



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 11:51 PM UTC

PDB ID : 5F98 / pdb_00005f98
Title : Crystal structure of RIG-I in complex with Cap-0 RNA
Authors : Wang, C.; Marcotrigiano, J.; Miller, M.; Jiang, F.
Deposited on : 2015-12-09
Resolution : 3.28 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

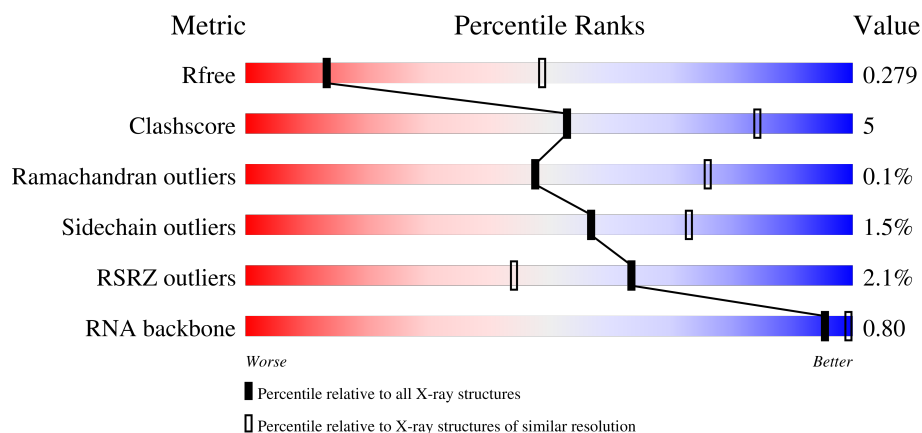
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.28 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.



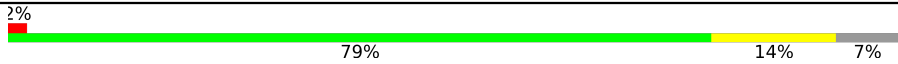
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1303 (3.30-3.26)
Clashscore	190562	1354 (3.30-3.26)
Ramachandran outliers	187476	1334 (3.30-3.26)
Sidechain outliers	187428	1333 (3.30-3.26)
RSRZ outliers	180081	1303 (3.30-3.26)
RNA backbone	3983	1020 (3.58-2.98)

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	695	80%13%6%
1	C	695	3%79%13%7%
1	E	695	3%78%14%8%
1	G	695	80%13%7%

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Mol	Chain	Length	Quality of chain
1	I	695	 2% 79% 14% 7%
1	K	695	 2% 83% 9% 7%
2	B	24	 75% 25%
2	D	24	 75% 25%
2	F	24	 83% 17%
2	H	24	 75% 25%
2	J	24	 83% 17%
2	L	24	 58% 42%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 32719 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 Probable ATP-dependent RNA helicase DDX58.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	650	Total	C	N	O	S	0	0	0
			5060	3237	855	938	30			
1	C	648	Total	C	N	O	S	0	0	0
			4949	3169	832	917	31			
1	E	641	Total	C	N	O	S	0	0	0
			4832	3087	822	894	29			
1	G	647	Total	C	N	O	S	0	1	0
			4965	3182	836	916	31			
1	I	647	Total	C	N	O	S	0	0	0
			4838	3093	810	906	29			
1	K	644	Total	C	N	O	S	0	0	0
			4859	3115	812	901	31			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	231	SER	-	expression tag	UNP O95786
C	231	SER	-	expression tag	UNP O95786
E	231	SER	-	expression tag	UNP O95786
G	231	SER	-	expression tag	UNP O95786
I	231	SER	-	expression tag	UNP O95786
K	231	SER	-	expression tag	UNP O95786

- Molecule 2 is a RNA chain called RNA (5'-R(P*GP*AP*AP*UP*AP*UP*AP*AP*UP*AP*GP*UP*GP*AP*UP*AP*UP*UP*AP*UP*AP*UP*UP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	24	Total	C	N	O	P	0	0	0
			509	229	88	168	24			
2	D	24	Total	C	N	O	P	0	0	0
			509	229	88	168	24			
2	F	24	Total	C	N	O	P	0	0	0
			509	229	88	168	24			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	24	Total	C	N	O	P	0	0	0
			509	229	88	168	24			
2	J	24	Total	C	N	O	P	0	0	0
			509	229	88	168	24			
2	L	24	Total	C	N	O	P	0	0	0
			509	229	88	168	24			

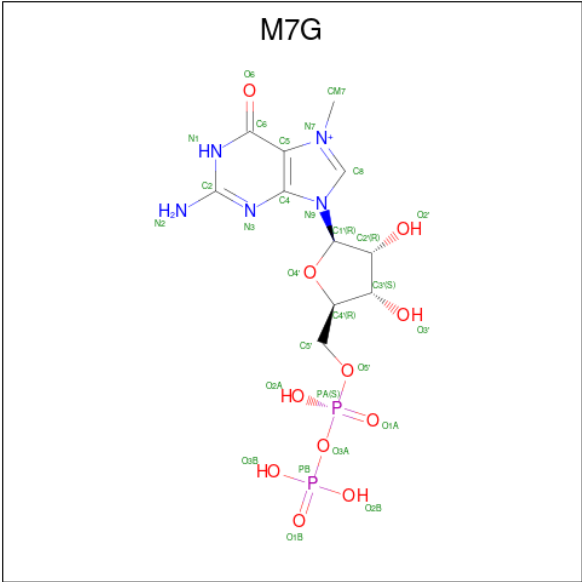
- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		
3	C	1	Total	Zn	0	0
			1	1		
3	E	1	Total	Zn	0	0
			1	1		
3	G	1	Total	Zn	0	0
			1	1		
3	I	1	Total	Zn	0	0
			1	1		
3	K	1	Total	Zn	0	0
			1	1		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	0
			1	1		
4	C	1	Total	Mg	0	0
			1	1		
4	E	1	Total	Mg	0	0
			1	1		
4	G	1	Total	Mg	0	0
			1	1		
4	I	1	Total	Mg	0	0
			1	1		
4	K	1	Total	Mg	0	0
			1	1		

- Molecule 5 is 7N-METHYL-8-HYDROGUANOSINE-5'-DIPHOSPHATE (CCD ID: M7G) (formula: C₁₁H₁₈N₅O₁₁P₂).

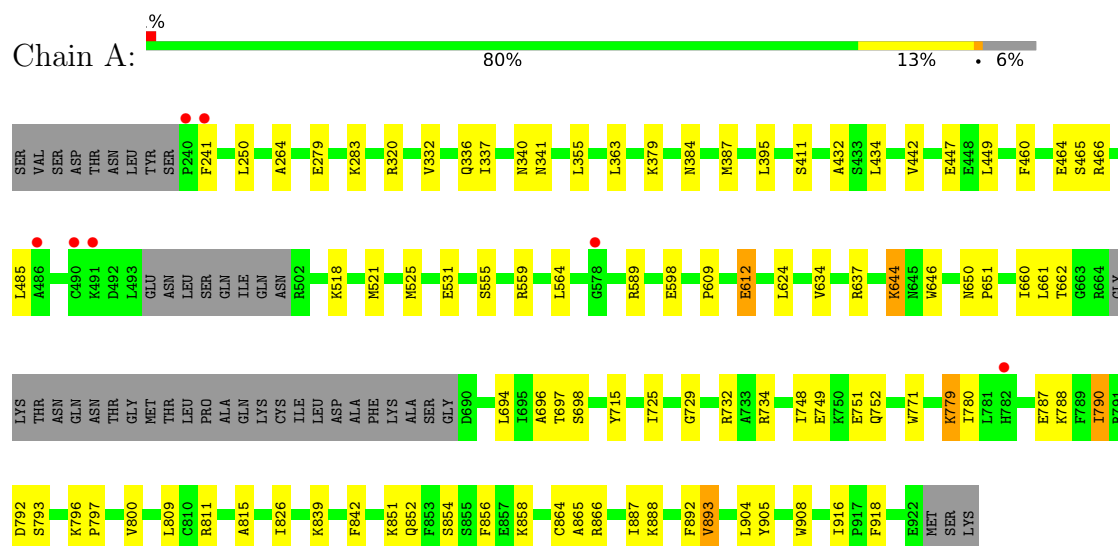


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	N	O	P	0	0
			29	11	5	11	2		
5	D	1	Total	C	N	O	P	0	0
			29	11	5	11	2		
5	F	1	Total	C	O	P		0	0
			17	5	10	2			
5	H	1	Total	C	N	O	P	0	0
			29	11	5	11	2		
5	J	1	Total	C	N	O	P	0	0
			29	11	5	11	2		
5	L	1	Total	C	O	P		0	0
			17	5	10	2			

