



# Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 12:55 am BST

PDB ID : 2IUA  
Title : C. trachomatis LpxD  
Authors : Buetow, L.; Smith, T.K.; Dawson, A.; Fyffe, S.; Hunter, W.N.  
Deposited on : 2006-05-30  
Resolution : 2.70 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 : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

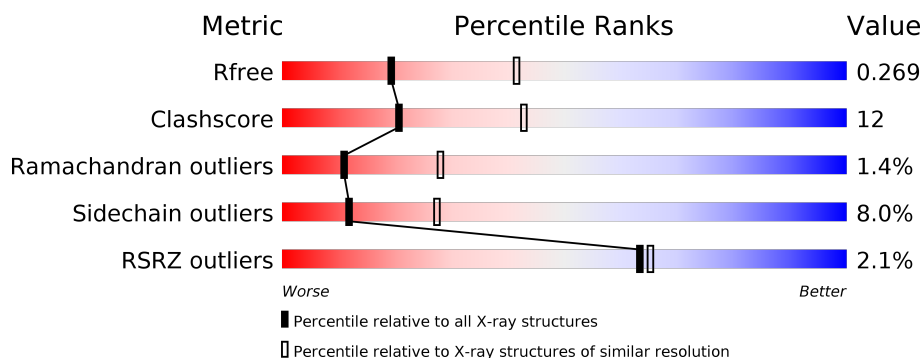
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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))
$R_{free}$	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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  $\leq 5\%$ . 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	374	<div> <div>2%</div> <div> <div></div> <div>72%</div> <div>18%</div> <div>• 7%</div> </div> </div>
1	B	374	<div> <div>2%</div> <div> <div></div> <div>72%</div> <div>18%</div> <div>• 8%</div> </div> </div>
1	C	374	<div> <div>2%</div> <div> <div></div> <div>71%</div> <div>19%</div> <div>• • 7%</div> </div> </div>

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
3	SO4	B	1346	-	-	X	-

## 2 Entry composition [i](#)

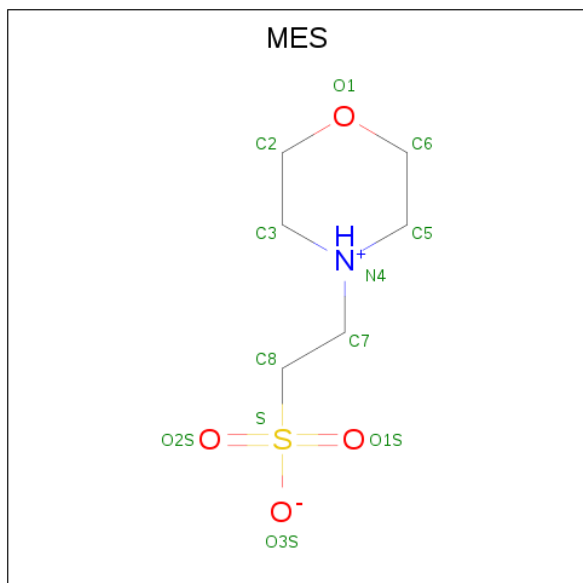
There are 5 unique types of molecules in this entry. The entry contains 8272 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 UDP-3-O-[3-HYDROXYMYRISTOYL] GLUCOSAMINE N-ACYLTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	346	Total	C	N	O	S	0	8	0
			2682	1693	484	495	10			
1	B	345	Total	C	N	O	S	0	5	0
			2658	1679	479	490	10			
1	C	346	Total	C	N	O	S	0	6	0
			2672	1689	481	492	10			

- Molecule 2 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C<sub>6</sub>H<sub>13</sub>NO<sub>4</sub>S).



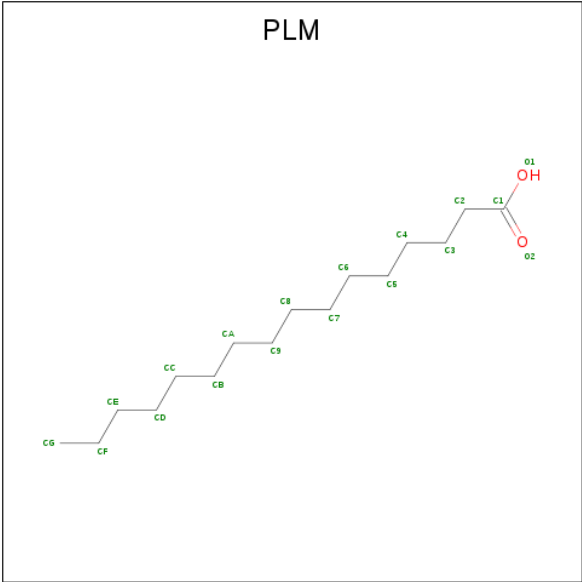
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is PALMITIC ACID (three-letter code: PLM) (formula: C<sub>16</sub>H<sub>32</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			18	16	2		
4	A	1	Total	C	O	0	0
			18	16	2		
4	B	1	Total	C	O	0	0
			18	16	2		

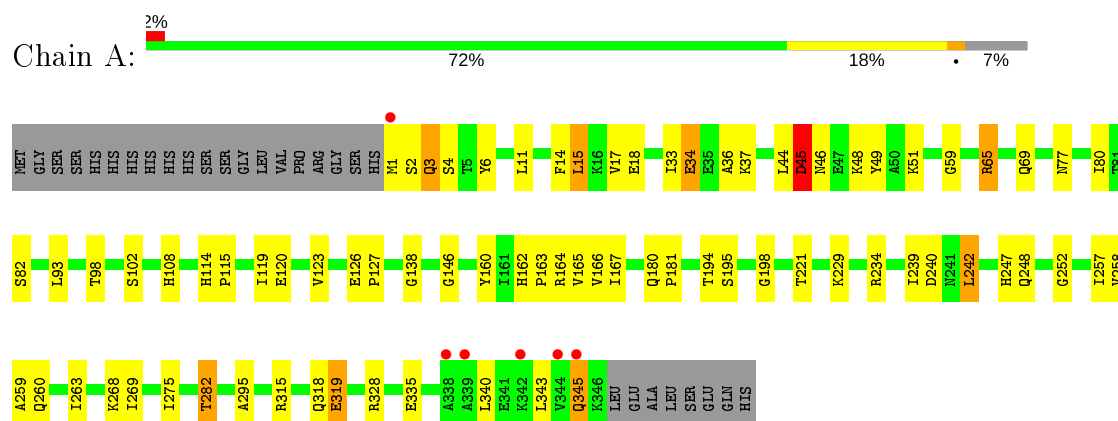
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	74	Total	O	0	0
			74	74		
5	B	46	Total	O	0	0
			46	46		
5	C	34	Total	O	0	0
			34	34		

