



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 01:25 PM UTC

PDB ID : 7CNY / pdb_00007cny
Title : Crystal structure of 8PE bound PSD from E. coli (2.12 Å)
Authors : Kim, J.; Cho, G.
Deposited on : 2020-08-03
Resolution : 2.12 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

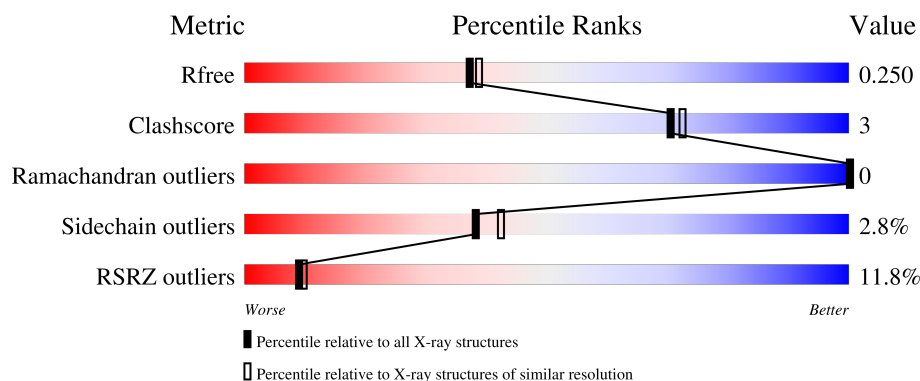
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.12 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	8290 (2.14-2.10)
Clashscore	190562	8817 (2.14-2.10)
Ramachandran outliers	187476	8738 (2.14-2.10)
Sidechain outliers	187428	8739 (2.14-2.10)
RSRZ outliers	180081	8294 (2.14-2.10)

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	253	2% 90% 9%
1	C	253	21% 87% 11%
2	B	42	79% 19%
2	D	42	24% 74% 7% 19%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4584 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 Phosphatidylserine decarboxylase beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	253	Total	C	N	O	S	0	1	0
			2004	1296	343	355	10			
1	C	247	Total	C	N	O	S	0	0	0
			1907	1231	323	344	9			

- Molecule 2 is a protein called Phosphatidylserine decarboxylase alpha chain.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	34	Total	C	N	O	0	0	0
			243	158	39	46			
2	D	34	Total	C	N	O	0	0	0
			232	152	37	43			

There are 18 discrepancies between the modelled and reference sequences:

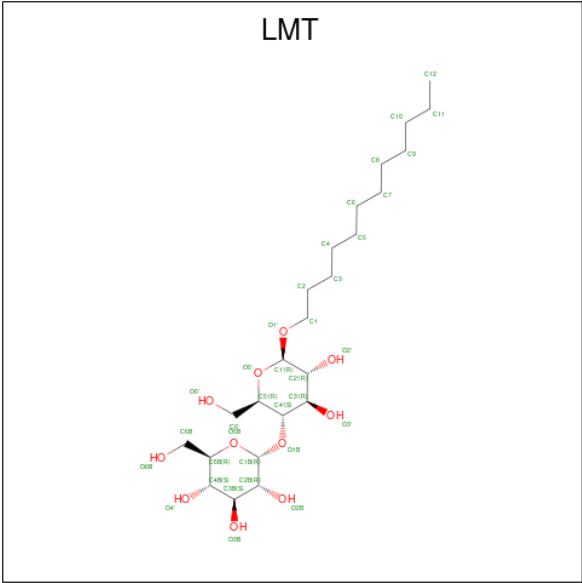
Chain	Residue	Modelled	Actual	Comment	Reference
B	254	PYR	SER	modified residue	UNP A0A6D2XQZ0
B	288	GLY	-	expression tag	UNP A0A6D2XQZ0
B	289	HIS	-	expression tag	UNP A0A6D2XQZ0
B	290	HIS	-	expression tag	UNP A0A6D2XQZ0
B	291	HIS	-	expression tag	UNP A0A6D2XQZ0
B	292	HIS	-	expression tag	UNP A0A6D2XQZ0
B	293	HIS	-	expression tag	UNP A0A6D2XQZ0
B	294	HIS	-	expression tag	UNP A0A6D2XQZ0
B	295	GLY	-	expression tag	UNP A0A6D2XQZ0
D	254	PYR	SER	modified residue	UNP A0A6D2XQZ0
D	288	GLY	-	expression tag	UNP A0A6D2XQZ0
D	289	HIS	-	expression tag	UNP A0A6D2XQZ0
D	290	HIS	-	expression tag	UNP A0A6D2XQZ0
D	291	HIS	-	expression tag	UNP A0A6D2XQZ0
D	292	HIS	-	expression tag	UNP A0A6D2XQZ0
D	293	HIS	-	expression tag	UNP A0A6D2XQZ0

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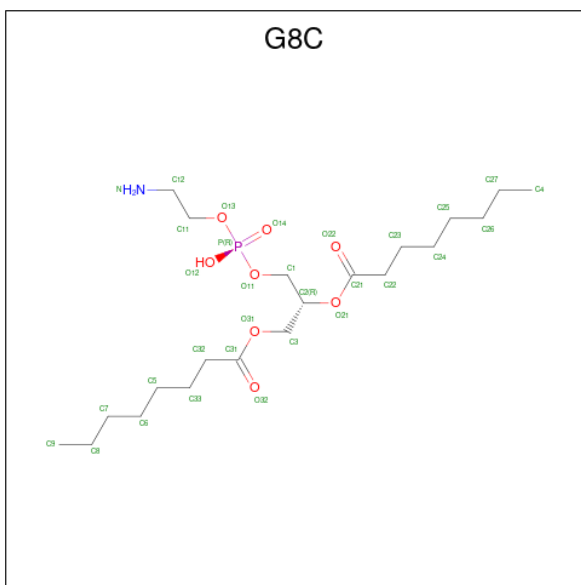
Chain	Residue	Modelled	Actual	Comment	Reference
D	294	HIS	-	expression tag	UNP A0A6D2XQZ0
D	295	GLY	-	expression tag	UNP A0A6D2XQZ0

