



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 14, 2020 – 03:02 AM BST

PDB ID : 6CD1  
Title : Crystal structure of Medicago truncatula serine hydroxymethyltransferase 3 (MtSHMT3), complexes with reaction intermediates  
Authors : Ruszkowski, M.; Sekula, B.; Ruszkowska, A.; Dauter, Z.  
Deposited on : 2018-02-07  
Resolution : 1.91 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](mailto: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.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : **FAILED**  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.14.4.dev1

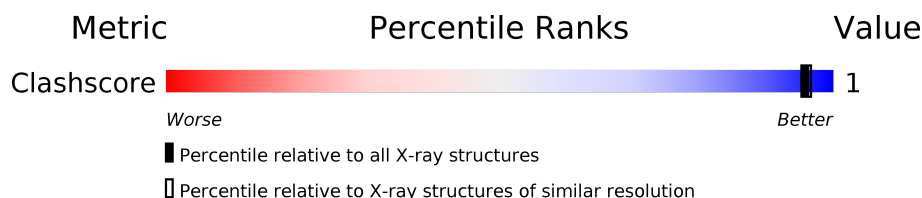
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.91 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))
Clashscore	141614	8644 (1.94-1.90)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$ .

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	455	 97% ..
1	B	455	 97% ..
1	C	455	 98% ..
1	D	455	 95% ..
1	F	455	 97% ..
2	E	455	 97% ..
2	G	455	 97% ..
2	H	455	 97% ..

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	ACT	C	601	-	-	X	-

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 29964 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	452	Total	C	N	O	S	0	0	0
			3468	2199	605	649	15			
1	B	451	Total	C	N	O	S	0	3	0
			3485	2207	611	652	15			
1	C	452	Total	C	N	O	S	0	1	0
			3477	2204	607	651	15			
1	D	445	Total	C	N	O	S	0	3	0
			3444	2182	604	643	15			
1	F	451	Total	C	N	O	S	0	1	0
			3466	2195	606	650	15			

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	79	SER	-	expression tag	UNP G7ILW0
A	80	ASN	-	expression tag	UNP G7ILW0
A	81	ALA	-	expression tag	UNP G7ILW0
B	79	SER	-	expression tag	UNP G7ILW0
B	80	ASN	-	expression tag	UNP G7ILW0
B	81	ALA	-	expression tag	UNP G7ILW0
C	79	SER	-	expression tag	UNP G7ILW0
C	80	ASN	-	expression tag	UNP G7ILW0
C	81	ALA	-	expression tag	UNP G7ILW0
D	79	SER	-	expression tag	UNP G7ILW0
D	80	ASN	-	expression tag	UNP G7ILW0
D	81	ALA	-	expression tag	UNP G7ILW0
F	79	SER	-	expression tag	UNP G7ILW0
F	80	ASN	-	expression tag	UNP G7ILW0
F	81	ALA	-	expression tag	UNP G7ILW0

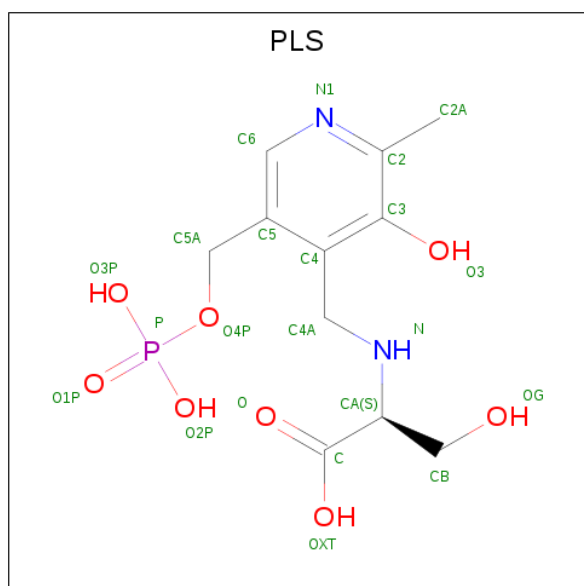
- Molecule 2 is a protein called Serine hydroxymethyltransferase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	E	451	Total	C	N	O	P	S	0	1	0
			3481	2203	607	655	1	15			
2	G	451	Total	C	N	O	P	S	0	1	0
			3481	2203	607	655	1	15			
2	H	452	Total	C	N	O	P	S	0	1	0
			3492	2212	608	656	1	15			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	79	SER	-	expression tag	UNP G7ILW0
E	80	ASN	-	expression tag	UNP G7ILW0
E	81	ALA	-	expression tag	UNP G7ILW0
G	79	SER	-	expression tag	UNP G7ILW0
G	80	ASN	-	expression tag	UNP G7ILW0
G	81	ALA	-	expression tag	UNP G7ILW0
H	79	SER	-	expression tag	UNP G7ILW0
H	80	ASN	-	expression tag	UNP G7ILW0
H	81	ALA	-	expression tag	UNP G7ILW0

- Molecule 3 is [3-HYDROXY-2-METHYL-5-PHOSPHONOOXYMETHYL-PYRIDIN-4-YL METHYL]-SERINE (three-letter code: PLS) (formula: C<sub>11</sub>H<sub>17</sub>N<sub>2</sub>O<sub>8</sub>P) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	N	O	P		0	0
			22	11	2	8	1			

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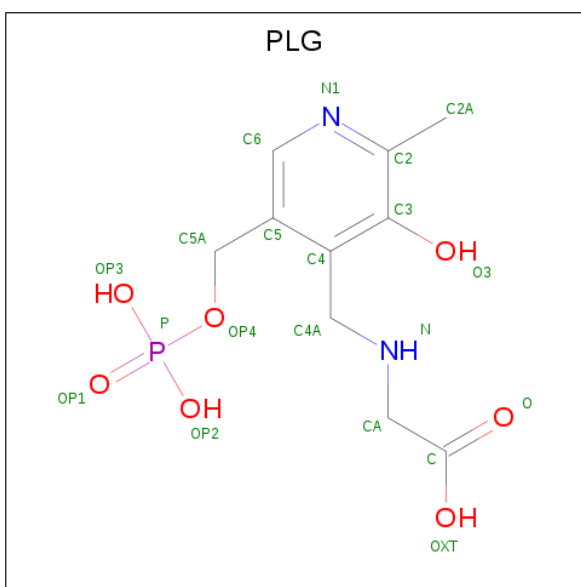
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	D	1	Total	C	N	O	P	0	0
			22	11	2	8	1		

