



Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 05:05 pm BST

PDB ID : 3EGL
Title : Crystal Structure of DegV Family Protein Cg2579 from *Corynebacterium glutamicum*
Authors : Kim, Y.; Tesar, C.; Abdullah, J.; Joachimiak, A.; Midwest Center for Structural Genomics (MCSG)
Deposited on : 2008-09-11
Resolution : 2.41 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

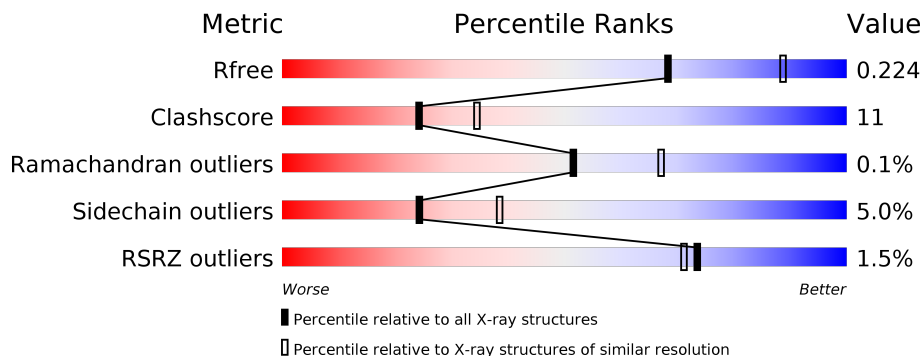
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.41 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4647 (2.44-2.40)
Clashscore	141614	5161 (2.44-2.40)
Ramachandran outliers	138981	5073 (2.44-2.40)
Sidechain outliers	138945	5074 (2.44-2.40)
RSRZ outliers	127900	4543 (2.44-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 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	277	<p>2% 78% 16% •• 5%</p>
1	B	277	<p>81% 13% • •</p>
1	C	277	<p>2% 71% 21% • 5%</p>

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
1	MLY	C	219	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6548 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.

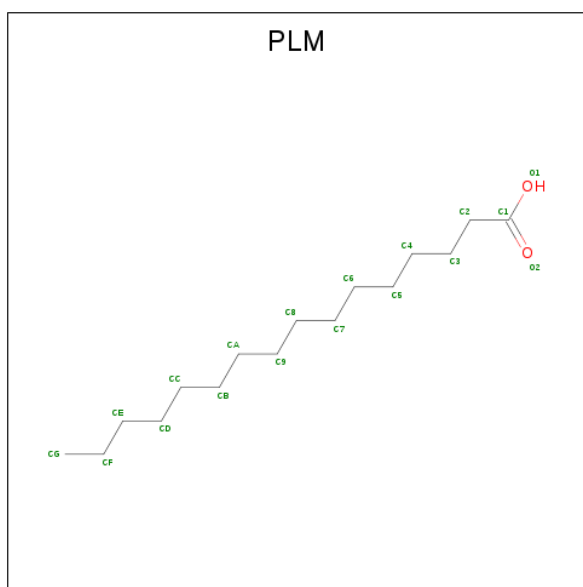
- Molecule 1 is a protein called DegV family protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	264	2008	1248	351	398	2	9	0	4	0
1	B	266	2025	1256	358	399	2	10	0	4	0
1	C	263	2003	1246	358	388	2	9	0	3	0

There are 9 discrepancies between the modelled and reference sequences:

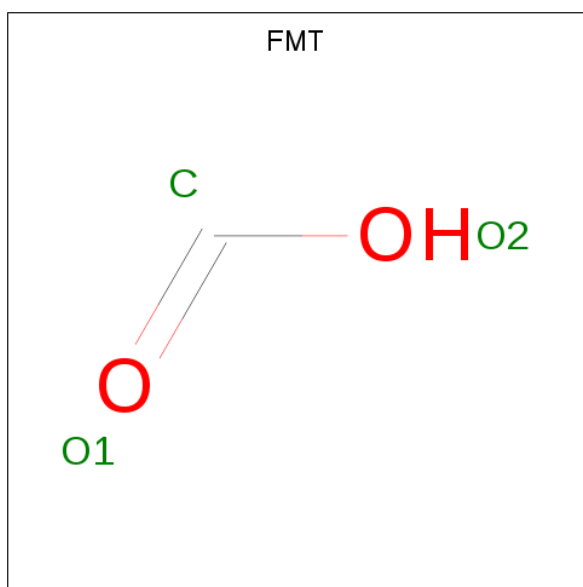
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP Q8NN60
A	-1	ASN	-	expression tag	UNP Q8NN60
A	0	ALA	-	expression tag	UNP Q8NN60
B	-2	SER	-	expression tag	UNP Q8NN60
B	-1	ASN	-	expression tag	UNP Q8NN60
B	0	ALA	-	expression tag	UNP Q8NN60
C	-2	SER	-	expression tag	UNP Q8NN60
C	-1	ASN	-	expression tag	UNP Q8NN60
C	0	ALA	-	expression tag	UNP Q8NN60

- Molecule 2 is PALMITIC ACID (three-letter code: PLM) (formula: C₁₆H₃₂O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			18	16	2		
2	B	1	Total	C	O	0	0
			18	16	2		
2	C	1	Total	C	O	0	0
			15	13	2		

- Molecule 3 is FORMIC ACID (three-letter code: FMT) (formula: CH₂O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total	C	O	0	0
			3	1	2		

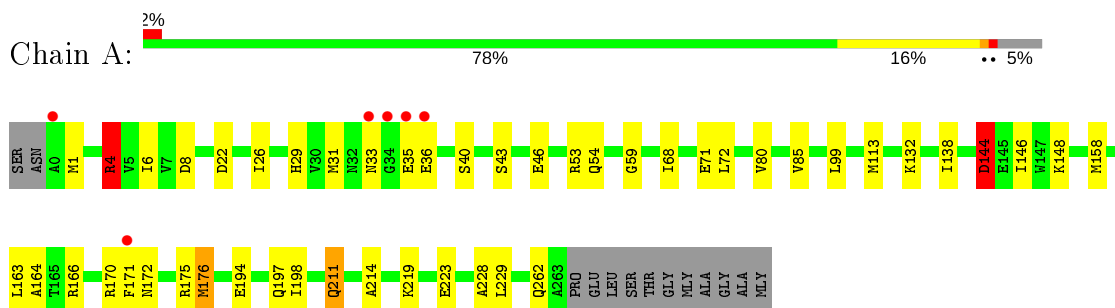
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	166	Total 166	O 166	0	0
4	B	165	Total 165	O 165	0	0
4	C	127	Total 127	O 127	0	0

