



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:59 AM UTC

PDB ID : 2IU8 / pdb_00002iu8
Title : Chlamydia trachomatis LpxD with 25mM UDPGlcNAc (Complex I)
Authors : Buetow, L.; Smith, T.K.; Dawson, A.; Fyffe, S.; Hunter, W.N.
Deposited on : 2006-05-30
Resolution : 2.20 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

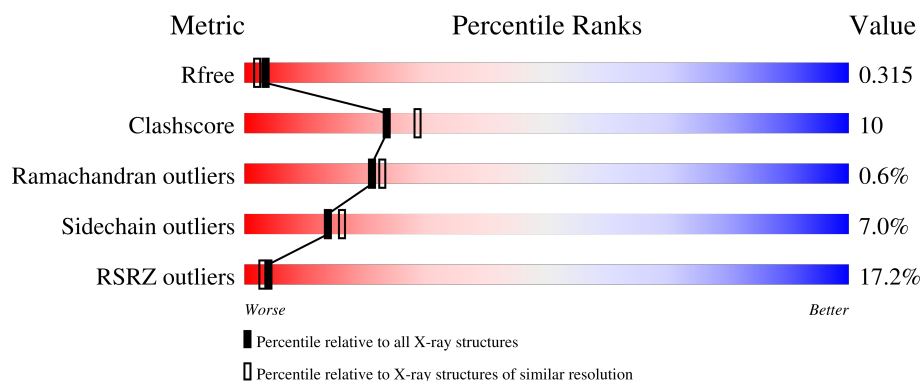
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	374	14% 72% 18% • 7%
1	B	374	14% 70% 19% • 8%
1	C	374	20% 73% 18% • 7%

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 8688 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	12	0
			2695	1700	485	498	12			
1	B	345	Total	C	N	O	S	0	9	0
			2676	1689	479	498	10			
1	C	346	Total	C	N	O	S	0	8	0
			2680	1693	481	496	10			

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



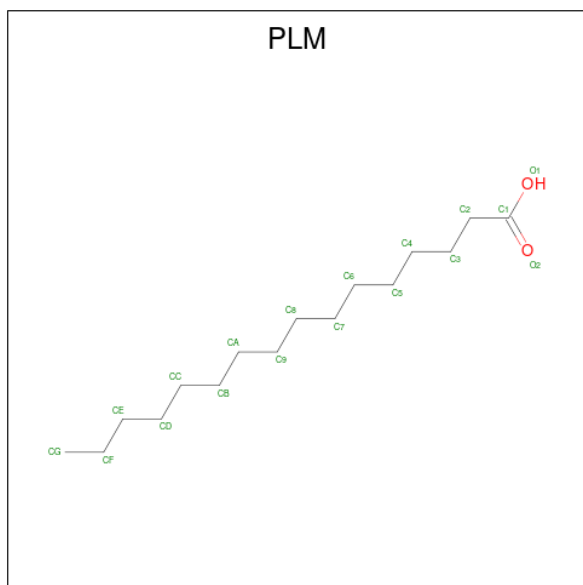
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

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

- Molecule 3 is PALMITIC ACID (CCD ID: PLM) (formula: $C_{16}H_{32}O_2$).



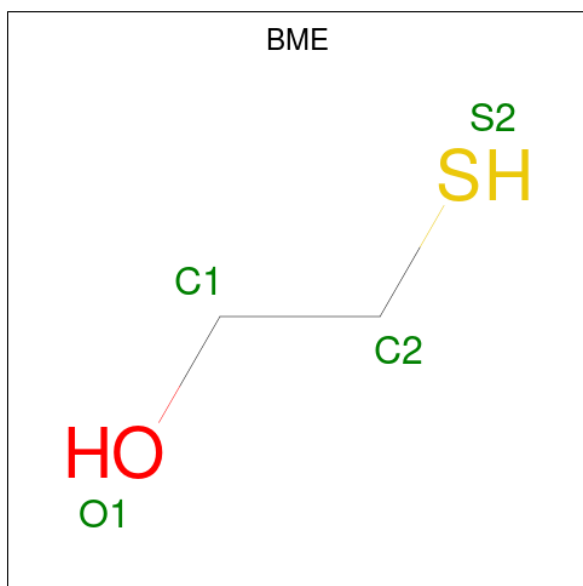
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			18	16	2		
3	B	1	Total	C	O	0	1
			25	23	2		
3	C	1	Total	C	O	0	0
			18	16	2		

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



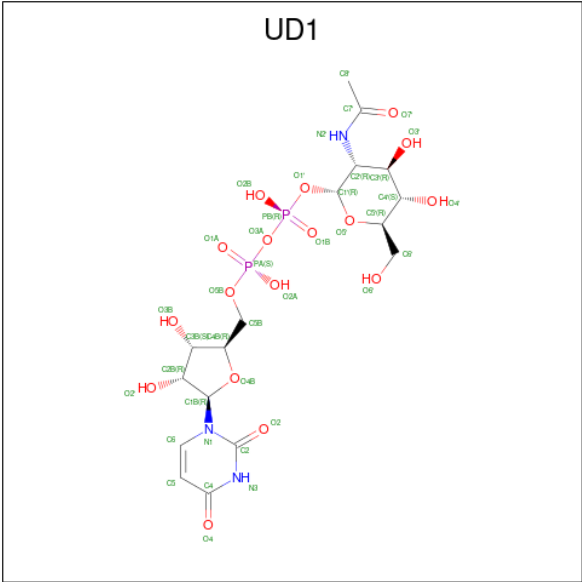
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is BETA-MERCAPTOETHANOL (CCD ID: BME) (formula: C_2H_6OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	O	S	0	1
			8	4	2	2		

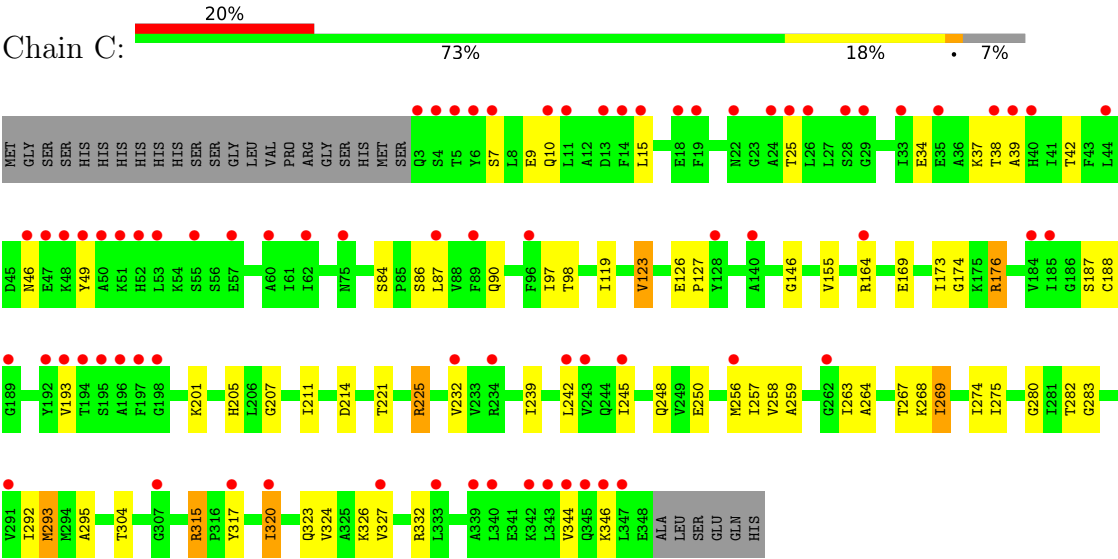
- Molecule 6 is URIDINE-DIPHOSPHATE-N-ACETYLGLUCOSAMINE (CCD ID: UD1) (formula: $C_{17}H_{27}N_3O_{17}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	B	1	Total	C	N	O	P	0	0
			39	17	3	17	2		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	209	Total	O	0	0
			209	209		
7	B	147	Total	O	0	0
			147	147		
7	C	139	Total	O	0	0
			139	139		