- Molecule 3 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			25	14	11		
3	A	1	Total	C	O	0	0
			35	24	11		

- Molecule 4 is 1,2-Dioctanoyl-SN-Glycero-3-Phosphoethanolamine (CCD ID: G8C) (formula: C₂₁H₄₂NO₈P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total 25	C 15	N 1	O 8	P 1	0	0
4	D	1	Total 23	C 13	N 1	O 8	P 1	0	0

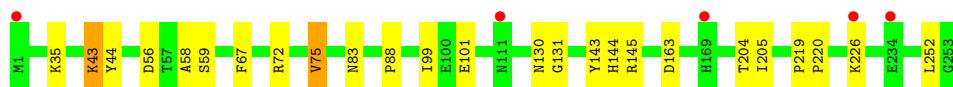
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	69	Total O 69 69	0	0
5	B	4	Total O 4 4	0	0
5	C	16	Total O 16 16	0	0
5	D	1	Total O 1 1	0	0

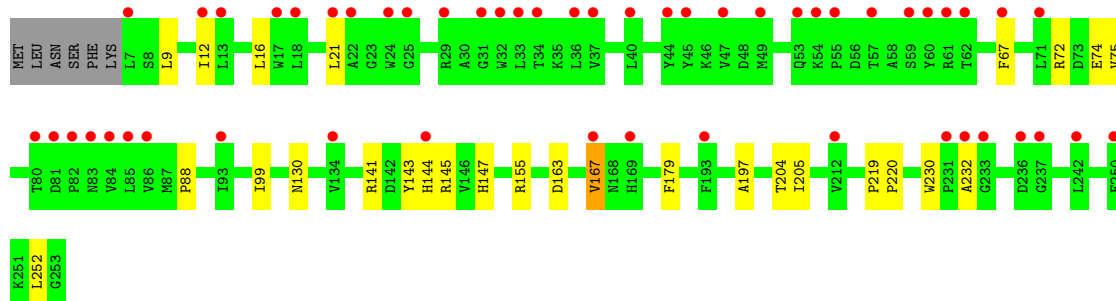
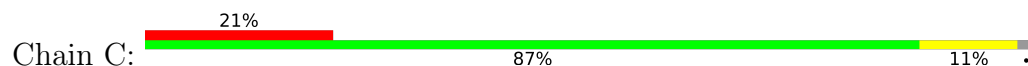
3 Residue-property plots [i](#)

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 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.

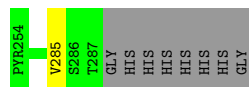
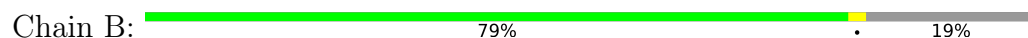
- Molecule 1: Phosphatidylserine decarboxylase beta chain



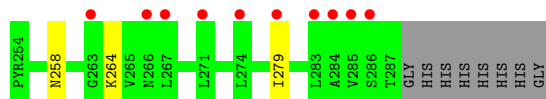
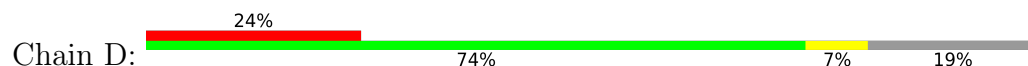
- Molecule 1: Phosphatidylserine decarboxylase beta chain



- Molecule 2: Phosphatidylserine decarboxylase alpha chain



- Molecule 2: Phosphatidylserine decarboxylase alpha chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	77.15Å 79.46Å 146.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.65 – 2.12 28.65 – 2.12	Depositor EDS
% Data completeness (in resolution range)	99.9 (28.65-2.12) 99.9 (28.65-2.12)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.65 (at 2.12Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.238 , 0.274 (Not available) , 0.250	Depositor DCC
R_{free} test set	2577 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	38.3	Xtriage
Anisotropy	0.474	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 34.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.005 for k,h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4584	wwPDB-VP
Average B, all atoms (Å ²)	51.0	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 23.58 % 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 4.5356e-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: PYR, G8C, LMT

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	1.02	1/2057 (0.0%)	1.35	0/2794
1	C	1.01	0/1955	1.34	2/2665 (0.1%)
2	B	1.00	0/241	1.27	0/329
2	D	1.07	0/230	1.27	0/316
All	All	1.02	1/4483 (0.0%)	1.34	2/6104 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	131	GLY	C-O	5.16	1.29	1.24

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	232	ALA	CA-C-N	5.52	125.22	119.92
1	C	232	ALA	C-N-CA	5.52	125.22	119.92

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	2004	0	2012	14	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1907	0	1857	16	0
2	B	243	0	259	1	0
2	D	232	0	240	2	0
3	A	60	0	69	0	1
4	B	25	0	0	0	0
4	D	23	0	0	0	0
5	A	69	0	0	2	0
5	B	4	0	0	0	0
5	C	16	0	0	1	0
5	D	1	0	0	0	0
All	All	4584	0	4437	30	1

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 3.