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



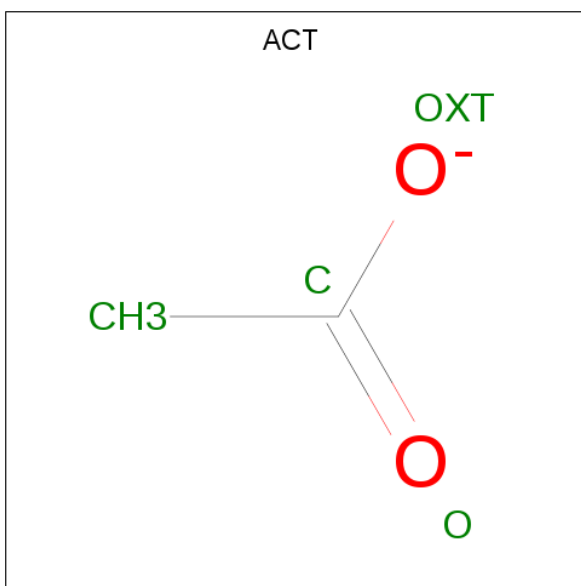
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	E	1	Total	C	O	0	0
			4	2	2		
4	F	1	Total	C	O	0	0
			4	2	2		
4	G	1	Total	C	O	0	0
			4	2	2		
4	H	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is N-GLYCINE-[3-HYDROXY-2-METHYL-5-PHOSPHONOOXYMETHYL-PYRIDIN-4-YL-METHANE] (three-letter code: PLG) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>2</sub>O<sub>7</sub>P) (labeled as "Ligand of Interest" by author).



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

- Molecule 6 is ACETATE ION (three-letter code: ACT) (formula:  $C_2H_3O_2$ ).



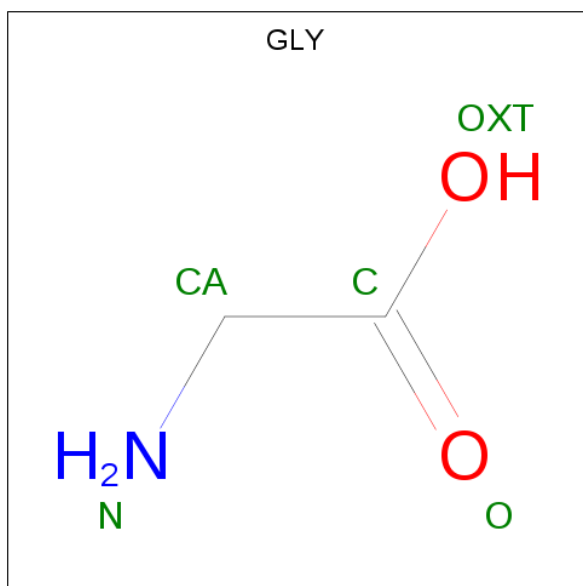
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	C	1	Total	C	O	0	0
			4	2	2		
6	C	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	H	1	Total	C	O	0	0
			4	2	2		

- Molecule 7 is GLYCINE (three-letter code: GLY) (formula:  $C_2H_5NO_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	E	1	Total	C	N	O	0	0
			5	2	1	2		
7	H	1	Total	C	N	O	0	0
			5	2	1	2		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	336	Total	O	0	0
			336	336		
8	B	229	Total	O	0	0
			229	229		
8	C	284	Total	O	0	0
			284	284		
8	D	200	Total	O	0	0
			200	200		
8	E	289	Total	O	0	0
			289	289		
8	F	199	Total	O	0	0
			199	199		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	G	279	Total 279	O 279	0	0
8	H	216	Total 216	O 216	0	0

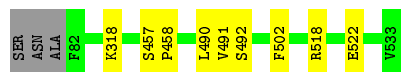
### 3 Residue-property plots [i](#)

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. 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. 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.

Note EDS failed to run properly.

- Molecule 1: Serine hydroxymethyltransferase

Chain A:  97%



- Molecule 1: Serine hydroxymethyltransferase

Chain B:  97%



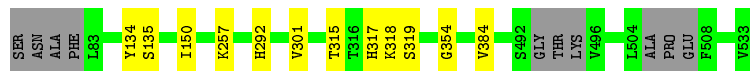
- Molecule 1: Serine hydroxymethyltransferase

Chain C:  98%



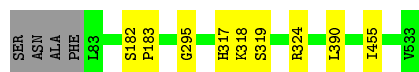
- Molecule 1: Serine hydroxymethyltransferase

Chain D:  95%



- Molecule 1: Serine hydroxymethyltransferase

Chain F:  97%



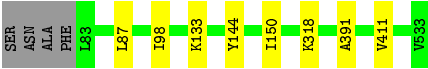
- Molecule 2: Serine hydroxymethyltransferase

Chain E:  97% ..



● Molecule 2: Serine hydroxymethyltransferase

Chain G:  97% ..



● Molecule 2: Serine hydroxymethyltransferase

Chain H:  97% ..



## 4 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	94.09Å 103.65Å 180.38Å 90.00° 97.38° 90.00°	Depositor
Resolution (Å)	46.65 – 1.91	Depositor
% Data completeness (in resolution range)	98.6 (46.65-1.91)	Depositor
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.01 (at 1.91Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, $R_{free}$	0.191 , 0.236	Depositor
Wilson B-factor (Å <sup>2</sup> )	35.1	Xtriage
Anisotropy	0.198	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	29964	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	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 52.82 % 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 4.6075e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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, LLP, PLS, EDO, ACT

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	0.68	0/3540	0.74	0/4788
1	B	0.64	0/3557	0.70	0/4810
1	C	0.63	0/3549	0.70	0/4800
1	D	0.63	0/3513	0.69	0/4747
1	F	0.59	0/3537	0.67	0/4784
2	E	0.59	0/3527	0.68	0/4770
2	G	0.62	0/3527	0.68	0/4770
2	H	0.60	0/3539	0.67	0/4786
All	All	0.62	0/28289	0.69	0/38255

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	3468	0	3467	10	0
1	B	3485	0	3484	11	0
1	C	3477	0	3474	5	0
1	D	3444	0	3441	11	0
1	F	3466	0	3465	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	3481	0	3469	6	0
2	G	3481	0	3469	4	0
2	H	3492	0	3478	8	0
3	A	22	0	14	6	0
3	D	22	0	13	4	0
4	A	4	0	6	0	0
4	B	4	0	6	0	0
4	C	4	0	6	1	0
4	D	4	0	6	0	0
4	E	4	0	6	0	0
4	F	4	0	6	0	0
4	G	4	0	6	0	0
4	H	4	0	6	0	0
5	B	20	0	12	5	0
5	F	20	0	12	2	0
6	C	8	0	6	2	0
6	H	4	0	3	0	0
7	E	5	0	2	0	0
7	H	5	0	2	1	0
8	A	336	0	0	1	0
8	B	229	0	0	1	0
8	C	284	0	0	2	0
8	D	200	0	0	1	0
8	E	289	0	0	1	0
8	F	199	0	0	0	0
8	G	279	0	0	0	0
8	H	216	0	0	0	0
All	All	29964	0	27859	62	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 1.

