271	ALA	3.2
1	E	272	VAL	3.2
1	A	427	GLY	3.2
1	C	427	GLY	3.2
1	C	424	LYS	3.2
1	E	306	ALA	3.2
1	E	352	PRO	3.2
1	D	348	TRP	3.2
1	B	113	ALA	3.2
1	C	421	GLU	3.2
1	E	415	ALA	3.2
1	B	439	ASN	3.2
1	E	360	VAL	3.2
1	B	129	LEU	3.2
1	E	303	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
1	E	354	GLY	3.2
1	D	377	PHE	3.2
1	C	37	ILE	3.1
1	D	358	ASN	3.1
1	E	144	GLY	3.1
1	C	145	LYS	3.1
1	E	207	LYS	3.1
1	D	65	GLY	3.1
1	D	430	LEU	3.1
1	C	417	THR	3.1
1	C	134	HIS	3.1
1	B	443	ILE	3.1
1	C	68	TYR	3.1
1	E	401	VAL	3.1
1	A	424	LYS	3.1
1	B	423	GLN	3.1
1	E	262	PRO	3.1
1	D	282	ALA	3.1
1	E	65	GLY	3.1
1	C	287	LEU	3.0
1	C	355	LEU	3.0
1	C	363	LEU	3.0
1	C	272	VAL	3.0
1	C	334	TYR	3.0
1	A	190	SER	3.0
1	E	164	THR	3.0
1	E	350	LEU	3.0
1	C	416	VAL	3.0
1	C	464	VAL	3.0
1	B	427	GLY	3.0
1	C	168	ILE	3.0
1	C	161	VAL	3.0
1	B	422	ILE	3.0
1	A	438	VAL	2.9
1	E	74	TYR	2.9
1	B	165	THR	2.9
1	E	133	GLY	2.9
1	D	442	ALA	2.9
1	E	271	ALA	2.9
1	E	424	LYS	2.9
1	E	209	GLY	2.9
1	E	281	PHE	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	329	LEU	2.9
1	C	326	GLY	2.9
1	B	428	LYS	2.9
1	E	421	GLU	2.9
1	C	365	ASP	2.8
1	A	147	ILE	2.8
1	A	386	GLY	2.8
1	E	434	ASN	2.8
1	E	273	TYR	2.8
1	A	84	SER	2.8
1	B	436	GLY	2.8
1	B	456	LEU	2.8
1	C	408	ILE	2.8
1	C	130	PRO	2.8
1	C	69	TYR	2.8
1	A	410	GLU	2.8
1	C	350	LEU	2.8
1	D	463	LEU	2.8
1	E	63	MET	2.8
1	D	139	TYR	2.7
1	A	439	ASN	2.7
1	C	271	ALA	2.7
1	A	470	LYS	2.7
1	B	435	LYS	2.7
1	E	411	PHE	2.7
1	E	386	GLY	2.7
1	A	366	LEU	2.7
1	A	437	LEU	2.7
1	A	450	VAL	2.7
1	B	376	VAL	2.7
1	C	337	VAL	2.7
1	C	225	ALA	2.7
1	E	61	GLU	2.7
1	E	307	ALA	2.7
1	A	456	LEU	2.7
1	B	418	LEU	2.7
1	B	260	PRO	2.7
1	D	421	GLU	2.7
1	B	272	VAL	2.7
1	E	47	VAL	2.7
1	C	469	TYR	2.7
1	E	469	TYR	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	347	LEU	2.7
1	A	355	LEU	2.7
1	A	363	LEU	2.7
1	E	334	TYR	2.6
1	E	32	ARG	2.6
1	C	411	PHE	2.6
1	D	425	GLU	2.6
1	E	81	LEU	2.6
1	E	4	VAL	2.6
1	B	307	ALA	2.6
1	B	328	TYR	2.6
1	D	431	LYS	2.6
1	C	0	ASN	2.6
1	D	66	ASN	2.6
1	A	350	LEU	2.6
1	B	353	LEU	2.6
1	C	446	LEU	2.6
1	B	259	GLY	2.6
1	E	373	LYS	2.6
1	E	275	PHE	2.6
1	E	7	TRP	2.6
1	D	418	LEU	2.6
1	E	456	LEU	2.6
1	C	166	GLY	2.6
1	C	297	GLY	2.6
1	E	132	GLY	2.6
1	B	415	ALA	2.6
1	B	455	ALA	2.6
1	C	163	SER	2.6
1	D	28	ARG	2.5
1	B	284	PHE	2.5
1	D	432	ASP	2.5
1	A	443	ILE	2.5
1	D	422	ILE	2.5
1	E	146	LYS	2.5
1	E	131	SER	2.5
1	A	134	HIS	2.5
1	B	99	VAL	2.5
1	A	87	LEU	2.5
1	C	357	GLY	2.5
1	C	450	VAL	2.5
1	D	360	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	133	GLY	2.5
1	D	62	GLY	2.5
1	A	422	ILE	2.5
1	E	19	ILE	2.5
1	E	175	GLU	2.5
1	C	136	THR	2.5
1	A	272	VAL	2.5
1	B	416	VAL	2.5
1	D	388	VAL	2.5
1	E	161	VAL	2.5
1	C	434	ASN	2.4
1	D	470	LYS	2.4
1	E	191	ALA	2.4
1	B	348	TRP	2.4
1	A	161	VAL	2.4
1	B	385	PRO	2.4
1	E	223	VAL	2.4
1	E	388	VAL	2.4
1	D	368	ASN	2.4
1	A	466	GLU	2.4
1	B	446	LEU	2.4
1	E	429	LEU	2.4
1	E	447	LYS	2.4
1	B	375	ALA	2.4
1	C	340	GLY	2.4
1	E	211	LEU	2.4
1	A	170	TYR	2.4
1	A	370	THR	2.4
1	E	136	THR	2.4
1	E	205	ALA	2.4
1	E	374	ASN	2.4
1	A	144	GLY	2.4
1	A	146	LYS	2.4
1	D	350	LEU	2.3
1	E	351	ARG	2.3
1	E	430	LEU	2.3
1	B	273	TYR	2.3
1	E	453	PHE	2.3
1	B	136	THR	2.3
1	B	141	THR	2.3
1	E	10	THR	2.3
1	E	141	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	296	ILE	2.3
1	D	89	ALA	2.3
1	D	137	HIS	2.3
1	B	331	GLY	2.3
1	B	386	GLY	2.3
1	A	431	LYS	2.3
1	C	371	VAL	2.3
1	D	371	VAL	2.3
1	A	420	LEU	2.3
1	B	69	TYR	2.3
1	B	411	PHE	2.3
1	C	285	PRO	2.3
1	A	432	ASP	2.3
1	E	31	CYS	2.3
1	C	463	LEU	2.3
1	D	412	LEU	2.3
1	D	9	ASN	2.3
1	E	440	ASN	2.3
1	E	467	MET	2.3
1	E	234	TYR	2.3
1	A	365	ASP	2.3
1	D	464	VAL	2.3
1	E	372	ASN	2.3
1	A	164	THR	2.3
1	B	441	LYS	2.3
1	E	196	TRP	2.2
1	E	70	GLY	2.2
1	E	84	SER	2.2
1	B	75	ILE	2.2
1	C	34	ILE	2.2
1	A	145	LYS	2.2
1	B	424	LYS	2.2
1	C	435	LYS	2.2
1	E	370	THR	2.2
1	E	461	GLY	2.2
1	D	365	ASP	2.2
1	C	97	TRP	2.2
1	C	234	TYR	2.2
1	E	147	ILE	2.2
1	C	327	LYS	2.2
1	B	32	ARG	2.2
1	C	346	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	61	GLU	2.2
1	E	444	GLU	2.2
1	A	95	GLN	2.2
1	D	366	LEU	2.2
1	E	463	LEU	2.2
1	A	458	ASP	2.2
1	C	94	ALA	2.2
1	A	469	TYR	2.2
1	D	433	PHE	2.2
1	E	390	ILE	2.2
1	B	358	ASN	2.2
1	C	66	ASN	2.2
1	C	270	ASN	2.2
1	B	323	VAL	2.2
1	B	128	ASP	2.2
1	E	93	ASP	2.2
1	E	432	ASP	2.2
1	B	70	GLY	2.2
1	B	178	LEU	2.2
1	C	366	LEU	2.2
1	A	260	PRO	2.2
1	D	64	PRO	2.2
1	A	415	ALA	2.2
1	D	394	ALA	2.2
1	C	362	LYS	2.2
1	A	139	TYR	2.1
1	D	469	TYR	2.1
1	B	97	TRP	2.1
1	A	2	ASP	2.1
1	B	274	ASP	2.1
1	A	464	VAL	2.1
1	B	161	VAL	2.1
1	D	47	VAL	2.1
1	B	143	GLY	2.1
1	C	209	GLY	2.1
1	E	387	GLY	2.1
1	B	309	PRO	2.1
1	D	347	LEU	2.1
1	E	36	LEU	2.1
1	C	40	GLU	2.1
1	C	330	MET	2.1
1	D	191	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	300	ALA	2.1
1	B	37	ILE	2.1
1	B	334	TYR	2.1
1	B	164	THR	2.1
1	C	141	THR	2.1
1	E	96	SER	2.1
1	C	6	VAL	2.1
1	D	133	GLY	2.1
1	C	25	LYS	2.1
1	C	470	LYS	2.1
1	A	425	GLU	2.1
1	B	130	PRO	2.1
1	C	211	LEU	2.1
1	D	434	ASN	2.1
1	E	12	LEU	2.1
1	E	130	PRO	2.1
1	B	453	PHE	2.1
1	D	23	ILE	2.1
1	E	75	ILE	2.1
1	C	359	LYS	2.1
1	D	164	THR	2.1
1	A	259	GLY	2.1
1	B	98	GLY	2.1
1	D	427	GLY	2.1
1	E	221	GLY	2.1
1	E	129	LEU	2.1
1	E	329	LEU	2.1
1	C	375	ALA	2.1
1	E	442	ALA	2.1
1	A	168	ILE	2.0
1	C	369	ILE	2.0
1	E	37	ILE	2.0
1	E	431	LYS	2.0
1	B	387	GLY	2.0
1	D	138	GLY	2.0
1	B	228	VAL	2.0
1	B	352	PRO	2.0
1	D	272	VAL	2.0
1	A	92	LEU	2.0
1	C	31	CYS	2.0
1	C	173	LEU	2.0
1	C	336	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	274	ASP	2.0
1	E	261	LYS	2.0
1	A	397	SER	2.0
1	B	186	ILE	2.0
1	C	390	ILE	2.0
1	C	144	GLY	2.0
1	E	166	GLY	2.0
1	D	263	PRO	2.0
1	D	385	PRO	2.0
1	D	416	VAL	2.0
1	E	416	VAL	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](#)