All (30) 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:C:155:ARG:NH1	1:C:230:TRP:O	2.31	0.64
1:A:226:LYS:HE3	5:A:404:HOH:O	2.03	0.59
1:C:167:VAL:HG22	1:C:179:PHE:HE1	1.73	0.54
1:C:143:TYR:CZ	1:C:145:ARG:HB2	2.43	0.53
1:C:88:PRO:HD2	5:C:311:HOH:O	2.08	0.53
1:A:143:TYR:CZ	1:A:145:ARG:HB2	2.44	0.53
1:C:9:LEU:HA	1:C:12:ILE:HG13	1.92	0.52
1:C:147:HIS:CD2	2:D:279:ILE:HD13	2.45	0.52
1:C:99:ILE:O	1:C:130:ASN:HA	2.09	0.51
1:A:56[B]:ASP:OD2	1:A:58:ALA:HB3	2.10	0.51
1:C:167:VAL:O	1:C:167:VAL:HG13	2.12	0.50
1:A:99:ILE:O	1:A:130:ASN:HA	2.13	0.49
1:C:197:ALA:O	2:D:258:ASN:HA	2.13	0.48
1:A:219:PRO:HB2	1:A:220:PRO:HA	1.96	0.47
1:A:35:LYS:HE3	1:A:58:ALA:HB2	1.97	0.46
1:C:219:PRO:HB2	1:C:220:PRO:HA	1.98	0.46
1:C:67:PHE:CZ	1:C:144:HIS:CE1	3.04	0.46
1:C:9:LEU:HA	1:C:12:ILE:CG1	2.46	0.45
1:A:43:LYS:HE3	1:A:44:TYR:N	2.32	0.45
1:A:205:ILE:HG22	1:A:252:LEU:HG	1.99	0.44
1:C:205:ILE:HG22	1:C:252:LEU:HG	1.99	0.44
1:A:35:LYS:CE	1:A:58:ALA:HB2	2.48	0.43
1:C:167:VAL:HG22	1:C:179:PHE:CE1	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:PHE:CZ	1:A:144:HIS:CE1	3.07	0.43
1:A:72:ARG:O	1:A:75:VAL:HG12	2.21	0.41
1:A:88:PRO:HD2	5:A:435:HOH:O	2.20	0.41
1:C:67:PHE:CE1	1:C:144:HIS:CE1	3.09	0.41
1:A:67:PHE:CE1	1:A:144:HIS:CE1	3.09	0.40
1:C:72:ARG:HB2	1:C:75:VAL:HG23	2.04	0.40
1:A:83:ASN:O	2:B:285:VAL:HA	2.20	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:GLU:OE1	3:A:302:LMT:O2'[4_455]	2.17	0.03

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	252/253 (100%)	245 (97%)	7 (3%)	0	100	100
1	C	245/253 (97%)	235 (96%)	10 (4%)	0	100	100
2	B	32/42 (76%)	31 (97%)	1 (3%)	0	100	100
2	D	32/42 (76%)	30 (94%)	2 (6%)	0	100	100
All	All	561/590 (95%)	541 (96%)	20 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	212/216 (98%)	207 (98%)	5 (2%)	43	48
1	C	195/216 (90%)	188 (96%)	7 (4%)	31	33
2	B	28/35 (80%)	28 (100%)	0	100	100
2	D	25/35 (71%)	24 (96%)	1 (4%)	28	28
All	All	460/502 (92%)	447 (97%)	13 (3%)	38	42

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	LYS
1	A	59	SER
1	A	75	VAL
1	A	163	ASP
1	A	204	THR
1	C	16	LEU
1	C	21	LEU
1	C	74	GLU
1	C	141	ARG
1	C	163	ASP
1	C	167	VAL
1	C	204	THR
2	D	264	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	174	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	LMT	A	302	-	36,36,36	0.68	1 (2%)	47,47,47	1.21	5 (10%)
3	LMT	A	301	-	26,26,36	0.76	1 (3%)	37,37,47	1.69	9 (24%)
4	G8C	D	301	2	22,22,30	1.47	2 (9%)	25,27,35	1.68	5 (20%)
4	G8C	B	301	2	24,24,30	1.27	3 (12%)	27,29,35	1.86	6 (22%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	LMT	A	302	-	-	7/21/61/61	0/2/2/2
3	LMT	A	301	-	-	8/11/51/61	0/2/2/2
4	G8C	D	301	2	-	9/26/26/34	-
4	G8C	B	301	2	-	8/28/28/34	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	301	G8C	O31-C31	4.61	1.46	1.33
4	B	301	G8C	O31-C31	4.48	1.46	1.33
4	D	301	G8C	O21-C21	4.22	1.46	1.34
4	B	301	G8C	O21-C21	2.96	1.42	1.34
3	A	301	LMT	O1'-C1'	2.46	1.44	1.40
4	B	301	G8C	O21-C2	-2.29	1.41	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	302	LMT	O1'-C1'	2.00	1.43	1.40