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	98.81Å 98.81Å 283.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.20 50.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	90.4 (50.00-2.20) 90.3 (50.00-2.20)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.89 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.206 , 0.256 0.273 , 0.315	Depositor DCC
R_{free} test set	3302 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	48.4	Xtriage
Anisotropy	0.292	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 48.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8688	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.59% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PLM, SO4, BME, EDO, UD1

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	0.70	4/2796 (0.1%)	0.89	0/3778
1	B	0.73	3/2763 (0.1%)	0.95	4/3737 (0.1%)
1	C	0.60	2/2763 (0.1%)	0.84	0/3736
All	All	0.68	9/8322 (0.1%)	0.90	4/11251 (0.0%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	45	ASP	CG-OD2	10.63	1.45	1.25
1	A	47	GLU	CD-OE1	8.73	1.42	1.25
1	A	47	GLU	CD-OE2	8.53	1.41	1.25
1	C	9	GLU	CD-OE2	7.59	1.39	1.25
1	B	197	PHE	N-CA	6.35	1.54	1.46
1	B	195	SER	CB-OG	5.91	1.53	1.42
1	A	47	GLU	CG-CD	5.63	1.66	1.52
1	C	9	GLU	CD-OE1	5.12	1.35	1.25
1	B	345	GLN	CD-OE1	5.05	1.33	1.23

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	33	ILE	N-CA-C	6.29	117.79	110.62
1	B	182	GLY	N-CA-C	5.45	122.78	115.59
1	B	108	HIS	CA-C-N	5.10	126.21	119.84
1	B	108	HIS	C-N-CA	5.10	126.21	119.84