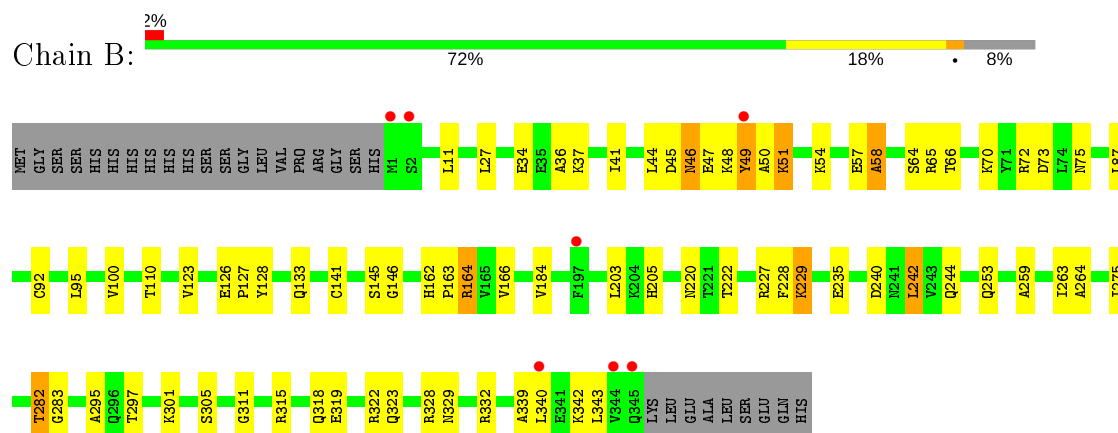
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

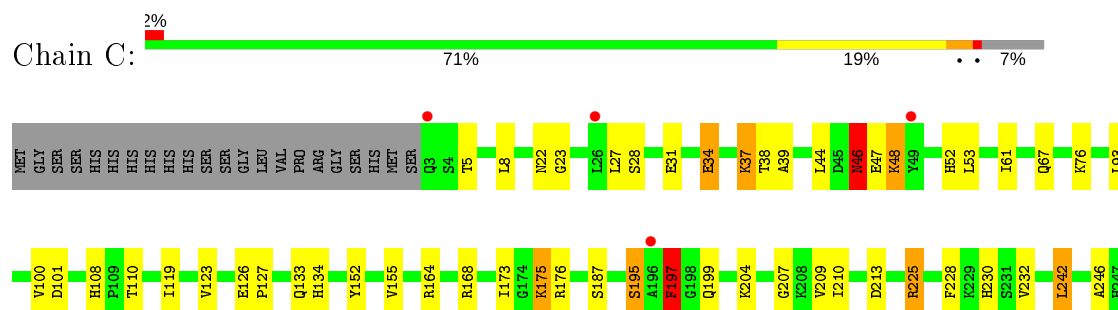
#### • Molecule 1: UDP-3-O-[3-HYDROXYMYRISTOYL] GLUCOSAMINE N-ACYLTRANSFERASE



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## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	98.68 Å 98.68 Å 284.50 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	93.25 – 2.70 39.22 – 2.70	Depositor EDS
% Data completeness (in resolution range)	96.3 (93.25-2.70) 96.4 (39.22-2.70)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.19 (at 2.69 Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.209 , 0.273 0.207 , 0.269	Depositor DCC
$R_{free}$ test set	1910 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	43.2	Xtriage
Anisotropy	0.121	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 32.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	8272	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.77% of the height of the origin peak. No significant pseudotranslation is detected.*

<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: PLM, SO4, MES

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	0.54	0/2766	0.66	0/3738
1	B	0.55	0/2729	0.69	0/3691
1	C	0.54	0/2747	0.68	0/3714
All	All	0.54	0/8242	0.68	0/11143

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	2682	0	2712	87	0
1	B	2658	0	2690	82	0
1	C	2672	0	2704	80	0
2	A	12	0	12	0	0
3	A	15	0	0	1	0
3	B	15	0	0	2	0
3	C	10	0	0	0	0
4	A	36	0	62	9	0
4	B	18	0	31	4	0
5	A	74	0	0	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	46	0	0	4	0
5	C	34	0	0	5	0
All	All	8272	0	8211	201	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 12.