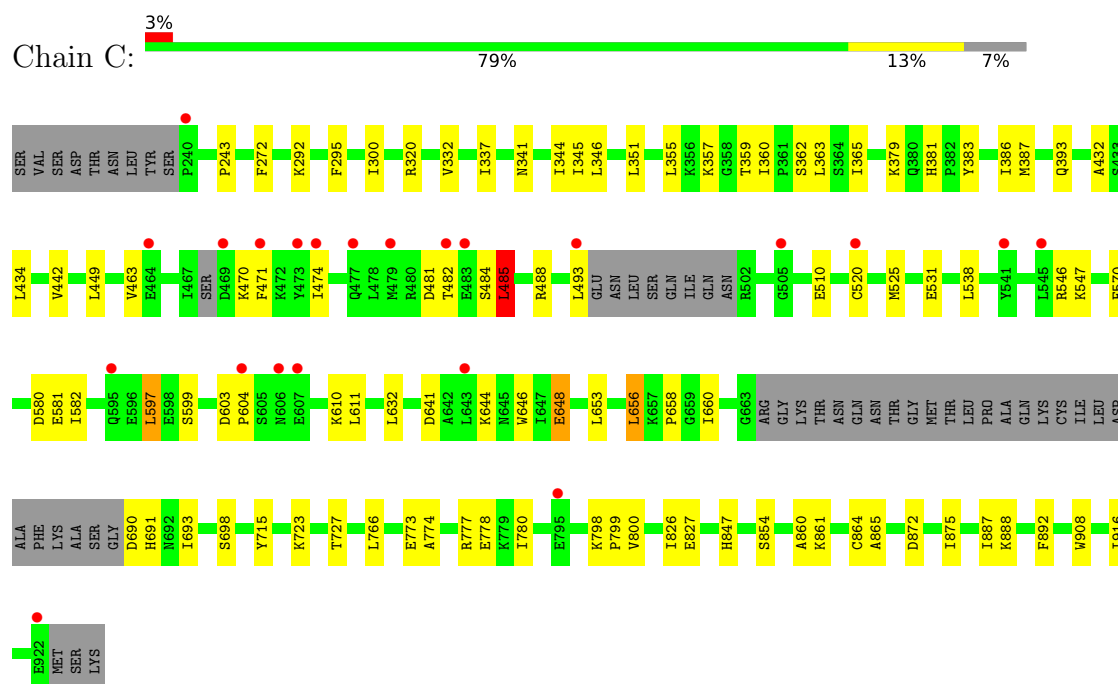
3 Residue-property plots [i](#)

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.

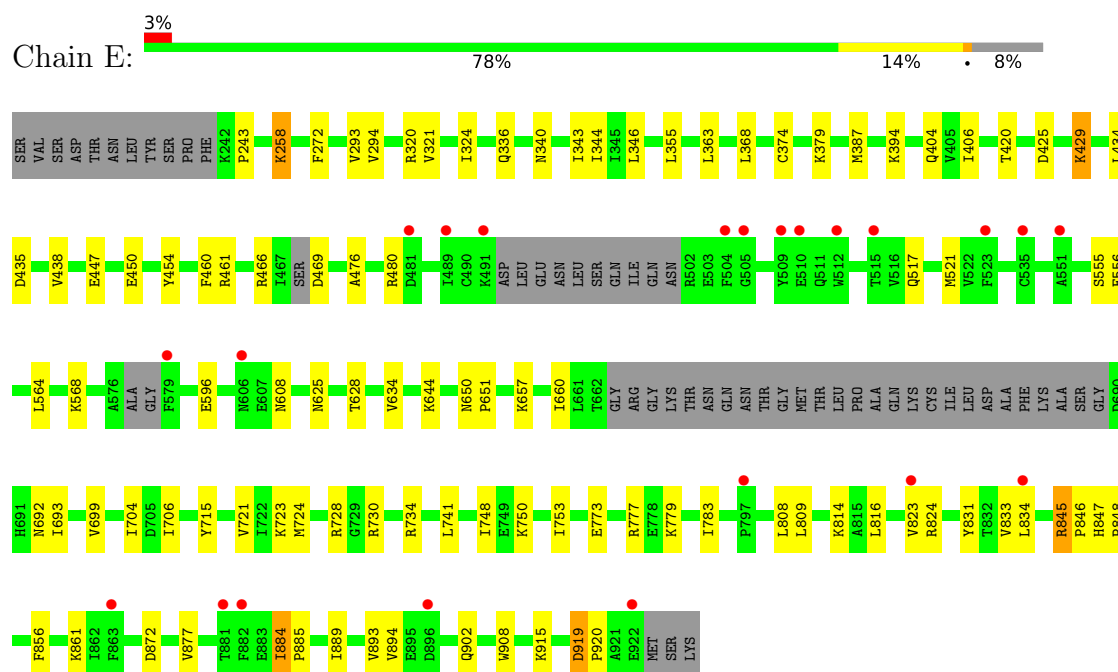
- Molecule 1: Probable ATP-dependent RNA helicase DDX58



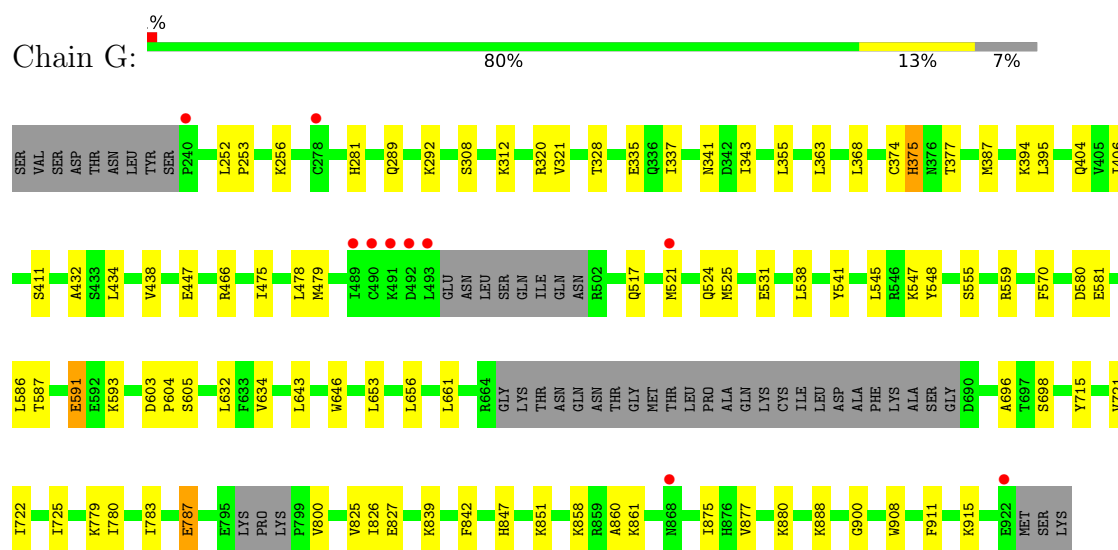
- Molecule 1: Probable ATP-dependent RNA helicase DDX58



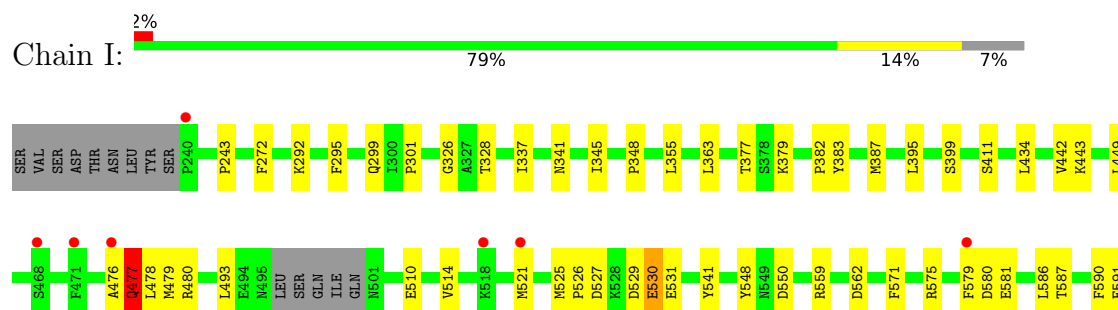
● Molecule 1: Probable ATP-dependent RNA helicase DDX58