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2695	0	2716	66	0
1	B	2676	0	2694	68	0
1	C	2680	0	2702	55	0
2	A	10	0	0	1	0
2	B	10	0	0	0	0
2	C	10	0	0	1	0
3	A	18	0	31	2	0
3	B	25	0	34	1	0
3	C	18	0	31	8	0
4	A	4	0	6	0	0
5	A	8	0	11	3	0
6	B	39	0	25	4	0
7	A	209	0	0	3	0
7	B	147	0	0	4	0
7	C	139	0	0	4	0
All	All	8688	0	8250	169	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (169) 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:164[A]:ARG:HD2	1:C:164[A]:ARG:CG	1.74	1.16
1:A:65:ARG:HH11	1:A:65:ARG:HG3	1.18	1.06
1:B:164[B]:ARG:HG2	1:B:164[B]:ARG:HH11	1.11	1.06
1:A:164[A]:ARG:CD	1:C:164[A]:ARG:HG2	1.91	1.01
1:A:164[A]:ARG:HD2	1:C:164[A]:ARG:HG2	0.95	0.94
1:A:164[B]:ARG:NE	1:C:164[B]:ARG:NH1	2.15	0.89
1:A:164[B]:ARG:HE	1:C:164[B]:ARG:NH1	1.69	0.88
1:A:148:VAL:HG23	1:B:164[B]:ARG:HH21	1.39	0.86
1:B:164[A]:ARG:HB2	1:C:164[A]:ARG:HD2	1.58	0.85
1:B:164[B]:ARG:HH11	1:B:164[B]:ARG:CG	1.89	0.84
1:A:164[B]:ARG:NH1	1:B:164[B]:ARG:NE	2.22	0.81
1:A:164[B]:ARG:NE	1:C:164[B]:ARG:HH12	1.79	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:178:ILE:HB	1:A:216:GLU:HG2	1.67	0.77
1:A:164[A]:ARG:HG2	1:B:164[A]:ARG:HD2	1.67	0.77
3:A:1349:PLM:H21	1:B:259:ALA:HB3	1.68	0.75
1:A:9:GLU:HG3	1:A:19:PHE:CE2	2.22	0.74
1:B:164[B]:ARG:HG2	1:B:164[B]:ARG:NH1	1.92	0.71
1:A:65:ARG:HH11	1:A:65:ARG:CG	2.00	0.71
1:B:319[A]:GLU:OE2	7:B:2143:HOH:O	2.12	0.68
1:A:295:ALA:CB	3:C:1351:PLM:H91	2.27	0.65
1:B:11:LEU:HD21	1:B:41:ILE:HD11	1.77	0.65
1:B:250[A]:GLU:OE2	1:B:268:LYS:HD3	1.97	0.64
1:B:257:ILE:HG12	1:B:275:ILE:HD12	1.79	0.64
1:A:193:VAL:HG23	1:A:201:LYS:HB2	1.81	0.63
1:A:65:ARG:HG3	1:A:65:ARG:NH1	1.99	0.62
1:A:259:ALA:HB3	3:C:1351:PLM:H32	1.81	0.62
1:A:126:GLU:HB3	1:A:127:PRO:HD2	1.82	0.61
1:A:164[A]:ARG:HG2	1:B:164[A]:ARG:CD	2.29	0.61
1:B:282:THR:HG23	7:C:2046:HOH:O	2.00	0.61
7:A:2206:HOH:O	6:B:1348:UD1:H8'2	2.01	0.59
1:B:126:GLU:HB3	1:B:127:PRO:HD2	1.85	0.58
1:B:247:HIS:H	1:B:247:HIS:CD2	2.22	0.58
1:C:146:GLY:O	1:C:164[B]:ARG:NH1	2.37	0.58
1:A:47:GLU:HB2	1:A:49:TYR:CE1	2.38	0.57
1:A:164[B]:ARG:HH12	1:B:164[B]:ARG:NE	1.97	0.57
1:B:315[A]:ARG:HH22	1:C:324:VAL:HG13	1.69	0.57
1:B:11:LEU:HD12	1:B:15:LEU:HD22	1.85	0.57
1:A:188[B]:CYS:HB2	5:A:1351[B]:BME:S2	2.44	0.57
1:C:7:SER:OG	1:C:10:GLN:HB2	2.05	0.57
1:C:119:ILE:HG22	1:C:123:VAL:HG11	1.87	0.57
1:A:32:GLU:HA	1:A:32:GLU:OE1	2.04	0.57
1:B:3:GLN:O	7:B:2003:HOH:O	2.17	0.57
1:B:189:GLY:HA3	1:B:205:HIS:CE1	2.40	0.57
1:A:162:HIS:HB3	1:A:163:PRO:HD2	1.88	0.56
1:C:239:ILE:HG12	1:C:257:ILE:HD12	1.86	0.56
1:A:315:ARG:HB2	1:A:320:ILE:HG23	1.87	0.56
1:C:207:GLY:O	1:C:225:ARG:NH1	2.40	0.55
1:A:164[B]:ARG:CD	1:C:164[B]:ARG:HH12	2.18	0.55
1:A:257:ILE:HG12	1:A:275:ILE:HD12	1.89	0.55
1:C:46:ASN:HB2	1:C:49:TYR:HB2	1.88	0.55
1:B:227:ARG:NH2	1:C:86:SER:OG	2.40	0.55
1:B:161:ILE:HD12	1:B:179:ILE:HD12	1.88	0.54
1:C:275:ILE:HG12	1:C:293:MET:CE	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:164[A]:ARG:HE	1:C:164[A]:ARG:NE	2.04	0.54
1:C:263:ILE:HD13	1:C:269:ILE:HD13	1.89	0.54
1:A:247:HIS:HD2	7:A:2155:HOH:O	1.91	0.54
1:B:2:SER:C	1:B:4:SER:H	2.15	0.54
1:C:245:ILE:HD13	1:C:263:ILE:HD12	1.91	0.53
3:B:1349[B]:PLM:HC2	1:C:295:ALA:HB3	1.91	0.53
1:A:38:THR:O	1:A:59:GLY:HA3	2.09	0.53
1:C:176:ARG:HG3	1:C:214:ASP:OD1	2.09	0.52
1:B:178:ILE:HB	1:B:216:GLU:HG2	1.91	0.52
1:A:146:GLY:O	1:A:164[B]:ARG:NH1	2.41	0.52
1:B:227:ARG:HB3	1:B:228:PHE:HD2	1.74	0.51
1:A:162:HIS:HB3	1:A:163:PRO:CD	2.40	0.51
1:A:47:GLU:C	1:A:49:TYR:H	2.18	0.51
1:A:164[A]:ARG:CG	1:B:164[A]:ARG:HD2	2.40	0.51
1:B:343:LEU:HD13	1:B:345:GLN:HB2	1.93	0.51
1:C:245:ILE:CD1	1:C:263:ILE:HD12	2.41	0.51
1:A:126:GLU:HB3	1:A:127:PRO:CD	2.41	0.50
1:C:126:GLU:HB3	1:C:127:PRO:CD	2.41	0.50
1:A:47:GLU:HB2	1:A:49:TYR:HE1	1.76	0.50
1:A:65:ARG:NH1	2:A:1347:SO4:O1	2.44	0.49
1:B:49:TYR:O	1:B:51:LYS:N	2.35	0.49
1:A:188[B]:CYS:SG	5:A:1351[B]:BME:S2	3.11	0.49
1:A:166:VAL:CG2	1:B:164[A]:ARG:HG2	2.43	0.49
1:C:248:GLN:NE2	7:C:2101:HOH:O	2.46	0.49
1:B:71:TYR:HB3	1:B:74:LEU:HD12	1.94	0.48
1:C:84:SER:HB3	1:C:87:LEU:HD12	1.94	0.48
1:B:164[B]:ARG:CG	1:B:164[B]:ARG:NH1	2.58	0.48
1:B:186:GLY:O	1:B:225:ARG:NH1	2.46	0.48
1:B:227:ARG:HD3	1:C:90:GLN:OE1	2.13	0.48
1:C:257:ILE:HG12	1:C:275:ILE:HD12	1.94	0.48
1:B:133:GLN:HG3	1:B:134:HIS:HD2	1.78	0.47
1:C:174:GLY:N	1:C:211:ILE:O	2.45	0.47
1:C:315:ARG:NH1	7:C:2125:HOH:O	2.48	0.47
1:B:36:ALA:HB3	7:B:2027:HOH:O	2.14	0.47
1:B:11:LEU:HD21	1:B:41:ILE:CD1	2.43	0.46
1:B:166:VAL:CG2	1:C:164[B]:ARG:HG2	2.44	0.46
1:C:126:GLU:HB3	1:C:127:PRO:HD2	1.97	0.46
1:A:191:GLY:HA2	6:B:1348:UD1:O4'	2.15	0.46
1:B:287:ILE:HD12	1:B:303:ILE:HD12	1.97	0.46
1:B:281:ILE:HG23	1:B:285:ILE:HD11	1.98	0.46
1:A:182:GLY:O	1:A:220:ASN:HA	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:LEU:HG	1:A:15:LEU:HD22	1.98	0.46
1:C:250:GLU:HB3	1:C:268:LYS:HG3	1.98	0.46
1:C:280:GLY:HA3	3:C:1351:PLM:H81	1.98	0.45
1:A:275:ILE:HG12	1:A:293:MET:CE	2.47	0.45
1:B:119:ILE:HG22	1:B:123:VAL:HG11	1.98	0.45
1:C:274:ILE:HD12	1:C:292:ILE:HG12	1.97	0.45
1:C:275:ILE:HG12	1:C:293:MET:HE1	1.97	0.45
1:A:277:GLY:HA3	3:C:1351:PLM:H71	1.98	0.45
1:A:226:GLY:HA3	1:A:229:LYS:O	2.17	0.45
1:B:193:VAL:HG23	1:B:203:LEU:HD21	1.98	0.45
1:A:295:ALA:HB3	3:C:1351:PLM:H91	1.99	0.44
1:B:151:ALA:O	1:B:152:TYR:HB2	2.17	0.44
1:A:15:LEU:HB3	1:A:17:VAL:HB	1.99	0.44
5:A:1351[A]:BME:H21	1:B:162:HIS:HE1	1.82	0.44
1:B:2:SER:C	1:B:4:SER:N	2.76	0.44
1:A:208:LYS:HG3	1:A:230:HIS:CE1	2.53	0.44
1:C:37:LYS:HE3	1:C:39:ALA:HB3	2.00	0.44
1:A:47:GLU:O	1:A:49:TYR:N	2.49	0.44
1:C:344:VAL:C	1:C:346:LYS:H	2.26	0.44
1:C:317:TYR:HA	1:C:320:ILE:HD11	1.98	0.43
3:A:1349:PLM:HF1	1:B:294:MET:HE2	1.99	0.43
1:B:76:LYS:HB2	1:B:78:PHE:CZ	2.53	0.43
1:C:7:SER:HA	1:C:25:THR:O	2.19	0.43
1:A:20:GLN:HG3	1:A:68:PHE:CZ	2.54	0.43
1:C:188:CYS:HB2	2:C:1350:SO4:O4	2.18	0.43
1:C:205:HIS:O	1:C:225:ARG:HD3	2.17	0.43
1:C:344:VAL:C	1:C:346:LYS:N	2.76	0.43
1:A:69[B]:GLN:HE22	1:A:72[B]:ARG:HH12	1.66	0.43
1:A:320:ILE:HA	1:A:323:GLN:HB2	2.00	0.43
1:C:256:MET:HE2	1:C:256:MET:HB3	1.91	0.43
3:C:1351:PLM:HF2	3:C:1351:PLM:HC1	1.57	0.43
1:C:258:VAL:HG12	1:C:259:ALA:N	2.34	0.43
1:B:169:GLU:O	1:B:225:ARG:NH2	2.51	0.43
1:B:49:TYR:CD1	1:B:49:TYR:N	2.87	0.42
1:B:190:PHE:HE2	1:C:256:MET:HE2	1.83	0.42
1:C:264:ALA:HB3	1:C:283:GLY:N	2.33	0.42
1:C:264:ALA:HB2	3:C:1351:PLM:H41	2.01	0.42
1:A:155:VAL:HA	1:A:173:ILE:HB	2.02	0.42
1:A:164[A]:ARG:NE	1:C:164[A]:ARG:HE	2.17	0.42
1:A:30:VAL:HG12	1:A:41:ILE:HB	2.02	0.42
1:C:155:VAL:HA	1:C:173:ILE:HB	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:193:VAL:HB	1:C:201:LYS:HB2	2.00	0.42
1:B:314:ALA:C	1:B:315[A]:ARG:HG2	2.45	0.42
1:A:295:ALA:HB1	3:C:1351:PLM:H91	2.00	0.42
1:B:132:CYS:O	1:B:133:GLN:C	2.61	0.41
1:A:265:GLY:O	6:B:1348:UD1:O7'	2.38	0.41
1:B:247:HIS:O	1:B:248:GLN:HB2	2.19	0.41
1:A:164[A]:ARG:CD	1:C:164[A]:ARG:CG	2.69	0.41
1:A:180:GLN:HB3	1:A:181:PRO:CD	2.50	0.41
1:B:247:HIS:H	1:B:247:HIS:HD2	1.65	0.41
1:A:250[A]:GLU:HB2	1:A:268:LYS:HG3	2.01	0.41
1:A:310:GLY:O	1:A:314:ALA:HA	2.20	0.41
1:B:344:VAL:O	1:B:345:GLN:C	2.63	0.41
1:C:323:GLN:O	1:C:327:VAL:HG23	2.21	0.41
1:B:63:ILE:HG12	1:B:67:GLN:HB2	2.03	0.41
1:A:234[B]:ARG:HD3	1:A:253:GLN:HG3	2.03	0.41
1:B:329:ASN:OD1	1:B:332:ARG:HD3	2.21	0.41
1:A:177:VAL:HG13	1:A:215:VAL:O	2.21	0.40
1:B:49:TYR:C	1:B:51:LYS:H	2.24	0.40
1:A:240:ASP:HB3	1:A:259:ALA:N	2.36	0.40
1:C:293:MET:HE2	1:C:293:MET:HB2	1.82	0.40
1:A:247:HIS:CD2	7:A:2155:HOH:O	2.72	0.40
1:A:284:HIS:CD2	6:B:1348:UD1:O7'	2.74	0.40
1:B:332:ARG:HH12	1:B:336:ARG:HH11	1.69	0.40
1:B:56:SER:OG	7:B:2027:HOH:O	2.22	0.40
1:B:205:HIS:O	1:B:206:LEU:HD23	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	356/374 (95%)	336 (94%)	19 (5%)	1 (0%)	36 42