All (201) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:164[B]:ARG:HE	1:C:164[B]:ARG:NH2	1.14	1.44
1:B:164[B]:ARG:NE	1:C:164[B]:ARG:NH2	1.76	1.32
1:A:164[B]:ARG:HH12	1:B:164[B]:ARG:CZ	1.43	1.31
1:A:164[B]:ARG:NH2	1:B:164[B]:ARG:NE	1.86	1.23
1:A:164[B]:ARG:CZ	1:B:164[B]:ARG:CD	2.27	1.11
1:A:164[B]:ARG:NH2	1:B:164[B]:ARG:CD	2.18	1.06
1:A:164[B]:ARG:NE	1:C:164[B]:ARG:HH12	0.88	1.06
1:B:329:ASN:HD21	1:B:332:ARG:HD3	1.20	1.05
1:A:65[A]:ARG:HG3	1:A:65[A]:ARG:HH11	1.22	1.04
1:B:164[A]:ARG:HH21	1:C:164[A]:ARG:NH2	1.53	1.04
1:A:164[A]:ARG:HD2	1:C:164[A]:ARG:CG	1.86	1.03
1:A:164[B]:ARG:HE	1:C:164[B]:ARG:NH1	1.30	1.03
1:A:164[B]:ARG:CZ	1:B:164[B]:ARG:HD3	1.87	1.03
1:A:164[B]:ARG:NH2	1:B:164[B]:ARG:HD3	1.74	1.02
1:A:164[B]:ARG:CZ	1:B:164[B]:ARG:NE	2.23	1.02
1:A:164[B]:ARG:NH1	1:B:164[B]:ARG:NE	2.09	0.99
1:B:164[A]:ARG:HE	1:C:164[A]:ARG:NE	1.61	0.99
1:A:164[A]:ARG:CD	1:C:164[A]:ARG:HG2	1.93	0.99
1:A:164[B]:ARG:NH1	1:B:164[B]:ARG:CZ	2.26	0.98
1:A:164[B]:ARG:HH12	1:B:164[B]:ARG:NE	1.63	0.97
1:A:3:GLN:HB3	5:A:2019:HOH:O	1.65	0.96
1:B:164[B]:ARG:HE	1:C:164[B]:ARG:HH21	1.12	0.95
1:A:164[A]:ARG:HD2	1:C:164[A]:ARG:HG2	0.97	0.94
1:A:164[B]:ARG:NE	1:C:164[B]:ARG:NH1	1.68	0.94
1:B:164[B]:ARG:HD3	1:C:164[B]:ARG:NH1	1.85	0.92
1:A:164[B]:ARG:NH2	1:B:164[B]:ARG:HE	1.48	0.90
1:B:164[B]:ARG:HD3	1:C:164[B]:ARG:CZ	2.02	0.89
1:B:164[B]:ARG:NE	1:C:164[B]:ARG:HH22	1.65	0.88
1:B:164[A]:ARG:HB2	1:C:164[A]:ARG:HD2	1.57	0.85
1:B:164[A]:ARG:HH21	1:C:164[A]:ARG:HH21	1.21	0.84
1:A:164[B]:ARG:NH1	1:B:164[B]:ARG:CD	2.42	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65[A]:ARG:HH11	1:A:65[A]:ARG:CG	1.92	0.82
4:B:1349:PLM:HE1	1:C:311:GLY:HA2	1.63	0.81
4:B:1349:PLM:HB1	4:B:1349:PLM:HF1	1.63	0.80
1:A:164[A]:ARG:NE	1:C:164[A]:ARG:HE	1.82	0.77
1:C:207:GLY:O	1:C:225:ARG:NH1	2.17	0.77
1:C:281:ILE:HD11	1:C:293:MET:CE	2.15	0.77
1:A:319:GLU:HG2	5:A:2066:HOH:O	1.84	0.76
1:A:257:ILE:HG12	1:A:275:ILE:HD12	1.67	0.76
1:B:146:GLY:HA3	1:B:164[B]:ARG:HH21	1.51	0.74
1:B:343:LEU:HA	5:B:2044:HOH:O	1.88	0.73
1:C:5:THR:HG22	1:C:28:SER:HB3	1.69	0.72
1:C:37:LYS:HG3	1:C:39:ALA:H	1.54	0.72
1:C:281:ILE:HD11	1:C:293:MET:HE3	1.71	0.72
1:A:282:THR:HG23	4:A:1351:PLM:H62	1.71	0.71
1:C:53:LEU:HD11	1:C:61:ILE:HD13	1.72	0.71
1:C:225:ARG:HG3	1:C:225:ARG:HH11	1.54	0.70
1:B:329:ASN:ND2	1:B:332:ARG:HD3	2.02	0.70
1:B:44:LEU:HD12	1:B:49:TYR:HD1	1.57	0.70
1:A:162:HIS:HB3	1:A:163:PRO:CD	2.23	0.69
1:B:164[B]:ARG:CD	1:C:164[B]:ARG:CZ	2.66	0.68
1:A:164[A]:ARG:HG2	1:B:164[A]:ARG:HD2	1.78	0.66
1:A:263:ILE:HG12	1:A:269:ILE:HD11	1.77	0.66
1:C:204:LYS:HE3	5:C:2012:HOH:O	1.94	0.66
1:B:229[A]:LYS:HE2	1:C:31:GLU:OE2	1.97	0.64
1:B:87:LEU:HD23	5:B:2013:HOH:O	1.98	0.64
1:B:45:ASP:H	1:B:49:TYR:HE1	1.42	0.64
1:B:164[A]:ARG:NE	1:C:164[A]:ARG:NE	2.43	0.63
1:A:18[A]:GLU:HG3	1:A:65[A]:ARG:HH21	1.64	0.63
4:A:1351:PLM:H61	1:B:295:ALA:HB3	1.81	0.62
1:C:336:ARG:O	1:C:340:LEU:HB2	1.99	0.61
1:B:164[A]:ARG:NH2	1:C:164[A]:ARG:HH21	1.96	0.61
1:A:263:ILE:HG12	1:A:269:ILE:CD1	2.31	0.60
1:C:8:LEU:HB3	1:C:23:GLY:HA2	1.83	0.60
1:A:162:HIS:HB3	1:A:163:PRO:HD2	1.83	0.60
1:C:53:LEU:CD1	1:C:61:ILE:HD13	2.31	0.59
1:A:82:SER:HA	3:A:1348:SO4:O2	2.03	0.59
1:A:180:GLN:HB3	1:A:181:PRO:HD2	1.83	0.58
4:A:1351:PLM:H52	4:A:1351:PLM:HA1	1.87	0.57
1:A:164[B]:ARG:NH1	1:B:164[B]:ARG:HD2	2.20	0.57
1:A:33:ILE:HG21	5:A:2011:HOH:O	2.04	0.57
4:A:1351:PLM:H91	4:A:1351:PLM:HE2	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:LEU:HG	1:A:15:LEU:HD22	1.87	0.57
1:C:257:ILE:HG12	1:C:275:ILE:HD12	1.87	0.56
1:A:295:ALA:H	4:A:1352:PLM:HG1	1.69	0.56
1:A:2:SER:O	1:A:4:SER:N	2.38	0.56
1:A:65[A]:ARG:NH1	1:A:65[A]:ARG:CG	2.61	0.56
1:A:164[B]:ARG:HH12	1:B:164[B]:ARG:NH1	1.97	0.55
1:A:45:ASP:HB2	1:A:48:LYS:HG3	1.89	0.55
1:B:64:SER:HB2	3:B:1346:SO4:O1	2.06	0.55
1:C:119:ILE:HG22	1:C:123:VAL:HG11	1.87	0.55
1:C:315:ARG:HB2	1:C:320:ILE:HG23	1.86	0.55
1:C:230:HIS:HB2	5:C:2018:HOH:O	2.06	0.55
1:A:126:GLU:HB3	1:A:127:PRO:HD2	1.88	0.55
1:A:65[A]:ARG:HD2	1:A:80:ILE:HG22	1.89	0.55
1:A:166:VAL:CG2	1:B:164[A]:ARG:HG2	2.36	0.54
1:C:134:HIS:O	1:C:152:TYR:HA	2.08	0.54
1:B:46:ASN:ND2	1:B:48:LYS:HG2	2.23	0.54
1:A:165:VAL:HG12	1:A:167:ILE:HD12	1.90	0.54
1:B:297:THR:HG23	1:B:311:GLY:O	2.07	0.53
1:A:180:GLN:HB3	1:A:181:PRO:CD	2.38	0.53
1:B:46:ASN:HD21	1:B:48:LYS:HE2	1.74	0.53
1:C:155:VAL:HA	1:C:173:ILE:HB	1.89	0.53
1:B:92:CYS:O	1:B:95:LEU:HB2	2.08	0.53
1:C:248:GLN:O	1:C:266:SER:HA	2.10	0.52
1:A:164[A]:ARG:NH2	1:C:164[A]:ARG:HH21	2.08	0.51
1:C:175:LYS:H	1:C:175:LYS:HE3	1.76	0.51
1:A:93:LEU:HD21	1:C:228:PHE:HB3	1.91	0.51
4:A:1351:PLM:C5	4:A:1351:PLM:HA1	2.40	0.51
1:A:108:HIS:CD2	1:A:127:PRO:HG3	2.46	0.50