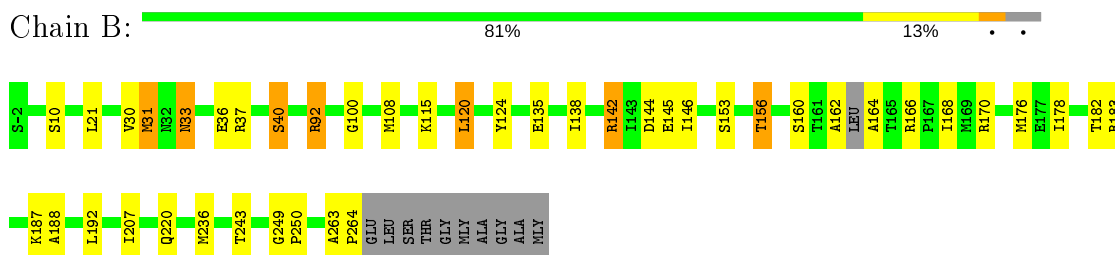
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

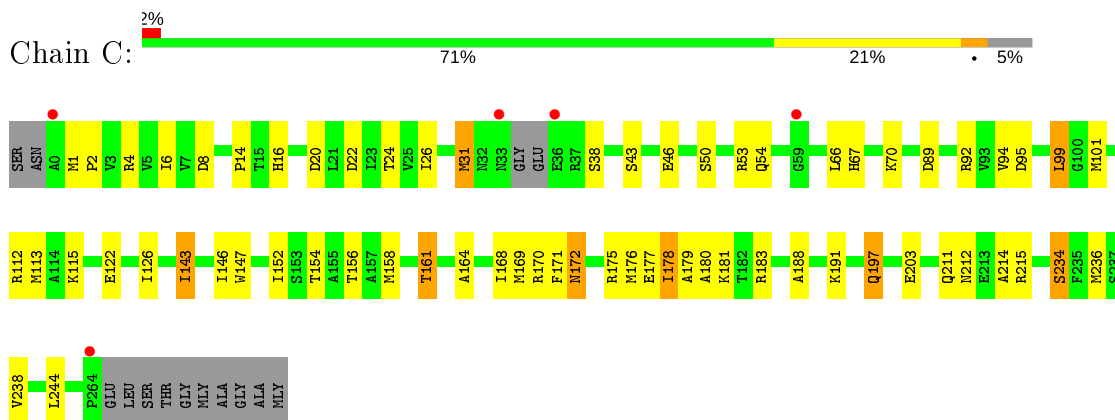
- Molecule 1: DegV family protein



- Molecule 1: DegV family protein



- Molecule 1: DegV family protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	104.25Å 151.67Å 76.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.30 – 2.41 45.49 – 2.41	Depositor EDS
% Data completeness (in resolution range)	99.6 (49.30-2.41) 99.6 (45.49-2.41)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.96 (at 2.42Å)	Xtrriage
Refinement program	REFMAC 5.5.0053	Depositor
R, R_{free}	0.179 , 0.218 0.187 , 0.224	Depositor DCC
R_{free} test set	2420 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	37.7	Xtrriage
Anisotropy	0.205	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 39.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6548	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.14% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: FMT, MLY, PLM

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	0.81	0/1937	0.83	5/2622 (0.2%)
1	B	0.73	0/1954	0.76	1/2643 (0.0%)
1	C	0.74	0/1931	0.79	0/2609
All	All	0.76	0/5822	0.79	6/7874 (0.1%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	4	ARG	NE-CZ-NH2	-6.15	117.22	120.30
1	B	142	ARG	NE-CZ-NH1	6.04	123.32	120.30
1	A	144[A]	ASP	CB-CG-OD1	5.48	123.23	118.30
1	A	144[B]	ASP	CB-CG-OD1	5.48	123.23	118.30
1	A	113	MSE	CG-SE-CE	5.21	110.37	98.90
1	A	176	MSE	CG-SE-CE	-5.09	87.71	98.90

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	2008	0	2005	36	0
1	B	2025	0	2023	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2003	0	2019	71	0
2	A	18	0	31	1	0
2	B	18	0	31	0	0
2	C	15	0	22	1	0
3	C	3	0	1	1	0
4	A	166	0	0	4	0
4	B	165	0	0	3	0
4	C	127	0	0	4	0
All	All	6548	0	6132	134	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 11.