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	352/374 (94%)	333 (95%)	14 (4%)	5 (1%)	9	7
1	C	352/374 (94%)	333 (95%)	19 (5%)	0	100	100
All	All	1060/1122 (94%)	1002 (94%)	52 (5%)	6 (1%)	21	23

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	48	LYS
1	B	3	GLN
1	B	49	TYR
1	B	50	ALA
1	B	197	PHE
1	B	259	ALA

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	297/309 (96%)	276 (93%)	21 (7%)	13	16
1	B	293/309 (95%)	273 (93%)	20 (7%)	14	17
1	C	293/309 (95%)	270 (92%)	23 (8%)	11	13
All	All	883/927 (95%)	819 (93%)	64 (7%)	14	15

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	LEU
1	A	17	VAL
1	A	45	ASP
1	A	46	ASN
1	A	52	HIS
1	A	65	ARG
1	A	69[A]	GLN
1	A	69[B]	GLN

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Mol	Chain	Res	Type
1	A	72[A]	ARG
1	A	72[B]	ARG
1	A	87	LEU
1	A	98	THR
1	A	123	VAL
1	A	168	ARG
1	A	193	VAL
1	A	242	LEU
1	A	266	SER
1	A	268	LYS
1	A	269	ILE
1	A	322	ARG
1	A	332	ARG
1	B	3	GLN
1	B	11	LEU
1	B	15	LEU
1	B	17	VAL
1	B	47	GLU
1	B	57[A]	GLU
1	B	57[B]	GLU
1	B	73	ASP
1	B	123	VAL
1	B	164[A]	ARG
1	B	164[B]	ARG
1	B	201	LYS
1	B	210	ILE
1	B	227	ARG
1	B	242	LEU
1	B	268	LYS
1	B	282	THR
1	B	318	GLN
1	B	322	ARG
1	B	340	LEU
1	C	15	LEU
1	C	34	GLU
1	C	38	THR
1	C	42	THR
1	C	97	ILE
1	C	98	THR
1	C	123	VAL
1	C	169	GLU
1	C	176	ARG

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Mol	Chain	Res	Type
1	C	187	SER
1	C	221	THR
1	C	225	ARG
1	C	232	VAL
1	C	242	LEU
1	C	267	THR
1	C	269	ILE
1	C	282	THR
1	C	293	MET
1	C	304	THR
1	C	315	ARG
1	C	320	ILE
1	C	326	LYS
1	C	332	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	ASN
1	A	247	HIS
1	A	253	GLN
1	A	284	HIS
1	A	290	HIS
1	A	329	ASN
1	B	134	HIS
1	B	162	HIS
1	B	247	HIS
1	B	318	GLN
1	C	134	HIS
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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

14 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	C	1349	-	4,4,4	0.21	0	6,6,6	0.23	0
2	SO4	B	1346	-	4,4,4	0.23	0	6,6,6	0.14	0
3	PLM	A	1349	-	17,17,17	0.73	0	17,17,17	0.71	0
5	BME	A	1351[B]	-	3,3,3	0.54	0	2,2,2	0.18	0
3	PLM	B	1349[A]	-	17,17,17	0.58	0	17,17,17	0.94	1 (5%)
4	EDO	A	1350	-	3,3,3	0.45	0	2,2,2	0.29	0
6	UD1	B	1348	-	40,41,41	1.21	2 (5%)	59,62,62	1.64	10 (16%)
3	PLM	B	1349[B]	-	17,17,17	0.56	0	17,17,17	0.97	1 (5%)
3	PLM	C	1351	-	17,17,17	0.61	0	17,17,17	0.73	1 (5%)
2	SO4	C	1350	-	4,4,4	0.23	0	6,6,6	0.24	0
5	BME	A	1351[A]	-	3,3,3	0.60	0	2,2,2	0.48	0
2	SO4	A	1348	-	4,4,4	0.28	0	6,6,6	0.18	0
2	SO4	B	1347	-	4,4,4	0.29	0	6,6,6	0.17	0
2	SO4	A	1347	-	4,4,4	0.19	0	6,6,6	0.39	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
3	PLM	A	1349	-	-	10/15/15/15	-
5	BME	A	1351[B]	-	-	1/1/1/1	-
3	PLM	B	1349[A]	-	-	10/15/15/15	-
4	EDO	A	1350	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	UD1	B	1348	-	-	9/26/63/63	0/3/3/3
3	PLM	C	1351	-	-	9/15/15/15	-
5	BME	A	1351[A]	-	-	1/1/1/1	-
3	PLM	B	1349[B]	-	-	13/15/15/15	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	1348	UD1	C2-N1	3.07	1.43	1.38
6	B	1348	UD1	O5'-C1'	2.62	1.48	1.41

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	1348	UD1	C4-N3-C2	-5.38	119.94	126.61
6	B	1348	UD1	C5-C4-N3	4.00	120.41	114.80
6	B	1348	UD1	N3-C2-N1	3.67	119.67	114.89
6	B	1348	UD1	O4-C4-C5	-3.43	119.25	125.16
6	B	1348	UD1	C4'-C3'-C2'	3.04	114.83	110.40
6	B	1348	UD1	C3'-C2'-N2'	-3.00	105.09	110.62
6	B	1348	UD1	O5'-C1'-O1'	2.94	115.21	111.36
6	B	1348	UD1	C1B-N1-C2	2.62	122.31	117.59
6	B	1348	UD1	C5B-C4B-C3B	-2.56	106.00	115.21
6	B	1348	UD1	O4'-C4'-C3'	-2.47	104.56	110.38
3	B	1349[A]	PLM	O1-C1-C2	2.47	121.80	114.00
3	B	1349[B]	PLM	O1-C1-C2	2.47	121.80	114.00
3	C	1351	PLM	O1-C1-O2	-2.15	117.79	123.33

There are no chirality outliers.

