



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:16 PM UTC

PDB ID : 2IUA / pdb_00002iua
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

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

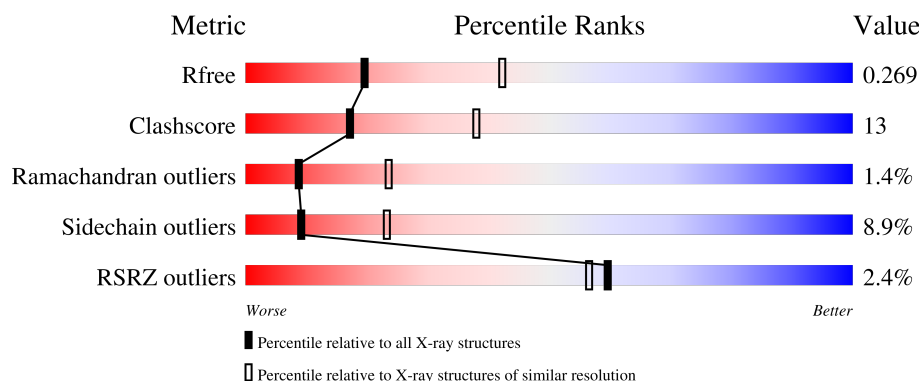
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (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 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	
1	B	374	
1	C	374	

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](#)

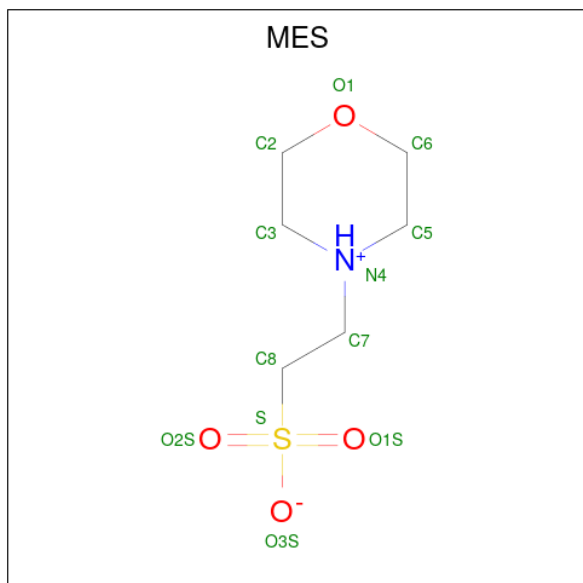
There are 5 unique types of molecules in this entry. The entry contains 8272 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

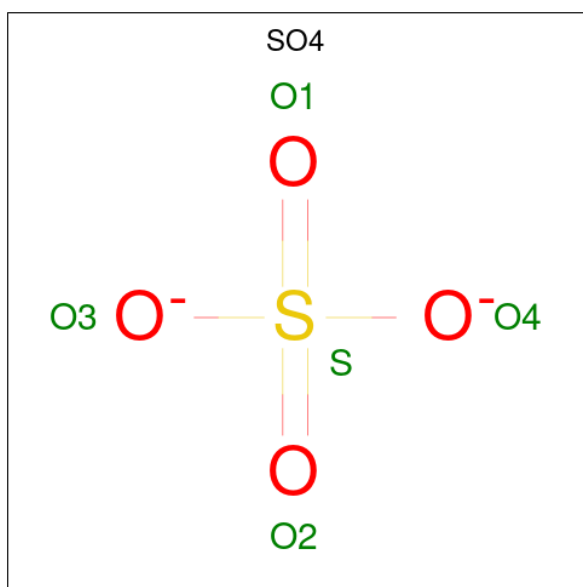
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	346	Total	C	N	O	S	0	8	0
			2682	1693	484	495	10			
1	B	345	Total	C	N	O	S	0	5	0
			2658	1679	479	490	10			
1	C	346	Total	C	N	O	S	0	6	0
			2672	1689	481	492	10			

- Molecule 2 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: $C_6H_{13}NO_4S$).



