



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:26 AM UTC

PDB ID : 5LOP / pdb_00005lop
Title : Structure of the active form of /K. lactis/ Dcp1-Dcp2-Edc3 decapping complex bound to m7GDP
Authors : Charenton, C.; Taverniti, V.; Gaudon-Plesse, C.; Back, R.; Seraphin, B.; Graille, M.
Deposited on : 2016-08-09
Resolution : 3.50 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

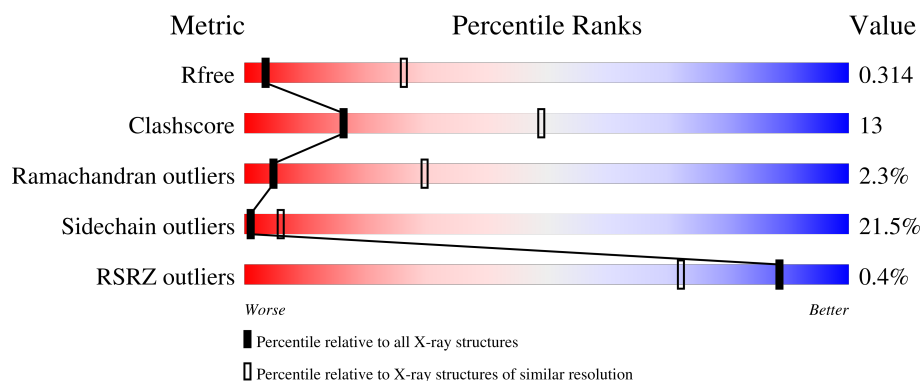
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)

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	281	
2	B	188	
3	C	66	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 4075 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 KLLA0F23980p.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	259	Total	C	N	O	S	0	0	0
			2121	1380	350	385	6			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	276	HIS	-	expression tag	UNP Q6CIU1
A	277	HIS	-	expression tag	UNP Q6CIU1
A	278	HIS	-	expression tag	UNP Q6CIU1
A	279	HIS	-	expression tag	UNP Q6CIU1
A	280	HIS	-	expression tag	UNP Q6CIU1
A	281	HIS	-	expression tag	UNP Q6CIU1

- Molecule 2 is a protein called KLLA0E01827p.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	173	Total	C	N	O	S	0	0	0
			1429	920	240	266	3			

- Molecule 3 is a protein called KLLA0A11308p.

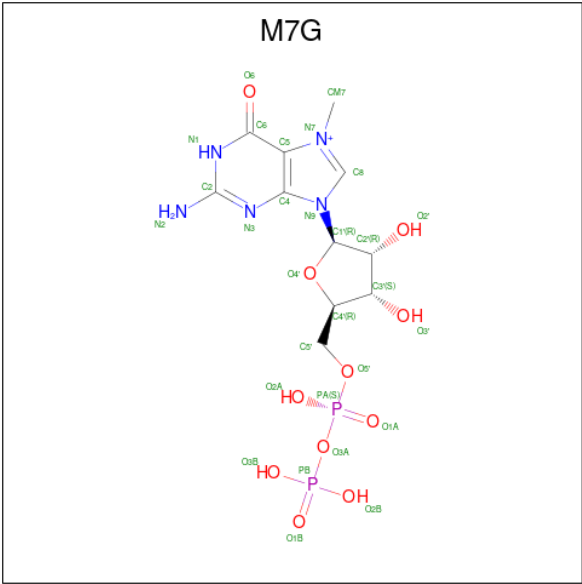
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	62	Total	C	N	O	0	0	0
			486	318	79	89			

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	3	Total	Mg	0	0
			3	3		

- Molecule 5 is 7N-METHYL-8-HYDROGUANOSINE-5'-DIPHOSPHATE (CCD ID: M7G)

(formula: C₁₁H₁₈N₅O₁₁P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			29	11	5	11	2		