1:B:164[A]:ARG:NH2	1:C:164[A]:ARG:NH2	2.39	0.50
1:C:209:VAL:HG23	1:C:225:ARG:HB2	1.94	0.50
1:A:328:ARG:HH21	1:C:315:ARG:NH1	2.09	0.50
1:B:110:THR:HB	1:B:128:TYR:CE2	2.47	0.49
1:B:166:VAL:CG2	1:C:164[B]:ARG:HG2	2.43	0.49
1:C:225:ARG:CG	1:C:225:ARG:HH11	2.25	0.49
1:A:146:GLY:O	1:A:164[B]:ARG:NH1	2.45	0.49
1:C:175:LYS:HE3	1:C:213:ASP:OD1	2.12	0.49
1:A:258:VAL:HG12	1:A:259:ALA:N	2.28	0.49
1:A:328:ARG:HH21	1:C:315:ARG:CZ	2.25	0.49
1:B:46:ASN:O	1:B:48:LYS:N	2.45	0.49
1:A:18[A]:GLU:HG3	1:A:65[A]:ARG:NH2	2.26	0.48
1:B:164[A]:ARG:HE	1:C:164[A]:ARG:CD	2.25	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:210:ILE:HB	1:C:232:VAL:HG22	1.95	0.48
1:C:281:ILE:CD1	1:C:293:MET:HE3	2.40	0.48
1:B:339:ALA:O	1:B:342:LYS:HB2	2.14	0.48
1:A:160:TYR:HE2	1:A:162:HIS:CE1	2.32	0.48
1:A:239:ILE:HG12	1:A:257:ILE:HD12	1.94	0.48
1:B:319[B]:GLU:HG3	5:B:2039:HOH:O	2.13	0.48
1:A:247:HIS:HD2	5:A:2046:HOH:O	1.95	0.48
1:C:250:GLU:HB2	5:C:2023:HOH:O	2.13	0.48
1:A:164[A]:ARG:HG2	1:B:164[A]:ARG:CD	2.42	0.47
1:A:258:VAL:HG12	1:A:259:ALA:H	1.78	0.47
1:A:343:LEU:HD13	1:B:343:LEU:HD11	1.97	0.47
1:B:315[B]:ARG:HH21	1:B:323:GLN:HB2	1.80	0.47
1:B:263:ILE:HD11	1:B:275:ILE:HD13	1.95	0.47
4:B:1349:PLM:CB	4:B:1349:PLM:HF1	2.40	0.47
1:B:240:ASP:HB3	1:B:259:ALA:N	2.30	0.47
1:C:168:ARG:NH1	1:C:187:SER:HA	2.30	0.46
1:A:4:SER:HB3	1:A:6:TYR:CE1	2.50	0.46
1:A:242:LEU:O	1:A:260:GLN:HA	2.16	0.46
1:C:339:ALA:HB3	5:C:2033:HOH:O	2.15	0.46
1:C:119:ILE:CG2	1:C:123:VAL:HG11	2.46	0.46
1:B:164[A]:ARG:HE	1:C:164[A]:ARG:HE	1.57	0.46
1:B:164[A]:ARG:HH21	1:C:164[A]:ARG:CZ	2.22	0.46
1:B:37:LYS:HA	1:B:57:GLU:HB2	1.97	0.46
1:A:102:SER:O	1:C:133:GLN:HG2	2.16	0.45
1:A:59:GLY:O	1:A:77:ASN:HB2	2.16	0.45
1:B:133:GLN:NE2	1:C:101:ASP:O	2.46	0.45
1:A:14:PHE:HD1	1:A:15:LEU:HD13	1.82	0.45
1:C:263:ILE:HD13	1:C:269:ILE:HD13	1.98	0.45
1:C:242:LEU:O	1:C:260:GLN:HA	2.16	0.45
1:C:195:SER:OG	1:C:197:PHE:HB2	2.17	0.45
1:B:164[B]:ARG:HE	1:C:164[B]:ARG:CZ	2.07	0.44
1:B:162:HIS:HB3	1:B:163:PRO:HD2	2.00	0.44
1:C:126:GLU:HB3	1:C:127:PRO:HD2	2.00	0.44
1:A:126:GLU:HB3	1:A:127:PRO:CD	2.47	0.44
1:A:119:ILE:CG2	1:A:123:VAL:HG21	2.48	0.44
1:A:234:ARG:HB2	1:A:252:GLY:C	2.37	0.44
1:B:184:VAL:HB	1:B:222:THR:HG22	2.00	0.44
1:A:120:GLU:HG3	1:A:138:GLY:HA2	2.00	0.43
1:B:65:ARG:NE	3:B:1346:SO4:O2	2.40	0.43
1:A:164[B]:ARG:NH1	1:C:164[B]:ARG:HH22	1.60	0.43
1:A:315:ARG:HD2	5:A:2065:HOH:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:GLN:HB2	5:A:2020:HOH:O	2.18	0.43
1:B:49:TYR:O	1:B:51:LYS:N	2.52	0.43
1:A:2:SER:C	1:A:4:SER:N	2.72	0.43
1:C:34:GLU:HG3	1:C:52:HIS:CG	2.54	0.43
1:A:65[A]:ARG:HG3	1:A:65[A]:ARG:NH1	2.03	0.43
1:C:46:ASN:HD22	1:C:48:LYS:HG3	1.83	0.43
1:A:34:GLU:H	1:A:34:GLU:CD	2.22	0.42
1:B:203:LEU:O	1:B:205:HIS:HD2	2.02	0.42
1:B:244:GLN:HA	1:B:244:GLN:OE1	2.19	0.42
1:B:27:LEU:HD13	1:B:41:ILE:HG12	2.01	0.42
4:A:1352:PLM:HA2	4:A:1352:PLM:HG3	2.01	0.42
1:A:160:TYR:CE2	1:A:162:HIS:CE1	3.07	0.42
1:A:164[B]:ARG:NH1	1:B:164[B]:ARG:NH1	2.64	0.42
1:A:2:SER:C	1:A:4:SER:H	2.23	0.42
1:B:57:GLU:O	1:B:58:ALA:C	2.57	0.42
1:A:194:THR:HG22	5:A:2038:HOH:O	2.18	0.42
1:C:258:VAL:HG12	1:C:259:ALA:N	2.35	0.42
1:B:66:THR:HG22	1:B:70:LYS:HD2	2.02	0.41
1:C:44:LEU:HD21	1:C:67:GLN:HE21	1.85	0.41
1:B:36:ALA:O	1:B:57:GLU:HB2	2.19	0.41
1:C:176:ARG:O	1:C:176:ARG:HG3	2.20	0.41
4:B:1349:PLM:HB1	4:B:1349:PLM:H82	1.78	0.41
1:B:264:ALA:HB3	1:B:283:GLY:N	2.35	0.41
1:C:246:ALA:O	1:C:249:VAL:HG23	2.20	0.41
1:A:114:HIS:HA	1:A:115:PRO:HD2	1.82	0.41
1:A:345:GLN:N	1:A:345:GLN:HE21	2.19	0.41
1:A:36:ALA:O	1:A:37:LYS:HE2	2.21	0.41
1:B:95:LEU:HD23	1:B:95:LEU:HA	1.95	0.41
4:A:1352:PLM:H61	1:C:300:THR:HG22	2.02	0.41
1:A:295:ALA:HB3	4:A:1352:PLM:H52	2.02	0.41
1:C:126:GLU:HB3	1:C:127:PRO:CD	2.51	0.41
1:B:220:ASN:HB2	1:B:242:LEU:HD13	2.03	0.41
1:A:269:ILE:HD13	1:A:275:ILE:HD11	2.02	0.41
1:B:203:LEU:O	1:B:205:HIS:CD2	2.74	0.41
1:B:49:TYR:HB3	5:B:2004:HOH:O	2.21	0.41
1:B:126:GLU:HB3	1:B:127:PRO:HD2	2.03	0.41
1:A:194:THR:CG2	1:A:198:GLY:HA2	2.50	0.40
1:B:228:PHE:HB3	1:C:93:LEU:HD13	2.03	0.40
1:B:44:LEU:HD12	1:B:49:TYR:CD1	2.46	0.40
1:C:108:HIS:CE1	1:C:110:THR:HG23	2.56	0.40
1:B:315[B]:ARG:NH1	1:C:328:ARG:HE	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:344:VAL:O	1:C:347:LEU:HB3	2.21	0.40
1:C:46:ASN:ND2	5:C:2002:HOH:O	2.53	0.40
1:A:258:VAL:CG1	1:A:259:ALA:H	2.35	0.40
1:B:264:ALA:HB3	1:B:282:THR:C	2.42	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	352/374 (94%)	333 (95%)	15 (4%)	4 (1%)	14	34
1	B	348/374 (93%)	326 (94%)	15 (4%)	7 (2%)	7	19
1	C	350/374 (94%)	329 (94%)	17 (5%)	4 (1%)	14	34
All	All	1050/1122 (94%)	988 (94%)	47 (4%)	15 (1%)	11	28