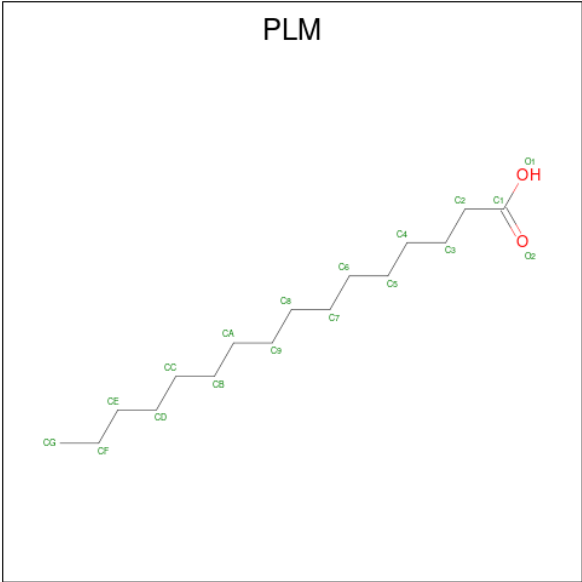
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



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 (CCD ID: PLM) (formula: C₁₆H₃₂O₂).



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		

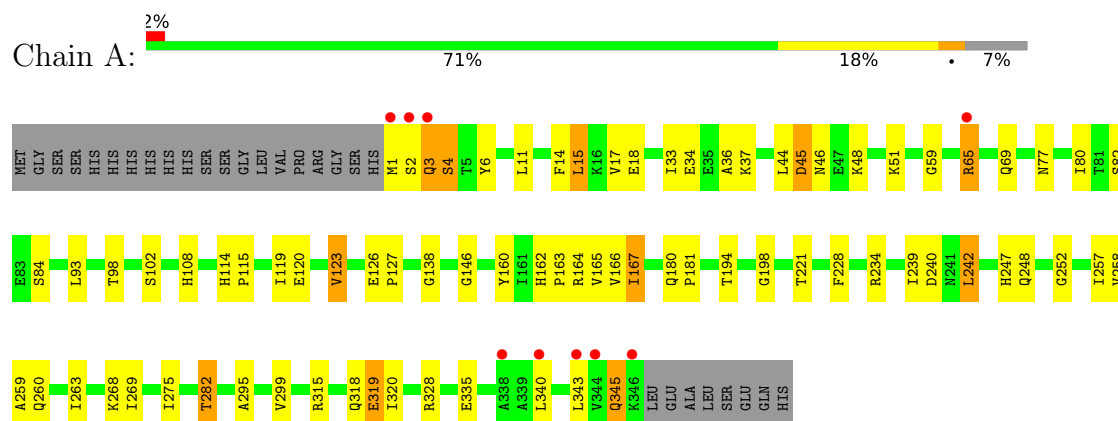
- Molecule 5 is water.

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		

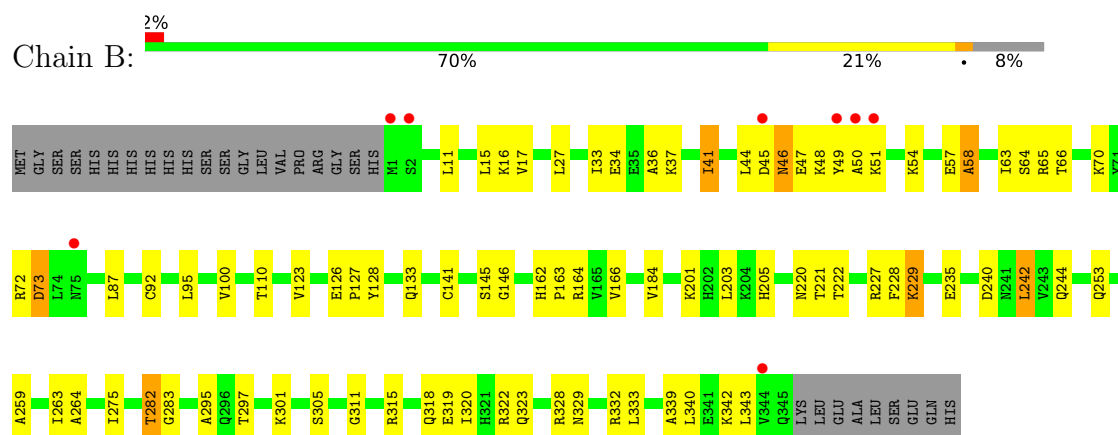
3 Residue-property plots

These plots are drawn for all protein, RNA, 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.

