



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:09 PM UTC

PDB ID : 2IU9 / pdb_00002iu9
Title : Chlamydia trachomatis LpxD with 100mM UDPGlcNAc (Complex II)
Authors : Buetow, L.; Smith, T.K.; Dawson, A.; Fyffe, S.; Hunter, W.N.
Deposited on : 2006-05-30
Resolution : 3.10 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

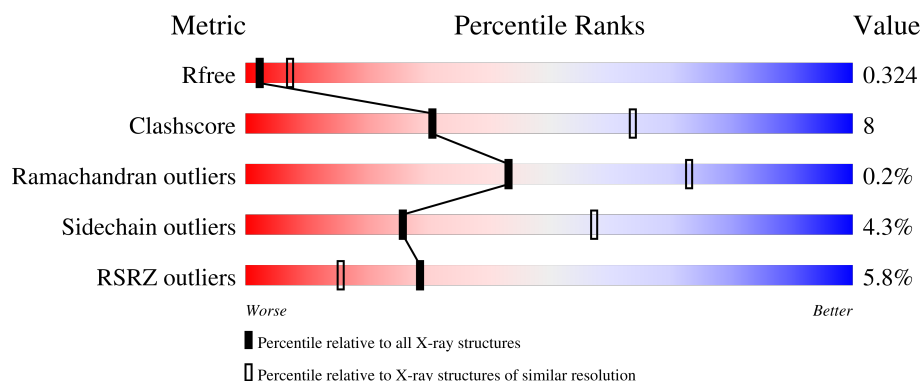
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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	374	 2% 74% 17% • 7%
1	B	374	 6% 76% 15% • 8%
1	C	374	 7% 77% 15% • 7%

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
4	PLM	C	1352	-	-	-	X

2 Entry composition [i](#)

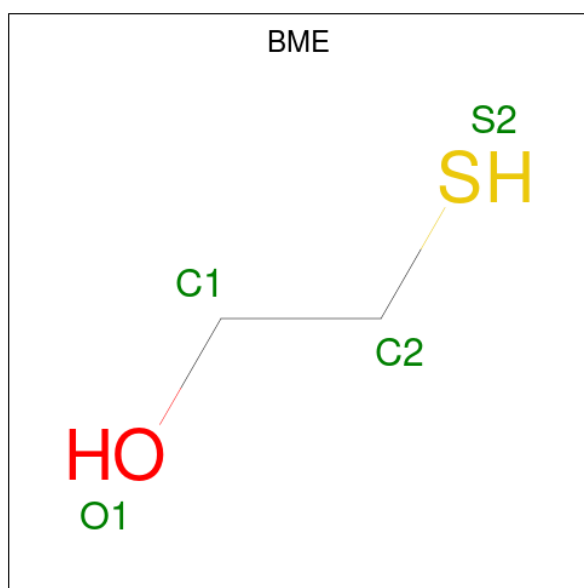
There are 6 unique types of molecules in this entry. The entry contains 8271 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
			2675	1688	480	495	12			
1	B	345	Total	C	N	O	S	0	7	0
			2665	1682	476	497	10			
1	C	346	Total	C	N	O	S	0	5	0
			2666	1684	479	493	10			

- Molecule 2 is BETA-MERCAPTOETHANOL (CCD ID: BME) (formula: C₂H₆OS).



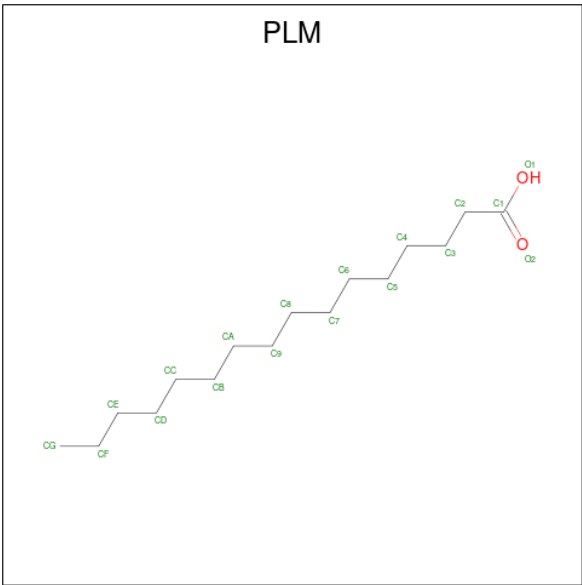
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



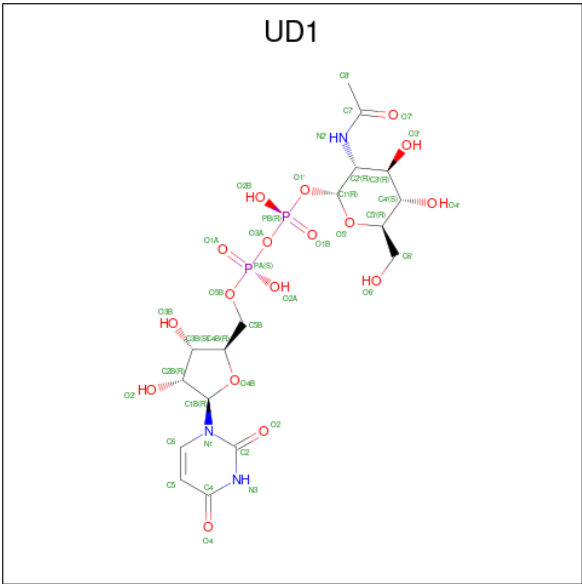
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is PALMITIC ACID (CCD ID: PLM) (formula: C₁₆H₃₂O₂).



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

- Molecule 5 is URIDINE-DIPHOSPHATE-N-ACETYLGLUCOSAMINE (CCD ID: UD1) (formula: C₁₇H₂₇N₃O₁₇P₂).



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

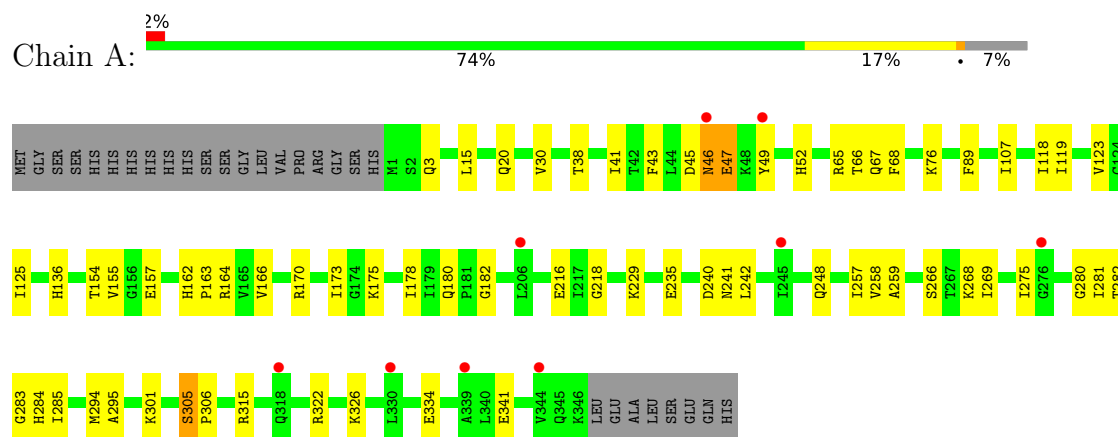
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	47	Total	O	0	0
			47	47		
6	B	32	Total	O	0	0
			32	32		
6	C	20	Total	O	0	0
			20	20		