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	301	G8C	O21-C21-C22	5.07	122.44	111.48
3	A	301	LMT	C1'-O5'-C5'	4.69	122.88	113.72
4	B	301	G8C	O21-C21-C22	4.47	121.15	111.48
4	B	301	G8C	O21-C21-O22	-3.92	114.55	123.70
4	B	301	G8C	O31-C31-C32	3.85	122.83	111.15
3	A	301	LMT	O1B-C4'-C5'	3.45	118.53	109.48
4	D	301	G8C	O31-C31-C32	3.39	121.43	111.15
4	D	301	G8C	O21-C21-O22	-3.16	116.31	123.70
4	B	301	G8C	O31-C31-O32	-3.13	115.81	123.63
4	B	301	G8C	C2-O21-C21	-3.11	110.36	117.80
3	A	301	LMT	O1B-C1B-C2B	2.77	114.90	108.09
4	D	301	G8C	C2-O21-C21	-2.72	111.28	117.80
3	A	301	LMT	C3B-C4B-C5B	2.69	115.12	110.23
3	A	302	LMT	O5B-C5B-C6B	2.66	113.03	106.44
3	A	302	LMT	O1'-C1'-C2'	2.48	112.03	108.27
3	A	301	LMT	O4'-C4B-C3B	-2.45	104.61	110.38
3	A	301	LMT	O5B-C1B-C2B	-2.37	105.51	110.37
3	A	302	LMT	O3B-C3B-C4B	-2.33	104.89	110.38
4	D	301	G8C	O31-C31-O32	-2.31	117.84	123.63
3	A	302	LMT	O5'-C5'-C4'	2.29	114.45	109.72
3	A	301	LMT	C1B-O1B-C4'	2.29	123.40	117.98
3	A	301	LMT	O5'-C5'-C4'	2.22	114.32	109.72
3	A	302	LMT	C6B-C5B-C4B	-2.22	107.57	113.02
4	B	301	G8C	O13-P-O14	-2.11	100.58	108.94
3	A	301	LMT	O2B-C2B-C3B	-2.11	105.41	110.38

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	301	LMT	O5'-C1'-O1'-C1
4	B	301	G8C	C1-O11-P-O14
4	D	301	G8C	C1-O11-P-O14
4	D	301	G8C	O13-C11-C12-N
3	A	301	LMT	C5'-C4'-O1B-C1B
3	A	302	LMT	O5'-C5'-C6'-O6'
3	A	301	LMT	C4B-C5B-C6B-O6B

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Mol	Chain	Res	Type	Atoms
3	A	301	LMT	O5B-C5B-C6B-O6B
3	A	301	LMT	C4'-C5'-C6'-O6'
3	A	302	LMT	C4'-C5'-C6'-O6'
3	A	301	LMT	O5'-C5'-C6'-O6'
3	A	302	LMT	O1'-C1-C2-C3
4	B	301	G8C	C22-C21-O21-C2
4	B	301	G8C	O22-C21-O21-C2
4	B	301	G8C	C21-C22-C23-C24
3	A	302	LMT	C3'-C4'-O1B-C1B
4	D	301	G8C	C1-C2-C3-O31
3	A	302	LMT	C5'-C4'-O1B-C1B
4	B	301	G8C	C22-C23-C24-C25
3	A	302	LMT	C2-C3-C4-C5
3	A	301	LMT	C2'-C1'-O1'-C1
4	B	301	G8C	C23-C24-C25-C26
4	D	301	G8C	O21-C2-C3-O31
4	D	301	G8C	C22-C21-O21-C2
4	D	301	G8C	O22-C21-O21-C2
4	D	301	G8C	C21-C22-C23-C24
4	B	301	G8C	C11-O13-P-O11
4	D	301	G8C	C1-O11-P-O12
3	A	301	LMT	C2-C1-O1'-C1'
4	B	301	G8C	C2-C1-O11-P
3	A	302	LMT	O5B-C5B-C6B-O6B
4	D	301	G8C	O11-C1-C2-C3