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	50	ALA
1	C	197	PHE
1	A	3	GLN
1	A	45	ASP
1	A	46	ASN
1	B	47	GLU
1	B	58	ALA
1	B	229[A]	LYS
1	B	229[B]	LYS
1	B	235	GLU
1	C	195	SER
1	B	72	ARG
1	A	240	ASP

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Mol	Chain	Res	Type
1	C	46	ASN
1	C	34	GLU

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	293/309 (95%)	270 (92%)	23 (8%)	12	29
1	B	289/309 (94%)	264 (91%)	25 (9%)	10	23
1	C	291/309 (94%)	268 (92%)	23 (8%)	12	28
All	All	873/927 (94%)	802 (92%)	71 (8%)	12	27

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	15	LEU
1	A	17	VAL
1	A	34	GLU
1	A	44	LEU
1	A	45	ASP
1	A	49	TYR
1	A	51	LYS
1	A	65[A]	ARG
1	A	65[B]	ARG
1	A	98	THR
1	A	195	SER
1	A	221	THR
1	A	229	LYS
1	A	242	LEU
1	A	248	GLN
1	A	268	LYS
1	A	282	THR
1	A	318	GLN
1	A	319	GLU

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Mol	Chain	Res	Type
1	A	335	GLU
1	A	340	LEU
1	A	345	GLN
1	B	11	LEU
1	B	34	GLU
1	B	46	ASN
1	B	49	TYR
1	B	51	LYS
1	B	54	LYS
1	B	73	ASP
1	B	75[A]	ASN
1	B	75[B]	ASN
1	B	100	VAL
1	B	123	VAL
1	B	141	CYS
1	B	145	SER
1	B	164[A]	ARG
1	B	164[B]	ARG
1	B	227	ARG
1	B	242	LEU
1	B	253	GLN
1	B	282	THR
1	B	301	LYS
1	B	305	SER
1	B	318	GLN
1	B	322	ARG
1	B	328	ARG
1	B	340	LEU
1	C	22	ASN
1	C	27	LEU
1	C	37	LYS
1	C	38	THR
1	C	46	ASN
1	C	47	GLU
1	C	48	LYS
1	C	76	LYS
1	C	100	VAL
1	C	175	LYS
1	C	197	PHE
1	C	199	GLN
1	C	225	ARG
1	C	242	LEU