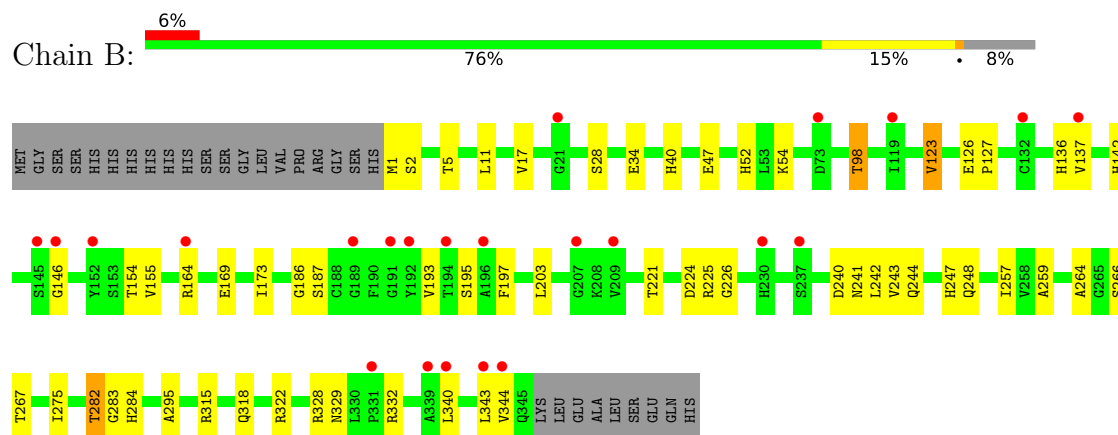
3 Residue-property plots

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.

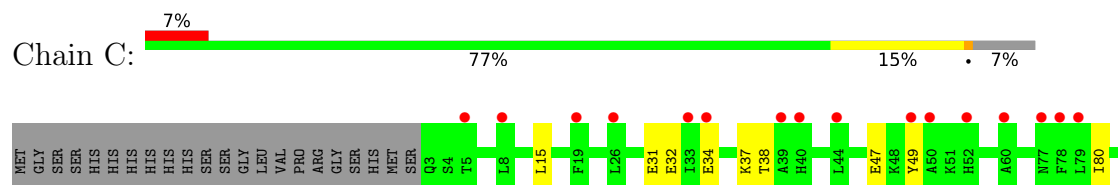
• Molecule 1: UDP-3-O-[3-HYDROXYMYRISTOYL] GLUCOSAMINE N-ACYLTRANSFERASE

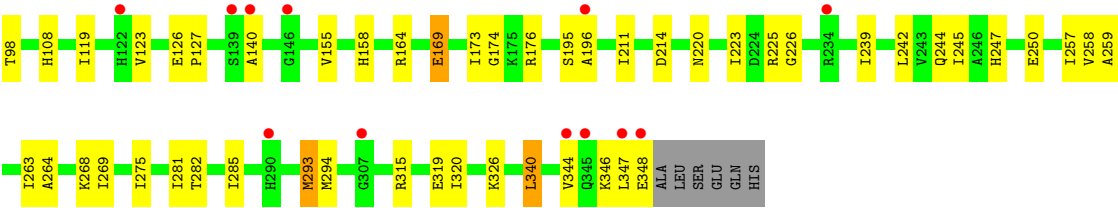


• Molecule 1: UDP-3-O-[3-HYDROXYMYRISTOYL] GLUCOSAMINE N-ACYLTRANSFERASE



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





4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	98.87Å 98.87Å 283.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.50 – 3.10 28.50 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.0 (28.50-3.10) 98.8 (28.50-3.10)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.72 (at 3.11Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.221 , 0.281 0.279 , 0.324	Depositor DCC
R_{free} test set	1323 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	80.4	Xtriage
Anisotropy	0.036	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 35.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.37$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	8271	wwPDB-VP
Average B, all atoms (Å ²)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.42% 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, UD1, BME, SO4

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	0.45	0/2758	0.78	0/3729
1	B	0.45	0/2744	0.81	1/3712 (0.0%)
1	C	0.49	1/2737 (0.0%)	0.79	0/3702
All	All	0.46	1/8239 (0.0%)	0.79	1/11143 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	348	GLU	C-O	6.99	1.37	1.23

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	40	HIS	N-CA-C	5.18	118.19	109.95

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	2675	0	2695	61	0
1	B	2665	0	2680	49	0
1	C	2666	0	2688	52	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	4	0	6	0	0
3	A	10	0	0	1	0
3	B	10	0	0	0	0
3	C	10	0	0	0	0
4	A	18	0	31	3	0
4	B	18	0	31	3	0
4	C	18	0	31	8	0
5	B	39	0	25	1	0
5	C	39	0	25	8	0
6	A	47	0	0	1	0
6	B	32	0	0	1	0
6	C	20	0	0	0	0
All	All	8271	0	8212	136	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 8.