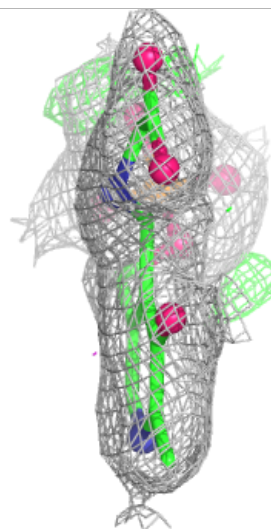
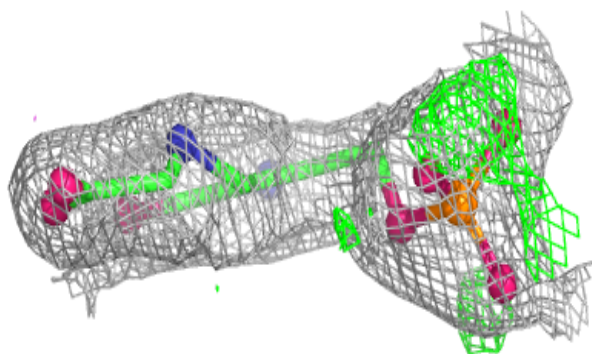
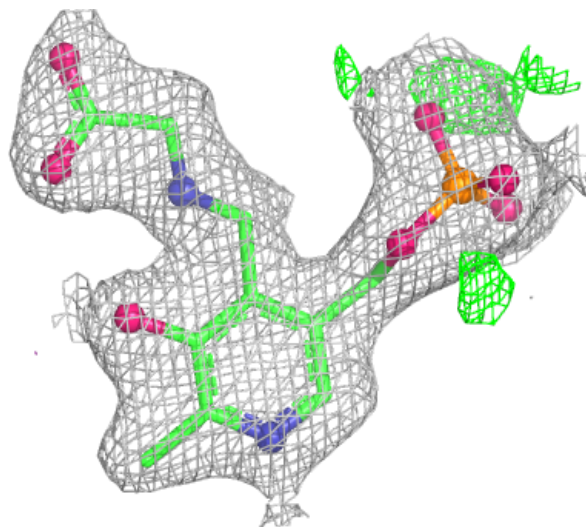
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	PLG	A	501	20/20	0.92	0.12	28,34,38,40	0
2	PLG	C	501	20/20	0.92	0.13	28,37,41,41	0
2	PLG	E	501	20/20	0.92	0.12	31,40,42,44	0
2	PLG	D	501	20/20	0.93	0.13	23,31,34,35	20
2	PLG	B	501	20/20	0.95	0.09	27,31,34,35	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.