All (134) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:236:MSE:HE3	1:C:238:VAL:CG1	1.84	1.07
1:C:112[B]:ARG:HG2	1:C:112[B]:ARG:HH11	1.24	1.02
1:C:211:GLN:HE21	1:C:214:ALA:H	0.97	0.95
1:B:21:LEU:HA	1:B:115:MLY:HH11	1.46	0.95
1:B:135:GLU:OE1	1:B:170:ARG:NH2	2.03	0.92
1:B:142:ARG:HD2	1:B:145:GLU:OE1	1.71	0.90
1:C:236:MSE:CE	1:C:238:VAL:CG1	2.52	0.87
1:B:162:ALA:O	1:B:183:ARG:NH2	2.08	0.86
1:C:146:ILE:HD11	1:C:176:MSE:HE1	1.58	0.84
1:B:146:ILE:HD11	1:B:176:MSE:HE2	1.64	0.79
1:A:4:ARG:HH11	1:A:54:GLN:NE2	1.81	0.79
1:A:175:ARG:HD3	4:A:382:HOH:O	1.82	0.78
1:C:146:ILE:CD1	1:C:176:MSE:HE1	2.15	0.76
1:B:160:SER:HA	1:B:164:ALA:HB3	1.68	0.76
1:C:112[B]:ARG:CG	1:C:112[B]:ARG:HH11	1.99	0.76
1:C:211:GLN:HE21	1:C:214:ALA:N	1.80	0.76
1:C:113:MSE:HE1	1:C:122:GLU:HB3	1.71	0.72
1:C:211:GLN:NE2	1:C:214:ALA:H	1.82	0.72
1:C:169:MSE:HE3	1:C:176:MSE:HG2	1.71	0.71
1:A:211:GLN:HE21	1:A:214:ALA:H	1.38	0.71
1:B:37:ARG:NH1	4:B:401:HOH:O	2.24	0.70
1:C:172:ASN:ND2	1:C:177:GLU:OE1	2.24	0.70
1:A:211:GLN:NE2	1:A:214:ALA:H	1.88	0.70
1:C:89:ASP:OD1	1:C:92[A]:ARG:NE	2.25	0.69
1:C:236:MSE:HE3	1:C:238:VAL:HG13	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:168:ILE:HD12	1:B:192:LEU:HD22	1.75	0.69
1:C:156:THR:HG23	1:C:178:ILE:HD12	1.75	0.69
1:C:236:MSE:CE	1:C:238:VAL:HG11	2.22	0.69
1:A:171:PHE:CZ	1:A:176:MSE:SE	2.97	0.68
1:A:35:GLU:O	4:A:357:HOH:O	2.12	0.68
1:C:158:MSE:O	1:C:161:THR:HB	1.92	0.67
1:C:70:MLY:HH12	1:C:95:ASP:OD2	1.95	0.66
1:A:138:ILE:HD11	1:A:171:PHE:HE2	1.60	0.66
1:C:6:ILE:HD11	1:C:54:GLN:HG3	1.76	0.66
1:C:169:MSE:HE2	1:C:176:MSE:HE3	1.75	0.66
1:B:166:ARG:O	1:B:182:THR:HG23	1.95	0.66
1:B:183:ARG:HH11	1:B:183:ARG:HG2	1.62	0.65
1:A:146:ILE:HD11	1:A:176:MSE:HE3	1.78	0.65
1:A:29:HIS:HB2	1:A:40:SER:HB3	1.79	0.65
1:C:236:MSE:HE3	1:C:238:VAL:HG12	1.76	0.64
1:A:1:MSE:HE2	1:A:1:MSE:HA	1.80	0.64
1:B:37:ARG:HG2	4:B:432:HOH:O	1.98	0.63
1:A:4:ARG:NH2	1:A:22:ASP:OD2	2.32	0.63
1:C:16:HIS:HD2	4:C:288:HOH:O	1.80	0.63
1:B:31:MSE:SE	1:B:40:SER:HB3	2.50	0.62
1:C:66:LEU:CD2	1:C:94:VAL:HG21	2.29	0.62
1:C:6:ILE:HD12	1:C:24:THR:HB	1.81	0.62
1:A:59:GLY:HA2	4:A:415:HOH:O	2.00	0.61
1:C:236:MSE:CE	1:C:238:VAL:HG13	2.29	0.61
1:C:31:MSE:HB2	1:C:38:SER:HB3	1.83	0.60
1:B:153:SER:HB2	4:B:441:HOH:O	2.00	0.60
1:B:263:ALA:HB1	1:B:264:PRO:HD2	1.84	0.59
1:A:138:ILE:HD11	1:A:171:PHE:CE2	2.37	0.59
1:B:156:THR:HG22	1:B:178:ILE:HG13	1.84	0.59
1:A:80[A]:VAL:HG11	1:B:250:PRO:HB3	1.84	0.59
1:B:92[A]:ARG:HD3	1:B:120:LEU:HD13	1.85	0.59
1:A:4:ARG:NH1	1:A:54:GLN:NE2	2.51	0.58
1:B:187:MLY:HH11	1:C:20:ASP:HA	1.86	0.58
1:A:4:ARG:HH11	1:A:54:GLN:HE21	1.49	0.57
1:B:183:ARG:NH1	1:B:183:ARG:HG2	2.19	0.57
1:A:146:ILE:HD11	1:A:176:MSE:CE	2.34	0.57
1:C:164:ALA:HB2	1:C:181:MLY:HA	1.86	0.56
1:C:146:ILE:CG1	1:C:176:MSE:HE1	2.35	0.56
1:A:194:GLU:O	1:A:198:ILE:HG12	2.06	0.55
1:B:92[B]:ARG:HG2	1:B:124:TYR:CD1	2.41	0.55
1:C:152:ILE:CG2	1:C:176:MSE:HE2	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:169:MSE:HE2	1:C:176:MSE:CE	2.36	0.55
1:C:66:LEU:HD23	1:C:94:VAL:CG2	2.37	0.54
1:C:1:MSE:CB	1:C:2:PRO:HD2	2.38	0.54
1:C:99:LEU:HD12	1:C:99:LEU:C	2.28	0.54
1:A:36:GLU:N	4:A:431:HOH:O	2.29	0.53
1:C:1:MSE:HB3	1:C:2:PRO:HD2	1.91	0.53
1:A:158:MSE:O	1:C:234:SER:HB2	2.10	0.52
1:C:170:ARG:NH1	1:C:171:PHE:O	2.43	0.52
1:A:99:LEU:HD21	1:A:171:PHE:CE2	2.45	0.52
1:A:132:MLY:HH22	1:A:262:GLN:OE1	2.08	0.52
1:A:163:LEU:O	1:A:164:ALA:HB3	2.10	0.51
1:C:1:MSE:HG2	1:C:2:PRO:HD2	1.92	0.51
1:A:138:ILE:HD13	2:A:275:PLM:HD2	1.91	0.51
1:C:244:LEU:HB3	2:C:275:PLM:HC2	1.93	0.51
1:A:171:PHE:CE1	1:A:176:MSE:SE	3.14	0.50
1:C:170:ARG:HG2	1:C:171:PHE:N	2.26	0.50
1:C:4:ARG:NH1	1:C:22:ASP:OD2	2.37	0.50
1:A:197:GLN:OE1	1:A:228:ALA:HB1	2.12	0.49
1:A:4:ARG:HD3	1:A:54:GLN:HE21	1.77	0.49
1:B:108:MSE:HE1	1:B:236:MSE:HE1	1.94	0.49
1:A:170:ARG:CZ	1:A:172:ASN:OD1	2.61	0.49
1:C:20:ASP:O	1:C:115:MLY:HH23	2.12	0.49
1:C:66:LEU:CD2	1:C:94:VAL:CG2	2.91	0.49
1:C:6:ILE:CD1	1:C:54:GLN:HG3	2.42	0.48
1:C:183[B]:ARG:HD2	4:C:400:HOH:O	2.13	0.48
1:C:143:ILE:HG23	1:C:147:TRP:HE3	1.78	0.48
1:B:182:THR:HG21	1:B:188:ALA:CB	2.44	0.48
1:C:197:GLN:HB3	1:C:197:GLN:HE21	1.38	0.47
1:C:146:ILE:HG12	1:C:176:MSE:HE1	1.94	0.47
1:C:170:ARG:HB2	1:C:179:ALA:HB2	1.97	0.47
1:C:99:LEU:HD12	1:C:99:LEU:O	2.14	0.47
1:B:182:THR:HG21	1:B:188:ALA:HB2	1.97	0.46
1:C:154:THR:HG22	3:C:276:FMT:H	1.98	0.46
1:B:135:GLU:CD	1:B:170:ARG:HH22	2.16	0.46
1:A:31:MSE:HB3	1:A:33:ASN:ND2	2.32	0.45
1:C:180:ALA:HB1	1:C:191:MLY:HG3	1.98	0.45
1:C:66:LEU:HD21	1:C:94:VAL:HG21	1.99	0.45
1:C:112[B]:ARG:HG2	1:C:112[B]:ARG:NH1	2.06	0.45
1:C:67:HIS:N	4:C:292:HOH:O	2.37	0.45
1:A:72:LEU:HD11	1:A:171:PHE:CE1	2.51	0.44
1:A:144[B]:ASP:OD2	1:A:148:MLY:HH12	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:10:SER:O	1:B:100:GLY:HA2	2.17	0.44
1:C:101:MSE:SE	1:C:236:MSE:HE1	2.68	0.43
1:A:4:ARG:HH22	1:A:22:ASP:CG	2.22	0.43
1:C:143:ILE:O	1:C:147:TRP:HB2	2.18	0.43
1:B:145:GLU:CG	1:B:249:GLY:CA	2.97	0.42
1:C:175:ARG:HE	1:C:175:ARG:HB2	1.69	0.42
1:C:14:PRO:HG3	1:C:238:VAL:HG12	2.01	0.42
1:C:8:ASP:HA	1:C:26:ILE:O	2.19	0.42
1:C:26:ILE:HD11	1:C:50:SER:OG	2.20	0.42
1:C:215:ARG:HG3	4:C:310:HOH:O	2.19	0.42
1:B:33:ASN:N	1:B:36:GLU:O	2.48	0.42
1:C:1:MSE:CB	1:C:2:PRO:CD	2.98	0.41
1:C:1:MSE:CG	1:C:2:PRO:HD2	2.49	0.41
1:B:176:MSE:HB3	1:B:176:MSE:HE3	1.88	0.41
1:C:112[B]:ARG:CG	1:C:112[B]:ARG:NH1	2.68	0.41
1:C:126:ILE:HD12	1:C:126:ILE:HA	1.87	0.41
1:A:8:ASP:HA	1:A:26:ILE:O	2.21	0.41
1:B:30:VAL:HG22	1:B:243:THR:HA	2.02	0.41
1:B:31:MSE:HE3	1:B:31:MSE:HB3	2.02	0.41
1:C:43:SER:OG	1:C:46:GLU:HG3	2.21	0.41
1:C:99:LEU:CD1	1:C:99:LEU:C	2.89	0.41
1:A:6:ILE:HD11	1:A:54:GLN:CG	2.51	0.41
1:C:168:ILE:HD11	1:C:188:ALA:HB1	2.03	0.41
1:A:219:MLY:HD2	1:A:219:MLY:HH12	1.93	0.40
1:A:43:SER:OG	1:A:46:GLU:HG3	2.22	0.40
1:C:169:MSE:CE	1:C:176:MSE:HG2	2.46	0.40
1:C:146:ILE:HA	1:C:146:ILE:HD12	1.93	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	258/277 (93%)	252 (98%)	5 (2%)	1 (0%)	34	47
1	B	258/277 (93%)	252 (98%)	6 (2%)	0	100	100
1	C	254/277 (92%)	248 (98%)	6 (2%)	0	100	100
All	All	770/831 (93%)	752 (98%)	17 (2%)	1 (0%)	51	67