All (136) 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	1.71	1.19
1:A:164[A]:ARG:CD	1:C:164[A]:ARG:HG2	1.89	1.02
1:A:164[A]:ARG:NE	1:C:164[A]:ARG:HE	1.61	0.97
1:A:164[A]:ARG:HD2	1:C:164[A]:ARG:HG2	0.97	0.96
1:B:164[A]:ARG:HB2	1:C:164[A]:ARG:HD2	1.48	0.96
1:B:164[B]:ARG:HG2	1:B:164[B]:ARG:HH11	1.30	0.94
1:A:164[A]:ARG:HG2	1:B:164[A]:ARG:HD2	1.53	0.90
1:A:46:ASN:HA	1:A:67:GLN:HE22	1.36	0.89
1:A:164[A]:ARG:HH21	1:B:164[A]:ARG:NH2	1.70	0.89
1:A:164[A]:ARG:NH2	1:C:164[A]:ARG:HH21	1.74	0.86
1:B:169:GLU:O	1:B:225:ARG:NH2	2.08	0.86
1:A:164[A]:ARG:HH21	1:B:164[A]:ARG:HH21	1.28	0.79
1:B:284:HIS:CD2	5:C:1351:UD1:H8'2	2.23	0.73
1:B:283:GLY:HA3	5:C:1351:UD1:H8'1	1.71	0.72
1:A:164[A]:ARG:HE	1:B:164[A]:ARG:NE	1.88	0.71
4:A:1350:PLM:HC1	1:B:295:ALA:HB3	1.71	0.70
1:B:257:ILE:HG12	1:B:275:ILE:HD12	1.72	0.70
1:B:248:GLN:O	1:B:266:SER:HA	1.92	0.69
1:A:164[A]:ARG:NE	1:C:164[A]:ARG:NE	2.39	0.69
1:B:247:HIS:HE2	5:C:1351:UD1:HO3'	1.42	0.67
1:B:247:HIS:NE2	5:C:1351:UD1:O3'	2.27	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:294:MET:HA	1:C:294:MET:HE2	1.76	0.66
1:A:45:ASP:O	1:A:47:GLU:N	2.27	0.66
1:B:164[B]:ARG:HG2	1:B:164[B]:ARG:NH1	2.06	0.65
1:C:257:ILE:HG12	1:C:275:ILE:HD12	1.80	0.64
1:A:164[A]:ARG:HD2	1:C:164[A]:ARG:CD	2.27	0.64
1:A:294:MET:HE2	4:C:1352:PLM:HE1	1.78	0.63
1:A:258:VAL:HG12	1:A:259:ALA:H	1.63	0.63
1:A:164[A]:ARG:CZ	1:C:164[A]:ARG:HE	2.11	0.62
1:A:170:ARG:NH2	1:B:98:THR:O	2.33	0.62
1:B:283:GLY:HA3	5:C:1351:UD1:C8'	2.29	0.62
1:A:178:ILE:HB	1:A:216:GLU:HG2	1.81	0.62
4:A:1350:PLM:HE2	1:B:295:ALA:H	1.65	0.61
1:A:281:ILE:HG23	1:A:285:ILE:HD11	1.82	0.61
1:C:263:ILE:HG12	1:C:281:ILE:HD12	1.84	0.60
1:B:264:ALA:HA	4:B:1348:PLM:H21	1.83	0.59
1:A:295:ALA:HB2	4:C:1352:PLM:H92	1.84	0.59
1:A:164[A]:ARG:CD	1:C:164[A]:ARG:HE	2.16	0.58
1:A:258:VAL:HG12	1:A:259:ALA:N	2.19	0.58
1:C:126:GLU:HB3	1:C:127:PRO:CD	2.34	0.58
1:A:162:HIS:HB3	1:A:163:PRO:CD	2.34	0.57
1:B:136:HIS:HB3	1:B:154:THR:HG22	1.85	0.57
1:B:1:MET:HG3	1:B:2:SER:H	1.70	0.57
1:A:157:GLU:HG2	1:A:175:LYS:HD3	1.87	0.57
1:C:37:LYS:HG2	1:C:38:THR:H	1.70	0.57
1:C:37:LYS:HG2	1:C:38:THR:N	2.20	0.56
1:B:164[A]:ARG:HH21	1:C:164[A]:ARG:NH2	2.03	0.55
1:A:164[A]:ARG:HE	1:B:164[A]:ARG:HE	1.53	0.55
1:C:264:ALA:HB2	4:C:1352:PLM:H82	1.89	0.55
1:B:247:HIS:CE1	5:C:1351:UD1:HO3'	2.24	0.55
1:A:282:THR:HG22	1:A:283:GLY:N	2.22	0.54
1:B:155:VAL:HA	1:B:173:ILE:HB	1.89	0.54
1:C:226:GLY:HA2	1:C:247:HIS:HB2	1.90	0.53
1:B:329:ASN:HD21	1:B:332:ARG:HD3	1.73	0.53
1:C:119:ILE:CG2	1:C:123:VAL:HG11	2.39	0.53
1:B:195:SER:C	1:B:197:PHE:H	2.17	0.53
1:B:284:HIS:HD2	5:C:1351:UD1:H8'2	1.72	0.52
1:B:187:SER:OG	1:B:224:ASP:OD1	2.26	0.52
1:B:126:GLU:HB3	1:B:127:PRO:HD2	1.92	0.52
1:A:269:ILE:HG12	1:A:275:ILE:HD11	1.92	0.51
4:B:1348:PLM:H31	1:C:259:ALA:HB3	1.92	0.51
1:A:229:LYS:HB2	1:A:248:GLN:HG3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:257:ILE:HG12	1:A:275:ILE:HD12	1.92	0.50
1:B:123:VAL:HG21	1:B:137:VAL:HG11	1.94	0.50
1:B:146:GLY:HA3	1:B:164[B]:ARG:CZ	2.41	0.50
1:C:155:VAL:HA	1:C:173:ILE:HB	1.93	0.50
1:A:164[A]:ARG:HG2	1:B:164[A]:ARG:CD	2.36	0.50
1:A:43:PHE:CE1	1:A:45:ASP:HB2	2.46	0.49
1:A:322:ARG:O	1:A:326:LYS:HG2	2.12	0.49
1:C:282:THR:HG22	4:C:1352:PLM:H91	1.94	0.49
1:A:166:VAL:CG2	1:B:164[A]:ARG:HG2	2.43	0.49
1:A:162:HIS:HB3	1:A:163:PRO:HD2	1.94	0.48
1:B:186:GLY:O	1:B:225:ARG:NH1	2.46	0.48
1:A:49:TYR:HA	1:A:52:HIS:CD2	2.49	0.48
1:C:281:ILE:HG22	1:C:285:ILE:HD11	1.96	0.48
1:A:341:GLU:HG2	1:C:340:LEU:HD21	1.94	0.48
1:C:223:ILE:HG12	1:C:245:ILE:HB	1.96	0.47
1:C:126:GLU:HB3	1:C:127:PRO:HD2	1.97	0.47
1:C:31:GLU:HG3	1:C:32:GLU:N	2.30	0.47
1:A:248:GLN:O	1:A:266:SER:HA	2.15	0.46
1:C:244:GLN:HG2	4:C:1352:PLM:H31	1.97	0.46
1:A:334:GLU:OE2	1:C:326:LYS:HD2	2.15	0.46
1:C:195:SER:OG	1:C:196:ALA:N	2.48	0.46
1:B:247:HIS:CE1	5:C:1351:UD1:O3'	2.69	0.46
1:A:164[A]:ARG:CZ	1:C:164[A]:ARG:HH21	2.28	0.46
1:A:280:GLY:C	4:A:1350:PLM:H92	2.41	0.46
1:C:108:HIS:CD2	1:C:127:PRO:HG3	2.51	0.46
1:C:119:ILE:HG22	1:C:123:VAL:HG11	1.98	0.46
1:C:239:ILE:HG12	1:C:257:ILE:HD12	1.98	0.45
1:C:344:VAL:C	1:C:346:LYS:H	2.25	0.45
1:C:264:ALA:HB3	1:C:282:THR:C	2.42	0.45
1:A:136:HIS:HB3	1:A:154:THR:HG22	1.97	0.45
1:C:174:GLY:N	1:C:211:ILE:O	2.50	0.44
1:A:240:ASP:CG	1:A:241:ASN:H	2.26	0.44
1:A:65:ARG:HB2	3:A:1348:SO4:O1	2.17	0.44
1:C:140:ALA:O	1:C:158:HIS:HA	2.17	0.44
1:C:47:GLU:C	1:C:49:TYR:H	2.25	0.44
1:B:244:GLN:CG	4:B:1348:PLM:H22	2.48	0.44
1:B:193:VAL:HG23	1:B:203:LEU:HD21	2.00	0.43
1:C:315:ARG:HB2	1:C:320:ILE:HG23	2.01	0.43
1:A:119:ILE:CG2	1:A:123:VAL:HG21	2.49	0.43
1:A:155:VAL:HA	1:A:173:ILE:HB	1.99	0.43
1:A:295:ALA:H	4:C:1352:PLM:HC2	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:264:ALA:HA	4:C:1352:PLM:H22	1.99	0.43
1:A:43:PHE:HD2	1:A:89:PHE:CD1	2.37	0.43
1:A:166:VAL:HG21	1:B:164[A]:ARG:HG2	2.00	0.43
1:A:107:ILE:HG23	1:A:125:ILE:HB	2.00	0.42
1:A:282:THR:HG22	1:A:283:GLY:H	1.83	0.42
1:A:118:ILE:HB	1:A:136:HIS:HD2	1.84	0.42
1:A:30:VAL:HG12	1:A:41:ILE:HB	2.00	0.42
1:B:34[A]:GLU:HG3	1:B:52:HIS:CD2	2.55	0.42
1:C:220:ASN:HB2	1:C:242:LEU:HD12	2.01	0.42
1:B:5:THR:HG23	1:B:28:SER:HB3	2.02	0.42
1:C:250:GLU:HB3	1:C:268:LYS:HG2	2.01	0.42
1:A:295:ALA:CB	4:C:1352:PLM:H92	2.49	0.42
1:B:282:THR:HG22	1:B:283:GLY:H	1.84	0.42
1:C:258:VAL:HG12	1:C:259:ALA:N	2.35	0.42
1:B:142:HIS:HD2	6:B:2010:HOH:O	2.02	0.41
1:B:226:GLY:HA2	1:B:247:HIS:HB2	2.01	0.41
1:B:241:ASN:O	1:B:243:VAL:HG23	2.20	0.41
1:C:281:ILE:HD11	1:C:293:MET:HE3	2.02	0.41
1:A:164[A]:ARG:HD2	1:C:164[A]:ARG:NE	2.35	0.41
1:A:284:HIS:NE2	5:B:1347:UD1:O2B	2.53	0.41
1:C:176:ARG:HD2	1:C:214:ASP:OD1	2.20	0.41
1:C:275:ILE:HG12	1:C:293:MET:HE2	2.03	0.41
1:A:164[A]:ARG:CD	1:C:164[A]:ARG:NE	2.82	0.41
1:A:305:SER:HA	1:A:306:PRO:HD3	1.88	0.41
1:A:20:GLN:HG3	1:A:68:PHE:CZ	2.56	0.40
1:B:240:ASP:HB3	1:B:259:ALA:N	2.36	0.40
1:B:315:ARG:HA	1:B:315:ARG:HD2	1.87	0.40
1:A:180:GLN:HB2	1:A:218:GLY:C	2.46	0.40
1:A:315:ARG:HG3	6:A:2047:HOH:O	2.21	0.40
1:B:164[B]:ARG:NH1	1:B:164[B]:ARG:CG	2.78	0.40
1:B:164[B]:ARG:HD3	1:C:164[B]:ARG:HE	1.69	0.40
1:C:169:GLU:H	1:C:169:GLU:HG3	1.63	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	352/374 (94%)	333 (95%)	17 (5%)	2 (1%)	21	52
1	B	350/374 (94%)	325 (93%)	25 (7%)	0	100	100
1	C	349/374 (93%)	332 (95%)	17 (5%)	0	100	100
All	All	1051/1122 (94%)	990 (94%)	59 (6%)	2 (0%)	43	73