All (62) 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:318:LYS:HZ3	3:A:601:PLS:H4A1	1.52	0.72
1:A:318:LYS:HZ3	3:A:601:PLS:C4A	2.03	0.71
1:F:318:LYS:NZ	5:F:601:PLG:H4A2	2.07	0.69
1:A:318:LYS:NZ	3:A:601:PLS:H4A1	2.09	0.67
1:A:318:LYS:NZ	3:A:601:PLS:C4A	2.59	0.65
1:F:318:LYS:HZ1	5:F:601:PLG:H4A2	1.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:301:VAL:HG11	1:D:384:VAL:HG21	1.80	0.62
1:D:318[B]:LYS:NZ	3:D:601:PLS:H4A1	2.16	0.61
2:E:468:LYS:CE	2:E:468:LYS:H	2.15	0.59
1:B:318[B]:LYS:HZ1	5:B:601:PLG:H4A2	1.68	0.58
8:C:710:HOH:O	3:D:601:PLS:H4A2	2.06	0.55
2:E:468:LYS:HE3	2:E:468:LYS:H	1.72	0.55
6:C:601:ACT:H2	1:D:134:TYR:OH	2.09	0.53
1:D:257:LYS:NZ	8:D:701:HOH:O	2.41	0.53
1:C:106:PHE:CE2	1:C:526:THR:HG22	2.44	0.53
2:E:482:ARG:NE	8:E:701:HOH:O	2.32	0.53
3:A:601:PLS:H4A2	8:B:706:HOH:O	2.08	0.53
1:D:315:THR:HB	1:D:317[B]:HIS:CE1	2.45	0.52
2:H:198:ARG:HB3	2:H:254:PHE:CE2	2.45	0.51
1:C:144:TYR:HD1	8:C:733:HOH:O	1.95	0.50
6:C:601:ACT:H1	1:D:354:GLY:HA3	1.94	0.49
1:B:503:VAL:HA	1:B:508:PHE:CD1	2.48	0.48
1:A:491:VAL:HG22	1:A:502:PHE:CD2	2.49	0.48
2:E:391:ALA:HB2	2:E:411:VAL:HG11	1.96	0.48
1:A:490:LEU:HD11	8:A:1032:HOH:O	2.15	0.47
1:A:318:LYS:NZ	3:A:601:PLS:N	2.62	0.47
1:D:318[B]:LYS:HZ3	3:D:601:PLS:H4A1	1.79	0.47
1:B:292:HIS:CD2	1:B:318[A]:LYS:HZ3	2.33	0.47
2:H:390:LEU:HD21	2:H:455:ILE:HG21	1.98	0.46
1:D:318[A]:LYS:NZ	3:D:601:PLS:H4A1	2.30	0.46
1:D:317[A]:HIS:O	1:D:318[A]:LYS:HB2	2.15	0.46
1:B:318[A]:LYS:HZ1	5:B:601:PLG:H4A2	1.81	0.45
1:A:518:ARG:O	1:A:522:GLU:HG3	2.15	0.45
1:B:318[B]:LYS:NZ	5:B:601:PLG:H4A2	2.32	0.45
2:H:103:ASP:OD2	2:H:107:ARG:NH2	2.50	0.45
1:F:390:LEU:HD21	1:F:455:ILE:HG21	1.98	0.44
1:B:315:THR:HB	1:B:317[B]:HIS:CE1	2.52	0.44
2:E:390:LEU:HD12	2:E:474:ALA:HB2	2.00	0.44
1:D:292:HIS:O	1:D:319:SER:HB2	2.17	0.44
2:E:387:CYS:SG	2:E:411:VAL:HG13	2.57	0.44
2:H:177:GLN:N	2:H:178:PRO:CD	2.81	0.43
1:F:317:HIS:ND1	1:F:324:ARG:HA	2.33	0.43
2:G:87:LEU:HD21	2:G:98:ILE:HD12	2.00	0.43
1:A:457:SER:N	1:A:458:PRO:CD	2.81	0.43
2:G:391:ALA:HB2	2:G:411:VAL:HG11	2.00	0.43
1:B:223:GLY:HA2	1:B:226:ILE:HD12	2.01	0.43
1:F:182:SER:HB2	1:F:183:PRO:HD3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:158:GLN:HB3	4:C:603:EDO:H12	2.01	0.42
2:G:144:TYR:HH	7:H:602:GLY:N	2.17	0.42
1:B:318[B]:LYS:HZ1	5:B:601:PLG:C4A	2.32	0.42
1:C:112:ILE:HB	1:C:115:GLU:HG3	2.02	0.42
2:H:410:LEU:C	2:H:410:LEU:HD12	2.40	0.41
1:B:409:HIS:CE1	1:B:410:LEU:HD23	2.56	0.41
2:H:114:SER:HB2	2:H:318:LLP:HE3	2.03	0.41
2:G:133:LYS:HG2	2:G:150:ILE:HG13	2.02	0.41
1:A:492:SER:O	2:H:519:ARG:CD	2.69	0.41
1:F:295:GLY:N	1:F:319:SER:OG	2.47	0.41
2:H:390:LEU:HD21	2:H:455:ILE:CG2	2.51	0.41
1:C:87:LEU:HD21	1:C:98:ILE:HD12	2.03	0.40
1:B:410:LEU:C	1:B:410:LEU:HD12	2.42	0.40
1:D:135:SER:CB	1:D:150:ILE:HG21	2.51	0.40
1:B:318[A]:LYS:NZ	5:B:601:PLG:H4A2	2.36	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

### 5.3.2 Protein sidechains [i](#)

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

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

3 non-standard protein/DNA/RNA residues 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	LLP	E	318	2	23,24,25	1.54	3 (13%)	25,32,34	2.31	9 (36%)
2	LLP	G	318	2	23,24,25	1.52	5 (21%)	25,32,34	1.97	7 (28%)
2	LLP	H	318	2	23,24,25	1.72	5 (21%)	25,32,34	2.30	8 (32%)