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Mol	Chain	Res	Type
1	C	256	MET
1	C	267	THR
1	C	282	THR
1	C	315	ARG
1	C	322	ARG
1	C	326	LYS
1	C	335	GLU
1	C	336	ARG
1	C	340	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	290	HIS
1	A	345	GLN
1	B	46	ASN
1	B	199	GLN
1	B	205	HIS
1	B	329	ASN
1	C	133	GLN
1	C	199	GLN
1	C	248	GLN
1	C	272	HIS
1	C	345	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

12 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	SO4	A	1348	-	4,4,4	0.13	0	6,6,6	0.23	0
3	SO4	C	1350	-	4,4,4	0.10	0	6,6,6	0.15	0
4	PLM	B	1349	-	14,17,17	0.37	0	13,17,17	0.51	0
3	SO4	C	1349	-	4,4,4	0.13	0	6,6,6	0.24	0
3	SO4	B	1346	-	4,4,4	0.12	0	6,6,6	0.30	0
4	PLM	A	1351	-	14,17,17	0.39	0	13,17,17	0.44	0
3	SO4	A	1349	-	4,4,4	0.17	0	6,6,6	0.09	0
4	PLM	A	1352	-	14,17,17	0.32	0	13,17,17	0.36	0
2	MES	A	1347	-	12,12,12	2.18	1 (8%)	14,16,16	2.49	7 (50%)
3	SO4	B	1348	-	4,4,4	0.15	0	6,6,6	0.31	0
3	SO4	B	1347	-	4,4,4	0.15	0	6,6,6	0.28	0
3	SO4	A	1350	-	4,4,4	0.12	0	6,6,6	0.18	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	PLM	B	1349	-	-	9/13/15/15	-
2	MES	A	1347	-	-	2/6/14/14	0/1/1/1
4	PLM	A	1352	-	-	12/13/15/15	-
4	PLM	A	1351	-	-	8/13/15/15	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1347	MES	C8-S	-7.20	1.67	1.77

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1347	MES	C5-N4-C3	5.63	121.50	108.83
2	A	1347	MES	C7-N4-C3	3.62	120.48	111.23
2	A	1347	MES	O3S-S-C8	2.71	110.15	105.77
2	A	1347	MES	C7-N4-C5	2.65	118.01	111.23
2	A	1347	MES	C2-C3-N4	-2.62	106.12	110.10
2	A	1347	MES	C6-C5-N4	-2.55	106.23	110.10
2	A	1347	MES	O2S-S-C8	2.29	109.68	106.92

There are no chirality outliers.

All (31) torsion outliers are listed below:

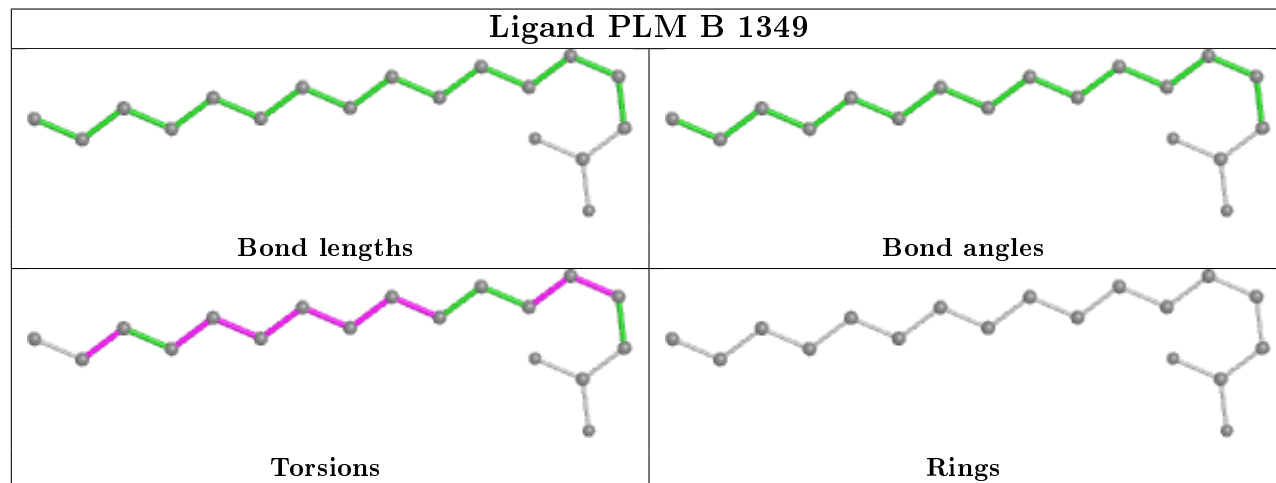
Mol	Chain	Res	Type	Atoms
2	A	1347	MES	N4-C7-C8-S
4	A	1351	PLM	C9-CA-CB-CC
4	A	1351	PLM	CB-CC-CD-CE
4	B	1349	PLM	CB-CC-CD-CE
4	A	1352	PLM	CB-CC-CD-CE
4	A	1352	PLM	CC-CD-CE-CF
4	A	1351	PLM	C7-C8-C9-CA
4	B	1349	PLM	C9-CA-CB-CC
4	B	1349	PLM	C2-C3-C4-C5
4	A	1351	PLM	C2-C3-C4-C5
4	B	1349	PLM	C7-C8-C9-CA
4	A	1352	PLM	C6-C7-C8-C9
4	A	1352	PLM	C2-C3-C4-C5
4	A	1352	PLM	C5-C6-C7-C8
4	A	1352	PLM	C8-C9-CA-CB
4	A	1352	PLM	C7-C8-C9-CA
4	A	1352	PLM	CA-CB-CC-CD
4	A	1352	PLM	CD-CE-CF-CG
4	A	1351	PLM	CC-CD-CE-CF
4	B	1349	PLM	C3-C4-C5-C6
4	B	1349	PLM	CD-CE-CF-CG
4	A	1351	PLM	C4-C5-C6-C7
4	B	1349	PLM	C8-C9-CA-CB
2	A	1347	MES	C8-C7-N4-C5
4	A	1352	PLM	C4-C5-C6-C7
4	A	1351	PLM	C6-C7-C8-C9
4	A	1352	PLM	C9-CA-CB-CC
4	A	1351	PLM	CA-CB-CC-CD
4	A	1352	PLM	C3-C4-C5-C6
4	B	1349	PLM	C6-C7-C8-C9
4	B	1349	PLM	CA-CB-CC-CD