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	46	ASN
1	A	47	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%)	283 (97%)	10 (3%)	32	63
1	B	291/309 (94%)	275 (94%)	16 (6%)	19	50
1	C	290/309 (94%)	279 (96%)	11 (4%)	29	60
All	All	874/927 (94%)	837 (96%)	37 (4%)	26	58

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	15	LEU
1	A	38	THR
1	A	66	THR
1	A	76	LYS
1	A	235	GLU
1	A	242	LEU

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Mol	Chain	Res	Type
1	A	268	LYS
1	A	301	LYS
1	A	305	SER
1	B	11	LEU
1	B	17	VAL
1	B	47	GLU
1	B	54	LYS
1	B	98	THR
1	B	123	VAL
1	B	221	THR
1	B	242	LEU
1	B	267	THR
1	B	282	THR
1	B	318	GLN
1	B	322	ARG
1	B	328	ARG
1	B	340	LEU
1	B	343	LEU
1	B	344	VAL
1	C	15	LEU
1	C	34	GLU
1	C	80	ILE
1	C	98	THR
1	C	169	GLU
1	C	225	ARG
1	C	269	ILE
1	C	293	MET
1	C	319	GLU
1	C	340	LEU
1	C	347	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	52	HIS
1	A	67	GLN
1	A	133	GLN
1	A	134	HIS
1	A	142	HIS
1	A	200	HIS
1	A	253	GLN
1	B	20	GLN

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Mol	Chain	Res	Type
1	B	52	HIS
1	B	133	GLN
1	B	134	HIS
1	B	162	HIS
1	B	202	HIS
1	B	290	HIS
1	B	329	ASN
1	C	10	GLN
1	C	134	HIS
1	C	260	GLN
1	C	272	HIS
1	C	318	GLN
1	C	345	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	$\# Z > 2$
4	PLM	C	1352	-	17,17,17	0.57	0	17,17,17	0.83	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	UD1	C	1351	-	40,41,41	1.12	2 (5%)	59,62,62	1.55	5 (8%)
5	UD1	B	1347	-	40,41,41	1.01	1 (2%)	59,62,62	1.56	9 (15%)
4	PLM	A	1350	-	17,17,17	0.57	0	17,17,17	0.77	0
3	SO4	C	1349	-	4,4,4	0.24	0	6,6,6	0.07	0
3	SO4	B	1346	-	4,4,4	0.25	0	6,6,6	0.15	0
2	BME	A	1347	-	3,3,3	0.33	0	2,2,2	0.67	0
3	SO4	C	1350	-	4,4,4	0.22	0	6,6,6	0.14	0
4	PLM	B	1348	-	17,17,17	0.54	0	17,17,17	0.90	1 (5%)
3	SO4	A	1348	-	4,4,4	0.25	0	6,6,6	0.08	0
3	SO4	A	1349	-	4,4,4	0.21	0	6,6,6	0.13	0
3	SO4	B	1351	-	4,4,4	0.26	0	6,6,6	0.09	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	C	1352	-	-	10/15/15/15	-
5	UD1	C	1351	-	-	7/26/63/63	0/3/3/3
5	UD1	B	1347	-	-	11/26/63/63	0/3/3/3
4	PLM	A	1350	-	-	11/15/15/15	-
2	BME	A	1347	-	-	0/1/1/1	-
4	PLM	B	1348	-	-	14/15/15/15	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	1351	UD1	O5'-C1'	2.61	1.48	1.41
5	B	1347	UD1	C8'-C7'	2.44	1.55	1.50
5	C	1351	UD1	PB-O3A	2.39	1.62	1.59