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	LLP	E	318	2	-	10/16/17/19	0/1/1/1
2	LLP	G	318	2	-	6/16/17/19	0/1/1/1
2	LLP	H	318	2	-	5/16/17/19	0/1/1/1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	318	LLP	C4-C4'	4.25	1.54	1.46
2	H	318	LLP	C4-C5	-4.18	1.36	1.42
2	G	318	LLP	C4-C4'	3.97	1.54	1.46
2	H	318	LLP	C4-C4'	3.67	1.53	1.46
2	H	318	LLP	C3-C2	-3.10	1.37	1.40
2	H	318	LLP	CB-CA	2.75	1.57	1.53
2	G	318	LLP	CB-CA	2.48	1.56	1.53
2	E	318	LLP	C4-C5	-2.48	1.38	1.42
2	G	318	LLP	C2'-C2	2.37	1.54	1.50
2	E	318	LLP	CB-CA	2.32	1.56	1.53
2	H	318	LLP	C4-C3	-2.08	1.37	1.40
2	G	318	LLP	P-OP4	2.06	1.66	1.60
2	G	318	LLP	C4-C3	-2.05	1.37	1.40

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	318	LLP	CE-NZ-C4'	6.95	140.23	118.90
2	H	318	LLP	OP4-C5'-C5	6.21	121.17	109.35
2	H	318	LLP	CE-NZ-C4'	5.57	136.02	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	318	LLP	CE-NZ-C4'	4.98	134.21	118.90
2	G	318	LLP	OP4-C5'-C5	4.34	117.62	109.35
2	E	318	LLP	C5'-C5-C6	-4.01	112.78	119.37
2	E	318	LLP	C4-C4'-NZ	-3.56	107.94	124.31
2	H	318	LLP	C4-C4'-NZ	-3.27	109.28	124.31
2	G	318	LLP	C4-C4'-NZ	-3.13	109.94	124.31
2	E	318	LLP	C5-C4-C4'	3.06	126.59	121.56
2	H	318	LLP	C3-C4-C5	2.99	120.56	118.26
2	E	318	LLP	OP4-C5'-C5	2.93	114.93	109.35
2	H	318	LLP	OP3-P-OP4	2.90	114.45	106.73
2	H	318	LLP	C3-C2-N1	-2.75	117.22	120.77
2	G	318	LLP	C5-C6-N1	-2.70	119.33	123.82
2	E	318	LLP	C3-C4-C4'	-2.68	115.43	120.41
2	G	318	LLP	C5'-C5-C6	-2.52	115.22	119.37
2	G	318	LLP	OP2-P-OP4	2.38	113.06	106.73
2	E	318	LLP	C4-C3-C2	2.32	121.62	120.19
2	H	318	LLP	C5-C6-N1	-2.29	120.00	123.82
2	E	318	LLP	C5-C6-N1	-2.22	120.12	123.82
2	H	318	LLP	C4-C3-C2	2.18	121.54	120.19
2	G	318	LLP	C3-C4-C4'	-2.12	116.46	120.41
2	E	318	LLP	C2'-C2-C3	2.02	123.39	120.89

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	318	LLP	C5-C4-C4'-NZ
2	E	318	LLP	C6-C5-C5'-OP4
2	E	318	LLP	C5'-OP4-P-OP3
2	E	318	LLP	O-C-CA-CB
2	E	318	LLP	CG-CD-CE-NZ
2	G	318	LLP	O-C-CA-CB
2	H	318	LLP	O-C-CA-CB
2	H	318	LLP	CG-CD-CE-NZ
2	G	318	LLP	CG-CD-CE-NZ
2	G	318	LLP	C3-C4-C4'-NZ
2	H	318	LLP	C5-C4-C4'-NZ
2	H	318	LLP	C3-C4-C4'-NZ
2	E	318	LLP	C3-C4-C4'-NZ
2	G	318	LLP	C5-C4-C4'-NZ
2	E	318	LLP	C5'-OP4-P-OP2
2	G	318	LLP	CD-CE-NZ-C4'

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Mol	Chain	Res	Type	Atoms
2	E	318	LLP	C4-C5-C5'-OP4
2	E	318	LLP	CD-CE-NZ-C4'
2	H	318	LLP	CD-CE-NZ-C4'
2	E	318	LLP	C5'-OP4-P-OP1
2	G	318	LLP	N-CA-CB-CG

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	318	LLP	1	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

17 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	$\# Z  > 2$
4	EDO	A	602	-	3,3,3	0.51	0	2,2,2	0.22	0
4	EDO	B	602	-	3,3,3	0.48	0	2,2,2	0.19	0
3	PLS	A	601	-	19,22,22	2.16	3 (15%)	25,31,31	2.15	7 (28%)
4	EDO	E	602	-	3,3,3	0.52	0	2,2,2	0.29	0
4	EDO	F	602	-	3,3,3	0.46	0	2,2,2	0.37	0
4	EDO	H	603	-	3,3,3	0.44	0	2,2,2	0.41	0
6	ACT	C	602	-	1,3,3	3.34	1 (100%)	0,3,3	0.00	-
4	EDO	C	603	-	3,3,3	0.32	0	2,2,2	0.36	0
3	PLS	D	601	-	19,22,22	1.81	3 (15%)	25,31,31	2.20	5 (20%)
6	ACT	C	601	-	1,3,3	0.94	0	0,3,3	0.00	-
7	GLY	E	601	-	1,4,4	0.10	0	0,4,4	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	GLY	H	602	-	1,4,4	0.11	0	0,4,4	0.00	-
4	EDO	G	601	-	3,3,3	0.47	0	2,2,2	0.33	0
6	ACT	H	601	-	1,3,3	3.66	1 (100%)	0,3,3	0.00	-
5	PLG	F	601	-	17,20,20	1.52	4 (23%)	23,28,28	1.96	6 (26%)
5	PLG	B	601	-	17,20,20	1.65	2 (11%)	23,28,28	2.01	6 (26%)
4	EDO	D	602	-	3,3,3	0.44	0	2,2,2	0.47	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	A	602	-	-	1/1/1/1	-
4	EDO	B	602	-	-	0/1/1/1	-
4	EDO	E	602	-	-	0/1/1/1	-
4	EDO	F	602	-	-	0/1/1/1	-
4	EDO	H	603	-	-	0/1/1/1	-
4	EDO	C	603	-	-	0/1/1/1	-
3	PLS	D	601	-	-	6/13/17/17	0/1/1/1
7	GLY	E	601	-	-	0/0/2/2	-
7	GLY	H	602	-	-	0/0/2/2	-
4	EDO	G	601	-	-	0/1/1/1	-
3	PLS	A	601	-	-	7/13/17/17	0/1/1/1
5	PLG	F	601	-	-	3/10/12/12	0/1/1/1
5	PLG	B	601	-	-	4/10/12/12	0/1/1/1
4	EDO	D	602	-	-	0/1/1/1	-