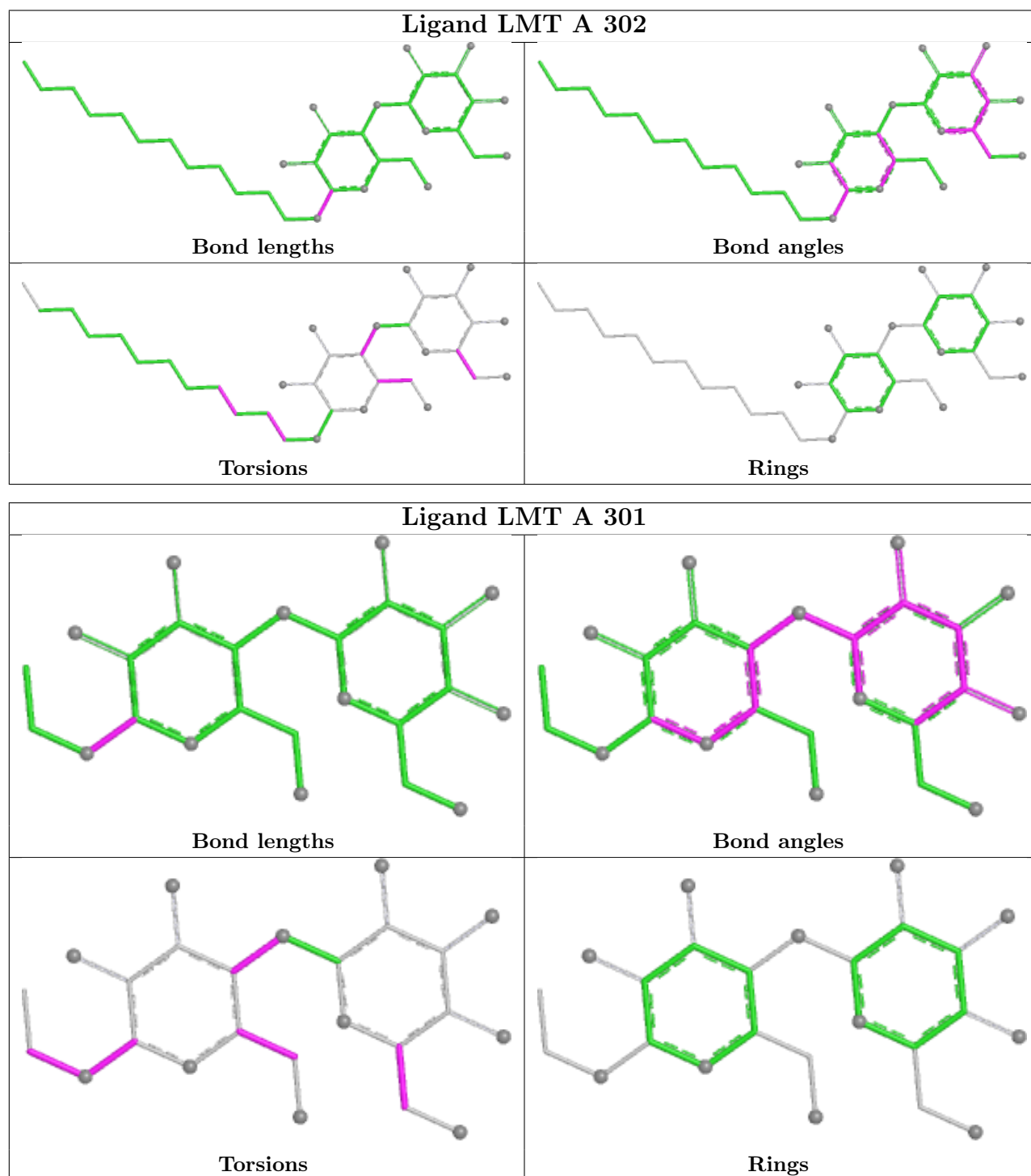
There are no ring outliers.

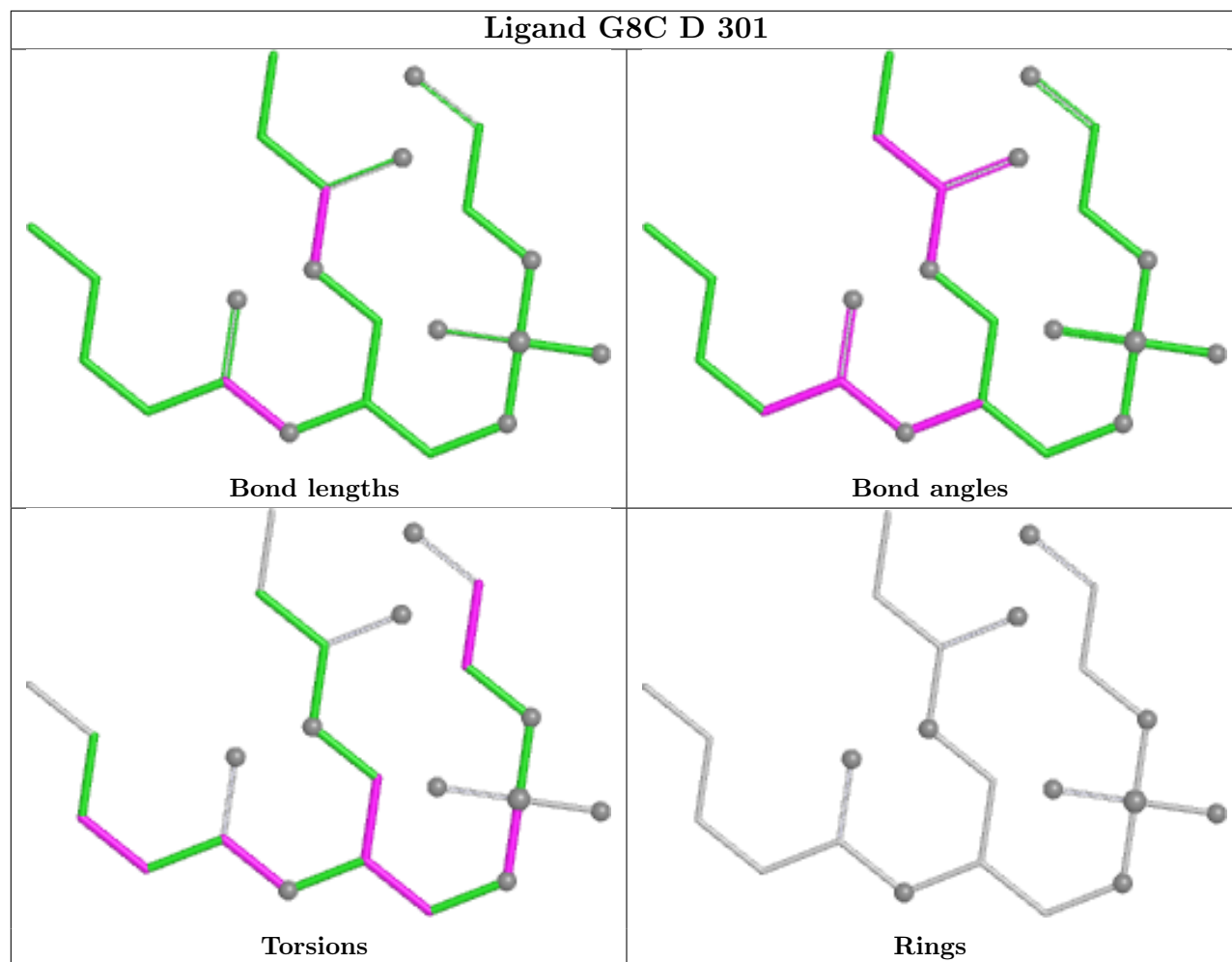
1 monomer is involved in 1 short contact:

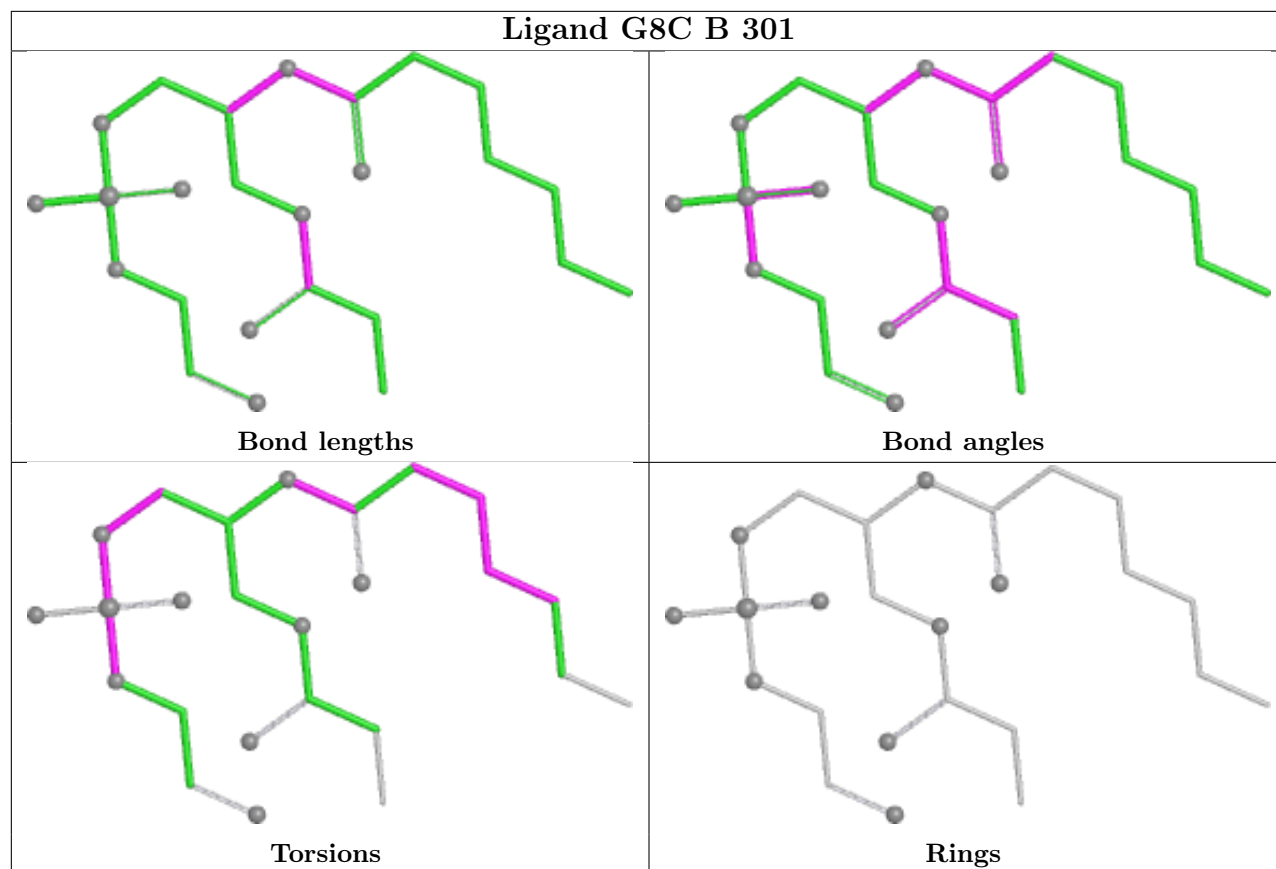
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	302	LMT	0	1

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	253/253 (100%)	0.31	5 (1%) 65 68	28, 40, 58, 74	1 (0%)
1	C	247/253 (97%)	1.23	52 (21%) 2 2	33, 59, 80, 97	0
2	B	33/42 (78%)	0.52	0 100 100	30, 42, 56, 61	0
2	D	33/42 (78%)	1.32	10 (30%) 1 1	42, 62, 76, 80	0
All	All	566/590 (95%)	0.78	67 (11%) 9 10	28, 49, 76, 97	1 (0%)