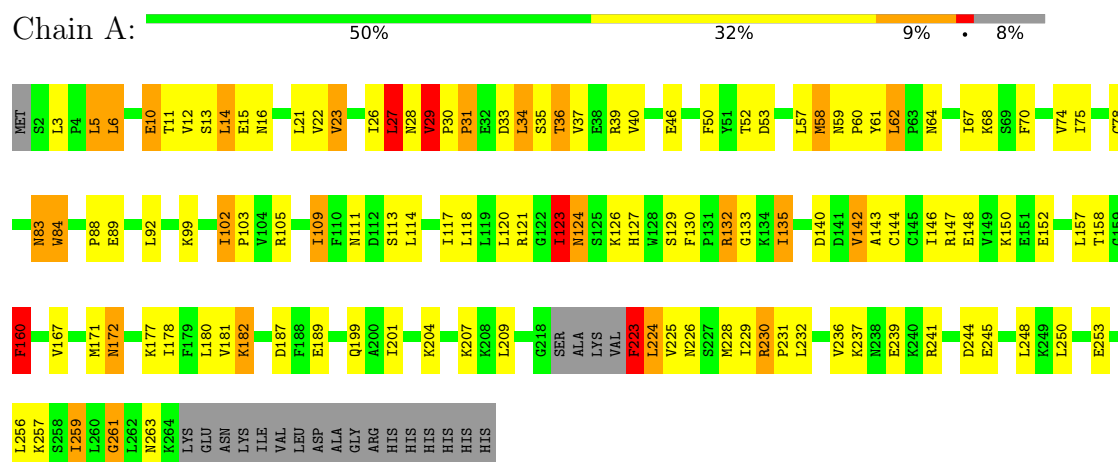
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	7	Total	O	0
			7	7	

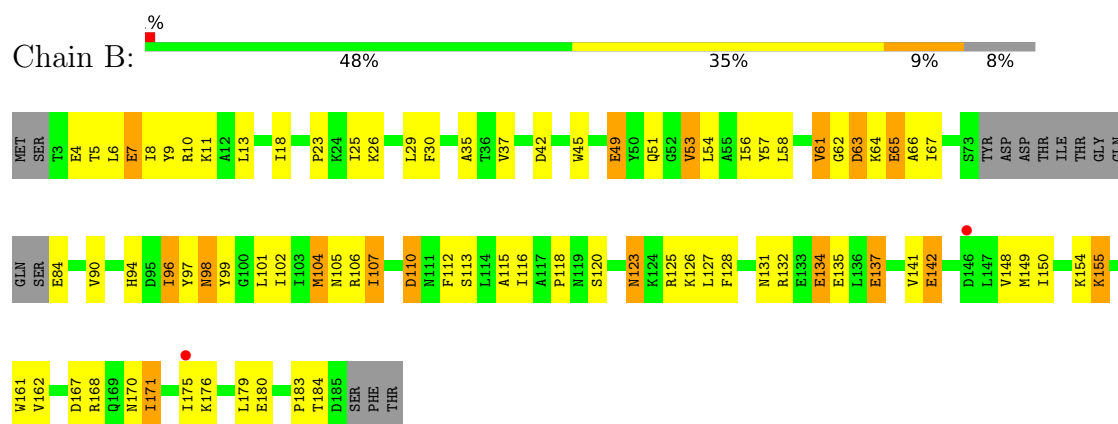
3 Residue-property plots

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.

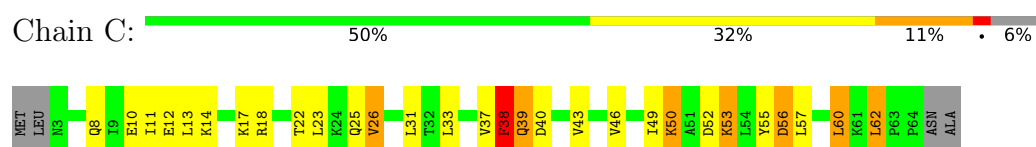
• Molecule 1: KLLA0F23980p



• Molecule 2: KLLA0E01827p



• Molecule 3: KLLA0A11308p



4 Data and refinement statistics

Property	Value	Source
Space group	P 64 2 2	Depositor
Cell constants a, b, c, α , β , γ	219.81Å 219.81Å 74.19Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.20 – 3.50 48.20 – 3.50	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.20-3.50) 99.9 (48.20-3.50)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.00 (at 3.48Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.200 , 0.266 0.274 , 0.314	Depositor DCC
R_{free} test set	697 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	201.6	Xtriage
Anisotropy	0.215	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 241.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4075	wwPDB-VP
Average B, all atoms (Å ²)	229.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.34% 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: M7G, MG