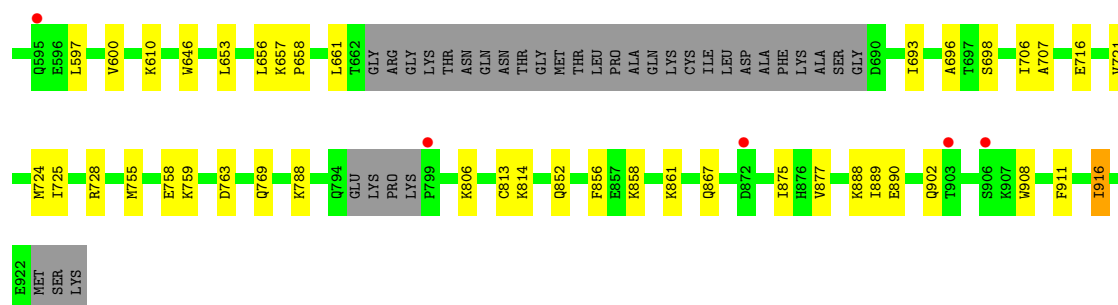


● Molecule 1: Probable ATP-dependent RNA helicase DDX58

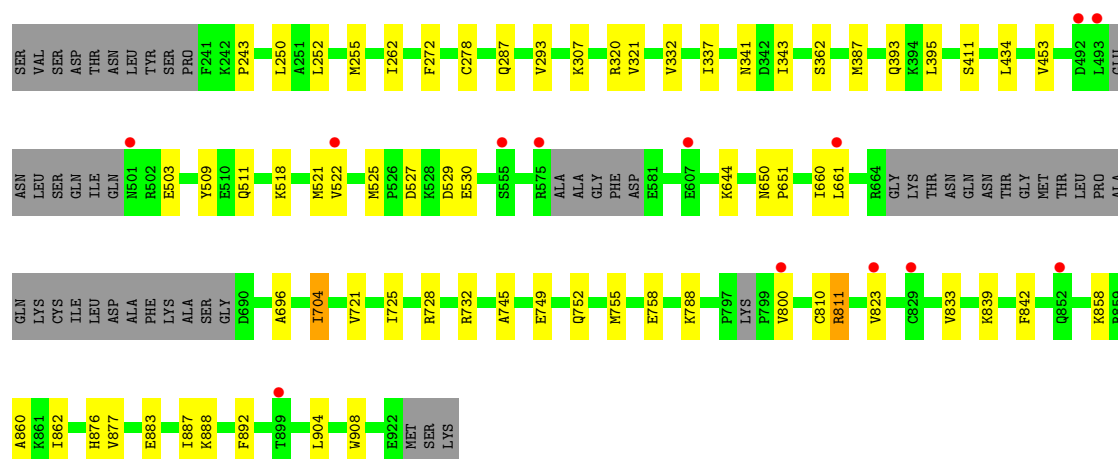
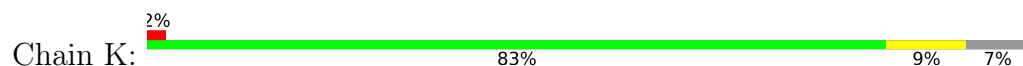


● Molecule 1: Probable ATP-dependent RNA helicase DDX58





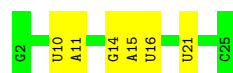
- Molecule 1: Probable ATP-dependent RNA helicase DDX58



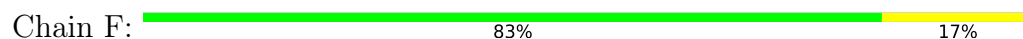
- Molecule 2: RNA (5'-R(P*GP*AP*AP*UP*AP*UP*AP*AP*UP*AP*GP*UP*GP*AP*UP*A P*UP*UP*AP*UP*AP*UP*UP*C)-3')



- Molecule 2: RNA (5'-R(P*GP*AP*AP*UP*AP*UP*AP*AP*UP*AP*GP*UP*GP*AP*UP*A P*UP*UP*AP*UP*AP*UP*UP*C)-3')



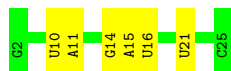
- Molecule 2: RNA (5'-R(P*GP*AP*AP*UP*AP*UP*AP*AP*UP*AP*GP*UP*GP*AP*UP*A P*UP*UP*AP*UP*AP*UP*UP*C)-3')





- Molecule 2: RNA (5'-R(P*GP*AP*AP*UP*AP*UP*AP*AP*UP*AP*GP*UP*GP*AP*UP*AP*UP*UP*AP*UP*AP*UP*UP*C)-3')

Chain H:  75% 25%



- Molecule 2: RNA (5'-R(P*GP*AP*AP*UP*AP*UP*AP*AP*UP*AP*GP*UP*GP*AP*UP*AP*UP*UP*AP*UP*AP*UP*UP*C)-3')

Chain J:  83% 17%



- Molecule 2: RNA (5'-R(P*GP*AP*AP*UP*AP*UP*AP*AP*UP*AP*GP*UP*GP*AP*UP*AP*UP*UP*AP*UP*AP*UP*UP*C)-3')

Chain L:  58% 42%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	111.18Å 174.57Å 309.26Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	84.00 – 3.28 84.00 – 3.28	Depositor EDS
% Data completeness (in resolution range)	99.3 (84.00-3.28) 92.1 (84.00-3.28)	Depositor EDS
R_{merge}	0.56	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.40 (at 3.26Å)	Xtriage
Refinement program	PHENIX 1.9_1690	Depositor
R, R_{free}	0.221 , 0.277 0.224 , 0.279	Depositor DCC
R_{free} test set	2000 reflections (2.15%)	wwPDB-VP
Wilson B-factor (Å ²)	51.9	Xtriage
Anisotropy	0.499	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 56.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	32719	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.75% 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: MG, ZN, M7G

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	0.27	0/5167	0.72	5/7005 (0.1%)
1	C	0.28	0/5052	0.75	6/6858 (0.1%)
1	E	0.26	0/4933	0.73	5/6708 (0.1%)
1	G	0.27	0/5069	0.71	0/6881
1	I	0.27	0/4942	0.73	6/6730 (0.1%)
1	K	0.27	0/4960	0.71	2/6745 (0.0%)
2	B	0.06	0/569	0.13	0/883
2	D	0.06	0/569	0.13	0/883
2	F	0.06	0/569	0.12	0/883
2	H	0.06	0/569	0.13	0/883
2	J	0.06	0/569	0.15	0/883
2	L	0.06	0/569	0.13	0/881
All	All	0.25	0/33537	0.68	24/46223 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	I	0	1

There are no bond length outliers.