All (53) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1351[A]	BME	O1-C1-C2-S2
6	B	1348	UD1	C5B-O5B-PA-O1A
6	B	1348	UD1	C5B-O5B-PA-O2A
6	B	1348	UD1	C5B-O5B-PA-O3A
6	B	1348	UD1	O5'-C5'-C6'-O6'
6	B	1348	UD1	C4'-C5'-C6'-O6'
6	B	1348	UD1	C8'-C7'-N2'-C2'
6	B	1348	UD1	O7'-C7'-N2'-C2'

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Mol	Chain	Res	Type	Atoms
3	B	1349[A]	PLM	C1-C2-C3-C4
3	B	1349[B]	PLM	C1-C2-C3-C4
3	C	1351	PLM	CC-CD-CE-CF
3	C	1351	PLM	C2-C3-C4-C5
3	C	1351	PLM	C9-CA-CB-CC
3	A	1349	PLM	C2-C3-C4-C5
3	A	1349	PLM	C4-C5-C6-C7
3	A	1349	PLM	C5-C6-C7-C8
3	B	1349[A]	PLM	CB-CC-CD-CE
3	C	1351	PLM	C4-C5-C6-C7
3	C	1351	PLM	CB-CC-CD-CE
3	C	1351	PLM	CA-CB-CC-CD
3	B	1349[A]	PLM	C2-C3-C4-C5
3	B	1349[B]	PLM	C2-C3-C4-C5
3	A	1349	PLM	CD-CE-CF-CG
3	C	1351	PLM	C8-C9-CA-CB
3	A	1349	PLM	CB-CC-CD-CE
3	B	1349[B]	PLM	CB-CC-CD-CE
6	B	1348	UD1	PA-O3A-PB-O1'
3	B	1349[A]	PLM	C4-C5-C6-C7
3	B	1349[B]	PLM	C4-C5-C6-C7
3	C	1351	PLM	C6-C7-C8-C9
3	B	1349[B]	PLM	C9-CA-CB-CC
3	B	1349[B]	PLM	CD-CE-CF-CG
5	A	1351[B]	BME	O1-C1-C2-S2
3	B	1349[B]	PLM	C8-C9-CA-CB
3	B	1349[A]	PLM	CD-CE-CF-CG
3	B	1349[A]	PLM	C3-C4-C5-C6
3	B	1349[A]	PLM	CC-CD-CE-CF
3	B	1349[B]	PLM	C3-C4-C5-C6
6	B	1348	UD1	C4B-C5B-O5B-PA
3	A	1349	PLM	C6-C7-C8-C9
3	A	1349	PLM	C8-C9-CA-CB
3	A	1349	PLM	C3-C4-C5-C6
3	A	1349	PLM	O1-C1-C2-C3
3	A	1349	PLM	O2-C1-C2-C3
3	B	1349[B]	PLM	CC-CD-CE-CF
3	B	1349[B]	PLM	CA-CB-CC-CD
3	B	1349[A]	PLM	C5-C6-C7-C8
3	B	1349[B]	PLM	C5-C6-C7-C8
3	C	1351	PLM	CD-CE-CF-CG
3	B	1349[A]	PLM	O1-C1-C2-C3

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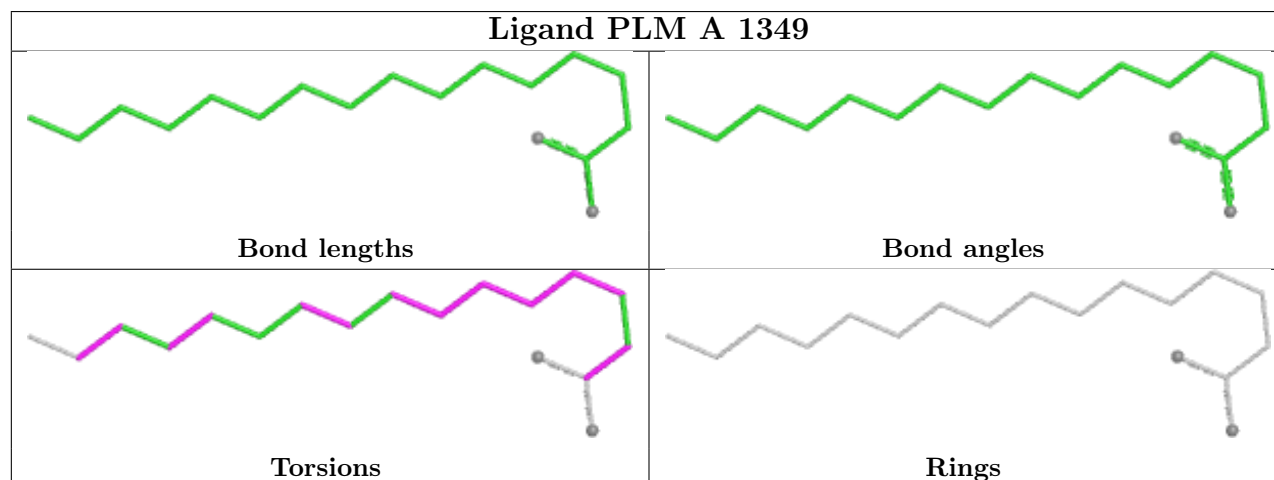
Mol	Chain	Res	Type	Atoms
3	B	1349[B]	PLM	O1-C1-C2-C3
3	B	1349[A]	PLM	O2-C1-C2-C3
3	B	1349[B]	PLM	O2-C1-C2-C3