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	0.90	1/2169 (0.0%)	1.49	20/2926 (0.7%)
2	B	0.89	0/1461	1.43	12/1983 (0.6%)
3	C	0.82	0/494	1.25	2/664 (0.3%)
All	All	0.88	1/4124 (0.0%)	1.44	34/5573 (0.6%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	29	VAL	CA-C	6.24	1.57	1.52

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	160	PHE	CA-CB-CG	7.74	121.54	113.80
3	C	38	PHE	CA-CB-CG	6.49	120.29	113.80
1	A	10	GLU	CB-CG-CD	6.28	123.28	112.60
1	A	60	PRO	CA-C-N	6.15	129.13	120.28
1	A	60	PRO	C-N-CA	6.15	129.13	120.28
1	A	160	PHE	CA-C-N	-6.14	114.80	122.48
1	A	160	PHE	C-N-CA	-6.14	114.80	122.48
1	A	226	ASN	CA-CB-CG	6.09	118.69	112.60
1	A	253	GLU	CA-C-N	6.04	129.20	120.38
1	A	253	GLU	C-N-CA	6.04	129.20	120.38
1	A	83	ASN	CA-C-N	6.03	130.41	120.94
1	A	83	ASN	C-N-CA	6.03	130.41	120.94
2	B	106	ARG	CA-C-N	5.96	128.15	120.88
2	B	106	ARG	C-N-CA	5.96	128.15	120.88
1	A	223	PHE	CA-CB-CG	5.93	119.73	113.80
1	A	53	ASP	CA-CB-CG	5.81	118.41	112.60
2	B	110	ASP	CA-CB-CG	5.74	118.34	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	46	GLU	CA-C-N	5.70	127.85	120.44
1	A	46	GLU	C-N-CA	5.70	127.85	120.44
2	B	96	ILE	CA-C-N	5.62	132.27	121.54
2	B	96	ILE	C-N-CA	5.62	132.27	121.54
2	B	123	ASN	CA-C-N	5.61	127.80	120.28
2	B	123	ASN	C-N-CA	5.61	127.80	120.28
3	C	56	ASP	CA-CB-CG	5.58	118.19	112.60
1	A	64	ASN	CA-C-N	-5.45	115.31	123.00
1	A	64	ASN	C-N-CA	-5.45	115.31	123.00
2	B	63	ASP	CA-CB-CG	5.42	118.02	112.60
2	B	107	ILE	N-CA-C	5.41	115.67	110.74
2	B	25	ILE	N-CA-CB	5.34	118.40	111.83
1	A	172	ASN	CA-CB-CG	5.33	117.93	112.60
2	B	184	THR	CB-CA-C	5.33	118.67	110.14
1	A	37	VAL	N-CA-C	-5.24	104.42	111.44
2	B	9	TYR	N-CA-C	-5.16	105.55	111.07
1	A	152	GLU	CB-CG-CD	5.02	121.14	112.60