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	601	PLS	C4A-N	-6.66	1.27	1.46
3	D	601	PLS	C4A-N	-6.11	1.28	1.46
5	B	601	PLG	C4A-N	-4.05	1.27	1.46
5	F	601	PLG	C4A-N	-3.92	1.27	1.46
6	H	601	ACT	CH3-C	3.66	1.53	1.48
3	A	601	PLS	C3-C2	-3.54	1.37	1.40
6	C	602	ACT	CH3-C	3.34	1.53	1.48
3	A	601	PLS	C2A-C2	2.90	1.55	1.50
5	F	601	PLG	C4A-C4	2.45	1.55	1.51
5	B	601	PLG	C2A-C2	2.37	1.54	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	601	PLS	P-O4P	2.18	1.67	1.60
5	F	601	PLG	P-OP4	2.15	1.67	1.60
3	D	601	PLS	C4A-C4	2.15	1.54	1.51
5	F	601	PLG	C2A-C2	2.02	1.53	1.50

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	601	PLS	C4A-N-CA	9.00	131.11	113.83
3	A	601	PLS	C4A-N-CA	5.92	125.19	113.83
5	F	601	PLG	C4-C4A-N	5.35	121.57	111.58
5	B	601	PLG	C4-C4A-N	4.97	120.86	111.58
5	B	601	PLG	CA-N-C4A	4.52	123.94	112.54
5	F	601	PLG	CA-N-C4A	4.42	123.68	112.54
3	A	601	PLS	O4P-C5A-C5	4.15	117.27	109.35
3	A	601	PLS	CB-CA-C	-3.49	102.08	110.97
5	F	601	PLG	OP4-C5A-C5	3.08	115.22	109.35
3	A	601	PLS	C5-C6-N1	-3.07	118.70	123.82
5	B	601	PLG	C5-C6-N1	-3.00	118.82	123.82
3	D	601	PLS	CB-CA-C	-2.99	103.37	110.97
3	A	601	PLS	C4-C4A-N	2.96	119.94	111.78
3	A	601	PLS	C6-N1-C2	2.77	124.29	119.17
3	D	601	PLS	C6-C5-C4	2.66	120.00	118.12
5	F	601	PLG	C5-C6-N1	-2.52	119.62	123.82
5	F	601	PLG	C5A-C5-C6	-2.47	115.30	119.37
3	D	601	PLS	C5-C6-N1	-2.44	119.75	123.82
5	B	601	PLG	OP4-P-OP1	2.29	112.91	106.47
5	F	601	PLG	C6-C5-C4	2.27	119.72	118.12
3	A	601	PLS	C5A-C5-C6	-2.27	115.64	119.37
3	D	601	PLS	C4-C4A-N	2.22	117.89	111.78
5	B	601	PLG	OP4-C5A-C5	2.19	113.52	109.35
5	B	601	PLG	C6-N1-C2	2.17	123.19	119.17

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	601	PLS	C-CA-N-C4A
3	D	601	PLS	C-CA-CB-OG
3	A	601	PLS	N-CA-CB-OG
3	A	601	PLS	C-CA-CB-OG
3	A	601	PLS	C3-C4-C4A-N

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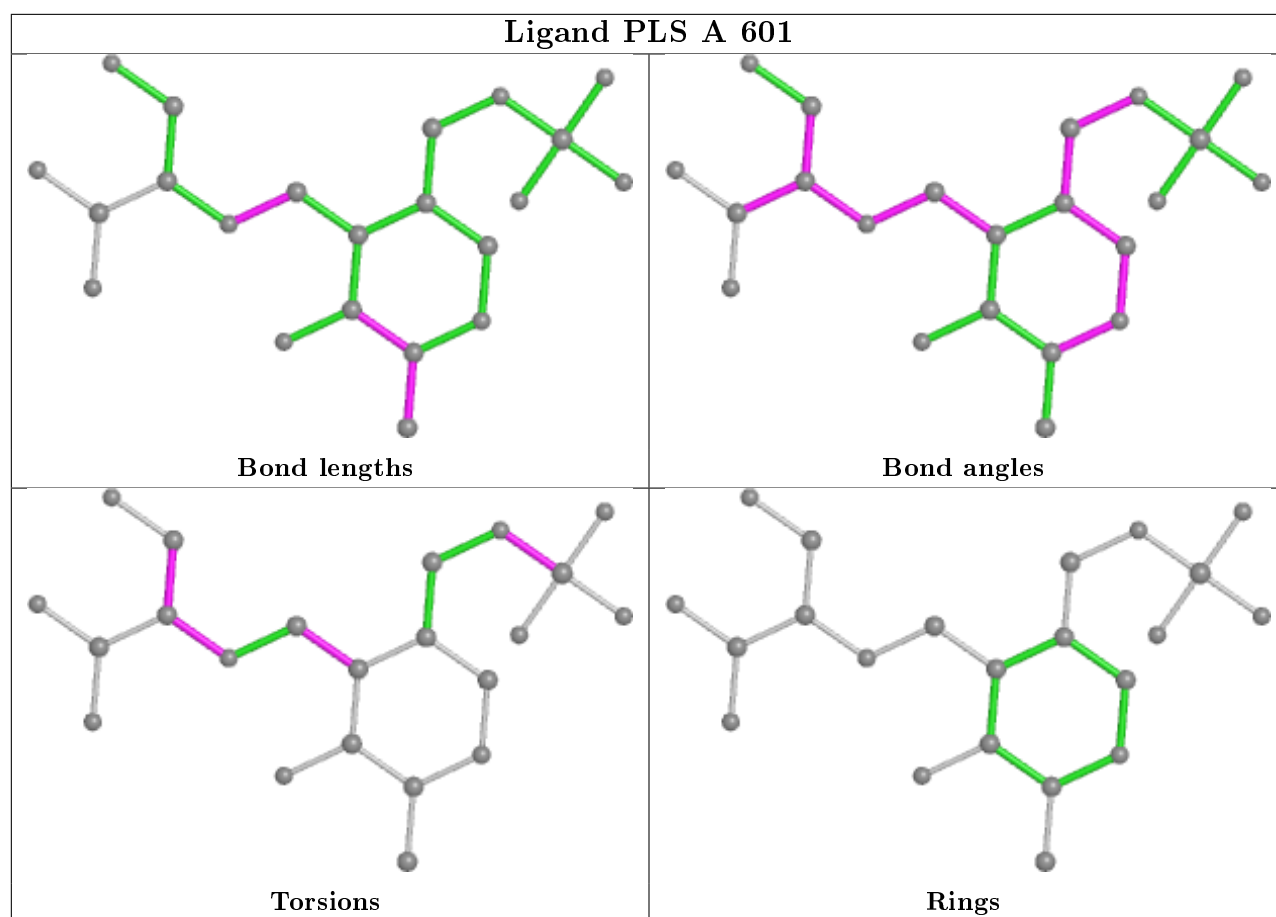
Mol	Chain	Res	Type	Atoms
5	F	601	PLG	C-CA-N-C4A
5	B	601	PLG	C-CA-N-C4A
3	D	601	PLS	C5-C4-C4A-N
3	A	601	PLS	C5-C4-C4A-N
5	F	601	PLG	C5-C4-C4A-N
5	B	601	PLG	C5-C4-C4A-N
5	F	601	PLG	C3-C4-C4A-N
3	A	601	PLS	C-CA-N-C4A
3	D	601	PLS	C3-C4-C4A-N
5	B	601	PLG	C3-C4-C4A-N
3	D	601	PLS	N-CA-CB-OG
3	D	601	PLS	CB-CA-N-C4A
3	A	601	PLS	CB-CA-N-C4A
3	A	601	PLS	C5A-O4P-P-O3P
5	B	601	PLG	C5A-OP4-P-OP3
4	A	602	EDO	O1-C1-C2-O2