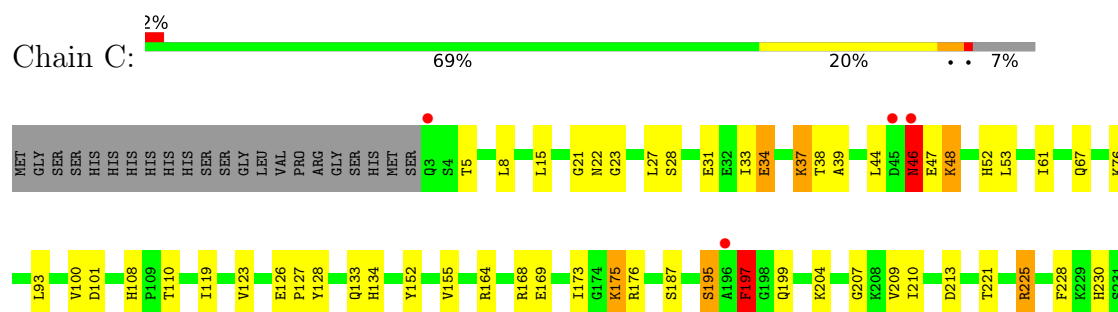
• Molecule 1: UDP-3-O-[3-HYDROXYMYRISTOYL] GLUCOSAMINE N-ACYLTRANSFERASE

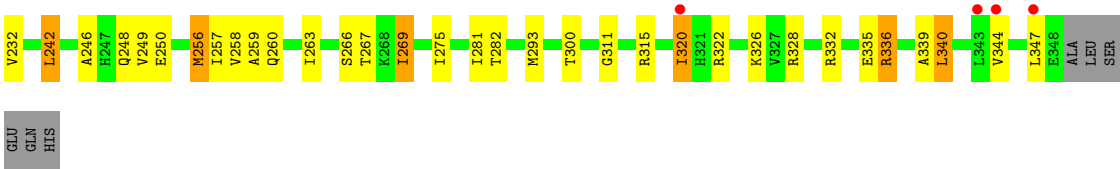


• Molecule 1: UDP-3-O-[3-HYDROXYMYRISTOYL] GLUCOSAMINE N-ACYLTRANSFERASE



• 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	98.68Å 98.68Å 284.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	93.25 – 2.70 93.23 – 2.70	Depositor EDS
% Data completeness (in resolution range)	96.3 (93.25-2.70) 96.3 (93.23-2.70)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.19 (at 2.69Å)	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 ²)	43.2	Xtriage
Anisotropy	0.121	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 26.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	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 ²)	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.*

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

5.1 Standard geometry

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	0.67	0/2766	0.92	4/3738 (0.1%)
1	B	0.68	0/2729	0.95	2/3691 (0.1%)
1	C	0.68	0/2747	0.95	2/3714 (0.1%)
All	All	0.67	0/8242	0.94	8/11143 (0.1%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	33	ILE	N-CA-C	6.63	117.38	110.62
1	A	4	SER	N-CA-C	6.16	119.29	108.75
1	C	33	ILE	N-CA-C	5.83	117.27	110.62
1	A	228	PHE	N-CA-C	-5.59	108.25	114.62
1	C	21	GLY	N-CA-C	-5.27	104.61	111.52
1	B	73	ASP	N-CA-C	5.21	117.87	111.82
1	A	84	SER	CA-C-N	5.08	124.52	119.24
1	A	84	SER	C-N-CA	5.08	124.52	119.24

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	2682	0	2712	87	0
1	B	2658	0	2690	84	0
1	C	2672	0	2704	84	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
5	B	46	0	0	4	0
5	C	34	0	0	5	0
All	All	8272	0	8211	206	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 13.