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	2121	0	2151	56	0
2	B	1429	0	1423	41	0
3	C	486	0	522	15	0
4	A	3	0	0	0	0
5	A	29	0	16	0	0
6	A	7	0	0	0	0
All	All	4075	0	4112	106	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 (106) 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:29:VAL:HG22	1:A:30:PRO:HD2	1.63	0.81
2:B:30:PHE:HE1	2:B:56:ILE:HD12	1.51	0.76
2:B:141:VAL:HG11	2:B:175:ILE:HG21	1.69	0.74
3:C:12:GLU:HB2	3:C:56:ASP:HB2	1.68	0.74
1:A:230:ARG:HG3	1:A:231:PRO:HD3	1.68	0.74
3:C:10:GLU:HB2	3:C:60:LEU:HD12	1.72	0.70
2:B:118:PRO:HG2	2:B:183:PRO:HG3	1.73	0.69
2:B:141:VAL:HG12	2:B:150:ILE:HG12	1.73	0.69
1:A:130:PHE:O	1:A:132:ARG:HD2	1.93	0.69
1:A:21:LEU:HD21	1:A:50:PHE:CD1	2.27	0.69
1:A:257:LYS:HB3	1:A:263:ASN:HD22	1.60	0.66
1:A:67:ILE:HD12	1:A:67:ILE:H	1.60	0.65
2:B:179:LEU:HD12	2:B:180:GLU:HG3	1.78	0.65
1:A:257:LYS:HA	1:A:261:GLY:HA3	1.77	0.65
1:A:130:PHE:HZ	1:A:232:LEU:HD21	1.62	0.65
1:A:160:PHE:HB2	1:A:181:VAL:HG13	1.77	0.64
1:A:10:GLU:HG3	1:A:11:THR:HG23	1.81	0.62
2:B:141:VAL:HG11	2:B:175:ILE:CG2	2.30	0.61
1:A:256:LEU:HA	1:A:259:ILE:HG22	1.82	0.60
1:A:228:MET:C	1:A:231:PRO:HD2	2.27	0.60
1:A:3:LEU:HB2	2:B:115:ALA:HB2	1.83	0.60
1:A:10:GLU:HA	1:A:58:MET:HB3	1.84	0.59
1:A:237:LYS:O	1:A:241:ARG:HB2	2.01	0.59
2:B:162:VAL:HG11	2:B:167:ASP:CB	2.32	0.59
2:B:162:VAL:HG11	2:B:167:ASP:HB2	1.84	0.59
2:B:137:GLU:OE1	2:B:155:LYS:HG3	2.01	0.59
1:A:245:GLU:HA	1:A:248:LEU:HD12	1.85	0.57
2:B:61:VAL:HG11	2:B:98:ASN:HA	1.87	0.56
1:A:5:LEU:HD11	2:B:113:SER:HB2	1.88	0.56
2:B:63:ASP:HB3	2:B:66:ALA:HB2	1.87	0.56
2:B:105:ASN:HD21	2:B:107:ILE:CG1	2.19	0.56
1:A:232:LEU:O	1:A:236:VAL:HG23	2.06	0.56
1:A:21:LEU:HD21	1:A:50:PHE:HD1	1.70	0.55
1:A:111:ASN:ND2	1:A:113:SER:HB3	2.22	0.54
2:B:45:TRP:HZ2	2:B:149:MET:HG2	1.72	0.54
2:B:64:LYS:HG3	2:B:65:GLU:HG2	1.90	0.54
1:A:6:LEU:HD23	1:A:6:LEU:H	1.72	0.53
1:A:103:PRO:HB2	1:A:105:ARG:NH2	2.24	0.53
3:C:18:ARG:HE	3:C:39:GLN:HB2	1.74	0.53
2:B:30:PHE:CZ	2:B:171:ILE:HG22	2.45	0.52
1:A:204:LYS:HB3	1:A:209:LEU:HD21	1.92	0.51
1:A:12:VAL:H	1:A:59:ASN:HD21	1.58	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:ILE:HD11	1:A:157:LEU:HD11	1.93	0.50
1:A:6:LEU:HD21	2:B:23:PRO:HD3	1.94	0.50
1:A:123:ILE:HA	1:A:199:GLN:HB2	1.93	0.50
1:A:22:VAL:HG12	1:A:27:LEU:HB2	1.93	0.50
2:B:167:ASP:O	2:B:171:ILE:HG23	2.12	0.50
1:A:29:VAL:HG22	1:A:30:PRO:CD	2.36	0.50
2:B:132:ARG:HD3	2:B:132:ARG:H	1.76	0.49
1:A:127:HIS:HD1	1:A:223:PHE:N	2.11	0.49
1:A:36:THR:HB	1:A:39:ARG:H	1.78	0.49