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	478	LEU	N-CA-C	-8.45	102.16	111.36
1	A	241	PHE	N-CA-C	6.94	119.48	109.14
1	A	790	ILE	N-CA-C	-6.73	105.55	113.42
1	E	919	ASP	CA-C-N	6.18	127.57	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	919	ASP	C-N-CA	6.18	127.57	119.84
1	C	798	LYS	CA-C-N	-5.87	112.50	119.84
1	C	798	LYS	C-N-CA	-5.87	112.50	119.84
1	A	854	SER	CB-CA-C	-5.58	110.12	116.54
1	I	379	LYS	CB-CA-C	-5.58	110.16	116.63
1	C	379	LYS	CB-CA-C	-5.55	110.19	116.63
1	E	379	LYS	CB-CA-C	-5.53	110.21	116.63
1	C	854	SER	CB-CA-C	-5.48	110.24	116.54
1	I	493	LEU	CB-CA-C	-5.47	109.79	117.23
1	E	845	ARG	CA-C-N	5.43	126.63	119.84
1	E	845	ARG	C-N-CA	5.43	126.63	119.84
1	I	867	GLN	CB-CA-C	-5.38	110.35	116.54
1	C	485	LEU	CA-CB-CG	5.31	134.89	116.30
1	C	300	ILE	CB-CA-C	-5.29	108.74	114.35
1	I	657	LYS	CA-C-N	5.14	125.13	119.89
1	I	657	LYS	C-N-CA	5.14	125.13	119.89
1	A	916	ILE	CA-C-N	5.09	125.09	119.90
1	A	916	ILE	C-N-CA	5.09	125.09	119.90
1	K	525	MET	CA-C-N	5.04	125.06	119.32
1	K	525	MET	C-N-CA	5.04	125.06	119.32

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	I	477	GLN	Peptide

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	5060	0	4907	55	0
1	C	4949	0	4755	51	0
1	E	4832	0	4529	54	0
1	G	4965	0	4768	52	0
1	I	4838	0	4460	58	0
1	K	4859	0	4582	37	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	509	0	255	3	0
2	D	509	0	255	3	0
2	F	509	0	255	2	0
2	H	509	0	255	3	0
2	J	509	0	255	4	0
2	L	509	0	255	7	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
3	E	1	0	0	0	0
3	G	1	0	0	0	0
3	I	1	0	0	0	0
3	K	1	0	0	0	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
4	E	1	0	0	0	0
4	G	1	0	0	0	0
4	I	1	0	0	0	0
4	K	1	0	0	0	0
5	B	29	0	15	0	0
5	D	29	0	16	0	0
5	F	17	0	7	0	0
5	H	29	0	16	0	0
5	J	29	0	15	1	0
5	L	17	0	7	0	0
All	All	32719	0	29607	310	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 5.