All (206) 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:HH11	1:A:65[A]:ARG:HG3	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:44:LEU:HD12	1:B:49:TYR:HD1	1.57	0.70
1:B:329:ASN:ND2	1:B:332:ARG:HD3	2.02	0.70
1:C:281:ILE:HD11	1:C:293:MET:HE3	1.75	0.69
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:11:LEU:HG	1:A:15:LEU:HD22	1.87	0.57
4:A:1351:PLM:H91	4:A:1351:PLM:HE2	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:CG	1:A:65[A]:ARG:NH1	2.61	0.56
1:A:45:ASP:HB2	1:A:48:LYS:HG3	1.89	0.55
1:A:164[B]:ARG:HH12	1:B:164[B]:ARG:NH1	1.97	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:275:ILE:HG12	1:C:293:MET:HE2	1.90	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:HE3	1:C:175:LYS:H	1.76	0.51
1:A:93:LEU:HD21	1:C:228:PHE:HB3	1.91	0.51
4:A:1351:PLM:HA1	4:A:1351:PLM:C5	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HH11	1:C:225:ARG:CG	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
1:C:210:ILE:HB	1:C:232:VAL:HG22	1.95	0.48
1:A:234:ARG:HB2	1:A:252:GLY:C	2.37	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:2:SER:C	1:A:4:SER:N	2.72	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:34:GLU:H	1:A:34:GLU:CD	2.22	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:A:2:SER:C	1:A:4:SER:H	2.23	0.47
1:B:57:GLU:O	1:B:58:ALA:C	2.57	0.47
1:B:263:ILE:HD11	1:B:275:ILE:HD13	1.95	0.47
1:B:240:ASP:HB3	1:B:259:ALA:N	2.30	0.47
4:B:1349:PLM:HF1	4:B:1349:PLM:CB	2.40	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:HH21	1:C:164[A]:ARG:CZ	2.22	0.46
1:B:164[A]:ARG:HE	1:C:164[A]:ARG:HE	1.57	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:C:256:MET:HE3	1:C:256:MET:HB3	1.82	0.45
1:B:34:GLU:CD	1:B:34:GLU:H	2.24	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:264:ALA:HB3	1:B:282:THR:C	2.42	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:B:110:THR:O	1:C:128:TYR:OH	2.27	0.44
1:A:119:ILE:CG2	1:A:123:VAL:HG21	2.48	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:A:164[B]:ARG:NH1	1:C:164[B]:ARG:HH22	1.60	0.43
1:B:65:ARG:NE	3:B:1346:SO4:O2	2.40	0.43
1:A:3:GLN:HB2	5:A:2020:HOH:O	2.18	0.43
1:A:315:ARG:HD2	5:A:2065:HOH:O	2.18	0.43
1:B:49:TYR:O	1:B:51:LYS:N	2.52	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:B:27:LEU:HD13	1:B:41:ILE:HG12	2.01	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: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
4:A:1352:PLM:HG3	4:A:1352:PLM:HA2	2.01	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:C:101:ASP:OD1	1:C:101:ASP:C	2.63	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:HG3	1:C:176:ARG:O	2.20	0.41
1:B:264:ALA:HB3	1:B:283:GLY:N	2.35	0.41
4:B:1349:PLM:HB1	4:B:1349:PLM:H82	1.78	0.41
1:C:246:ALA:O	1:C:249:VAL:HG23	2.20	0.41
1:A:36:ALA:O	1:A:37:LYS:HE2	2.21	0.41
1:A:114:HIS:HA	1:A:115:PRO:HD2	1.82	0.41
1:A:345:GLN:HE21	1:A:345:GLN:N	2.19	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:203:LEU:O	1:B:205:HIS:CD2	2.74	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:B:315[B]:ARG:NH1	1:C:328:ARG:HE	2.20	0.40
1:C:46:ASN:ND2	5:C:2002:HOH:O	2.53	0.40
1:C:108:HIS:CE1	1:C:110:THR:HG23	2.56	0.40
1:C:344:VAL:O	1:C:347:LEU:HB3	2.21	0.40
1:A:258:VAL:CG1	1:A:259:ALA:H	2.35	0.40
1:C:281:ILE:CD1	1:C:293:MET:HE3	2.49	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%)	11	29
1	B	348/374 (93%)	326 (94%)	15 (4%)	7 (2%)	6	16
1	C	350/374 (94%)	329 (94%)	17 (5%)	4 (1%)	11	29
All	All	1050/1122 (94%)	988 (94%)	47 (4%)	15 (1%)	9	23

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
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%)	271 (92%)	22 (8%)	12	31
1	B	289/309 (94%)	262 (91%)	27 (9%)	8	21
1	C	291/309 (94%)	263 (90%)	28 (10%)	8	20
All	All	873/927 (94%)	796 (91%)	77 (9%)	9	23