2:B:26:LYS:HB3	2:B:58:LEU:HG	1.94	0.49
1:A:123:ILE:HD12	1:A:124:ASN:HD22	1.77	0.48
2:B:37:VAL:HG11	2:B:112:PHE:CE1	2.48	0.48
1:A:105:ARG:NE	1:A:177:LYS:HB3	2.29	0.48
1:A:84:TRP:CD1	1:A:84:TRP:H	2.26	0.48
1:A:230:ARG:CG	1:A:231:PRO:HD3	2.43	0.48
2:B:118:PRO:HA	2:B:179:LEU:HA	1.95	0.47
2:B:45:TRP:CZ2	2:B:149:MET:HG2	2.49	0.47
2:B:105:ASN:HD21	2:B:107:ILE:HG12	1.78	0.47
1:A:167:VAL:HG23	1:A:180:LEU:HD11	1.97	0.47
3:C:18:ARG:NE	3:C:39:GLN:HB2	2.29	0.47
2:B:7:GLU:HA	2:B:10:ARG:HB3	1.96	0.47
3:C:23:LEU:HD11	3:C:26:VAL:HG13	1.97	0.47
1:A:121:ARG:HD2	1:A:126:LYS:HA	1.97	0.46
1:A:120:LEU:HB3	1:A:201:ILE:HG12	1.97	0.46
3:C:38:PHE:C	3:C:40:ASP:H	2.24	0.45
1:A:114:LEU:HD21	1:A:182:LYS:HG3	1.98	0.45
1:A:143:ALA:O	1:A:146:ILE:HG13	2.17	0.44
3:C:17:LYS:HG3	3:C:40:ASP:OD2	2.17	0.44
3:C:50:LYS:H	3:C:53:LYS:HZ3	1.64	0.44
2:B:51:GLN:H	2:B:105:ASN:ND2	2.16	0.44
2:B:58:LEU:HA	2:B:99:TYR:HD1	1.82	0.44
1:A:70:PHE:O	1:A:74:VAL:HG23	2.17	0.44
1:A:12:VAL:H	1:A:59:ASN:ND2	2.16	0.43
1:A:31:PRO:HA	1:A:34:LEU:HB2	2.00	0.43
2:B:54:LEU:HD21	2:B:101:LEU:HD11	1.99	0.43
3:C:37:VAL:HG13	3:C:43:VAL:HG22	1.99	0.43
2:B:126:LYS:HE2	2:B:134:GLU:O	2.19	0.43
3:C:13:LEU:HD22	3:C:55:TYR:HD2	1.84	0.43
2:B:35:ALA:HA	2:B:161:TRP:O	2.18	0.42
1:A:256:LEU:HD13	3:C:57:LEU:HD11	2.01	0.42
2:B:99:TYR:HB2	2:B:116:ILE:HG23	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:ASP:OD2	1:A:142:VAL:HG23	2.19	0.42
2:B:61:VAL:HA	2:B:62:GLY:HA3	1.88	0.42
1:A:13:SER:C	1:A:14:LEU:N	2.78	0.42
1:A:103:PRO:HG2	1:A:135:ILE:HG12	2.00	0.42
2:B:29:LEU:HG	2:B:57:TYR:HA	2.01	0.42
1:A:13:SER:C	1:A:16:ASN:H	2.28	0.42
2:B:142:GLU:HG2	2:B:149:MET:HB2	2.00	0.41
1:A:23:VAL:HG22	1:A:27:LEU:HD12	2.02	0.41
1:A:27:LEU:HG	2:B:13:LEU:HD23	2.03	0.41
1:A:245:GLU:HG2	3:C:62:LEU:HD21	2.03	0.41
2:B:18:ILE:HG23	2:B:102:ILE:HD13	2.03	0.41
2:B:105:ASN:ND2	2:B:107:ILE:HG12	2.36	0.41
1:A:133:GLY:HA3	1:A:148:GLU:HG3	2.03	0.41
3:C:8:GLN:HA	3:C:22:THR:HA	2.03	0.41
1:A:171:MET:HE2	1:A:224:LEU:HD13	2.03	0.41
2:B:5:THR:HA	2:B:8:ILE:HG12	2.03	0.41
1:A:75:ILE:HD12	1:A:88:PRO:HG3	2.03	0.40
3:C:14:LYS:HB2	3:C:55:TYR:CD1	2.55	0.40
2:B:116:ILE:HD11	2:B:179:LEU:HB3	2.03	0.40
1:A:59:ASN:HB3	1:A:62:LEU:HG	2.03	0.40
1:A:99:LYS:HA	1:A:102:ILE:HG12	2.03	0.40
3:C:23:LEU:HA	3:C:33:LEU:HD23	2.03	0.40
2:B:53:VAL:HG13	2:B:104:MET:HB2	2.03	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	253/281 (90%)	224 (88%)	23 (9%)	6 (2%)	4	29
2	B	167/188 (89%)	141 (84%)	22 (13%)	4 (2%)	4	29