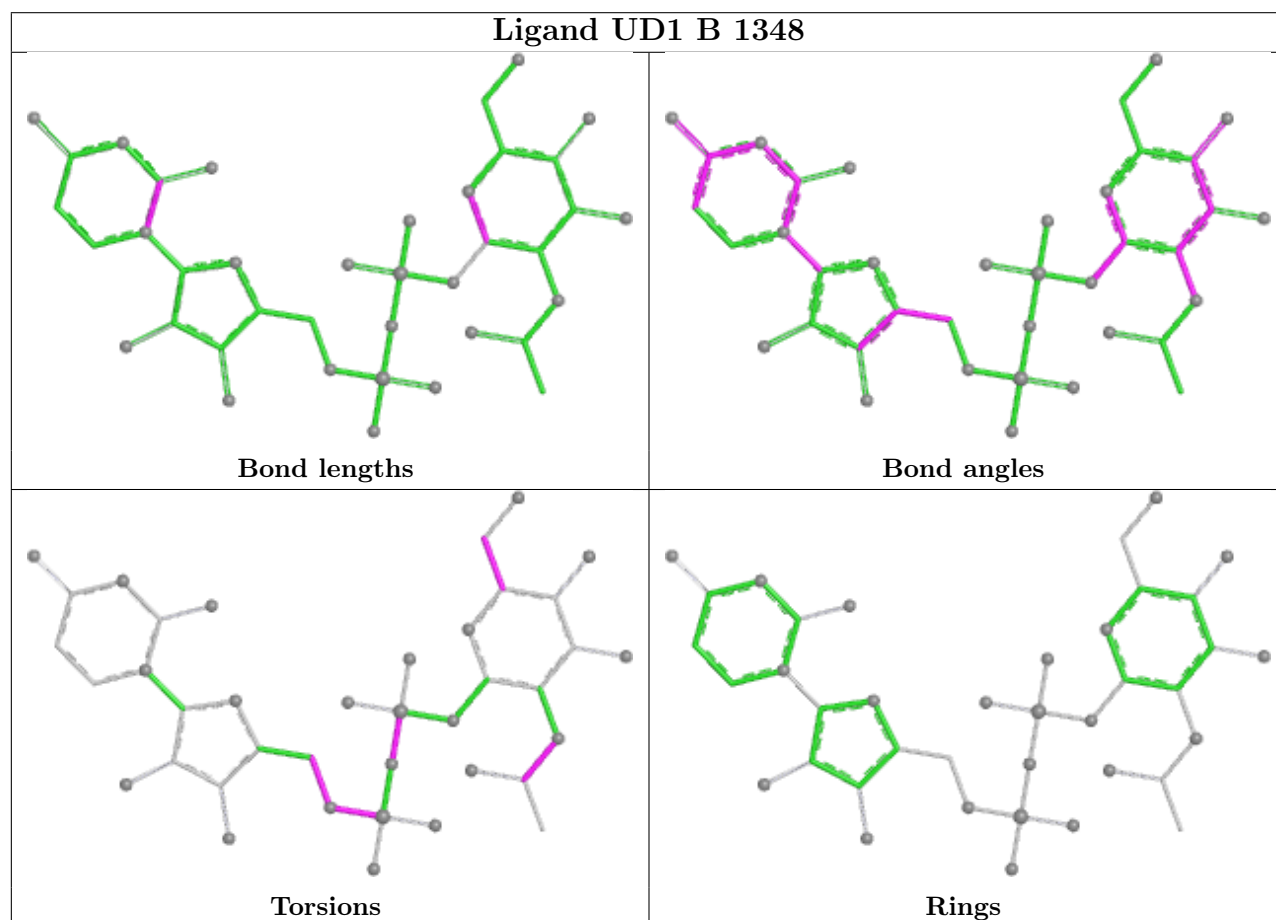
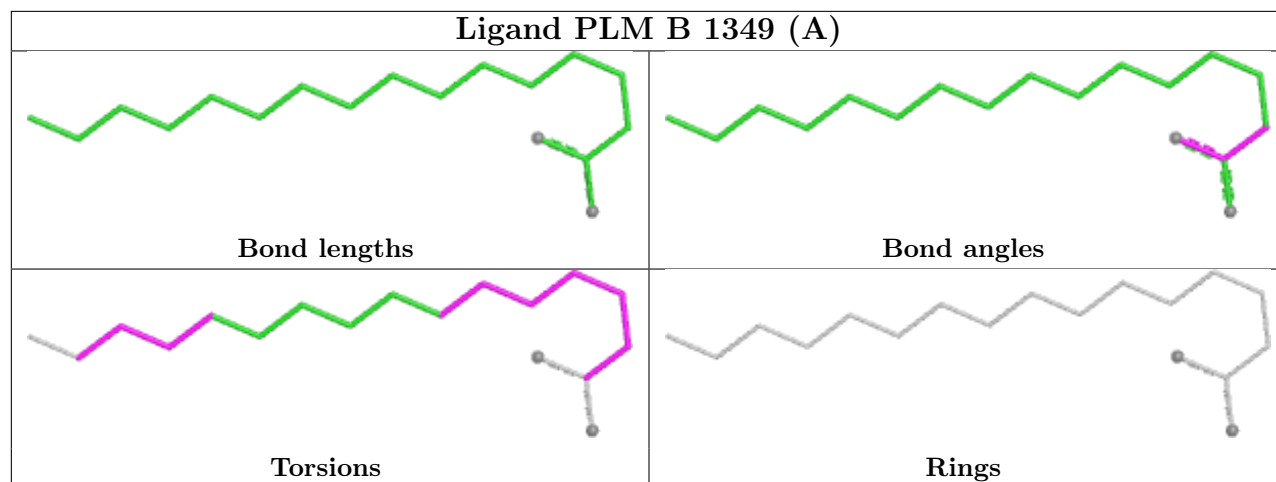
There are no ring outliers.

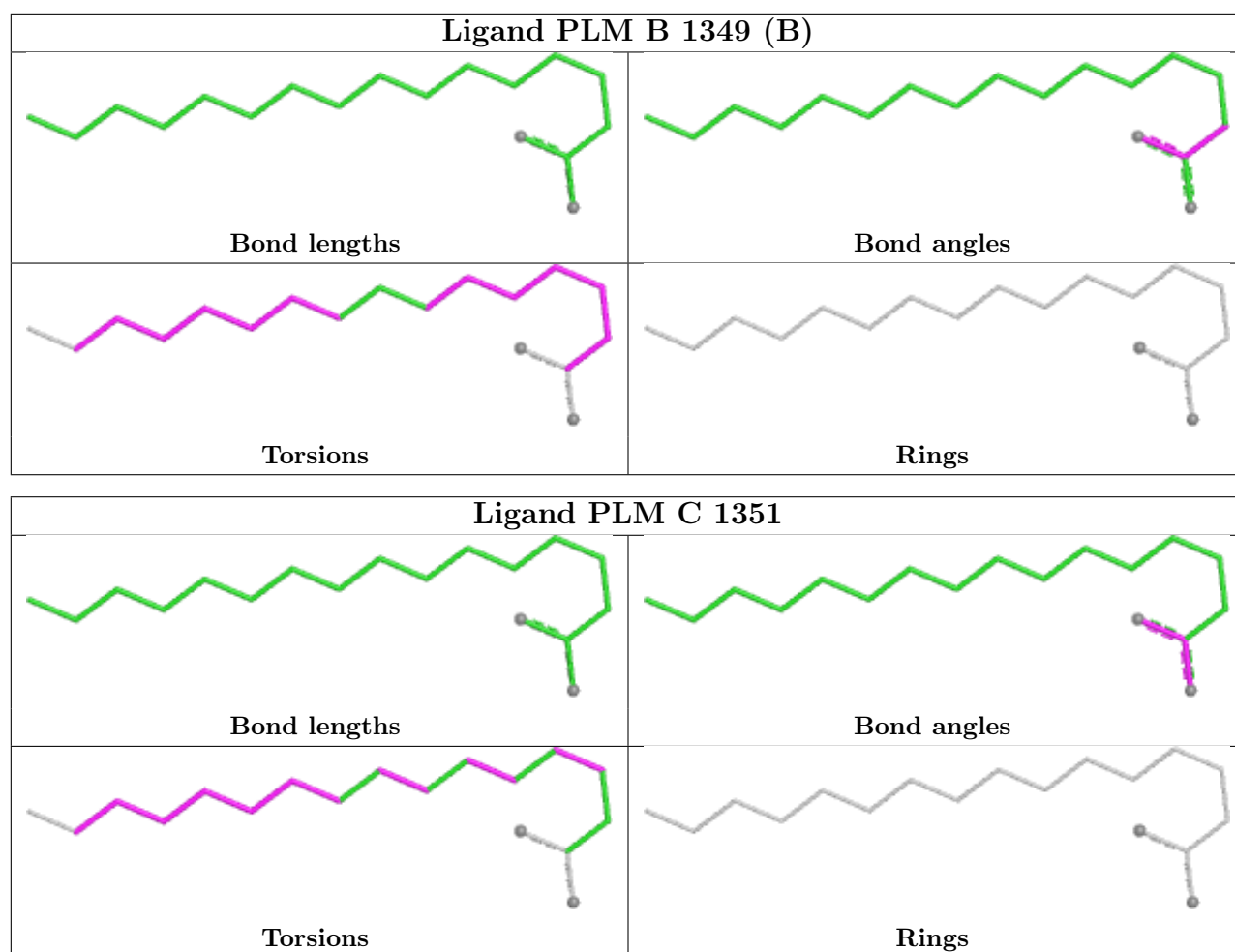
8 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1349	PLM	2	0
5	A	1351[B]	BME	2	0
6	B	1348	UD1	4	0
3	B	1349[B]	PLM	1	0
3	C	1351	PLM	8	0
2	C	1350	SO4	1	0
5	A	1351[A]	BME	1	0
2	A	1347	SO4	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	346/374 (92%)	1.26	51 (14%) 6 4	31, 62, 66, 72	12 (3%)
1	B	345/374 (92%)	1.28	53 (15%) 5 4	37, 61, 65, 78	9 (2%)
1	C	346/374 (92%)	1.33	74 (21%) 2 2	37, 62, 65, 72	8 (2%)
All	All	1037/1122 (92%)	1.29	178 (17%) 4 3	31, 61, 66, 78	29 (2%)