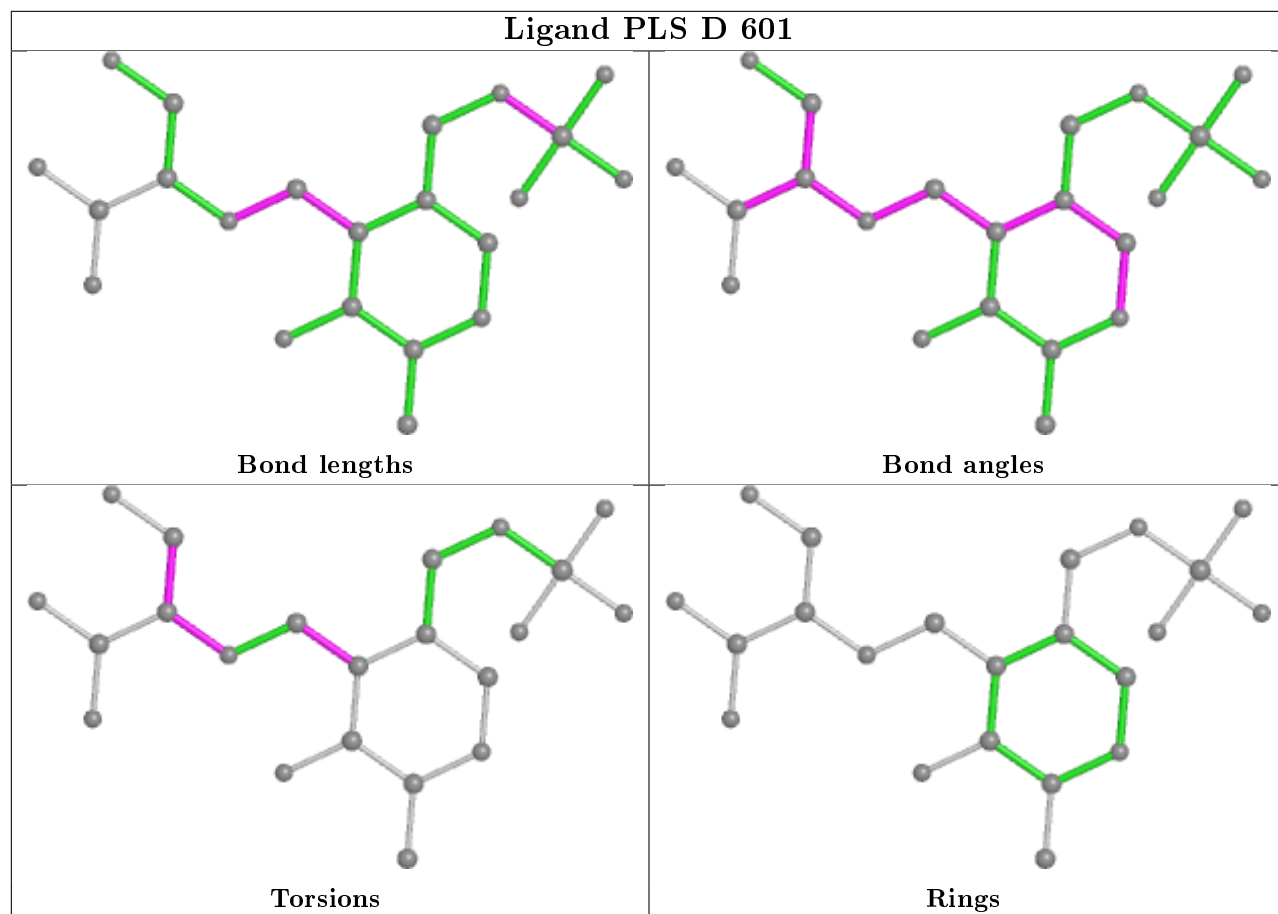
There are no ring outliers.

7 monomers are involved in 21 short contacts:

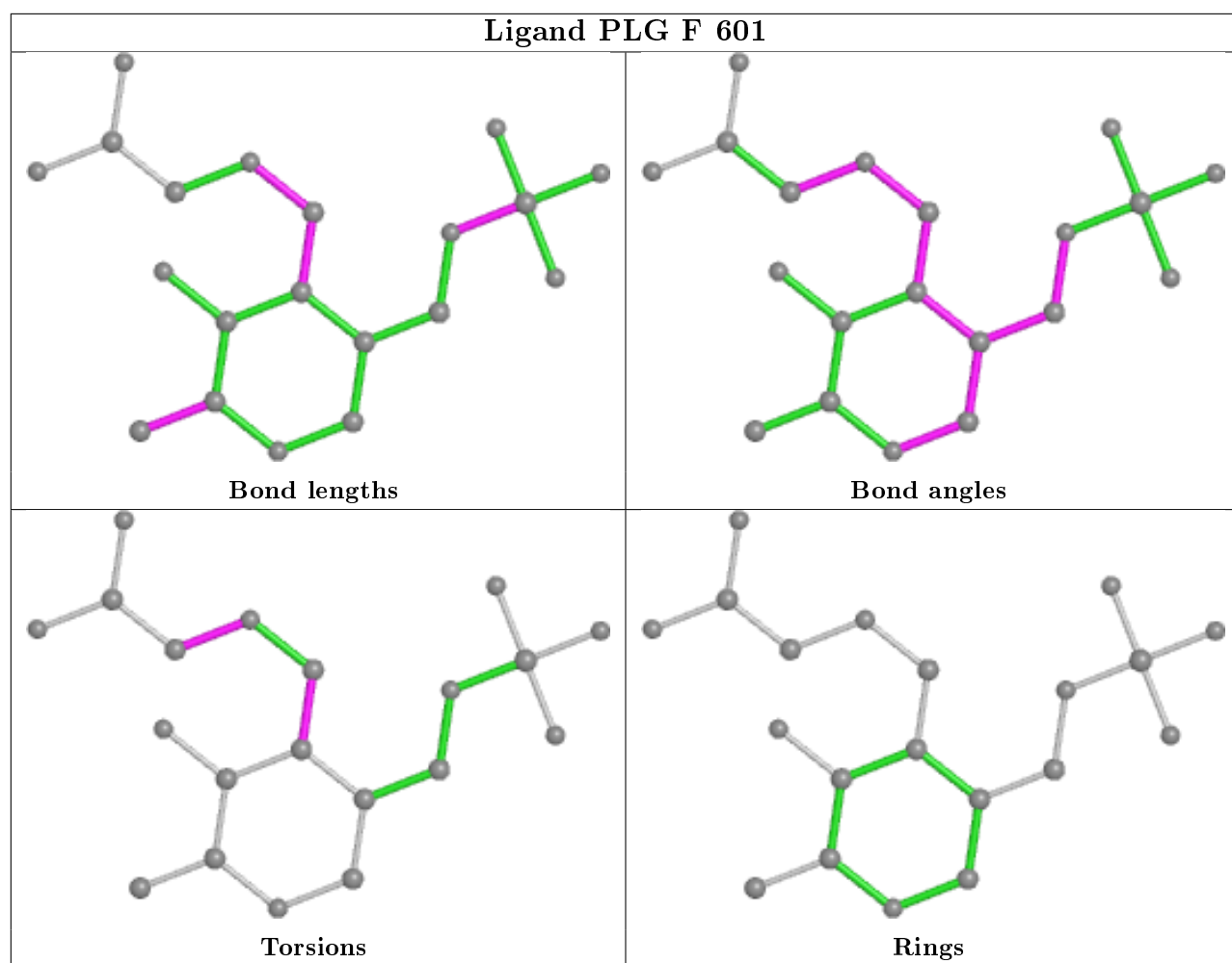
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	601	PLS	6	0
4	C	603	EDO	1	0
3	D	601	PLS	4	0
6	C	601	ACT	2	0
7	H	602	GLY	1	0
5	F	601	PLG	2	0
5	B	601	PLG	5	0

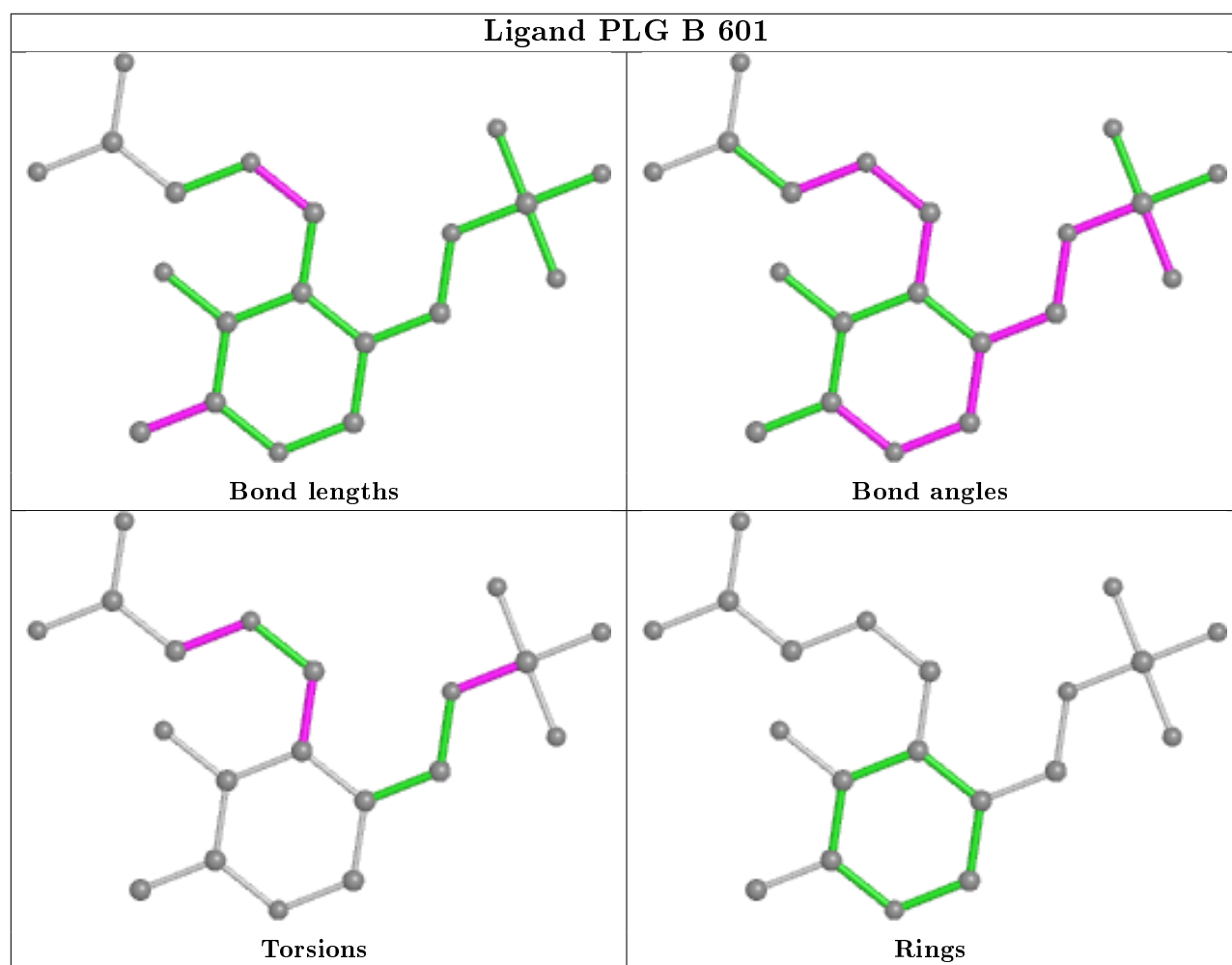
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

### 6.3 Carbohydrates ⓘ

EDS failed to run properly - this section is therefore empty.