All (310) 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:I:477:GLN:HA	1:I:480:ARG:H	1.54	0.72
1:E:644:LYS:HD2	1:E:660:ILE:HD11	1.73	0.71
1:E:258:LYS:HE3	1:E:438:VAL:HG21	1.72	0.71
1:I:443:LYS:NZ	1:I:769:GLN:OE1	2.21	0.69
1:E:831:TYR:OH	1:E:915:LYS:NZ	2.21	0.69
1:A:432:ALA:HA	1:A:780:ILE:HG23	1.76	0.68
1:G:783:ILE:HG22	1:G:787:GLU:OE2	1.94	0.68
1:I:476:ALA:O	1:I:479:MET:HB2	1.94	0.67
1:A:609:PRO:HA	1:A:612:GLU:HG3	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:466:ARG:NH1	1:A:555:SER:O	2.27	0.67
1:G:698:SER:HG	2:H:21:U:HO2'	1.43	0.65
1:C:432:ALA:HA	1:C:780:ILE:HG23	1.77	0.64
1:K:888:LYS:HA	1:K:908:TRP:HE1	1.62	0.64
1:G:559:ARG:HD3	1:G:646:TRP:HD1	1.63	0.64
1:E:466:ARG:NH2	1:E:555:SER:O	2.31	0.63
1:A:518:LYS:HA	1:A:521:MET:HE2	1.79	0.63
1:C:644:LYS:HD3	1:C:660:ILE:HD11	1.81	0.63
1:G:861:LYS:HD2	1:G:875:ILE:HG22	1.81	0.63
1:A:395:LEU:HD12	1:A:788:LYS:HD3	1.81	0.62
1:A:442:VAL:HG21	1:A:449:LEU:HD22	1.81	0.62
1:G:779:LYS:O	1:G:783:ILE:HG13	2.00	0.62
1:A:644:LYS:HD3	1:A:660:ILE:HD11	1.82	0.61
1:A:564:LEU:HD21	1:A:598:GLU:HG2	1.82	0.61
1:A:734:ARG:NH1	1:E:450:GLU:OE2	2.33	0.61
1:G:524:GLN:NE2	1:G:900:GLY:O	2.34	0.61
1:I:559:ARG:HD3	1:I:646:TRP:HD1	1.65	0.61
1:E:425:ASP:O	1:E:429:LYS:HG2	2.01	0.60
1:G:355:LEU:HD11	1:G:363:LEU:HD21	1.83	0.60
1:I:395:LEU:O	1:I:788:LYS:NZ	2.33	0.60
1:K:337:ILE:O	1:K:341:ASN:ND2	2.27	0.60
1:I:861:LYS:HD2	1:I:875:ILE:HG22	1.84	0.60
1:C:861:LYS:HD2	1:C:875:ILE:HG22	1.83	0.59
1:E:773:GLU:OE2	1:E:777:ARG:NH2	2.36	0.59
1:K:644:LYS:HD2	1:K:660:ILE:HD11	1.84	0.59
1:G:377:THR:HG21	1:G:434:LEU:HG	1.84	0.59
1:G:475:ILE:HG22	1:G:479:MET:HE2	1.83	0.59
1:G:525:MET:HB2	1:G:531:GLU:HB2	1.84	0.59
1:A:792:ASP:OD1	1:A:793:SER:N	2.36	0.58
2:F:12:G:N2	2:F:15:A:OP2	2.36	0.58
1:I:355:LEU:HD11	1:I:363:LEU:HD21	1.85	0.58
1:C:482:THR:HA	1:C:485:LEU:HD12	1.85	0.58
1:A:559:ARG:HD3	1:A:646:TRP:HD1	1.69	0.58
1:I:858:LYS:HA	1:I:877:VAL:HG12	1.86	0.57
1:A:771:TRP:HZ3	1:A:779:LYS:HE3	1.69	0.57
1:G:466:ARG:NH2	1:G:555:SER:O	2.38	0.57
1:E:556:GLU:O	1:E:608:ASN:ND2	2.35	0.57
1:A:355:LEU:HD11	1:A:363:LEU:HD21	1.87	0.56
1:E:699:VAL:O	1:E:723:LYS:NZ	2.37	0.56
1:I:295:PHE:HB3	1:I:345:ILE:HG13	1.87	0.56
1:I:521:MET:O	1:I:814:LYS:NZ	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:811:ARG:HD3	1:K:892:PHE:C	2.31	0.56
1:I:377:THR:HG21	1:I:434:LEU:HD21	1.87	0.56
1:C:485:LEU:HA	1:C:488:ARG:CG	2.36	0.55
1:G:374:CYS:O	1:G:377:THR:HG22	2.07	0.55
1:I:597:LEU:HA	1:I:600:VAL:HG22	1.88	0.55
1:G:826:ILE:HG22	1:G:827:GLU:HG3	1.88	0.55
1:A:337:ILE:O	1:A:341:ASN:ND2	2.32	0.55
1:I:377:THR:HG22	1:I:383:TYR:HB3	1.88	0.55
1:K:860:ALA:HB3	1:K:876:HIS:HB3	1.89	0.55
1:E:814:LYS:NZ	1:E:902:GLN:OE1	2.36	0.55
1:I:337:ILE:O	1:I:341:ASN:ND2	2.34	0.55
1:G:587:THR:O	1:G:591:GLU:HG2	2.08	0.54
1:A:748:ILE:O	1:A:752:GLN:HG2	2.07	0.54
1:C:698:SER:OG	2:D:21:U:O2'	2.25	0.54
1:A:379:LYS:O	1:A:384:ASN:ND2	2.36	0.54
1:I:442:VAL:HG21	1:I:449:LEU:HD22	1.90	0.54
1:G:661:LEU:HB3	1:G:696:ALA:HB2	1.90	0.54
1:I:888:LYS:HG2	1:I:890:GLU:H	1.71	0.54
1:A:279:GLU:O	1:A:283:LYS:HG3	2.08	0.53
1:E:517:GLN:HG2	1:E:521:MET:HE3	1.90	0.53
1:G:387:MET:HE2	1:G:434:LEU:HA	1.90	0.53
1:A:888:LYS:HA	1:A:908:TRP:HE1	1.72	0.53
1:G:632:LEU:HD21	1:G:643:LEU:HD13	1.90	0.53
1:I:580:ASP:OD1	1:I:581:GLU:N	2.42	0.53
1:I:292:LYS:NZ	1:I:341:ASN:O	2.41	0.53
1:E:634:VAL:HG12	1:E:715:TYR:HB3	1.90	0.53
1:K:527:ASP:O	1:K:529:ASP:N	2.41	0.53
1:E:324:ILE:HB	1:E:346:LEU:HD23	1.92	0.52
1:G:394:LYS:HG2	1:G:395:LEU:HD12	1.92	0.52
1:G:880:LYS:O	1:K:287:GLN:NE2	2.39	0.52
1:G:580:ASP:OD1	1:G:581:GLU:N	2.42	0.52
1:G:411:SER:HB3	1:G:722:ILE:HG23	1.91	0.52
1:I:477:GLN:HB3	1:I:480:ARG:CB	2.40	0.52
1:C:381:HIS:HD1	1:C:383:TYR:H	1.56	0.52
1:E:808:LEU:HG	1:E:894:VAL:HG22	1.92	0.51
1:A:634:VAL:HG12	1:A:715:TYR:HB3	1.91	0.51
1:C:337:ILE:O	1:C:341:ASN:ND2	2.33	0.51
1:G:328:THR:HB	1:K:320:ARG:HG2	1.93	0.51
1:A:752:GLN:OE1	1:E:460:PHE:HB2	2.11	0.51
1:A:811:ARG:NH2	1:A:905:TYR:O	2.43	0.51
1:C:580:ASP:OD1	1:C:581:GLU:N	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:858:LYS:HA	1:G:877:VAL:HG12	1.92	0.51
1:A:729:GLY:O	1:A:732:ARG:NH1	2.44	0.51
1:K:321:VAL:HG22	1:K:343:ILE:HB	1.93	0.51
1:E:657:LYS:H	1:E:692:ASN:HB3	1.76	0.51
1:A:661:LEU:HD22	1:A:694:LEU:HD21	1.92	0.50
1:I:477:GLN:HA	1:I:480:ARG:N	2.23	0.50
1:G:517:GLN:HG2	1:G:521:MET:HE3	1.92	0.50
1:E:293:VAL:HG22	1:E:368:LEU:HB3	1.92	0.50
1:I:724:MET:HE1	1:I:755:MET:HG2	1.93	0.50
1:C:723:LYS:O	1:C:727:THR:OG1	2.24	0.50
1:K:250:LEU:HD22	1:K:262:ILE:HG23	1.94	0.50
1:C:243:PRO:HB3	1:C:272:PHE:CE2	2.47	0.50
1:C:481:ASP:OD1	1:C:484:SER:HB2	2.11	0.49
1:K:362:SER:OG	1:K:393:GLN:OE1	2.30	0.49
1:I:861:LYS:NZ	5:J:101:M7G:O1B	2.45	0.49
1:G:320:ARG:HD2	1:K:332:VAL:HG11	1.94	0.49
2:L:14:G:H2'	2:L:15:A:C8	2.47	0.49
1:G:337:ILE:O	1:G:341:ASN:ND2	2.32	0.49
1:A:336:GLN:O	1:A:340:ASN:ND2	2.45	0.49
1:C:864:CYS:SG	1:C:865:ALA:N	2.86	0.49
1:E:809:LEU:HB3	1:E:816:LEU:HA	1.95	0.49
1:K:661:LEU:HB3	1:K:696:ALA:HB2	1.95	0.49
1:C:690:ASP:OD1	1:C:691:HIS:N	2.39	0.49
1:E:258:LYS:HD2	1:E:773:GLU:OE2	2.13	0.48
1:E:706:ILE:HD11	1:E:730:ARG:HD3	1.94	0.48
1:C:357:LYS:HD2	1:C:359:THR:HG23	1.95	0.48
1:K:529:ASP:OD1	1:K:530:GLU:N	2.46	0.48
1:K:752:GLN:HA	1:K:755:MET:HE2	1.94	0.48
1:E:564:LEU:O	1:E:568:LYS:HG3	2.14	0.48
1:I:387:MET:HE2	1:I:434:LEU:HA	1.94	0.48
1:A:336:GLN:HG2	1:A:340:ASN:HD21	1.78	0.48
1:A:387:MET:HE2	1:A:434:LEU:HA	1.94	0.48
1:A:864:CYS:SG	1:A:865:ALA:N	2.86	0.48
1:C:355:LEU:HD11	1:C:363:LEU:HD21	1.94	0.48
1:C:888:LYS:HA	1:C:908:TRP:HE1	1.78	0.48
1:G:888:LYS:HA	1:G:908:TRP:HE1	1.77	0.48
1:C:525:MET:HB3	1:C:531:GLU:HB2	1.96	0.48
1:C:774:ALA:O	1:C:778:GLU:HG2	2.12	0.48
1:E:461:ARG:HB2	1:E:741:LEU:HD12	1.95	0.48
1:I:525:MET:HE1	1:I:530:GLU:HG2	1.95	0.48
1:C:773:GLU:OE2	1:C:777:ARG:NH2	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:253:PRO:HB3	1:G:438:VAL:HG11	1.95	0.48
1:C:471:PHE:HA	1:C:474:ILE:HD13	1.96	0.47
1:E:521:MET:O	1:E:814:LYS:NZ	2.44	0.47
1:A:787:GLU:HA	1:A:790:ILE:HG22	1.96	0.47
1:I:575:ARG:HA	1:I:579:PHE:CE1	2.49	0.47
1:C:292:LYS:NZ	1:C:341:ASN:O	2.48	0.47
1:K:887:ILE:HB	1:K:892:PHE:HE2	1.79	0.47
1:E:394:LYS:NZ	1:E:435:ASP:OD1	2.46	0.47
1:E:919:ASP:HB2	1:E:920:PRO:HD2	1.96	0.47
1:A:809:LEU:HB2	1:A:893:VAL:HG13	1.97	0.46
1:E:823:VAL:HG22	1:E:833:VAL:HG22	1.96	0.46
1:C:295:PHE:HB3	1:C:345:ILE:HG13	1.97	0.46
1:C:362:SER:OG	1:C:393:GLN:OE1	2.32	0.46
1:G:292:LYS:NZ	1:G:341:ASN:O	2.48	0.46
1:I:653:LEU:HB3	1:I:656:LEU:HD12	1.97	0.46
1:C:611:LEU:HD13	1:C:646:TRP:CD1	2.51	0.46
1:E:861:LYS:NZ	1:E:872:ASP:OD2	2.47	0.46
2:H:10:U:H2'	2:H:11:A:C8	2.50	0.46
1:G:404:GLN:HE21	1:G:406:ILE:HD11	1.81	0.46
1:I:814:LYS:NZ	1:I:902:GLN:OE1	2.41	0.46
1:A:411:SER:HB2	1:A:725:ILE:HD12	1.98	0.46
1:I:571:PHE:CD1	1:I:587:THR:HG22	2.51	0.46
2:L:19:U:H2'	2:L:20:A:C8	2.50	0.46
1:I:243:PRO:HB3	1:I:272:PHE:CE2	2.51	0.45
1:I:706:ILE:HG22	1:I:707:ALA:H	1.81	0.45
1:K:810:CYS:SG	1:K:811:ARG:N	2.90	0.45
1:A:332:VAL:HG11	1:C:320:ARG:HD2	1.97	0.45