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	60/66 (91%)	54 (90%)	5 (8%)	1 (2%)	7	35
All	All	480/535 (90%)	419 (87%)	50 (10%)	11 (2%)	5	30

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	123	ILE
1	A	158	THR
2	B	49	GLU
2	B	97	TYR
2	B	104	MET
2	B	155	LYS
1	A	27	LEU
3	C	39	GLN
1	A	31	PRO
1	A	261	GLY
1	A	26	ILE

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	238/257 (93%)	185 (78%)	53 (22%)	1	5
2	B	158/172 (92%)	126 (80%)	32 (20%)	1	7
3	C	55/58 (95%)	43 (78%)	12 (22%)	1	6
All	All	451/487 (93%)	354 (78%)	97 (22%)	1	6

All (97) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LEU
1	A	6	LEU
1	A	14	LEU
1	A	15	GLU

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Mol	Chain	Res	Type
1	A	23	VAL
1	A	27	LEU
1	A	28	ASN
1	A	29	VAL
1	A	33	ASP
1	A	34	LEU
1	A	35	SER
1	A	36	THR
1	A	40	VAL
1	A	52	THR
1	A	57	LEU
1	A	58	MET
1	A	61	TYR
1	A	62	LEU
1	A	68	LYS
1	A	78	CYS
1	A	83	ASN
1	A	84	TRP
1	A	89	GLU
1	A	92	LEU
1	A	102	ILE
1	A	109	ILE
1	A	117	ILE
1	A	118	LEU
1	A	123	ILE
1	A	124	ASN
1	A	129	SER
1	A	132	ARG
1	A	135	ILE
1	A	142	VAL
1	A	144	CYS
1	A	147	ARG
1	A	150	LYS
1	A	160	PHE
1	A	172	ASN
1	A	178	ILE
1	A	182	LYS
1	A	187	ASP
1	A	189	GLU
1	A	207	LYS
1	A	223	PHE
1	A	224	LEU

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Mol	Chain	Res	Type
1	A	225	VAL
1	A	229	ILE
1	A	230	ARG
1	A	239	GLU
1	A	244	ASP
1	A	250	LEU
1	A	259	ILE
2	B	4	GLU
2	B	6	LEU
2	B	7	GLU
2	B	11	LYS
2	B	42	ASP
2	B	49	GLU
2	B	53	VAL
2	B	61	VAL
2	B	65	GLU
2	B	67	ILE
2	B	84	GLU
2	B	90	VAL
2	B	94	HIS
2	B	96	ILE
2	B	98	ASN
2	B	110	ASP
2	B	120	SER
2	B	123	ASN
2	B	125	ARG
2	B	127	LEU
2	B	128	PHE
2	B	131	ASN
2	B	134	GLU
2	B	135	GLU
2	B	137	GLU
2	B	142	GLU
2	B	148	VAL
2	B	154	LYS
2	B	168	ARG
2	B	170	ASN
2	B	171	ILE
2	B	176	LYS
3	C	11	ILE
3	C	25	GLN
3	C	26	VAL

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Mol	Chain	Res	Type
3	C	31	LEU
3	C	38	PHE
3	C	46	VAL
3	C	49	ILE
3	C	50	LYS
3	C	52	ASP
3	C	53	LYS
3	C	60	LEU
3	C	62	LEU

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

Mol	Chain	Res	Type
1	A	16	ASN
1	A	59	ASN
1	A	124	ASN
1	A	165	GLN
1	A	170	ASN
1	A	194	HIS
1	A	216	ASN
1	A	263	ASN
2	B	31	HIS
2	B	51	GLN
2	B	105	ASN
2	B	131	ASN
3	C	25	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 4 ligands modelled in this entry, 3 are monoatomic - leaving 1 for Mogul analysis.

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
5	M7G	A	303	4	30,31,31	1.64	3 (10%)	47,49,49	1.33	5 (10%)

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
5	M7G	A	303	4	-	5/16/32/32	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	303	M7G	C8-N7	7.17	1.45	1.33
5	A	303	M7G	C8-N9	3.82	1.46	1.35
5	A	303	M7G	C5-N7	-2.53	1.36	1.39

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	303	M7G	N9-C8-N7	-4.06	102.63	112.48
5	A	303	M7G	CM7-N7-C5	-3.64	122.26	126.80
5	A	303	M7G	CM7-N7-C8	-3.41	119.63	124.79
5	A	303	M7G	O4'-C1'-N9	2.79	114.67	108.36
5	A	303	M7G	C5-C4-N9	2.12	110.41	105.88

There are no chirality outliers.