All (178) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	188[A]	CYS	8.1
1	A	48	LYS	6.6
1	B	46	ASN	6.0
1	B	338	ALA	5.9
1	C	347	LEU	4.9
1	B	340	LEU	4.9
1	B	198	GLY	4.7
1	C	47	GLU	4.5
1	A	46	ASN	4.3
1	A	50	ALA	4.2
1	B	197	PHE	4.2
1	B	344	VAL	4.1
1	A	49	TYR	4.0
1	A	339	ALA	4.0
1	A	1	MET	3.9
1	C	14	PHE	3.9
1	B	345	GLN	3.9
1	C	344	VAL	3.8
1	B	47	GLU	3.7
1	A	45	ASP	3.7
1	C	48	LYS	3.7
1	C	75	ASN	3.7
1	C	49	TYR	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	337	ILE	3.6
1	A	47	GLU	3.6
1	C	15	LEU	3.6
1	C	26	LEU	3.6
1	C	50	ALA	3.5
1	A	344	VAL	3.3
1	C	307	GLY	3.3
1	C	11	LEU	3.3
1	C	7	SER	3.3
1	C	196	ALA	3.3
1	C	96	PHE	3.3
1	A	36	ALA	3.3
1	B	151	ALA	3.2
1	B	164[A]	ARG	3.2
1	B	21	GLY	3.2
1	C	339	ALA	3.2
1	B	45	ASP	3.2
1	C	46	ASN	3.1
1	C	140	ALA	3.1
1	B	49	TYR	3.1
1	C	22	ASN	3.1
1	C	39	ALA	3.1
1	C	342	LYS	3.1
1	A	286[A]	CYS	3.1
1	B	252	GLY	3.1
1	B	331	PRO	3.0
1	A	340	LEU	3.0
1	C	243	VAL	3.0
1	C	198	GLY	3.0
1	B	343	LEU	2.9
1	B	141	CYS	2.9
1	C	317	TYR	2.9
1	C	197	PHE	2.9
1	C	242	LEU	2.9
1	B	1	MET	2.9
1	C	320	ILE	2.8
1	A	51	LYS	2.8
1	A	346	LYS	2.8
1	A	241	ASN	2.8
1	B	190	PHE	2.8
1	A	155	VAL	2.8
1	C	345	GLN	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	53	LEU	2.8
1	C	35	GLU	2.8
1	C	44	LEU	2.8
1	B	179	ILE	2.7
1	A	198	GLY	2.7
1	B	242	LEU	2.7
1	C	24	ALA	2.7
1	C	51	LYS	2.7
1	C	340	LEU	2.7
1	C	327	VAL	2.7
1	B	304	THR	2.6
1	B	48	LYS	2.6
1	C	62	ILE	2.6
1	C	40	HIS	2.6
1	C	57	GLU	2.6
1	C	164[A]	ARG	2.6
1	C	291	VAL	2.6
1	B	152	TYR	2.6
1	C	6	TYR	2.6
1	C	33	ILE	2.6
1	A	52	HIS	2.6
1	C	3	GLN	2.5
1	B	74	LEU	2.5
1	C	343	LEU	2.5
1	B	219	ALA	2.5
1	C	193	VAL	2.5
1	C	232	VAL	2.5
1	A	320	ILE	2.5
1	A	338	ALA	2.5
1	A	301[A]	LYS	2.5
1	C	28	SER	2.5
1	C	53	LEU	2.5
1	C	25	THR	2.5
1	A	263	ILE	2.5
1	A	269	ILE	2.5
1	C	13	ASP	2.5
1	B	50	ALA	2.5
1	C	234[A]	ARG	2.4
1	A	17	VAL	2.4
1	C	19	PHE	2.4
1	A	285	ILE	2.4
1	B	178	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	29	GLY	2.4
1	B	194	THR	2.4
1	A	139	SER	2.4
1	A	232	VAL	2.4
1	B	337	ILE	2.4
1	A	71	TYR	2.4
1	B	75[A]	ASN	2.4
1	A	43	PHE	2.4
1	B	274	ILE	2.4
1	A	203	LEU	2.4
1	C	52	HIS	2.4
1	B	218	GLY	2.4
1	A	97	ILE	2.4
1	A	189	GLY	2.3
1	A	294	MET	2.3
1	A	330	LEU	2.3
1	C	10	GLN	2.3
1	A	60	ALA	2.3
1	A	261	ALA	2.3
1	C	194	THR	2.3
1	C	55	SER	2.3
1	B	292	ILE	2.3
1	C	87	LEU	2.3
1	C	128	TYR	2.3
1	B	71	TYR	2.3
1	C	5	THR	2.3
1	A	172	SER	2.3
1	A	165	VAL	2.3
1	C	333	LEU	2.2
1	A	259	ALA	2.2
1	C	195	SER	2.2
1	A	161	ILE	2.2
1	B	223	ILE	2.2
1	B	123	VAL	2.2
1	C	89	PHE	2.2
1	A	5	THR	2.2
1	A	210	ILE	2.2
1	A	245	ILE	2.2
1	B	239	ILE	2.2
1	A	343	LEU	2.2
1	B	276	GLY	2.2
1	C	262	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	18	GLU	2.2
1	B	339	ALA	2.2
1	B	206	LEU	2.2
1	B	217	ILE	2.2
1	C	184	VAL	2.2
1	C	38	THR	2.2
1	B	67	GLN	2.1
1	A	217	ILE	2.1
1	C	245	ILE	2.1
1	B	251	VAL	2.1
1	A	72[A]	ARG	2.1
1	B	234	ARG	2.1
1	C	60	ALA	2.1
1	C	256	MET	2.1
1	B	73	ASP	2.1
1	B	317	TYR	2.1
1	C	189	GLY	2.1
1	B	297	THR	2.1
1	C	4	SER	2.1
1	C	346	LYS	2.1
1	C	192	TYR	2.1
1	A	183	ALA	2.0
1	A	334	GLU	2.0
1	B	341	GLU	2.0
1	B	258	VAL	2.0
1	B	221	THR	2.0
1	B	11	LEU	2.0
1	B	275	ILE	2.0
1	C	185	ILE	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands