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	68	ILE

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	202/196 (103%)	191 (95%)	11 (5%)	22	34
1	B	204/196 (104%)	193 (95%)	11 (5%)	22	34
1	C	201/196 (103%)	190 (94%)	11 (6%)	21	33
All	All	607/588 (103%)	574 (95%)	33 (5%)	24	34

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ARG
1	A	53	ARG
1	A	71	GLU
1	A	85	VAL
1	A	144[A]	ASP
1	A	144[B]	ASP
1	A	166	ARG
1	A	211	GLN
1	A	223[A]	GLU
1	A	223[B]	GLU
1	A	229	LEU
1	B	31	MSE

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Mol	Chain	Res	Type
1	B	33	ASN
1	B	40	SER
1	B	92[A]	ARG
1	B	92[B]	ARG
1	B	120	LEU
1	B	138	ILE
1	B	144	ASP
1	B	156	THR
1	B	207	ILE
1	B	220	GLN
1	C	31	MSE
1	C	53	ARG
1	C	99	LEU
1	C	143	ILE
1	C	161	THR
1	C	172	ASN
1	C	178	ILE
1	C	197	GLN
1	C	203	GLU
1	C	212	ASN
1	C	234	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	ASN
1	A	54	GLN
1	A	211	GLN
1	C	197	GLN
1	C	211	GLN
1	C	262	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](#)