All (77) 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	44	LEU
1	A	51	LYS
1	A	65[A]	ARG
1	A	65[B]	ARG
1	A	98	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	123	VAL
1	A	167	ILE
1	A	221	THR
1	A	242	LEU
1	A	248	GLN
1	A	268	LYS
1	A	282	THR
1	A	299	VAL
1	A	318	GLN
1	A	319	GLU
1	A	320	ILE
1	A	335	GLU
1	A	340	LEU
1	A	345	GLN
1	B	11	LEU
1	B	15	LEU
1	B	16	LYS
1	B	17	VAL
1	B	41	ILE
1	B	46	ASN
1	B	54	LYS
1	B	63	ILE
1	B	73	ASP
1	B	100	VAL
1	B	123	VAL
1	B	141	CYS
1	B	145	SER
1	B	201	LYS
1	B	221	THR
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	320	ILE
1	B	322	ARG
1	B	328	ARG
1	B	333	LEU
1	B	340	LEU
1	C	15	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	169	GLU
1	C	175	LYS
1	C	197	PHE
1	C	199	GLN
1	C	221	THR
1	C	225	ARG
1	C	242	LEU
1	C	256	MET
1	C	267	THR
1	C	269	ILE
1	C	282	THR
1	C	320	ILE
1	C	322	ARG
1	C	326	LYS
1	C	332	ARG
1	C	335	GLU
1	C	336	ARG
1	C	340	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	248	GLN
1	A	290	HIS
1	A	345	GLN
1	B	46	ASN
1	B	199	GLN
1	B	205	HIS
1	B	230	HIS
1	B	329	ASN
1	B	345	GLN
1	C	67	GLN
1	C	133	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	199	GLN
1	C	248	GLN
1	C	272	HIS
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	$\# Z > 2$
3	SO4	A	1350	-	4,4,4	0.23	0	6,6,6	0.16	0
3	SO4	B	1346	-	4,4,4	0.19	0	6,6,6	0.29	0
3	SO4	C	1349	-	4,4,4	0.25	0	6,6,6	0.25	0
3	SO4	A	1349	-	4,4,4	0.28	0	6,6,6	0.09	0
3	SO4	B	1348	-	4,4,4	0.26	0	6,6,6	0.33	0
4	PLM	A	1351	-	17,17,17	0.63	0	17,17,17	0.93	2 (11%)
3	SO4	B	1347	-	4,4,4	0.19	0	6,6,6	0.27	0
4	PLM	B	1349	-	17,17,17	0.65	0	17,17,17	0.91	1 (5%)
3	SO4	C	1350	-	4,4,4	0.22	0	6,6,6	0.14	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MES	A	1347	-	12,12,12	2.22	1 (8%)	15,16,16	2.37	6 (40%)
4	PLM	A	1352	-	17,17,17	0.59	0	17,17,17	0.94	2 (11%)
3	SO4	A	1348	-	4,4,4	0.21	0	6,6,6	0.27	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	A	1352	-	-	12/15/15/15	-
4	PLM	A	1351	-	-	8/15/15/15	-
4	PLM	B	1349	-	-	9/15/15/15	-
2	MES	A	1347	-	-	2/6/14/14	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1347	MES	C8-S	-7.35	1.67	1.77

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1347	MES	C5-N4-C3	5.88	121.50	108.84
2	A	1347	MES	C7-N4-C3	3.47	120.48	111.24
4	B	1349	PLM	O1-C1-O2	-2.75	116.27	123.33
4	A	1351	PLM	O1-C1-O2	-2.74	116.29	123.33
2	A	1347	MES	C2-C3-N4	-2.63	106.12	110.12
4	A	1352	PLM	O1-C1-C2	2.60	122.22	114.00
2	A	1347	MES	C6-C5-N4	-2.56	106.23	110.12
2	A	1347	MES	C7-N4-C5	2.54	118.01	111.24
4	A	1352	PLM	O1-C1-O2	-2.37	117.23	123.33
4	A	1351	PLM	O1-C1-C2	2.14	120.76	114.00
2	A	1347	MES	O3S-S-C8	2.12	110.15	106.00

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1351	PLM	C9-CA-CB-CC

Continued on next page...

Continued from previous page...