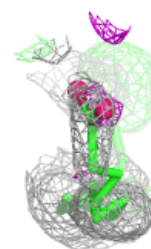
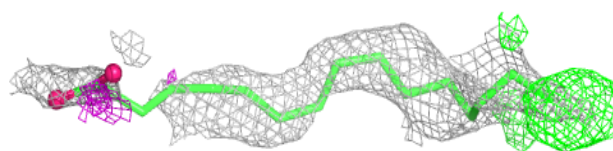
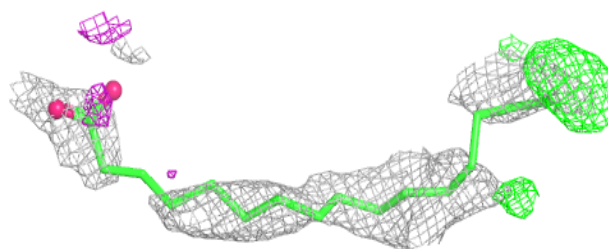
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	PLM	B	1349[A]	18/18	0.71	0.35	52,60,69,70	7
3	PLM	B	1349[B]	18/18	0.71	0.35	57,60,69,70	7
2	SO4	A	1348	5/5	0.75	0.15	66,67,68,68	5
6	UD1	B	1348	39/39	0.82	0.24	56,70,73,74	39
3	PLM	C	1351	18/18	0.83	0.20	70,72,77,77	0
3	PLM	A	1349	18/18	0.83	0.21	54,61,69,69	0
4	EDO	A	1350	4/4	0.90	0.09	61,63,65,66	0
2	SO4	B	1346	5/5	0.91	0.09	79,79,80,80	0
2	SO4	C	1349	5/5	0.91	0.11	77,78,78,78	0
2	SO4	A	1347	5/5	0.92	0.08	70,70,71,72	0
2	SO4	C	1350	5/5	0.92	0.12	71,72,72,73	5
2	SO4	B	1347	5/5	0.93	0.20	49,49,50,50	5
5	BME	A	1351[B]	4/4	0.94	0.08	73,75,76,77	4
5	BME	A	1351[A]	4/4	0.94	0.08	37,40,41,46	4

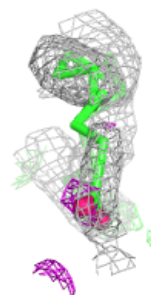
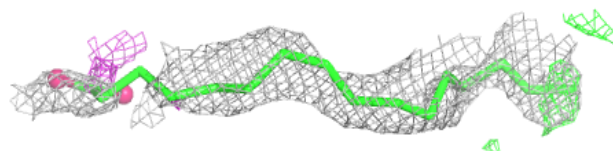
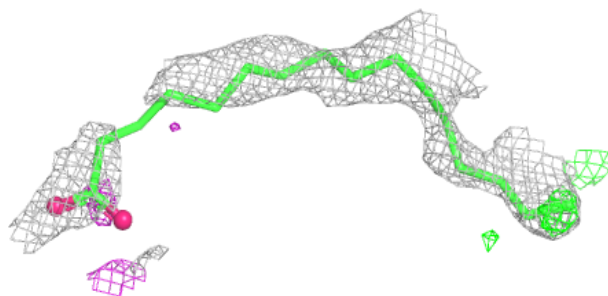
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around PLM B 1349 (A):

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

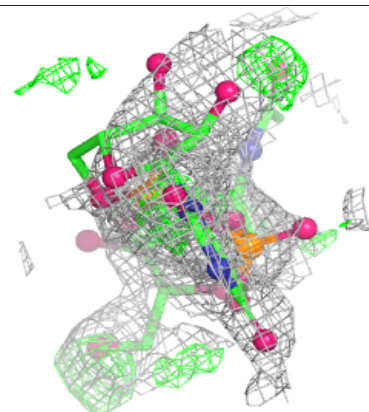
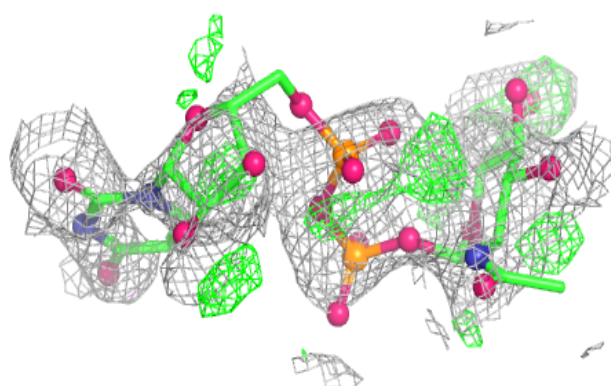
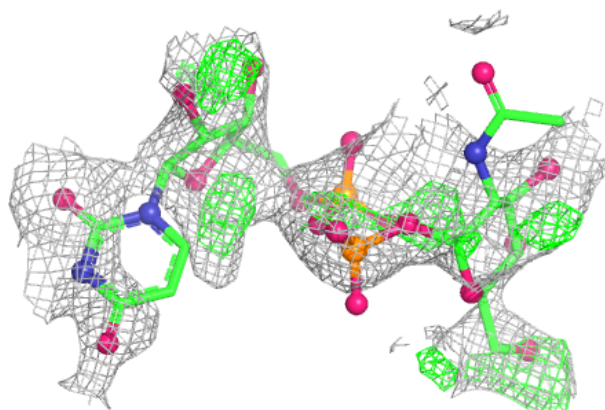
**Electron density around PLM B 1349 (B):**

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

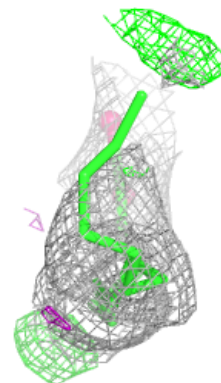
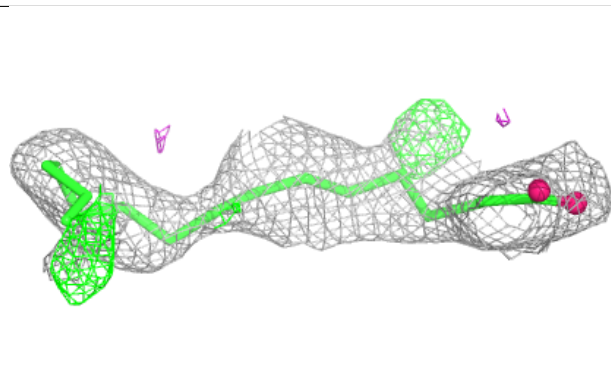
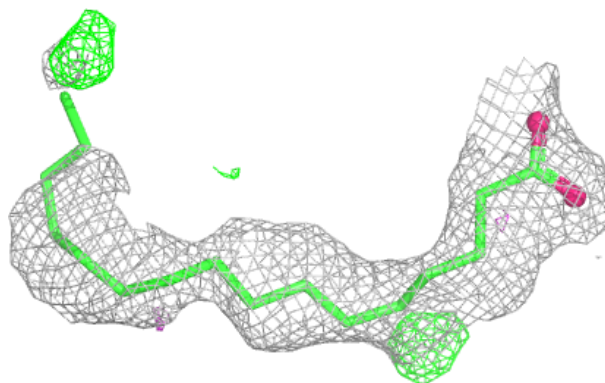


Electron density around UD1 B 1348:

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

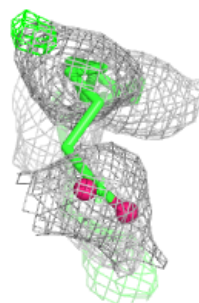
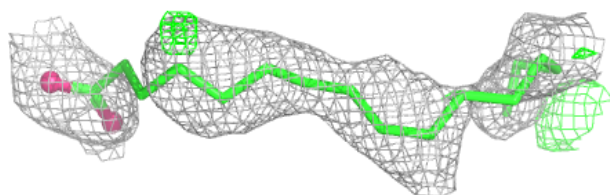
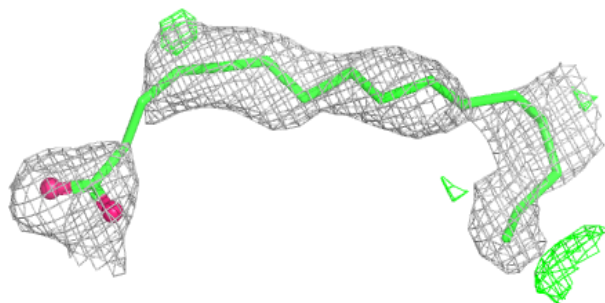
**Electron density around PLM C 1351:**

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



Electron density around PLM A 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 [i](#)

There are no such residues in this entry.