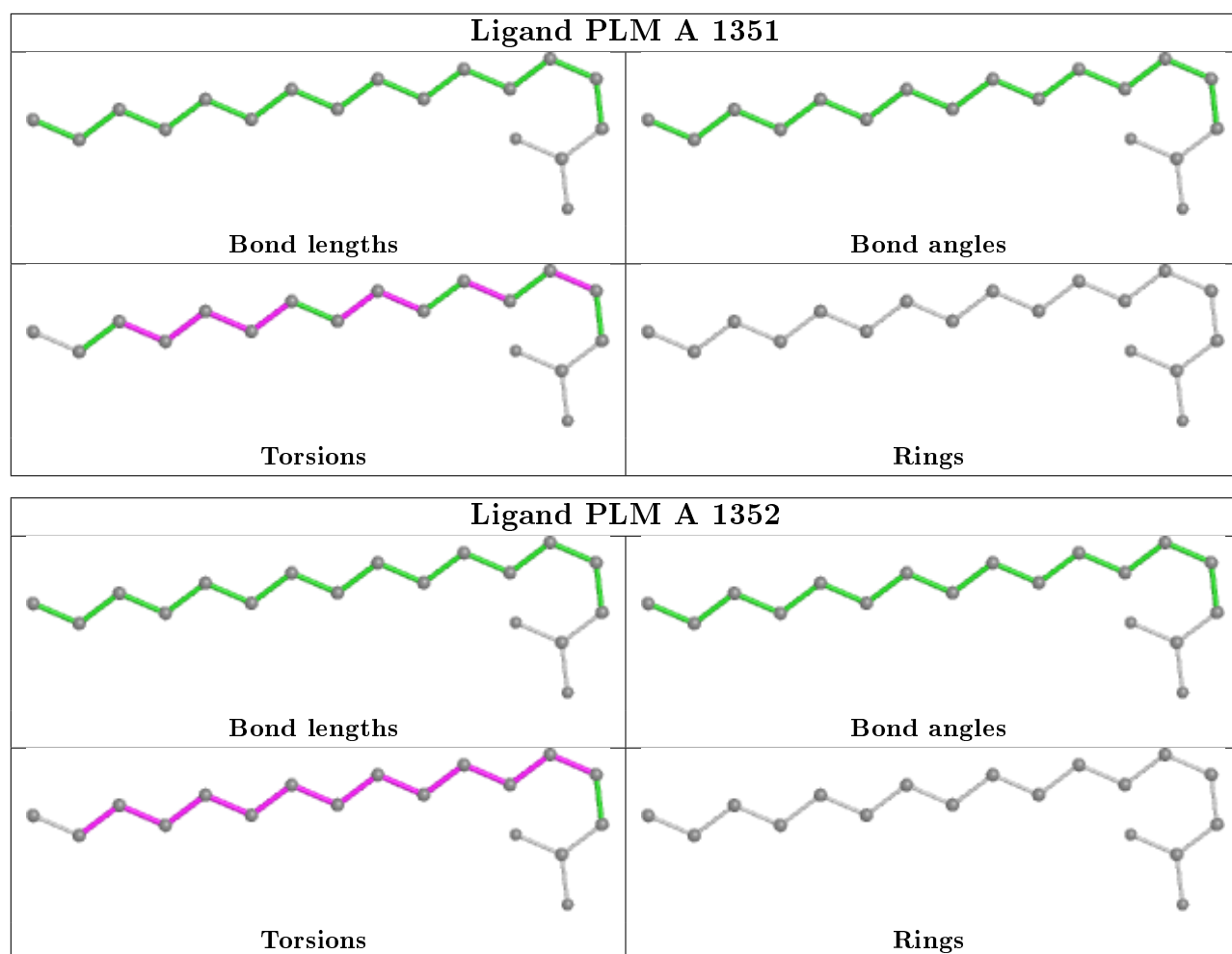
There are no ring outliers.

5 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1348	SO4	1	0
4	B	1349	PLM	4	0
3	B	1346	SO4	2	0
4	A	1351	PLM	5	0
4	A	1352	PLM	4	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	346/374 (92%)	-0.20	6 (1%) 70 72	23, 36, 67, 94	0
1	B	345/374 (92%)	-0.22	7 (2%) 65 67	22, 34, 71, 94	0
1	C	346/374 (92%)	-0.08	9 (2%) 56 57	24, 40, 78, 99	0
All	All	1037/1122 (92%)	-0.16	22 (2%) 63 65	22, 37, 75, 99	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	347	LEU	4.9
1	A	1	MET	4.9
1	A	338	ALA	4.8
1	B	1	MET	4.1
1	B	345	GLN	3.9
1	C	342	LYS	3.8
1	A	344	VAL	3.6
1	C	348	GLU	3.3
1	C	345	GLN	3.2
1	B	49	TYR	3.1
1	B	340	LEU	2.8
1	C	343	LEU	2.6
1	A	339	ALA	2.5
1	C	3	GLN	2.5
1	B	2	SER	2.4
1	C	196	ALA	2.4
1	C	49	TYR	2.2
1	A	342	LYS	2.2
1	B	197	PHE	2.1
1	C	26	LEU	2.0
1	B	344	VAL	2.0
1	A	345	GLN	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 carbohydrates in this entry.