24 non-standard protein/DNA/RNA residues 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$
1	MLY	B	115	1	9,10,11	0.73	0	6,11,13	0.94	0
1	MLY	B	132	1	9,10,11	0.88	0	6,11,13	1.60	1 (16%)
1	MLY	B	148	1	9,10,11	0.57	0	6,11,13	0.68	0
1	MLY	A	70	1	9,10,11	0.80	0	6,11,13	1.30	0
1	MLY	A	187	1	9,10,11	0.66	0	6,11,13	1.15	0
1	MLY	B	191	1	9,10,11	0.94	0	6,11,13	0.60	0
1	MLY	B	219	1	9,10,11	0.78	0	6,11,13	0.72	0
1	MLY	C	70	1	9,10,11	0.61	0	6,11,13	0.79	0
1	MLY	B	70	1	9,10,11	0.58	0	6,11,13	1.11	0
1	MLY	C	115	1	9,10,11	0.76	0	6,11,13	0.94	0
1	MLY	A	219	1	9,10,11	0.88	0	6,11,13	0.64	0
1	MLY	B	187	1	9,10,11	0.83	0	6,11,13	1.56	2 (33%)
1	MLY	A	191	1	9,10,11	0.86	0	6,11,13	1.22	0
1	MLY	A	132	1	9,10,11	0.90	0	6,11,13	0.70	0
1	MLY	A	181	1	9,10,11	0.90	0	6,11,13	0.41	0
1	MLY	C	148	1	9,10,11	0.61	0	6,11,13	0.92	0
1	MLY	C	181	1	9,10,11	0.93	0	6,11,13	0.68	0
1	MLY	B	181	1	9,10,11	0.75	0	6,11,13	0.75	0
1	MLY	C	132	1	9,10,11	0.78	0	6,11,13	0.80	0
1	MLY	A	115	1	9,10,11	0.88	0	6,11,13	0.67	0
1	MLY	C	187	1	9,10,11	0.93	0	6,11,13	0.36	0
1	MLY	A	148	1	9,10,11	0.74	0	6,11,13	0.75	0
1	MLY	C	219	1	9,10,11	0.78	0	6,11,13	1.36	1 (16%)
1	MLY	C	191	1	9,10,11	0.78	0	6,11,13	0.89	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
1	MLY	B	115	1	-	4/8/9/11	-
1	MLY	B	132	1	-	7/8/9/11	-
1	MLY	B	148	1	-	3/8/9/11	-
1	MLY	A	70	1	-	0/8/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	A	187	1	-	3/8/9/11	-
1	MLY	B	191	1	-	4/8/9/11	-
1	MLY	B	219	1	-	3/8/9/11	-
1	MLY	C	70	1	-	0/8/9/11	-
1	MLY	B	70	1	-	0/8/9/11	-
1	MLY	C	115	1	-	4/8/9/11	-
1	MLY	A	219	1	-	4/8/9/11	-
1	MLY	B	187	1	-	3/8/9/11	-
1	MLY	A	191	1	-	1/8/9/11	-
1	MLY	A	132	1	-	5/8/9/11	-
1	MLY	A	181	1	-	1/8/9/11	-
1	MLY	C	148	1	-	1/8/9/11	-
1	MLY	C	181	1	-	1/8/9/11	-
1	MLY	B	181	1	-	5/8/9/11	-
1	MLY	C	132	1	-	2/8/9/11	-
1	MLY	A	115	1	-	2/8/9/11	-
1	MLY	C	187	1	-	2/8/9/11	-
1	MLY	A	148	1	-	2/8/9/11	-
1	MLY	C	219	1	-	1/8/9/11	-
1	MLY	C	191	1	-	0/8/9/11	-

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	132	MLY	CH2-NZ-CH1	-3.39	100.97	109.73
1	B	187	MLY	CH2-NZ-CH1	2.67	116.63	109.73
1	B	187	MLY	CH2-NZ-CE	2.33	119.98	110.74
1	C	219	MLY	CD-CG-CB	-2.09	106.22	113.62

There are no chirality outliers.

All (58) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	132	MLY	N-CA-CB-CG
1	B	132	MLY	C-CA-CB-CG
1	B	132	MLY	O-C-CA-CB
1	B	191	MLY	C-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
1	C	115	MLY	N-CA-CB-CG
1	C	115	MLY	C-CA-CB-CG
1	A	132	MLY	N-CA-CB-CG
1	A	132	MLY	C-CA-CB-CG
1	B	181	MLY	N-CA-CB-CG
1	B	181	MLY	C-CA-CB-CG
1	B	191	MLY	CA-CB-CG-CD
1	B	115	MLY	CD-CE-NZ-CH2
1	B	148	MLY	CD-CE-NZ-CH1
1	B	148	MLY	CD-CE-NZ-CH2
1	A	187	MLY	CD-CE-NZ-CH1
1	A	219	MLY	CD-CE-NZ-CH1
1	A	115	MLY	CD-CE-NZ-CH1
1	A	115	MLY	CD-CE-NZ-CH2
1	A	148	MLY	CD-CE-NZ-CH1
1	A	148	MLY	CD-CE-NZ-CH2
1	C	115	MLY	CG-CD-CE-NZ
1	B	115	MLY	CG-CD-CE-NZ
1	B	132	MLY	CD-CE-NZ-CH1
1	A	187	MLY	CD-CE-NZ-CH2
1	A	219	MLY	CD-CE-NZ-CH2
1	C	148	MLY	CD-CE-NZ-CH2
1	C	219	MLY	CD-CE-NZ-CH2
1	B	219	MLY	CA-CB-CG-CD
1	B	115	MLY	CD-CE-NZ-CH1
1	B	132	MLY	CD-CE-NZ-CH2
1	B	219	MLY	CD-CE-NZ-CH2
1	B	181	MLY	CD-CE-NZ-CH2
1	C	115	MLY	CA-CB-CG-CD
1	A	132	MLY	CG-CD-CE-NZ
1	A	191	MLY	CD-CE-NZ-CH1
1	B	115	MLY	CE-CD-CG-CB
1	C	187	MLY	CA-CB-CG-CD
1	B	187	MLY	CD-CE-NZ-CH1
1	A	219	MLY	CE-CD-CG-CB
1	A	132	MLY	CA-CB-CG-CD
1	B	181	MLY	CA-CB-CG-CD
1	B	219	MLY	CE-CD-CG-CB
1	B	181	MLY	CE-CD-CG-CB
1	B	148	MLY	CE-CD-CG-CB
1	B	132	MLY	CA-CB-CG-CD
1	A	219	MLY	CA-CB-CG-CD

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Mol	Chain	Res	Type	Atoms
1	A	187	MLY	C-CA-CB-CG
1	A	132	MLY	CE-CD-CG-CB
1	C	132	MLY	CD-CE-NZ-CH2
1	B	191	MLY	N-CA-CB-CG
1	B	191	MLY	CE-CD-CG-CB
1	B	132	MLY	CG-CD-CE-NZ
1	C	181	MLY	CE-CD-CG-CB
1	C	132	MLY	CE-CD-CG-CB
1	B	187	MLY	C-CA-CB-CG
1	C	187	MLY	CG-CD-CE-NZ
1	B	187	MLY	CD-CE-NZ-CH2
1	A	181	MLY	CE-CD-CG-CB

There are no ring outliers.