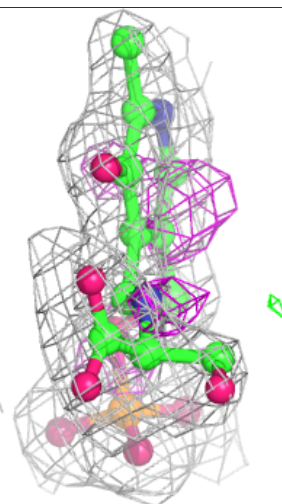
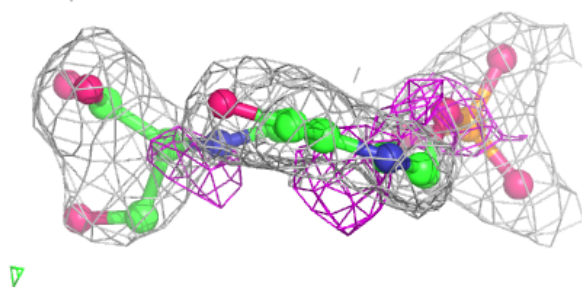
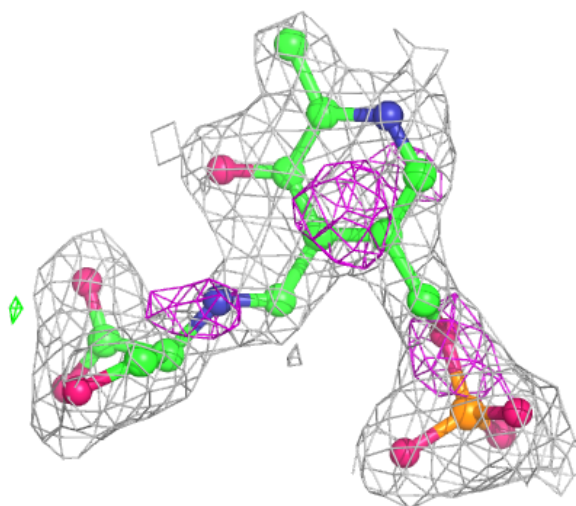
### 6.4 Ligands ⓘ

EDS failed to run properly - this section is therefore empty.

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.

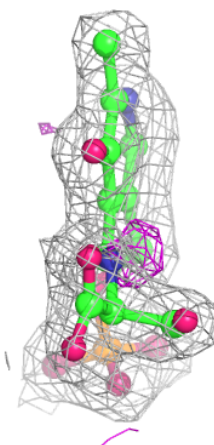
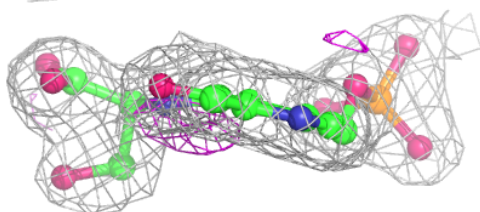
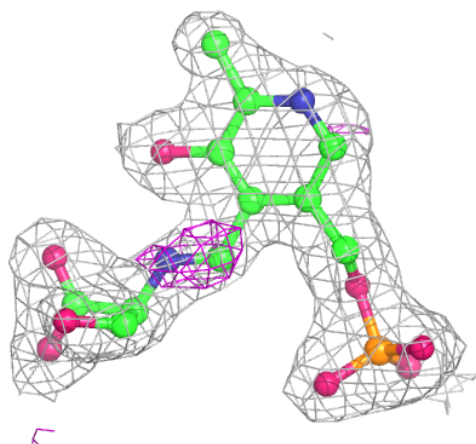
**Electron density around PLS D 601:**

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



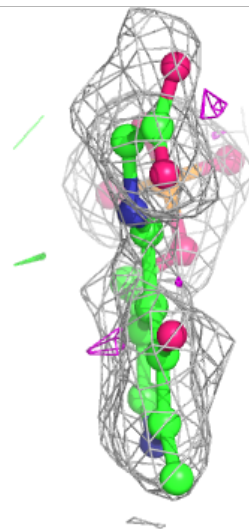
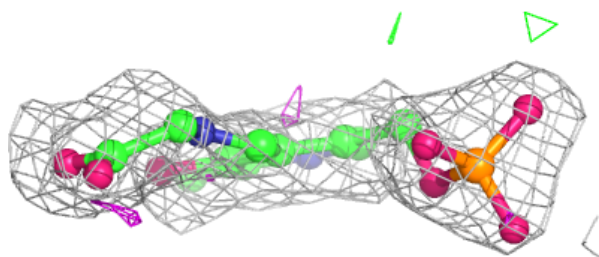
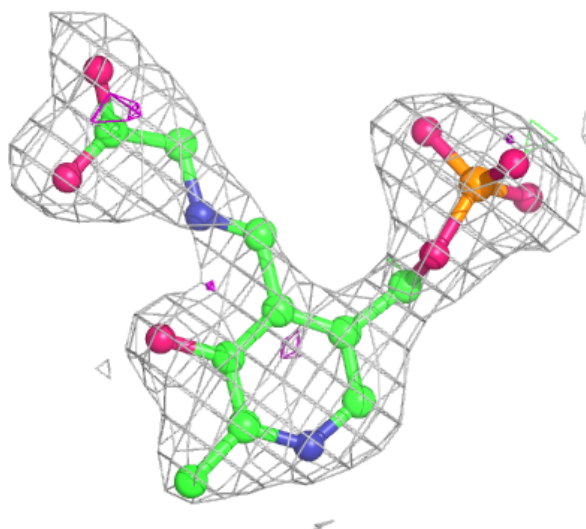
**Electron density around PLS A 601:**

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



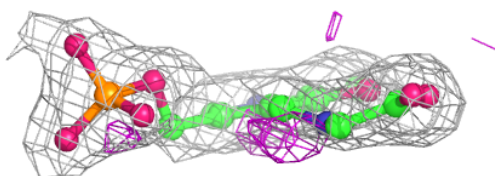
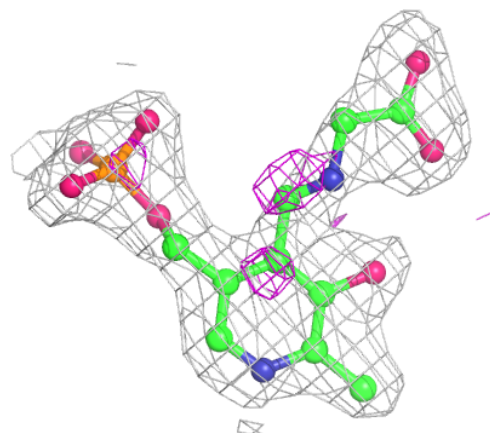
**Electron density around PLG F 601:**

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



**Electron density around PLG B 601:**

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



## 6.5 Other polymers ⓘ

EDS failed to run properly - this section is therefore empty.