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1347	UD1	C4-N3-C2	-5.34	119.98	126.61
5	C	1351	UD1	C4-N3-C2	-5.05	120.35	126.61
5	C	1351	UD1	O5'-C1'-O1'	4.88	117.74	111.36
5	B	1347	UD1	C5-C4-N3	3.99	120.39	114.80
5	C	1351	UD1	C5-C4-N3	3.73	120.02	114.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	1351	UD1	N3-C2-N1	3.65	119.64	114.89
5	B	1347	UD1	N3-C2-N1	3.61	119.59	114.89
5	B	1347	UD1	O5'-C5'-C4'	3.39	115.81	109.70
5	B	1347	UD1	O4-C4-C5	-3.18	119.68	125.16
5	C	1351	UD1	O4-C4-C5	-3.13	119.77	125.16
5	B	1347	UD1	C4B-O4B-C1B	-2.51	103.92	109.47
5	B	1347	UD1	C4'-C3'-C2'	2.26	113.69	110.40
5	B	1347	UD1	O4B-C1B-C2B	-2.22	101.86	106.62
4	B	1348	PLM	O1-C1-C2	2.21	121.00	114.00
4	C	1352	PLM	O1-C1-O2	-2.16	117.77	123.33
5	B	1347	UD1	C5B-C4B-C3B	-2.08	107.71	115.21

There are no chirality outliers.

All (53) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	1347	UD1	C1'-O1'-PB-O3A
5	B	1347	UD1	O4B-C4B-C5B-O5B
5	B	1347	UD1	C5B-O5B-PA-O1A
5	B	1347	UD1	C5B-O5B-PA-O3A
5	B	1347	UD1	PA-O3A-PB-O1'
5	C	1351	UD1	O5'-C1'-O1'-PB
5	C	1351	UD1	O4B-C4B-C5B-O5B
5	C	1351	UD1	C5B-O5B-PA-O1A
5	B	1347	UD1	C3B-C4B-C5B-O5B
5	C	1351	UD1	C4'-C5'-C6'-O6'
5	B	1347	UD1	C8'-C7'-N2'-C2'
5	B	1347	UD1	O7'-C7'-N2'-C2'
5	C	1351	UD1	C4B-C5B-O5B-PA
4	C	1352	PLM	C1-C2-C3-C4
5	C	1351	UD1	C3B-C4B-C5B-O5B
4	B	1348	PLM	C1-C2-C3-C4
4	B	1348	PLM	C5-C6-C7-C8
4	A	1350	PLM	C3-C4-C5-C6
4	C	1352	PLM	C2-C3-C4-C5
4	C	1352	PLM	CA-CB-CC-CD
4	B	1348	PLM	CA-CB-CC-CD
4	C	1352	PLM	C4-C5-C6-C7
5	C	1351	UD1	O5'-C5'-C6'-O6'
4	C	1352	PLM	C8-C9-CA-CB
4	A	1350	PLM	C1-C2-C3-C4
4	B	1348	PLM	C9-CA-CB-CC

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Mol	Chain	Res	Type	Atoms
4	A	1350	PLM	C5-C6-C7-C8
4	C	1352	PLM	CC-CD-CE-CF
4	B	1348	PLM	CC-CD-CE-CF
4	A	1350	PLM	CA-CB-CC-CD
4	A	1350	PLM	C2-C3-C4-C5
4	B	1348	PLM	C6-C7-C8-C9
4	A	1350	PLM	C8-C9-CA-CB
4	B	1348	PLM	C4-C5-C6-C7
4	C	1352	PLM	C6-C7-C8-C9
4	C	1352	PLM	C3-C4-C5-C6
4	C	1352	PLM	CD-CE-CF-CG
5	B	1347	UD1	C1'-O1'-PB-O2B
4	C	1352	PLM	C9-CA-CB-CC
4	B	1348	PLM	C3-C4-C5-C6
4	A	1350	PLM	CB-CC-CD-CE
5	B	1347	UD1	C5B-O5B-PA-O2A
4	A	1350	PLM	C7-C8-C9-CA
5	B	1347	UD1	C4B-C5B-O5B-PA
4	B	1348	PLM	C8-C9-CA-CB
4	B	1348	PLM	C2-C3-C4-C5
4	B	1348	PLM	CD-CE-CF-CG
4	B	1348	PLM	O1-C1-C2-C3
4	B	1348	PLM	O2-C1-C2-C3
4	A	1350	PLM	C9-CA-CB-CC
4	A	1350	PLM	CC-CD-CE-CF
4	A	1350	PLM	C4-C5-C6-C7
4	B	1348	PLM	CB-CC-CD-CE