9 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	115	MLY	1	0
1	C	70	MLY	1	0
1	C	115	MLY	1	0
1	A	219	MLY	1	0
1	B	187	MLY	1	0
1	A	132	MLY	1	0
1	C	181	MLY	1	0
1	A	148	MLY	1	0
1	C	191	MLY	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	FMT	C	276	-	0,2,2	0.00	-	0,1,1	0.00	-
2	PLM	C	275	-	11,14,17	0.26	0	10,14,17	0.82	0
2	PLM	A	275	-	14,17,17	0.29	0	13,17,17	0.72	0
2	PLM	B	275	-	14,17,17	0.31	0	13,17,17	0.79	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
2	PLM	C	275	-	-	5/10/12/15	-
2	PLM	A	275	-	-	5/13/15/15	-
2	PLM	B	275	-	-	8/13/15/15	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	275	PLM	C8-C9-CA-CB
2	A	275	PLM	CC-CD-CE-CF
2	C	275	PLM	C7-C8-C9-CA
2	B	275	PLM	CA-CB-CC-CD
2	B	275	PLM	C6-C7-C8-C9
2	B	275	PLM	C5-C6-C7-C8
2	C	275	PLM	C6-C7-C8-C9
2	C	275	PLM	C9-CA-CB-CC
2	B	275	PLM	CC-CD-CE-CF
2	A	275	PLM	CA-CB-CC-CD
2	A	275	PLM	CD-CE-CF-CG
2	C	275	PLM	C1-C2-C3-C4
2	B	275	PLM	CB-CC-CD-CE
2	B	275	PLM	C9-CA-CB-CC
2	A	275	PLM	CB-CC-CD-CE
2	C	275	PLM	C2-C3-C4-C5

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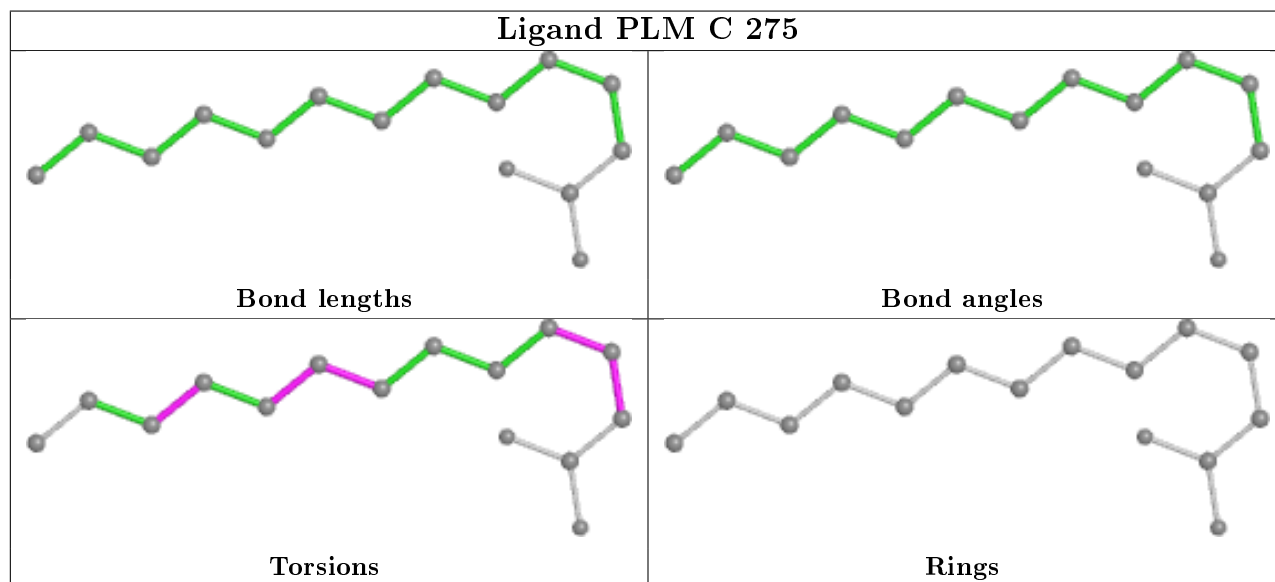
Mol	Chain	Res	Type	Atoms
2	A	275	PLM	C1-C2-C3-C4
2	B	275	PLM	C1-C2-C3-C4