1:A:624:LEU:HD11	1:E:420:THR:HG21	1.98	0.45
1:A:779:LYS:HB3	1:A:779:LYS:HE2	1.65	0.45
1:G:404:GLN:NE2	1:G:406:ILE:HD11	2.32	0.45
2:L:5:U:H2'	2:L:6:A:C8	2.52	0.45
1:G:447:GLU:OE1	1:G:447:GLU:N	2.45	0.45
1:E:856:PHE:HD2	1:E:877:VAL:HG21	1.81	0.45
1:A:464:GLU:CD	1:A:465:SER:H	2.25	0.45
1:I:411:SER:HB2	1:I:725:ILE:HD12	1.98	0.45
1:K:511:GLN:NE2	2:L:10:U:O2'	2.50	0.45
1:C:510:GLU:OE2	1:C:546:ARG:NH1	2.49	0.45
1:C:520:CYS:SG	1:C:538:LEU:HD23	2.57	0.44
1:C:547:LYS:HD2	1:C:570:PHE:CD1	2.53	0.44
1:C:644:LYS:HG2	1:C:648:GLU:OE2	2.17	0.44
1:E:447:GLU:H	1:E:447:GLU:CD	2.25	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:404:GLN:HE21	1:E:406:ILE:HD11	1.83	0.44
1:G:432:ALA:HA	1:G:780:ILE:HG23	1.98	0.44
1:I:326:GLY:N	2:J:25:C:OP1	2.49	0.44
1:E:454:TYR:OH	1:E:734:ARG:NH2	2.50	0.44
1:E:884:ILE:HG13	1:E:885:PRO:HD2	1.99	0.44
1:I:610:LYS:NZ	1:I:716:GLU:OE1	2.37	0.44
1:C:861:LYS:NZ	1:C:872:ASP:OD1	2.35	0.44
1:E:387:MET:HE2	1:E:434:LEU:HA	1.98	0.44
1:E:750:LYS:HD2	1:E:753:ILE:HD11	2.00	0.44
1:G:281:HIS:CE1	1:G:368:LEU:HB2	2.52	0.44
1:E:344:ILE:HG22	1:E:346:LEU:HG	2.00	0.44
1:G:308:SER:O	1:G:312:LYS:HG2	2.17	0.44
1:G:321:VAL:HG22	1:G:343:ILE:HB	1.99	0.44
1:I:479:MET:HE2	1:I:548:TYR:HB3	2.00	0.44
1:C:641:ASP:OD1	1:C:641:ASP:N	2.50	0.44
1:I:728:ARG:NH2	1:I:758:GLU:OE1	2.50	0.44
2:F:19:U:H2'	2:F:20:A:C8	2.53	0.44
1:I:587:THR:O	1:I:590:PHE:N	2.50	0.44
1:A:464:GLU:O	1:A:609:PRO:HG2	2.17	0.44
1:I:889:ILE:HB	1:I:908:TRP:CE2	2.52	0.44
1:E:320:ARG:HG2	1:I:328:THR:HB	1.98	0.44
1:E:336:GLN:HG2	1:E:340:ASN:HD21	1.83	0.44
1:I:299:GLN:HB3	1:I:301:PRO:HD2	1.98	0.43
1:C:826:ILE:HG22	1:C:827:GLU:HG3	2.00	0.43
2:L:6:A:H2'	2:L:7:U:C6	2.53	0.43
1:C:351:LEU:HD23	1:C:386:ILE:HD13	1.99	0.43
1:E:650:ASN:HA	1:E:651:PRO:HD3	1.86	0.43
1:K:307:LYS:HZ3	1:K:307:LYS:HB3	1.82	0.43
1:C:485:LEU:HA	1:C:488:ARG:HG3	1.99	0.43
2:D:10:U:H2'	2:D:11:A:C8	2.54	0.43
1:G:653:LEU:HB3	1:G:656:LEU:HD12	1.99	0.43
1:I:527:ASP:O	1:I:529:ASP:N	2.44	0.43
1:K:503:GLU:O	1:K:509:TYR:HB2	2.18	0.43
1:A:852:GLN:HG3	1:A:856:PHE:O	2.17	0.43
1:C:653:LEU:HD23	1:C:656:LEU:HD22	2.00	0.43
1:E:321:VAL:HG22	1:E:343:ILE:HB	2.01	0.43
1:K:278:CYS:SG	1:K:293:VAL:HG11	2.59	0.43
1:K:704:ILE:H	1:K:704:ILE:HG13	1.52	0.43
1:A:661:LEU:HB3	1:A:696:ALA:HB2	2.01	0.43
1:C:485:LEU:HA	1:C:488:ARG:HG2	2.01	0.43
1:C:632:LEU:HD11	1:C:715:TYR:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:806:LYS:HD2	1:I:911:PHE:HZ	1.84	0.43
1:A:250:LEU:HD21	1:A:264:ALA:HB2	2.00	0.43
1:G:541:TYR:HD1	1:G:586:LEU:HD11	1.84	0.43
1:I:888:LYS:HZ1	2:J:2:G:P	2.41	0.43
1:K:387:MET:HE2	1:K:434:LEU:HA	2.00	0.43
1:K:728:ARG:HH22	1:K:758:GLU:CD	2.27	0.43
2:L:19:U:H2'	2:L:20:A:H8	1.82	0.43
1:G:368:LEU:HD11	1:G:406:ILE:HG12	2.01	0.43
1:G:545:LEU:HA	1:G:548:TYR:HD2	1.84	0.43
1:I:243:PRO:HB3	1:I:272:PHE:HE2	1.83	0.43
1:I:658:PRO:HA	1:I:693:ILE:HG23	2.01	0.43
1:A:826:ILE:HG12	1:A:918:PHE:HB2	2.01	0.42
1:C:387:MET:HE2	1:C:434:LEU:HA	2.01	0.42
1:G:478:LEU:HD21	1:G:593:LYS:HG3	2.01	0.42
1:K:858:LYS:HA	1:K:877:VAL:HG12	2.01	0.42
1:E:429:LYS:HG2	1:E:429:LYS:H	1.65	0.42
1:G:547:LYS:HG3	1:G:570:PHE:CE1	2.54	0.42
1:K:411:SER:HB2	1:K:725:ILE:HD12	2.00	0.42
1:E:460:PHE:HB3	1:E:748:ILE:HD12	2.00	0.42
2:H:14:G:H2'	2:H:15:A:C8	2.54	0.42
1:I:348:PRO:HB2	1:I:382:PRO:HB2	2.00	0.42
1:C:847:HIS:H	1:C:860:ALA:HA	1.85	0.42
1:K:243:PRO:HB3	1:K:272:PHE:CE2	2.55	0.42
1:A:796:LYS:N	1:A:797:PRO:HD3	2.34	0.42
2:B:24:U:H2'	2:B:25:C:C6	2.54	0.42
1:G:847:HIS:H	1:G:860:ALA:HA	1.83	0.42
1:K:252:LEU:HA	1:K:255:MET:HE2	2.02	0.42
1:A:815:ALA:HB2	1:A:866:ARG:HD2	2.02	0.42
1:E:847:HIS:HA	1:E:848:PRO:HD3	1.92	0.42
1:G:252:LEU:O	1:G:256:LYS:HG3	2.19	0.42
1:G:634:VAL:HG12	1:G:715:TYR:HB3	2.00	0.42
1:K:745:ALA:O	1:K:749:GLU:HG3	2.19	0.42
1:A:662:THR:HG22	1:A:697:THR:HG23	2.02	0.42
1:I:852:GLN:HG3	1:I:856:PHE:O	2.20	0.42
1:C:603:ASP:HA	1:C:604:PRO:HD3	1.92	0.42
1:E:476:ALA:O	1:E:480:ARG:HG3	2.20	0.42
1:G:911:PHE:O	1:G:915:LYS:NZ	2.46	0.42
1:I:698:SER:OG	2:J:21:U:O2'	2.20	0.42
1:K:842:PHE:CD1	1:K:862:ILE:HG23	2.55	0.42
1:A:525:MET:HB2	1:A:531:GLU:HB2	2.02	0.42
1:I:541:TYR:HD1	1:I:586:LEU:HD11	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:336:GLN:HG2	1:A:340:ASN:ND2	2.35	0.41
1:I:916:ILE:H	1:I:916:ILE:HG13	1.63	0.41
1:K:650:ASN:HA	1:K:651:PRO:HD3	1.91	0.41
1:E:845:ARG:HA	1:E:846:PRO:HD3	1.96	0.41
1:I:525:MET:HE3	1:I:527:ASP:HB3	2.02	0.41
1:A:320:ARG:HD2	1:C:332:VAL:HG11	2.02	0.41
1:E:355:LEU:HD11	1:E:363:LEU:HD21	2.02	0.41
1:C:360:ILE:HG23	1:C:365:ILE:HD12	2.01	0.41
1:I:525:MET:HA	1:I:526:PRO:HD3	1.94	0.41
1:I:759:LYS:NZ	1:I:763:ASP:OD2	2.48	0.41
2:D:14:G:H2'	2:D:15:A:C8	2.56	0.41
1:E:824:ARG:HD2	1:E:834:LEU:HD12	2.02	0.41
1:E:889:ILE:HB	1:E:908:TRP:CE2	2.56	0.41
1:G:374:CYS:SG	1:G:375:HIS:N	2.93	0.41
1:G:851:LYS:H	1:G:858:LYS:HB2	1.86	0.41
1:A:485:LEU:HD11	1:A:589:ARG:CZ	2.51	0.41
1:A:650:ASN:HA	1:A:651:PRO:HD3	1.88	0.41
1:E:884:ILE:HD12	1:E:884:ILE:HA	1.96	0.41
1:A:637:ARG:NH2	2:B:22:A:OP2	2.51	0.41
1:A:698:SER:HG	2:B:21:U:HO2'	1.54	0.41
1:A:851:LYS:H	1:A:858:LYS:HB2	1.86	0.41
1:C:344:ILE:HG22	1:C:346:LEU:HG	2.03	0.41
1:C:597:LEU:O	1:C:599:SER:N	2.44	0.41
1:E:625:ASN:O	1:E:628:THR:OG1	2.38	0.41
1:G:603:ASP:HA	1:G:604:PRO:HD3	1.86	0.41
1:K:521:MET:HB2	1:K:904:LEU:HD21	2.02	0.41
1:K:823:VAL:HG22	1:K:833:VAL:HG22	2.01	0.41
1:A:447:GLU:H	1:A:447:GLU:HG2	1.61	0.41
1:C:463:VAL:HG21	1:C:610:LYS:HG2	2.02	0.41
1:C:470:LYS:O	1:C:471:PHE:HD1	2.03	0.41
1:C:887:ILE:HB	1:C:892:PHE:HE2	1.86	0.41
1:E:724:MET:HE2	1:E:728:ARG:HH21	1.85	0.41
1:I:550:ASP:OD1	1:I:550:ASP:N	2.52	0.41
1:G:603:ASP:OD2	1:G:605:SER:OG	2.27	0.41
1:I:559:ARG:NH2	1:I:562:ASP:OD1	2.42	0.41
1:I:661:LEU:HB3	1:I:696:ALA:HB2	2.03	0.41
1:K:518:LYS:HE3	2:L:18:U:H5''	2.03	0.41
1:K:839:LYS:HA	1:K:842:PHE:CE2	2.56	0.41
1:C:442:VAL:HG21	1:C:449:LEU:HD22	2.02	0.40
1:G:411:SER:HB2	1:G:725:ILE:HD12	2.03	0.40
1:A:839:LYS:HA	1:A:842:PHE:CE2	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:582:ILE:HD12	1:C:582:ILE:H	1.87	0.40
1:E:779:LYS:O	1:E:783:ILE:HG13	2.21	0.40
1:I:514:VAL:HG11	2:J:18:U:H4'	2.02	0.40
1:I:559:ARG:HD3	1:I:646:TRP:CD1	2.50	0.40
1:K:453:VAL:HG13	1:K:732:ARG:HB2	2.03	0.40
1:E:374:CYS:HB2	1:E:434:LEU:HD11	2.04	0.40
1:A:521:MET:SD	1:A:811:ARG:HB3	2.61	0.40
1:C:658:PRO:HA	1:C:693:ILE:HG23	2.04	0.40
1:E:243:PRO:HB3	1:E:272:PHE:CE2	2.56	0.40
1:K:395:LEU:HD12	1:K:788:LYS:HD2	2.03	0.40
1:A:460:PHE:HE2	1:A:751:GLU:HG2	1.87	0.40
1:A:887:ILE:HB	1:A:892:PHE:HE2	1.86	0.40
1:G:839:LYS:HA	1:G:842:PHE:CE2	2.57	0.40
1:I:525:MET:HB3	1:I:531:GLU:HB2	2.04	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	644/695 (93%)	602 (94%)	42 (6%)	0	100	100
1	C	640/695 (92%)	595 (93%)	44 (7%)	1 (0%)	43	71
1	E	631/695 (91%)	588 (93%)	42 (7%)	1 (0%)	43	71
1	G	640/695 (92%)	596 (93%)	43 (7%)	1 (0%)	43	71
1	I	639/695 (92%)	588 (92%)	51 (8%)	0	100	100
1	K	634/695 (91%)	596 (94%)	38 (6%)	0	100	100
All	All	3828/4170 (92%)	3565 (93%)	260 (7%)	3 (0%)	48	76