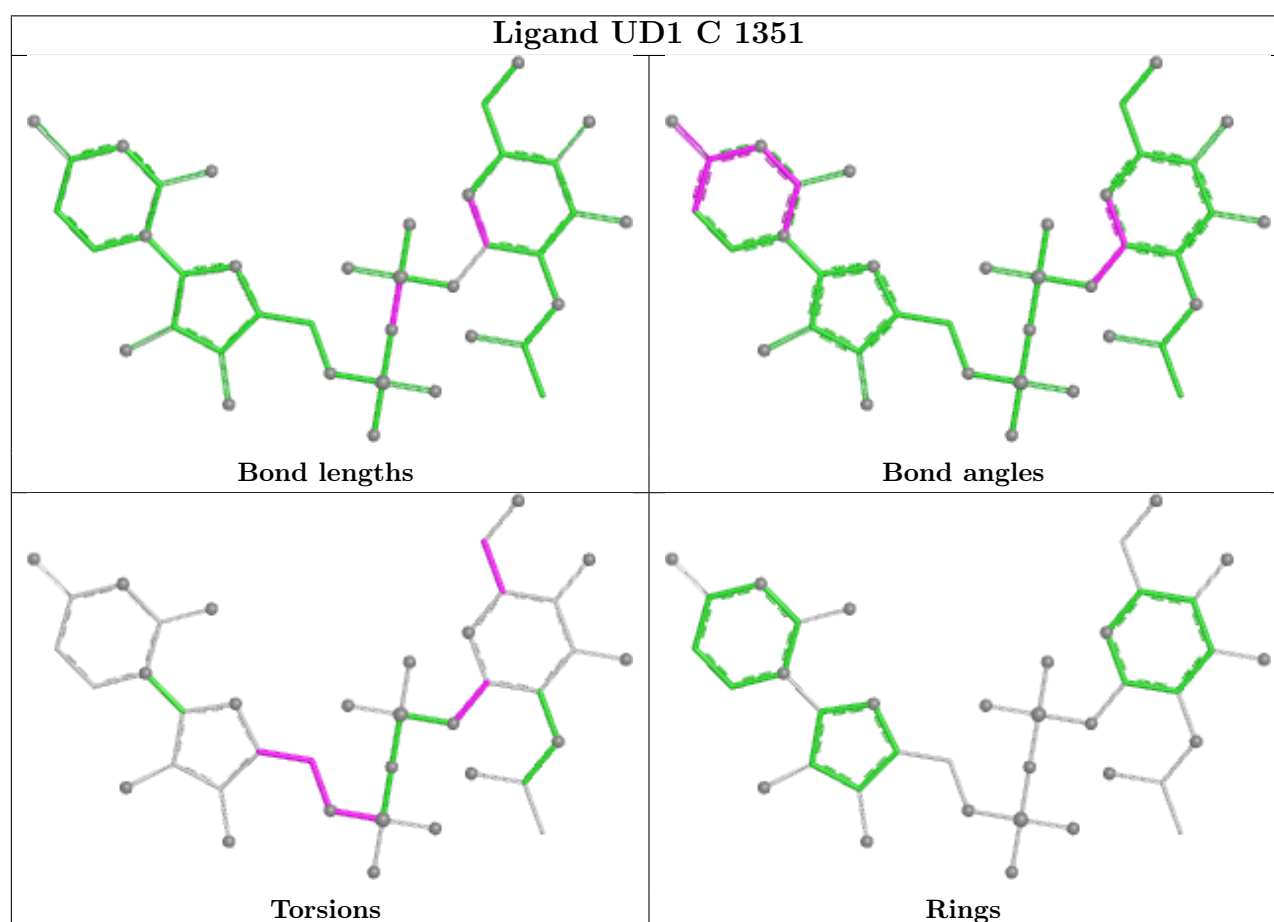
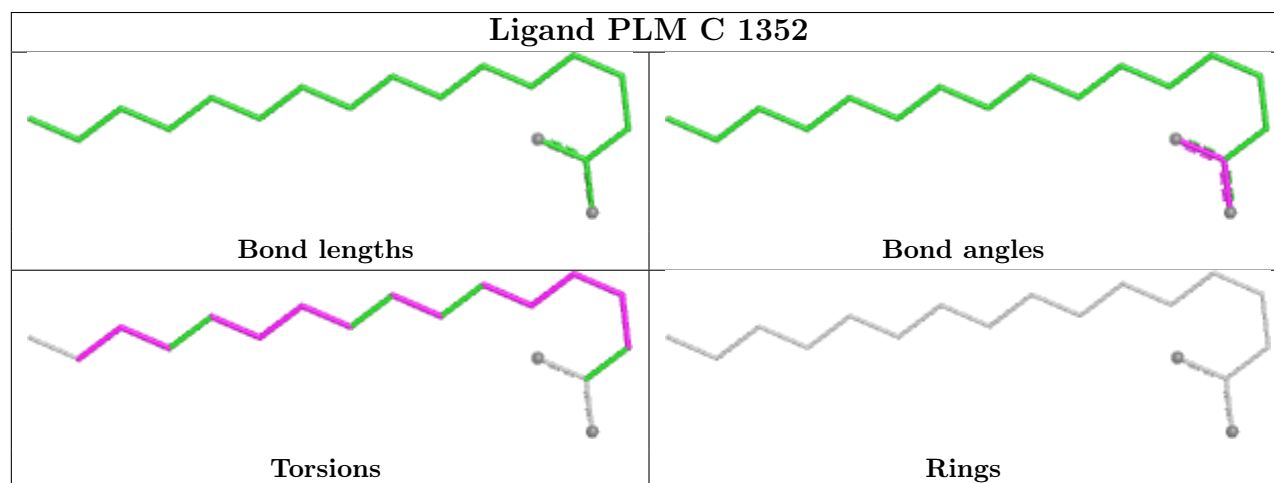
There are no ring outliers.

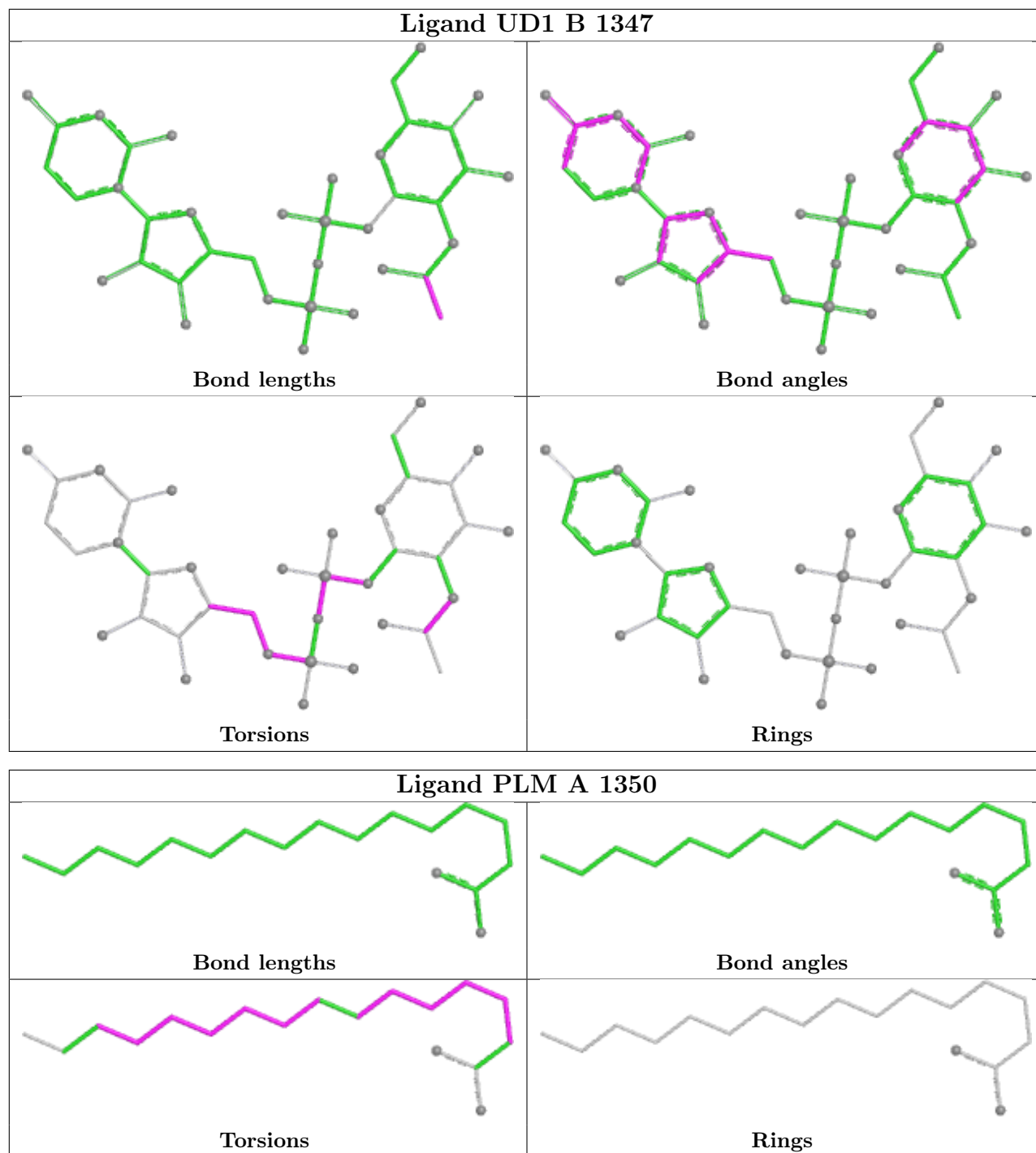
6 monomers are involved in 24 short contacts:

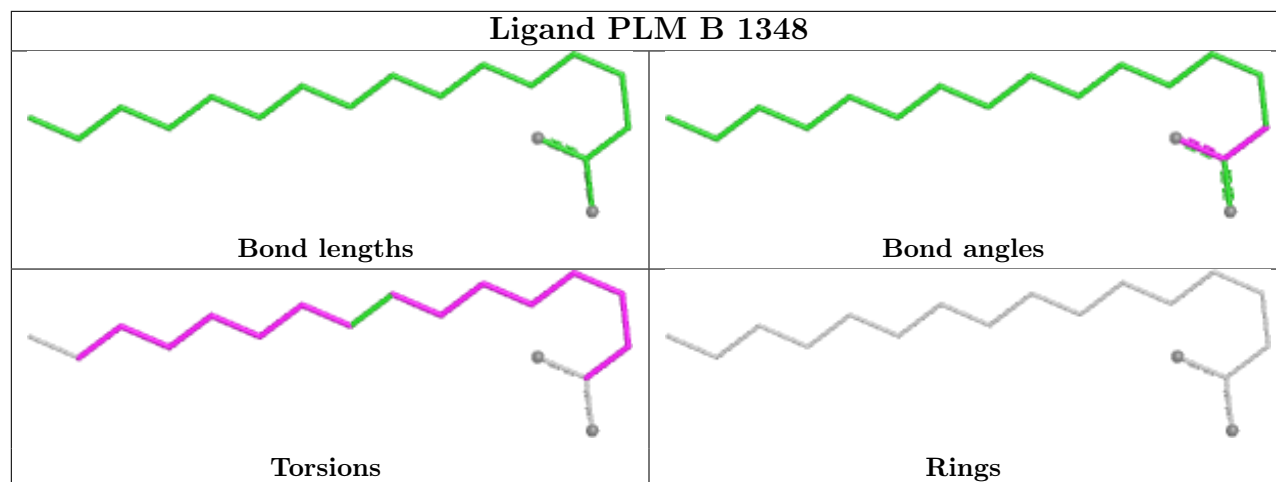
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	1352	PLM	8	0
5	C	1351	UD1	8	0
5	B	1347	UD1	1	0
4	A	1350	PLM	3	0
4	B	1348	PLM	3	0
3	A	1348	SO4	1	0

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%)	0.63	9 (2%)	57 36	46, 76, 82, 92	8 (2%)
1	B	345/374 (92%)	0.70	23 (6%)	24 13	48, 77, 81, 95	7 (2%)
1	C	346/374 (92%)	0.78	28 (8%)	18 10	46, 76, 81, 84	5 (1%)
All	All	1037/1122 (92%)	0.70	60 (5%)	29 16	46, 76, 81, 95	20 (1%)

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	39	ALA	4.7
1	C	344	VAL	4.1
1	B	191	GLY	3.8
1	C	196	ALA	3.8
1	C	26	LEU	3.7
1	C	77	ASN	3.5
1	B	145	SER	3.4
1	B	237	SER	3.4
1	A	344	VAL	3.1
1	B	164[A]	ARG	3.1
1	A	276	GLY	3.0
1	B	73	ASP	3.0
1	C	60	ALA	3.0
1	B	344	VAL	2.8
1	C	52	HIS	2.7
1	A	318	GLN	2.7
1	C	34	GLU	2.7
1	C	345	GLN	2.6
1	B	189	GLY	2.6
1	A	339	ALA	2.5
1	B	152	TYR	2.5
1	C	49	TYR	2.5
1	B	209	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	40	HIS	2.5
1	C	140	ALA	2.4
1	B	339	ALA	2.3
1	B	340	LEU	2.3
1	C	5	THR	2.3
1	B	119	ILE	2.3
1	C	122	HIS	2.3
1	C	348	GLU	2.3
1	A	245	ILE	2.3
1	C	146	GLY	2.3
1	C	33	ILE	2.2
1	B	207	GLY	2.2
1	B	137	VAL	2.2
1	C	44	LEU	2.2
1	C	50	ALA	2.2
1	B	132	CYS	2.2
1	B	21	GLY	2.2
1	B	230	HIS	2.2
1	C	290	HIS	2.2
1	C	78	PHE	2.2
1	C	347	LEU	2.2
1	A	46	ASN	2.2
1	A	49	TYR	2.1
1	B	331	PRO	2.1
1	B	192	TYR	2.1
1	C	19	PHE	2.1
1	A	206	LEU	2.1
1	C	307	GLY	2.1
1	C	79	LEU	2.1
1	C	139	SER	2.1
1	B	343	LEU	2.1
1	C	8	LEU	2.1
1	C	234[A]	ARG	2.1
1	B	194	THR	2.1
1	B	146	GLY	2.0
1	A	330	LEU	2.0
1	B	196	ALA	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 ⓘ

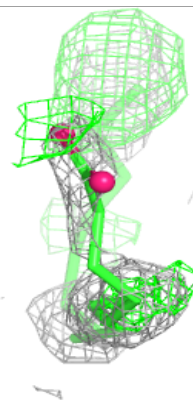
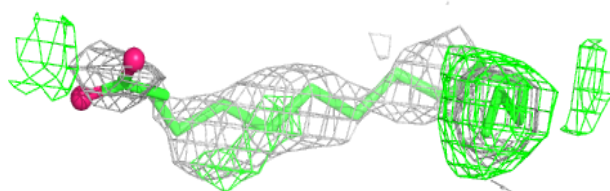
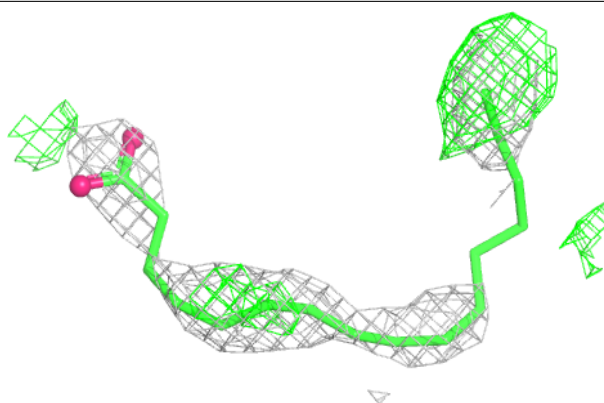
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
4	PLM	A	1350	18/18	0.66	0.38	35,35,38,38	18
3	SO4	B	1351	5/5	0.76	0.17	67,68,68,68	5
4	PLM	C	1352	18/18	0.78	0.43	55,58,60,60	18
3	SO4	A	1348	5/5	0.79	0.10	80,80,80,80	5
3	SO4	C	1349	5/5	0.81	0.21	70,71,71,71	5
5	UD1	B	1347	39/39	0.83	0.16	71,78,86,86	39
2	BME	A	1347	4/4	0.84	0.32	38,38,38,39	4
4	PLM	B	1348	18/18	0.84	0.30	47,48,48,48	18
5	UD1	C	1351	39/39	0.85	0.28	72,75,77,77	39
3	SO4	C	1350	5/5	0.91	0.11	75,75,75,75	5
3	SO4	A	1349	5/5	0.91	0.20	74,74,75,75	5
3	SO4	B	1346	5/5	0.96	0.08	83,83,84,84	0