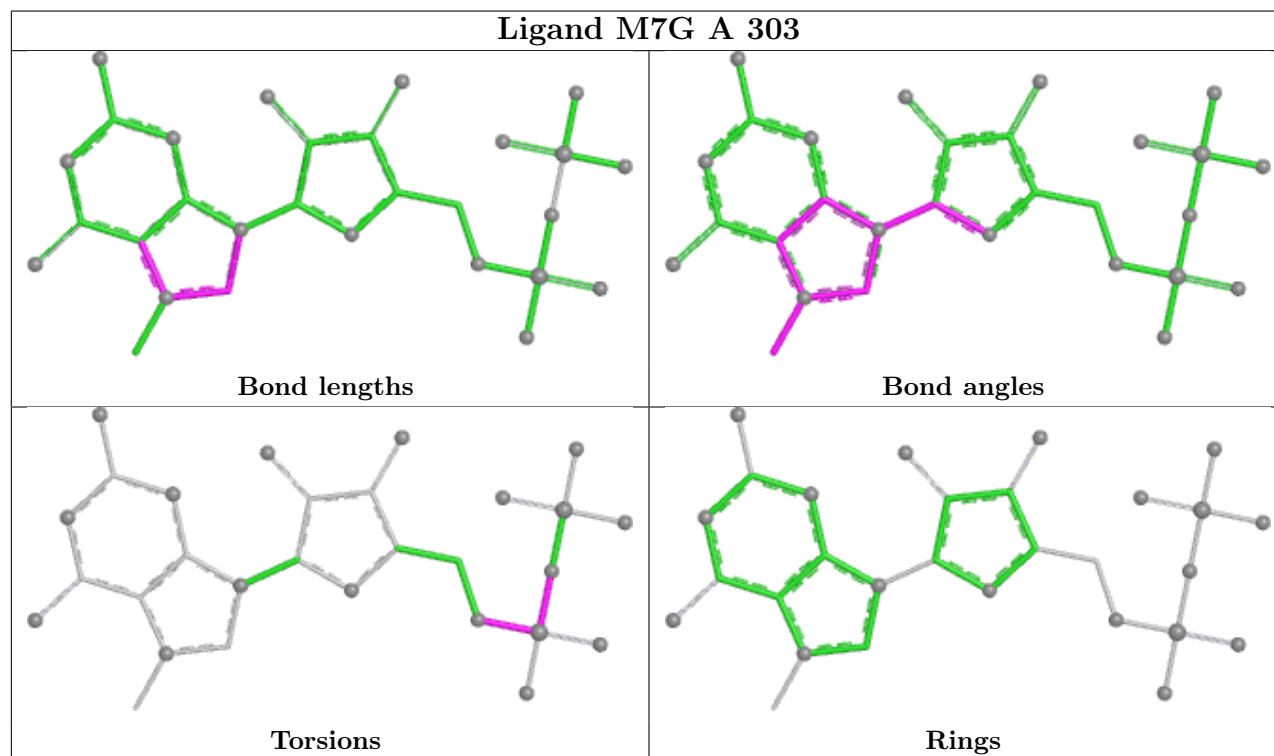
All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	303	M7G	C5'-O5'-PA-O1A
5	A	303	M7G	C5'-O5'-PA-O2A
5	A	303	M7G	C5'-O5'-PA-O3A
5	A	303	M7G	PB-O3A-PA-O2A
5	A	303	M7G	PB-O3A-PA-O1A

There are no ring outliers.

No monomer is involved in short contacts.

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	B	1
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	59:ARG	C	60:ASP	N	2.97
1	A	13:SER	C	14:LEU	N	2.78

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	259/281 (92%)	-0.62	0 100 100	163, 213, 264, 286	0
2	B	173/188 (92%)	-0.56	2 (1%) 76 52	128, 248, 282, 297	0
3	C	62/66 (93%)	-0.68	0 100 100	221, 246, 269, 280	0
All	All	494/535 (92%)	-0.61	2 (0%) 88 72	128, 231, 279, 297	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	146	ASP	3.5
2	B	175	ILE	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.