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	17	TRP	4.4
1	C	33	LEU	3.7
1	C	29	ARG	3.7
1	C	7	LEU	3.6
1	C	47	VAL	3.5
1	A	111	ASN	3.5
1	C	233	GLY	3.4
1	C	21	LEU	3.4
1	C	24	TRP	3.3
1	C	232	ALA	3.3
1	C	55	PRO	3.2
2	D	267	LEU	3.2
1	C	32	TRP	3.1
1	C	45	TYR	3.1
1	A	1	MET	3.1
1	C	80	THR	3.0
1	A	234	GLU	3.0
1	C	85	LEU	3.0
1	C	237	GLY	2.9
1	C	236	ASP	2.9
1	C	61	ARG	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	57	THR	2.8
1	C	81	ASP	2.8
1	C	59	SER	2.7
2	D	286	SER	2.7
1	C	18	LEU	2.6
2	D	285	VAL	2.6
1	C	31	GLY	2.6
1	C	167	VAL	2.5
2	D	266	ASN	2.5
2	D	274	LEU	2.5
1	C	144	HIS	2.4
1	C	71	LEU	2.4
1	C	12	ILE	2.4
1	C	82	PRO	2.4
1	C	37	VAL	2.4
2	D	279	ILE	2.4
2	D	271	LEU	2.3
1	C	25	GLY	2.3
1	C	193	PHE	2.3
1	C	36	LEU	2.3
1	C	54	LYS	2.3
1	C	67	PHE	2.3
1	C	62	THR	2.3
1	C	40	LEU	2.3
1	C	86	VAL	2.3
1	C	250	PHE	2.2
1	C	169	HIS	2.2
1	C	34	THR	2.2
1	C	93	ILE	2.2
1	C	22	ALA	2.2
1	C	242	LEU	2.2
1	A	226	LYS	2.2
1	C	212	VAL	2.2
2	D	283	LEU	2.2
1	C	231	PRO	2.1
1	C	53	GLN	2.1
1	C	84	VAL	2.1
1	C	13	LEU	2.1
1	C	134	VAL	2.1
1	C	83	ASN	2.0
1	C	44	TYR	2.0
1	C	49	MET	2.0

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Mol	Chain	Res	Type	RSRZ
2	D	284	ALA	2.0
1	A	169	HIS	2.0
2	D	263	GLY	2.0
1	C	60	TYR	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](#)

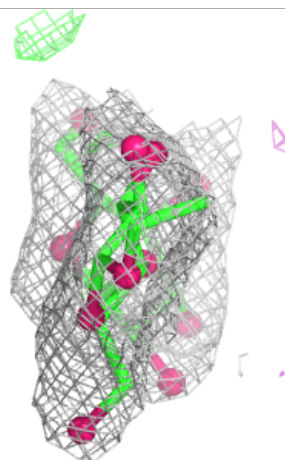
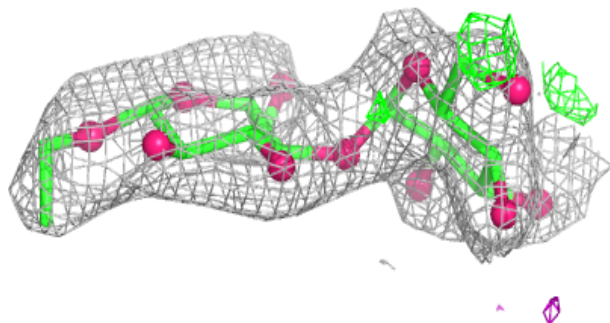
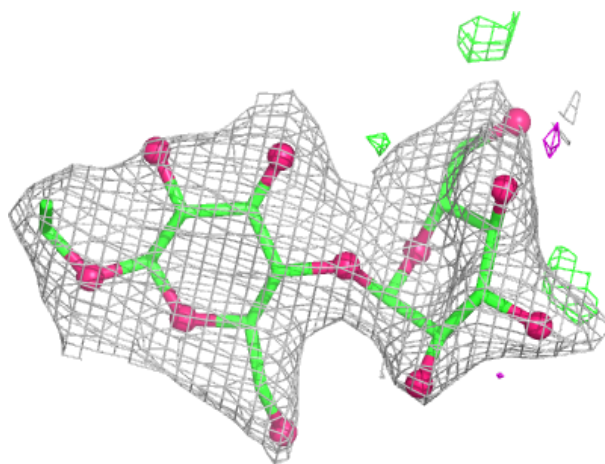
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	LMT	A	301	25/35	0.82	0.15	52,64,70,75	25
3	LMT	A	302	35/35	0.85	0.14	47,68,84,88	0
4	G8C	D	301	23/31	0.93	0.13	54,74,83,84	0
4	G8C	B	301	25/31	0.96	0.10	28,53,64,68	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.

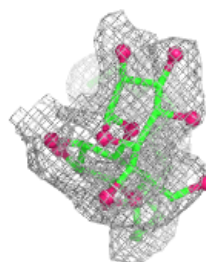
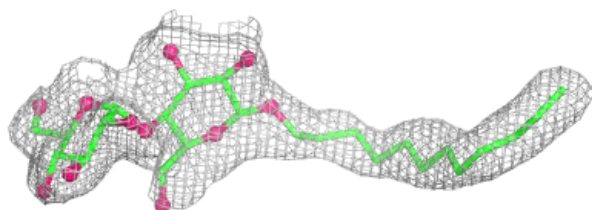
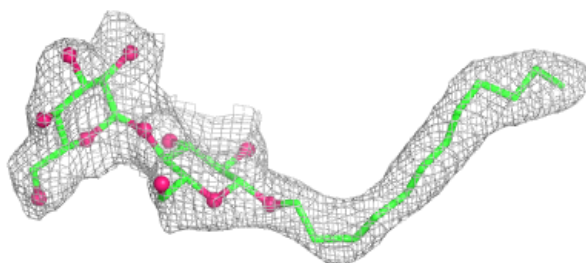
Electron density around LMT A 301:

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



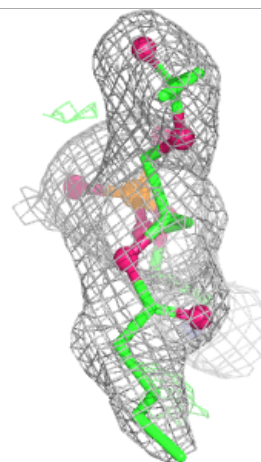
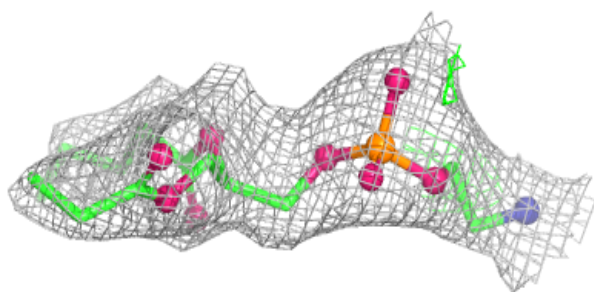
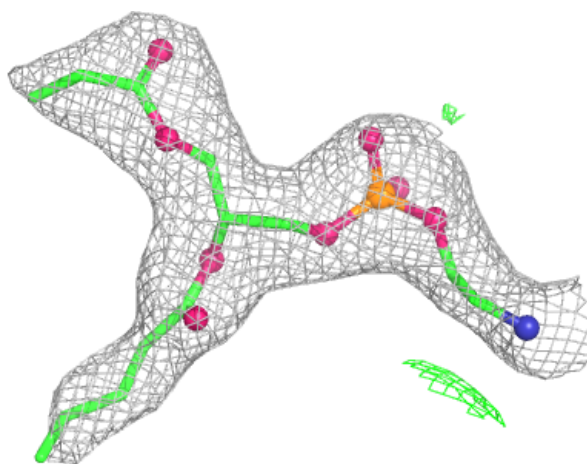
Electron density around LMT A 302:

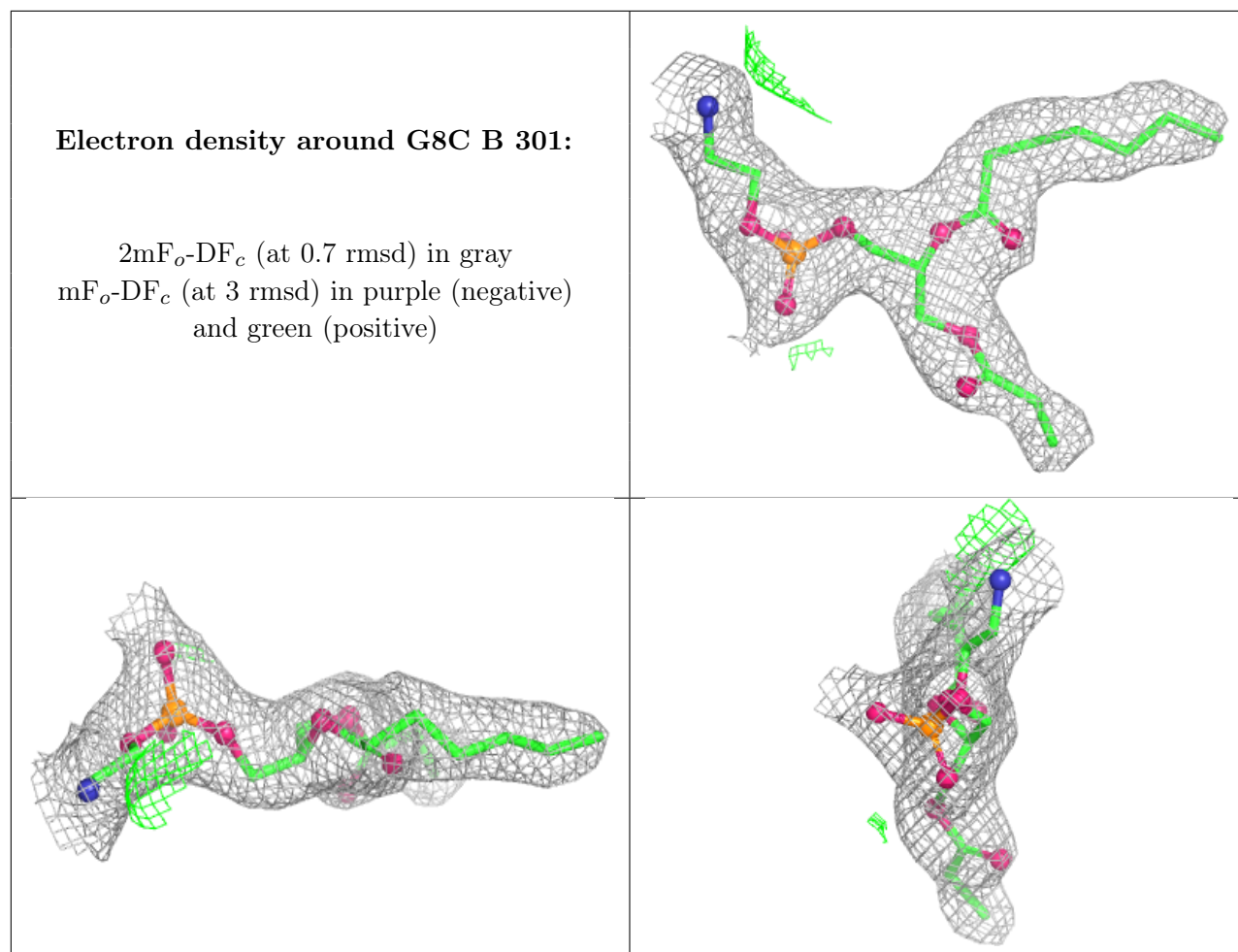
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around G8C D 301:

$2mF_o-DF_c$ (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.