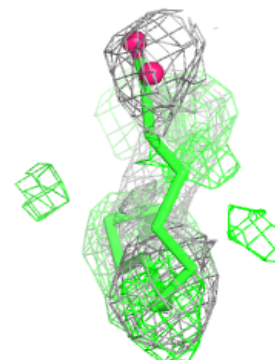
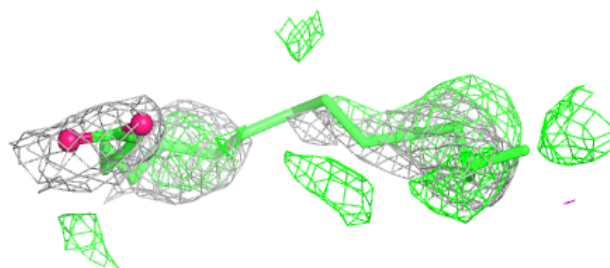
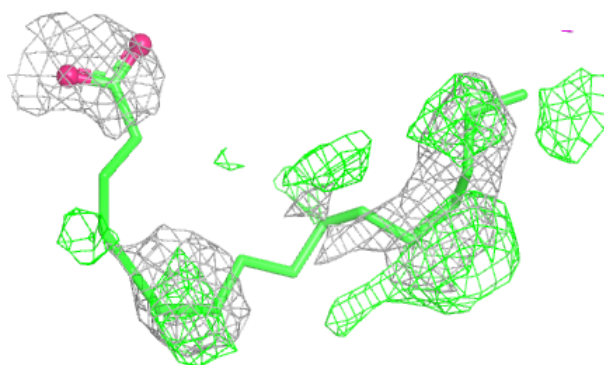
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around PLM A 1350:

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

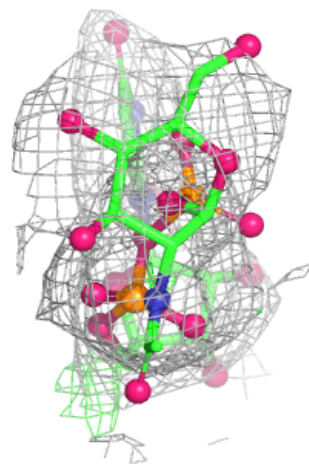
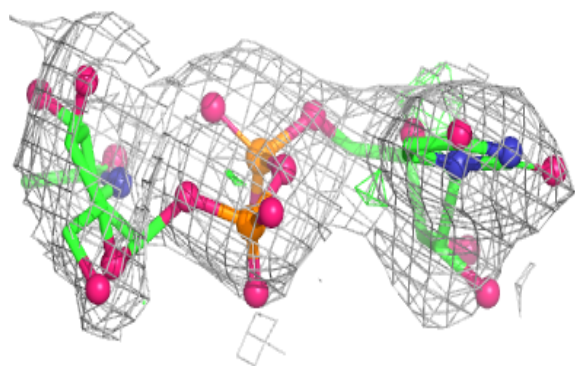
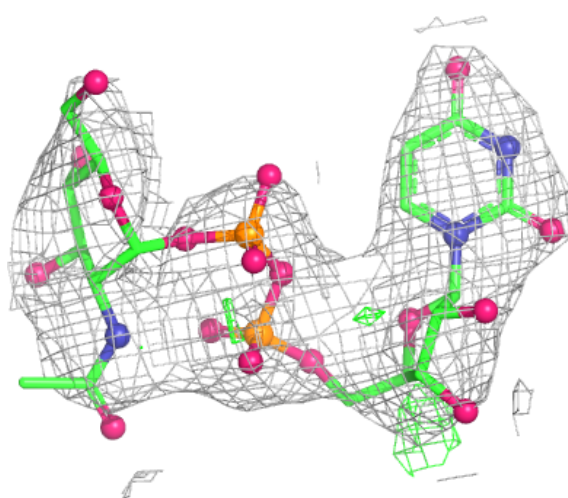
**Electron density around PLM C 1352:**

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



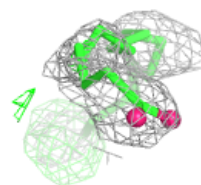
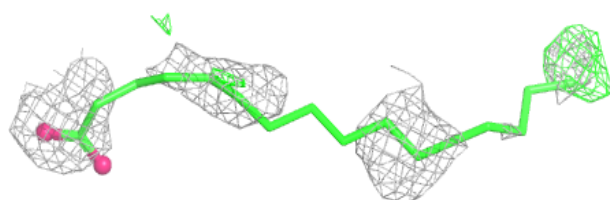
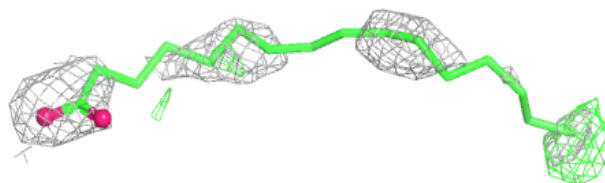
Electron density around UD1 B 1347:

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

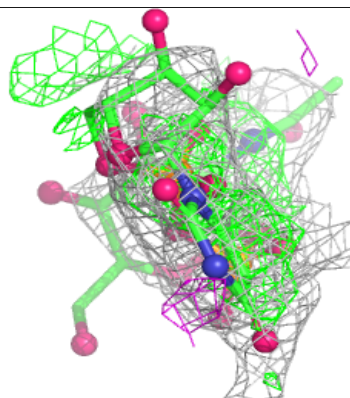
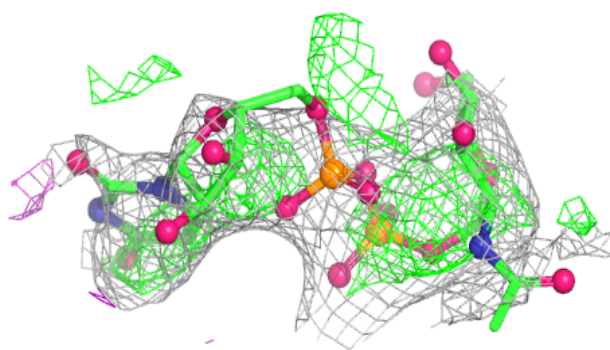
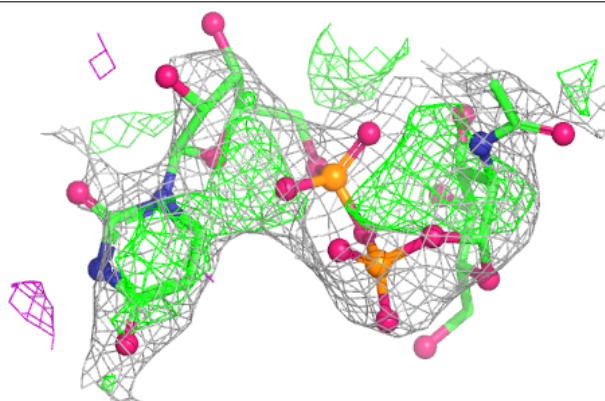


Electron density around PLM B 1348:

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

**Electron density around UD1 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.