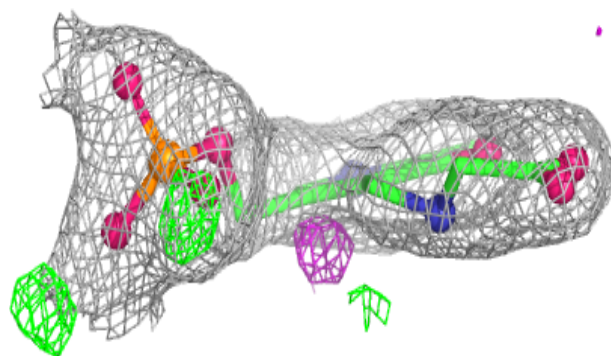
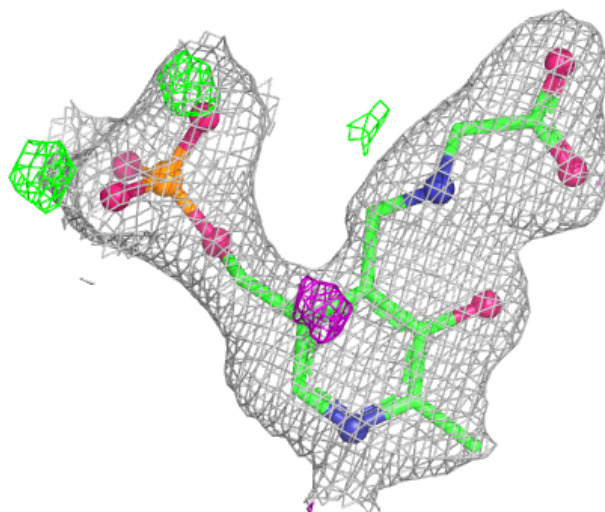
Electron density around PLG A 501:

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



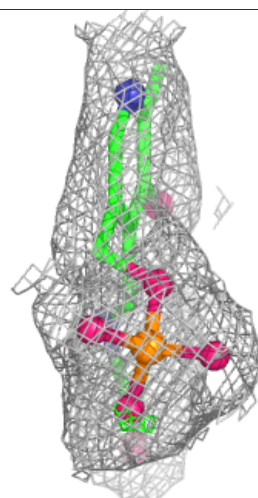
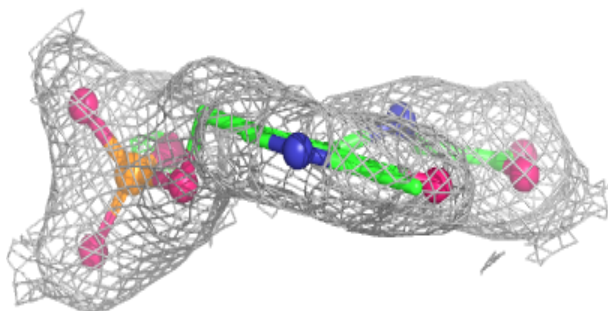
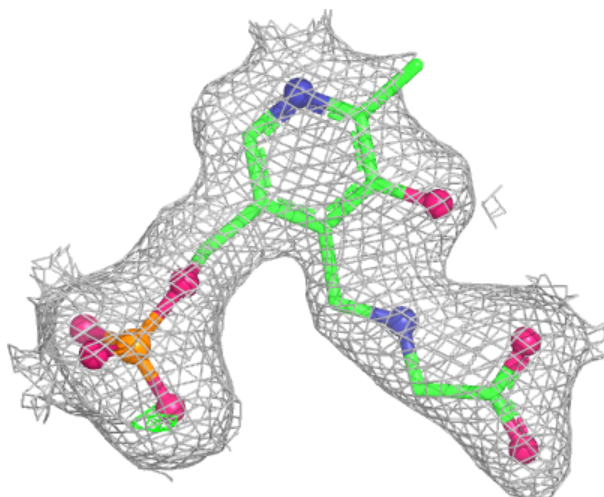
Electron density around PLG C 501:

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



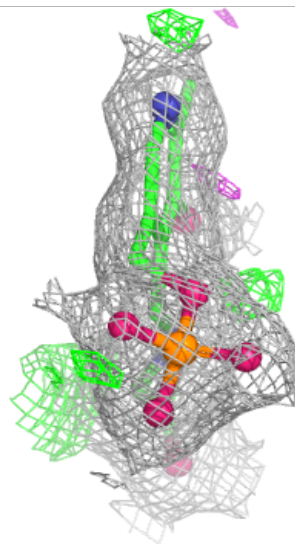
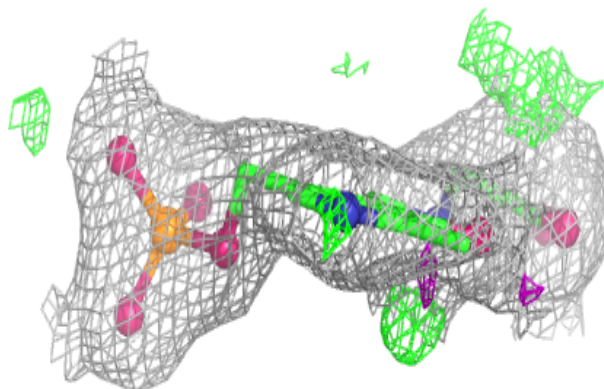
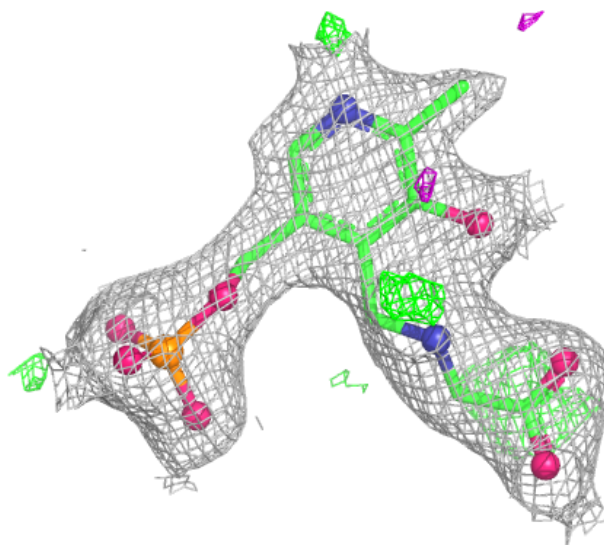
Electron density around PLG E 501:

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



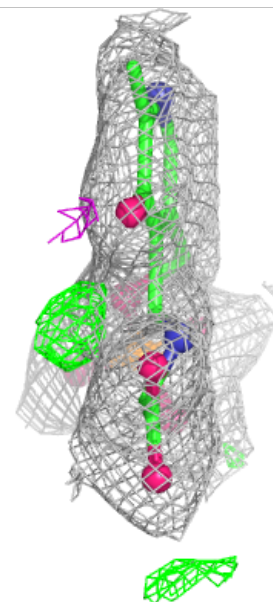
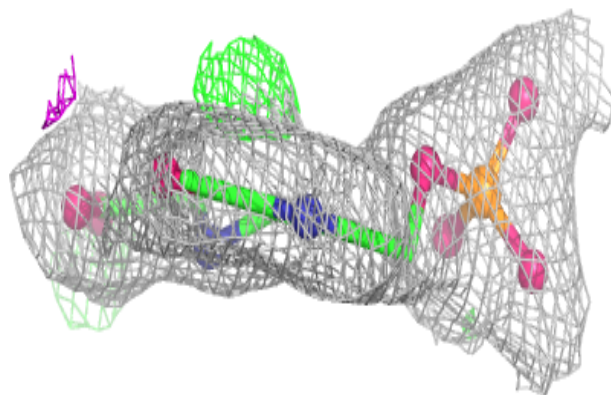
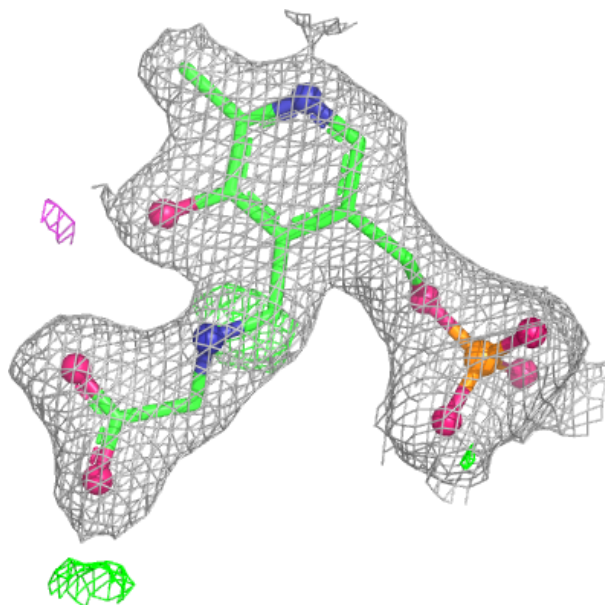
Electron density around PLG D 501:

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



Electron density around PLG B 501:

$2mF_o-DF_c$ (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.