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

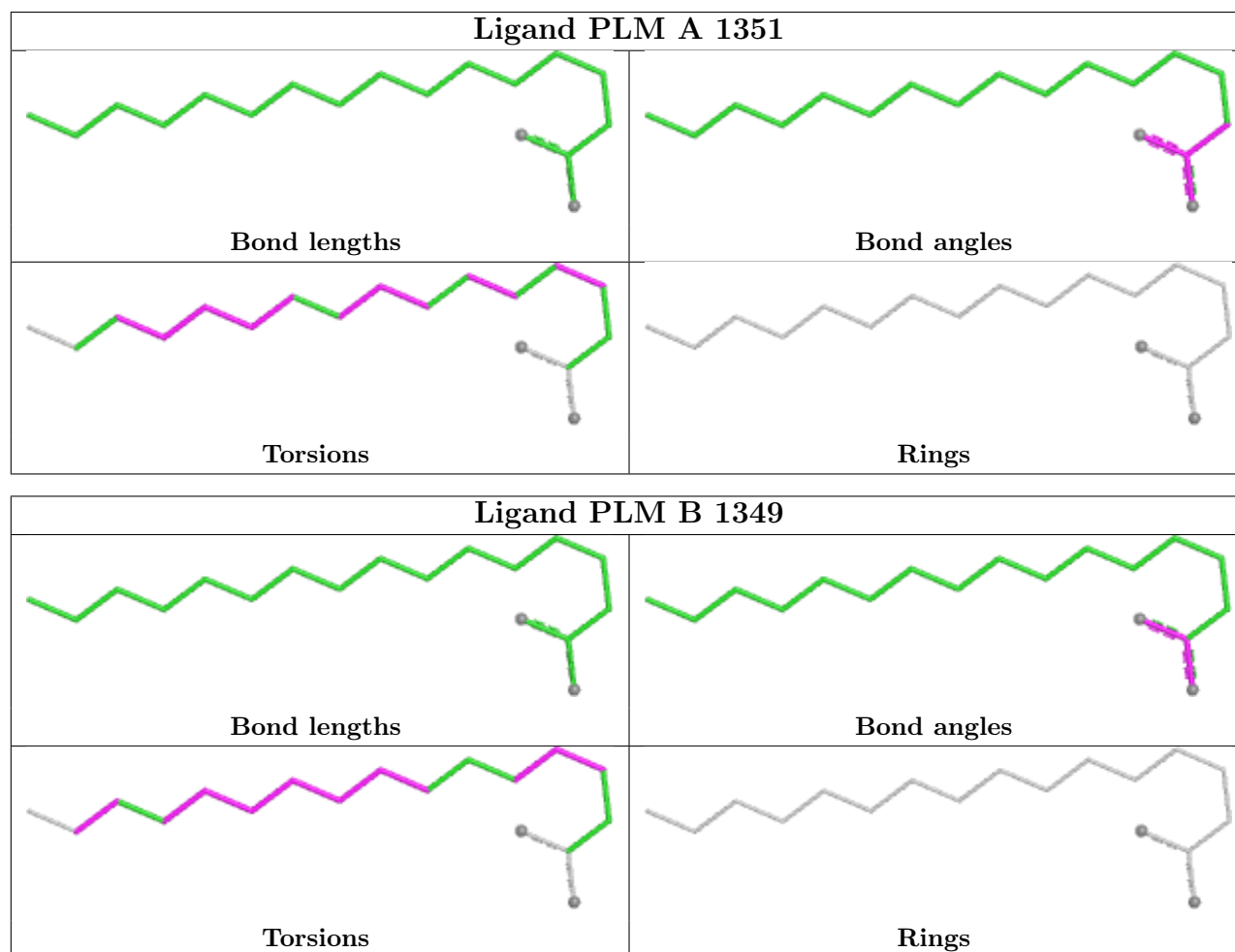
There are no ring outliers.