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	799	PRO
1	G	375	HIS
1	E	704	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	537/623 (86%)	530 (99%)	7 (1%)	61	75
1	C	516/623 (83%)	508 (98%)	8 (2%)	55	72
1	E	487/623 (78%)	478 (98%)	9 (2%)	51	70
1	G	517/623 (83%)	509 (98%)	8 (2%)	57	73
1	I	480/623 (77%)	472 (98%)	8 (2%)	53	71
1	K	495/623 (80%)	489 (99%)	6 (1%)	63	75
All	All	3032/3738 (81%)	2986 (98%)	46 (2%)	57	73

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	612	GLU
1	A	644	LYS
1	A	749	GLU
1	A	779	LYS
1	A	800	VAL
1	A	893	VAL
1	A	904	LEU
1	C	485	LEU
1	C	493	LEU
1	C	597	LEU
1	C	648	GLU
1	C	656	LEU
1	C	766	LEU
1	C	800	VAL
1	C	916	ILE
1	E	258	LYS

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Mol	Chain	Res	Type
1	E	294	VAL
1	E	429	LYS
1	E	469	ASP
1	E	596	GLU
1	E	693	ILE
1	E	721	VAL
1	E	884	ILE
1	E	893	VAL
1	G	289	GLN
1	G	335	GLU
1	G	538	LEU
1	G	591	GLU
1	G	721	VAL
1	G	787	GLU
1	G	800	VAL
1	G	825	VAL
1	I	399	SER
1	I	477	GLN
1	I	510	GLU
1	I	530	GLU
1	I	591	GLU
1	I	721	VAL
1	I	813	CYS
1	I	916	ILE
1	K	522	VAL
1	K	704	ILE
1	K	721	VAL
1	K	800	VAL
1	K	811	ARG
1	K	883	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	331	ASN
1	A	340	ASN
1	A	517	GLN
1	A	557	HIS
1	A	619	GLN
1	A	692	ASN
1	A	782	HIS
1	C	298	ASN

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Mol	Chain	Res	Type
1	C	331	ASN
1	C	376	ASN
1	C	380	GLN
1	C	507	GLN
1	C	511	GLN
1	E	287	GLN
1	E	289	GLN
1	E	305	GLN
1	E	340	ASN
1	E	389	ASN
1	E	876	HIS
1	G	573	ASN
1	G	691	HIS
1	G	708	GLN
1	G	912	HIS
1	I	306	GLN
1	I	340	ASN
1	I	380	GLN
1	I	389	ASN
1	I	584	GLN
1	I	708	GLN
1	I	752	GLN
1	I	912	HIS
1	K	404	GLN
1	K	511	GLN
1	K	708	GLN
1	K	782	HIS
1	K	876	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	23/24 (95%)	2 (8%)	0
2	D	23/24 (95%)	1 (4%)	0
2	F	23/24 (95%)	0	0
2	H	23/24 (95%)	1 (4%)	0
2	J	23/24 (95%)	0	0
2	L	23/24 (95%)	1 (4%)	0
All	All	138/144 (95%)	5 (3%)	0

All (5) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	11	A
2	B	16	U
2	D	16	U
2	H	16	U
2	L	16	U

There are no RNA pucker outliers to report.