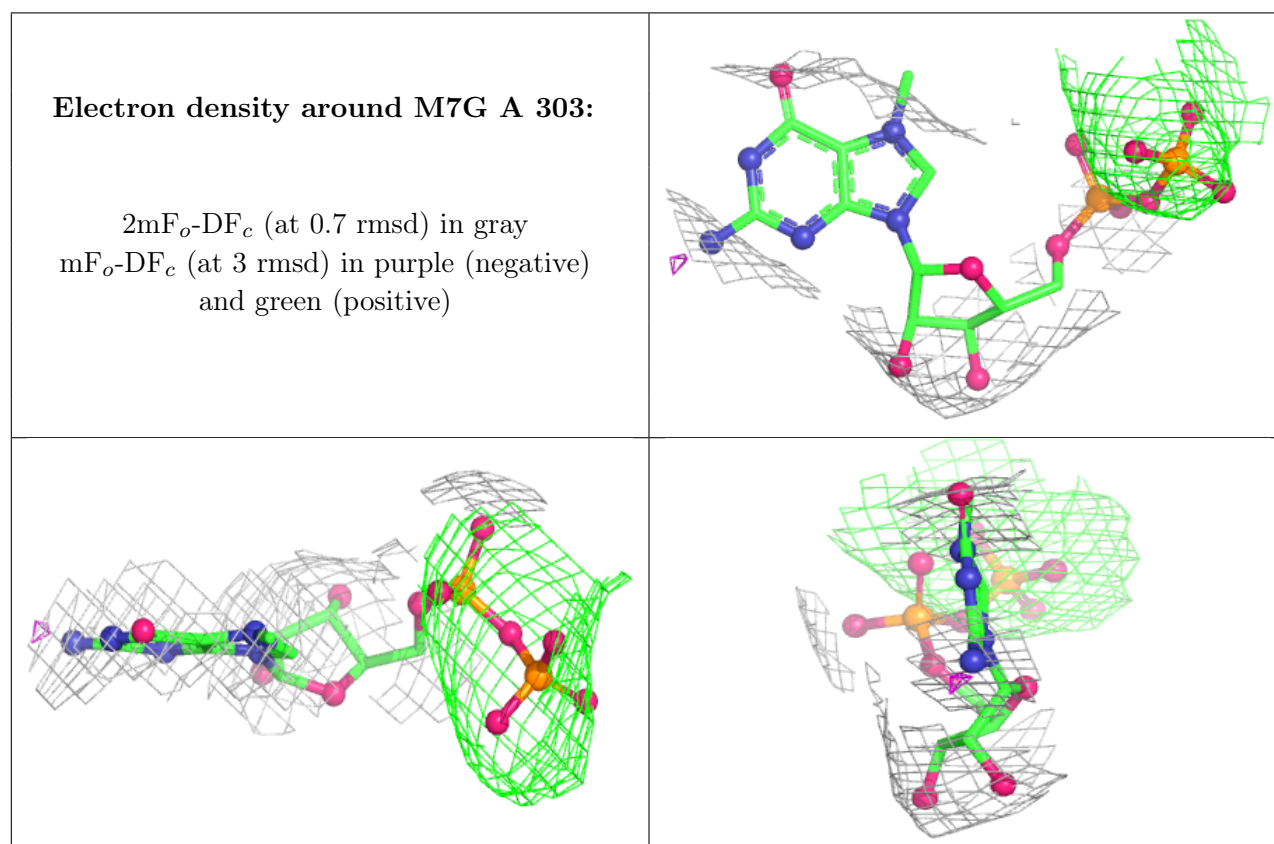
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	MG	A	304	1/1	0.91	0.19	131,131,131,131	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	M7G	A	303	29/29	0.94	0.08	191,206,223,227	0
4	MG	A	301	1/1	1.00	0.09	139,139,139,139	0
4	MG	A	302	1/1	1.00	0.09	130,130,130,130	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.



6.5 Other polymers ⓘ

There are no such residues in this entry.