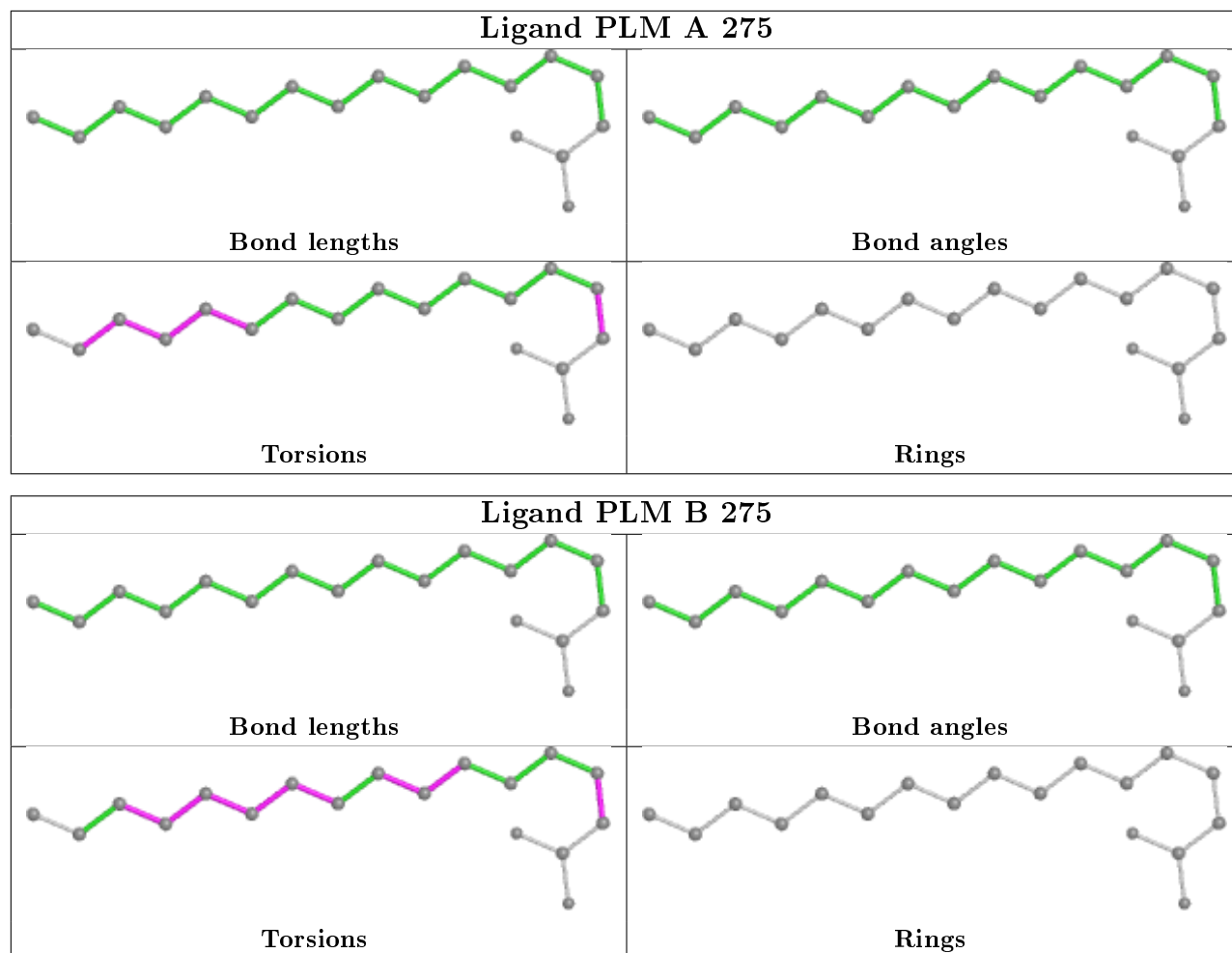
There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	276	FMT	1	0
2	C	275	PLM	1	0
2	A	275	PLM	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	247/277 (89%)	-0.49	6 (2%) 59 56	19, 27, 43, 60	0
1	B	249/277 (89%)	-0.38	0 100 100	17, 27, 46, 55	1 (0%)
1	C	246/277 (88%)	-0.26	5 (2%) 65 62	21, 30, 46, 58	1 (0%)
All	All	742/831 (89%)	-0.38	11 (1%) 73 71	17, 28, 46, 60	2 (0%)

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	264	PRO	4.6
1	A	35	GLU	4.2
1	A	33	ASN	3.5
1	C	0	ALA	3.3
1	C	33	ASN	2.8
1	C	36	GLU	2.8
1	A	0	ALA	2.6
1	A	171	PHE	2.6
1	A	36	GLU	2.5
1	C	59	GLY	2.4
1	A	34	GLY	2.3

6.2 Non-standard residues in protein, DNA, RNA chains [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(Å ²)	Q<0.9
1	MLY	C	219	11/12	0.48	0.63	26,28,51,51	7
1	MLY	B	181	11/12	0.89	0.29	35,37,47,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
1	MLY	C	187	11/12	0.92	0.20	29,32,47,48	0
1	MLY	B	132	11/12	0.92	0.16	26,28,47,47	0
1	MLY	C	115	11/12	0.93	0.23	38,40,55,55	0
1	MLY	A	191	11/12	0.94	0.15	27,30,42,43	0
1	MLY	A	132	11/12	0.94	0.17	26,27,49,50	0
1	MLY	A	181	11/12	0.94	0.11	27,29,42,43	0
1	MLY	C	181	11/12	0.94	0.15	32,34,46,47	0
1	MLY	B	191	11/12	0.94	0.19	26,28,44,44	0
1	MLY	C	132	11/12	0.94	0.19	24,26,45,46	0
1	MLY	B	219	11/12	0.94	0.16	25,28,53,53	0
1	MLY	B	115	11/12	0.94	0.23	29,32,52,53	0
1	MLY	B	187	11/12	0.95	0.16	21,23,36,37	0
1	MLY	B	148	11/12	0.95	0.12	30,32,48,48	0
1	MLY	A	219	11/12	0.95	0.19	31,33,51,51	0
1	MLY	C	70	11/12	0.96	0.16	27,29,37,37	0
1	MLY	A	148	11/12	0.96	0.11	25,26,41,42	0
1	MLY	A	187	11/12	0.96	0.15	29,30,37,38	0
1	MLY	C	191	11/12	0.96	0.15	27,28,45,45	0
1	MLY	C	148	11/12	0.97	0.14	26,27,30,31	0
1	MLY	A	115	11/12	0.97	0.10	21,22,34,36	0
1	MLY	B	70	11/12	0.98	0.11	22,23,24,27	0
1	MLY	A	70	11/12	0.98	0.11	21,24,28,28	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