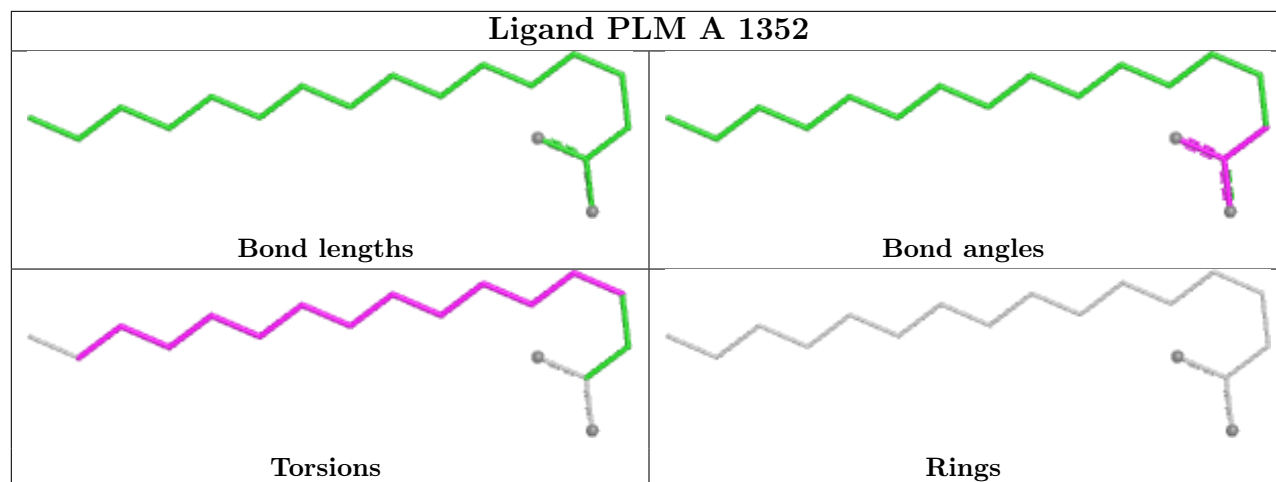
5 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1346	SO4	2	0
4	A	1351	PLM	5	0
4	B	1349	PLM	4	0
4	A	1352	PLM	4	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%)	-0.21	9 (2%) 57 54	19, 35, 67, 94	8 (2%)
1	B	345/374 (92%)	-0.20	8 (2%) 61 58	17, 34, 71, 94	5 (1%)
1	C	346/374 (92%)	-0.04	8 (2%) 61 58	16, 39, 78, 99	6 (1%)
All	All	1037/1122 (92%)	-0.15	25 (2%) 59 56	16, 36, 75, 99	19 (1%)

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	49	TYR	4.1
1	C	344	VAL	3.8
1	A	1	MET	3.7
1	B	45	ASP	3.4
1	B	50	ALA	3.2
1	C	196	ALA	3.1
1	A	338	ALA	3.1
1	B	344	VAL	3.1
1	A	2	SER	3.0
1	C	45	ASP	2.9
1	C	347	LEU	2.9
1	C	3	GLN	2.8
1	A	343	LEU	2.7
1	C	46	ASN	2.6
1	B	51	LYS	2.6
1	B	75[A]	ASN	2.6
1	B	2	SER	2.5
1	A	346	LYS	2.4
1	B	1	MET	2.3
1	C	343	LEU	2.3
1	A	65[A]	ARG	2.2
1	C	320	ILE	2.2
1	A	3	GLN	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	340	LEU	2.1
1	A	344	VAL	2.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

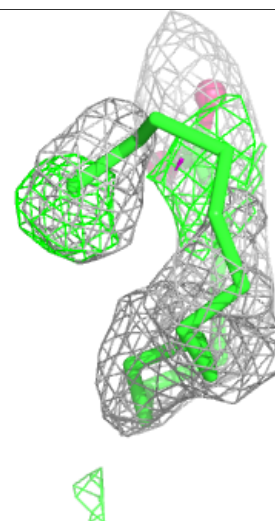
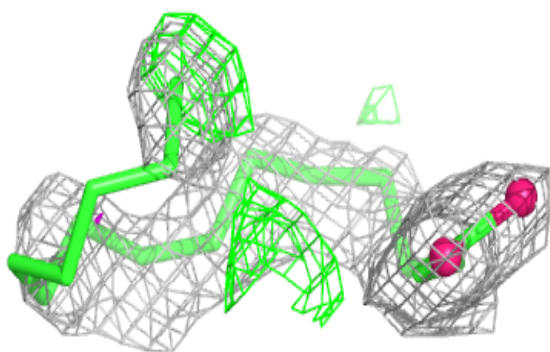
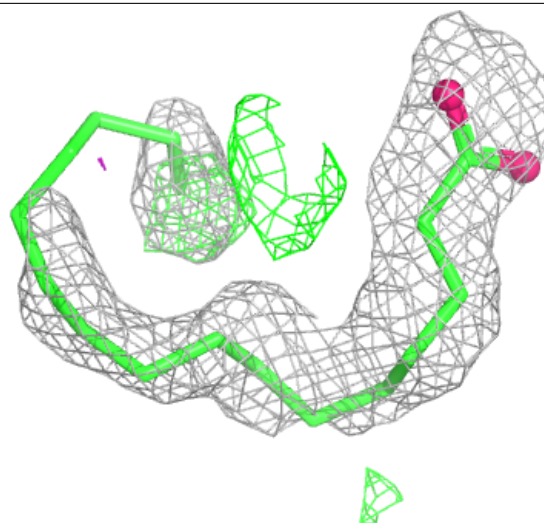
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	SO4	A	1350	5/5	0.72	0.22	37,39,39,39	5
3	SO4	B	1347	5/5	0.73	0.16	34,35,36,37	5
3	SO4	C	1349	5/5	0.74	0.21	36,36,37,38	5
4	PLM	A	1352	18/18	0.78	0.28	71,73,75,76	0
4	PLM	A	1351	18/18	0.79	0.23	48,53,59,59	0
3	SO4	A	1349	5/5	0.82	0.17	32,32,33,33	5
2	MES	A	1347	12/12	0.82	0.26	66,67,69,69	12
3	SO4	B	1348	5/5	0.86	0.14	32,32,34,34	5
4	PLM	B	1349	18/18	0.87	0.17	47,52,54,54	0
3	SO4	A	1348	5/5	0.92	0.13	42,43,44,45	5
3	SO4	C	1350	5/5	0.96	0.06	47,47,48,48	0
3	SO4	B	1346	5/5	0.98	0.04	44,44,45,46	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.