## 6.4 Ligands [i](#)

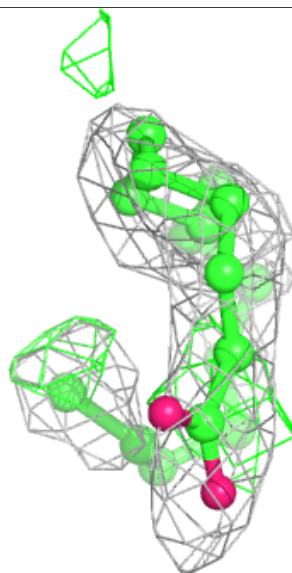
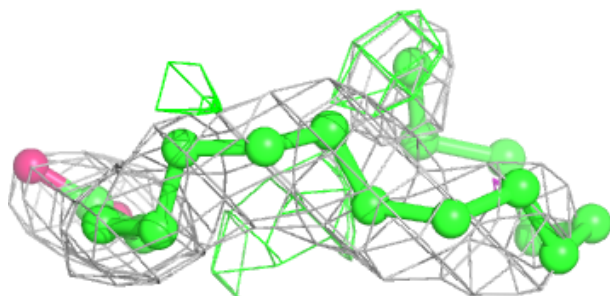
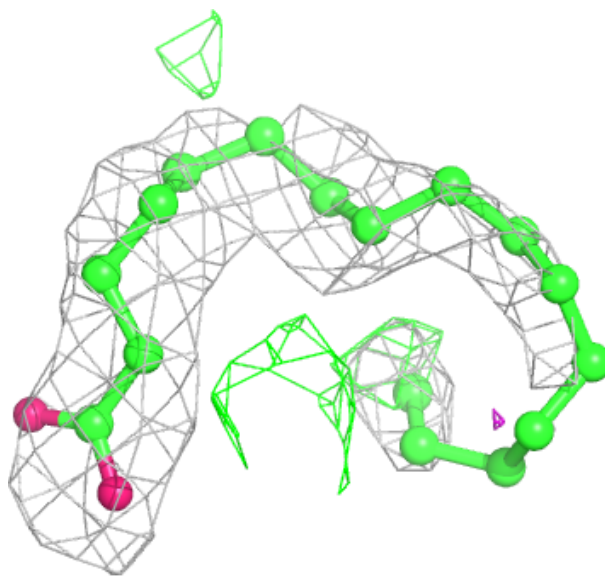
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
4	PLM	A	1352	18/18	0.72	0.35	71,73,75,76	0
3	SO4	B	1347	5/5	0.79	0.27	34,35,36,37	5
3	SO4	A	1350	5/5	0.85	0.21	37,39,39,39	5
2	MES	A	1347	12/12	0.86	0.31	66,67,69,69	12
4	PLM	A	1351	18/18	0.87	0.24	48,53,59,59	0
3	SO4	C	1349	5/5	0.90	0.18	36,36,37,38	5
4	PLM	B	1349	18/18	0.90	0.22	47,52,54,54	0
3	SO4	A	1349	5/5	0.93	0.13	32,32,33,33	5
3	SO4	B	1348	5/5	0.94	0.15	32,32,34,34	5
3	SO4	A	1348	5/5	0.96	0.17	42,43,44,45	5
3	SO4	B	1346	5/5	0.99	0.11	44,44,45,46	0
3	SO4	C	1350	5/5	0.99	0.05	47,47,48,48	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.

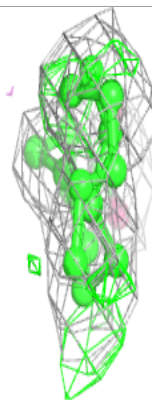
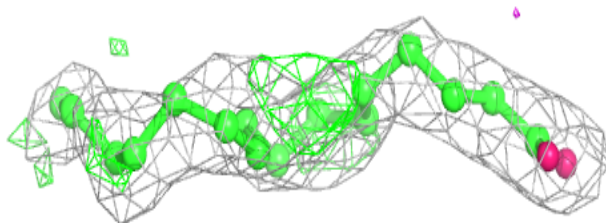
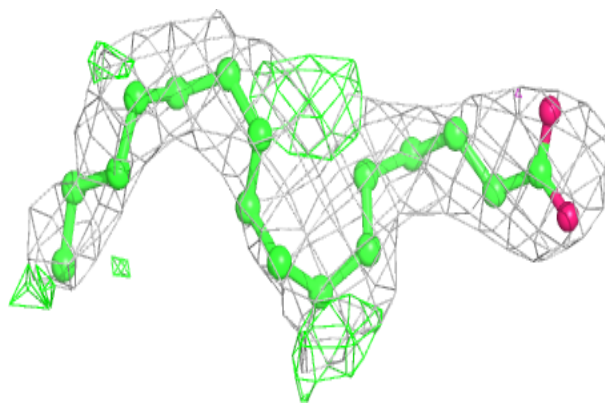
**Electron density around PLM A 1352:**

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

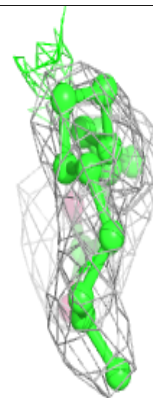
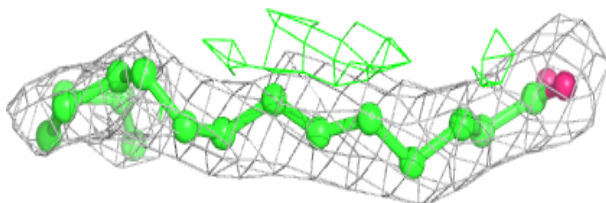
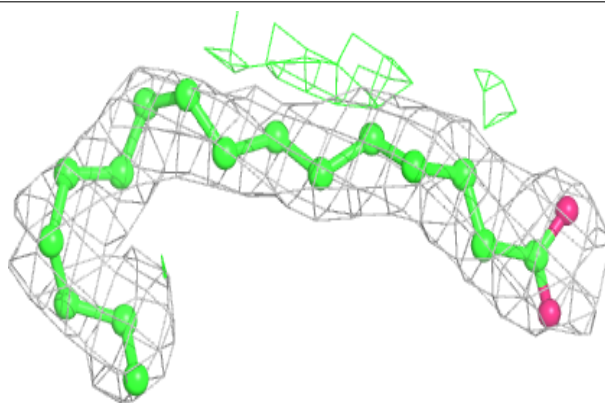


**Electron density around PLM A 1351:**

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

**Electron density around PLM B 1349:**

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



## 6.5 Other polymers

There are no such residues in this entry.