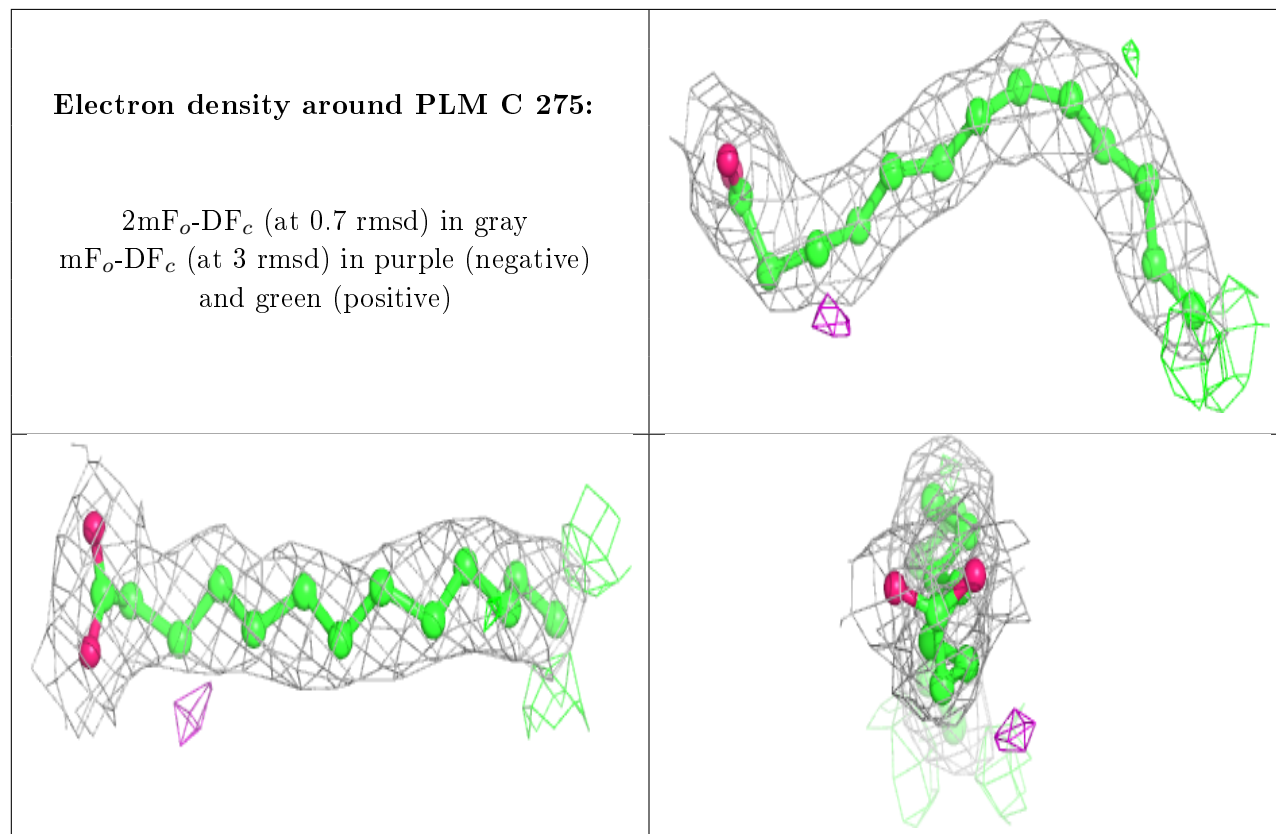
6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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(\AA^2)	Q<0.9
2	PLM	C	275	15/18	0.90	0.21	35,40,42,42	0
3	FMT	C	276	3/3	0.94	0.10	47,47,49,49	0
2	PLM	A	275	18/18	0.95	0.15	29,35,43,43	0
2	PLM	B	275	18/18	0.97	0.15	35,37,40,40	0

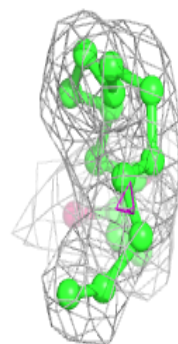
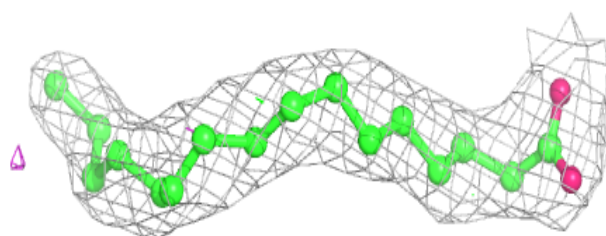
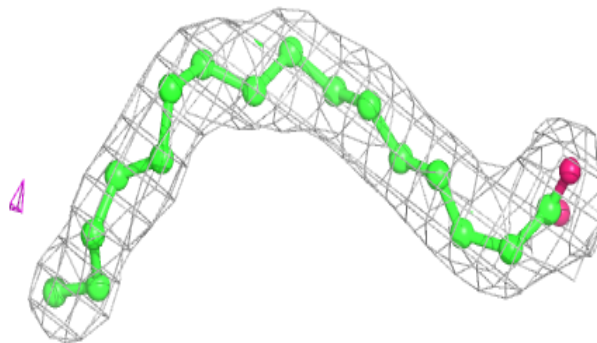
The following is a graphical depiction of the model fit to experimental electron density of all

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.

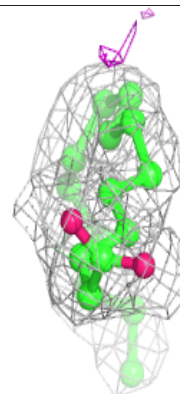
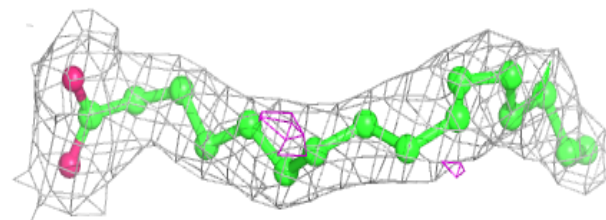
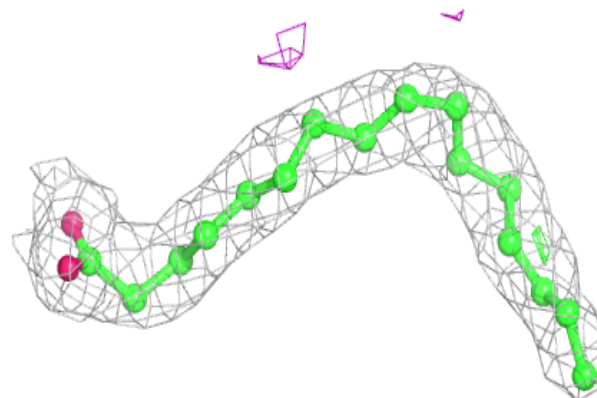


Electron density around PLM A 275:

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

**Electron density around PLM B 275:**

$2mF_o-DF_c$ (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.