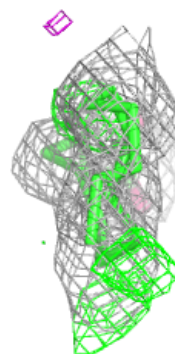
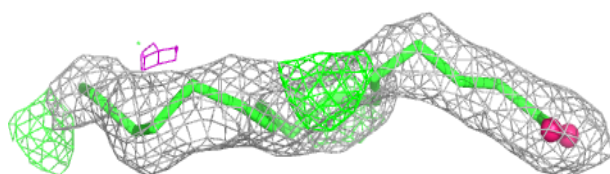
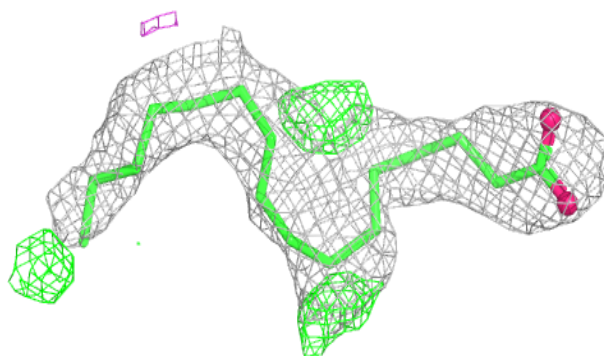
Electron density around PLM A 1352:

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

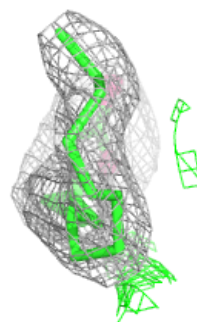
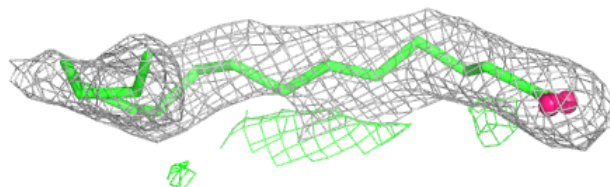
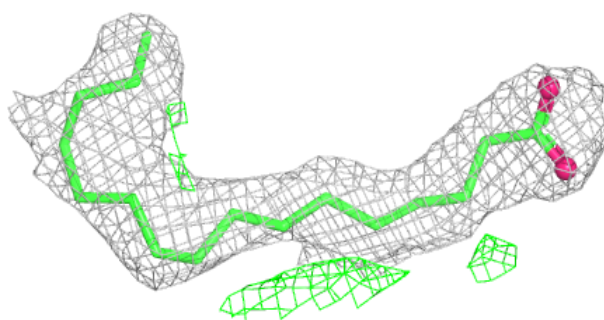


Electron density around PLM A 1351:

$2mF_o-DF_c$ (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 [i](#)

There are no such residues in this entry.