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](#)

Of 18 ligands modelled in this entry, 12 are monoatomic - leaving 6 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	B	101	2	30,31,31	3.65	15 (50%)	47,49,49	1.54	7 (14%)
5	M7G	L	101	2	16,17,31	3.85	6 (37%)	22,26,49	1.04	2 (9%)
5	M7G	D	101	2	30,31,31	3.65	15 (50%)	47,49,49	1.60	9 (19%)
5	M7G	J	101	2	30,31,31	3.66	15 (50%)	47,49,49	1.57	7 (14%)
5	M7G	H	101	2	30,31,31	3.63	15 (50%)	47,49,49	1.70	10 (21%)
5	M7G	F	101	2	16,17,31	3.86	6 (37%)	22,26,49	0.95	1 (4%)

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	B	101	2	-	6/16/32/32	0/3/3/3
5	M7G	L	101	2	-	3/12/25/32	0/1/1/3
5	M7G	D	101	2	-	5/16/32/32	0/3/3/3
5	M7G	J	101	2	-	4/16/32/32	0/3/3/3
5	M7G	H	101	2	-	4/16/32/32	0/3/3/3
5	M7G	F	101	2	-	3/12/25/32	0/1/1/3

All (72) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	101	M7G	C8-N7	9.69	1.49	1.33
5	J	101	M7G	C8-N7	9.68	1.49	1.33
5	D	101	M7G	C8-N7	9.61	1.49	1.33
5	H	101	M7G	C8-N7	9.55	1.49	1.33
5	L	101	M7G	O4'-C4'	9.54	1.60	1.44
5	F	101	M7G	O4'-C4'	9.47	1.59	1.44
5	F	101	M7G	C3'-C4'	-8.78	1.30	1.53
5	D	101	M7G	C3'-C4'	-8.68	1.31	1.53
5	L	101	M7G	C3'-C4'	-8.64	1.31	1.53
5	B	101	M7G	C3'-C4'	-8.62	1.31	1.53
5	H	101	M7G	C3'-C4'	-8.62	1.31	1.53
5	J	101	M7G	C3'-C4'	-8.57	1.31	1.53
5	D	101	M7G	O4'-C4'	6.91	1.60	1.45
5	J	101	M7G	O4'-C4'	6.91	1.60	1.45
5	B	101	M7G	O4'-C4'	6.91	1.60	1.45
5	H	101	M7G	O4'-C4'	6.83	1.60	1.45
5	F	101	M7G	O4'-C1'	-6.52	1.29	1.43
5	L	101	M7G	O4'-C1'	-6.50	1.30	1.43
5	D	101	M7G	C2-N3	5.30	1.46	1.33
5	H	101	M7G	C2-N3	5.27	1.46	1.33
5	J	101	M7G	C2-N3	5.27	1.46	1.33
5	B	101	M7G	C2-N3	5.25	1.45	1.33
5	B	101	M7G	C8-N9	5.22	1.49	1.35
5	J	101	M7G	O4'-C1'	-5.21	1.30	1.42
5	H	101	M7G	C8-N9	5.20	1.49	1.35
5	D	101	M7G	C8-N9	5.20	1.49	1.35
5	B	101	M7G	O4'-C1'	-5.20	1.30	1.42
5	J	101	M7G	C8-N9	5.18	1.49	1.35
5	D	101	M7G	O4'-C1'	-5.11	1.30	1.42
5	H	101	M7G	O4'-C1'	-5.09	1.30	1.42
5	H	101	M7G	C4-N3	4.99	1.45	1.34
5	D	101	M7G	C4-N3	4.85	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	101	M7G	C4-N3	4.84	1.45	1.34
5	J	101	M7G	C4-N3	4.81	1.45	1.34
5	B	101	M7G	C2-N2	3.96	1.43	1.34
5	D	101	M7G	C2-N2	3.94	1.43	1.34
5	J	101	M7G	C2-N2	3.93	1.43	1.34
5	H	101	M7G	C2-N2	3.90	1.43	1.34
5	J	101	M7G	PA-O3A	3.25	1.63	1.59
5	B	101	M7G	C5-N7	3.10	1.42	1.39
5	L	101	M7G	O2'-C2'	-3.09	1.36	1.43
5	F	101	M7G	O2'-C2'	-3.08	1.36	1.43
5	J	101	M7G	C5-N7	3.05	1.42	1.39
5	D	101	M7G	C5-N7	2.97	1.42	1.39
5	H	101	M7G	C5-N7	2.96	1.42	1.39
5	D	101	M7G	PA-O3A	2.90	1.62	1.59
5	D	101	M7G	C2-N1	2.89	1.44	1.37
5	L	101	M7G	O3'-C3'	2.88	1.50	1.43
5	B	101	M7G	C2-N1	2.88	1.44	1.37
5	B	101	M7G	O3'-C3'	2.87	1.50	1.43
5	H	101	M7G	O3'-C3'	2.86	1.50	1.43
5	D	101	M7G	O3'-C3'	2.86	1.50	1.43
5	J	101	M7G	C2-N1	2.85	1.44	1.37
5	H	101	M7G	C5-C6	2.84	1.51	1.43
5	F	101	M7G	O3'-C3'	2.84	1.50	1.43
5	J	101	M7G	O3'-C3'	2.82	1.49	1.43
5	F	101	M7G	PA-O3A	2.82	1.62	1.59
5	J	101	M7G	C5-C6	2.81	1.51	1.43
5	H	101	M7G	C2-N1	2.81	1.44	1.37
5	D	101	M7G	C5-C6	2.80	1.51	1.43
5	B	101	M7G	C5-C6	2.78	1.51	1.43
5	B	101	M7G	PA-O3A	2.78	1.62	1.59
5	H	101	M7G	PA-O3A	2.76	1.62	1.59
5	L	101	M7G	PA-O3A	2.75	1.62	1.59
5	J	101	M7G	C6-N1	2.53	1.43	1.38
5	B	101	M7G	C6-N1	2.50	1.43	1.38
5	J	101	M7G	O2'-C2'	-2.49	1.36	1.43
5	B	101	M7G	O2'-C2'	-2.48	1.36	1.43
5	D	101	M7G	C6-N1	2.48	1.43	1.38
5	H	101	M7G	O2'-C2'	-2.45	1.36	1.43
5	H	101	M7G	C6-N1	2.44	1.43	1.38
5	D	101	M7G	O2'-C2'	-2.41	1.37	1.43

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	101	M7G	C2-N3-C4	5.12	121.12	112.30
5	H	101	M7G	C5-C4-N3	-4.69	119.28	128.15
5	D	101	M7G	C2-N3-C4	4.65	120.30	112.30
5	J	101	M7G	C2-N3-C4	4.62	120.26	112.30
5	B	101	M7G	C2-N3-C4	4.57	120.17	112.30
5	D	101	M7G	C5-C4-N3	-4.18	120.26	128.15
5	J	101	M7G	C5-C4-N3	-4.08	120.45	128.15
5	B	101	M7G	C5-C4-N3	-4.03	120.53	128.15
5	H	101	M7G	C5-C6-N1	3.95	120.00	111.84
5	B	101	M7G	C5-C6-N1	3.82	119.73	111.84
5	J	101	M7G	C5-C6-N1	3.80	119.70	111.84
5	D	101	M7G	C5-C6-N1	3.79	119.67	111.84
5	H	101	M7G	O6-C6-C5	-3.22	120.82	128.01
5	J	101	M7G	O6-C6-C5	-3.21	120.85	128.01
5	B	101	M7G	O6-C6-C5	-3.19	120.89	128.01
5	D	101	M7G	O6-C6-C5	-3.17	120.93	128.01
5	H	101	M7G	C2-N1-C6	-2.87	119.90	125.11
5	D	101	M7G	C2-N1-C6	-2.75	120.12	125.11
5	B	101	M7G	C2-N1-C6	-2.75	120.13	125.11
5	J	101	M7G	C2-N1-C6	-2.74	120.14	125.11
5	L	101	M7G	O4'-C4'-C3'	2.57	107.01	104.63
5	F	101	M7G	C1'-C2'-C3'	2.51	105.65	101.63
5	D	101	M7G	C3'-C2'-C1'	2.45	106.10	101.46
5	D	101	M7G	C2'-C3'-C4'	2.44	107.31	102.61
5	H	101	M7G	C2'-C3'-C4'	2.42	107.29	102.61
5	B	101	M7G	N9-C8-N7	-2.42	106.60	112.48
5	J	101	M7G	N9-C8-N7	-2.39	106.68	112.48
5	L	101	M7G	C1'-C2'-C3'	2.33	105.35	101.63
5	H	101	M7G	C3'-C2'-C1'	2.29	105.80	101.46
5	D	101	M7G	N9-C8-N7	-2.26	107.00	112.48
5	H	101	M7G	N9-C4-N3	2.25	130.45	125.95
5	D	101	M7G	C5-C4-N9	2.18	110.54	105.88
5	B	101	M7G	C5-C4-N9	2.14	110.45	105.88
5	H	101	M7G	N9-C8-N7	-2.14	107.29	112.48
5	J	101	M7G	C5-C4-N9	2.11	110.39	105.88
5	H	101	M7G	C5-C4-N9	2.05	110.26	105.88

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	101	M7G	C5'-O5'-PA-O1A
5	B	101	M7G	C5'-O5'-PA-O3A

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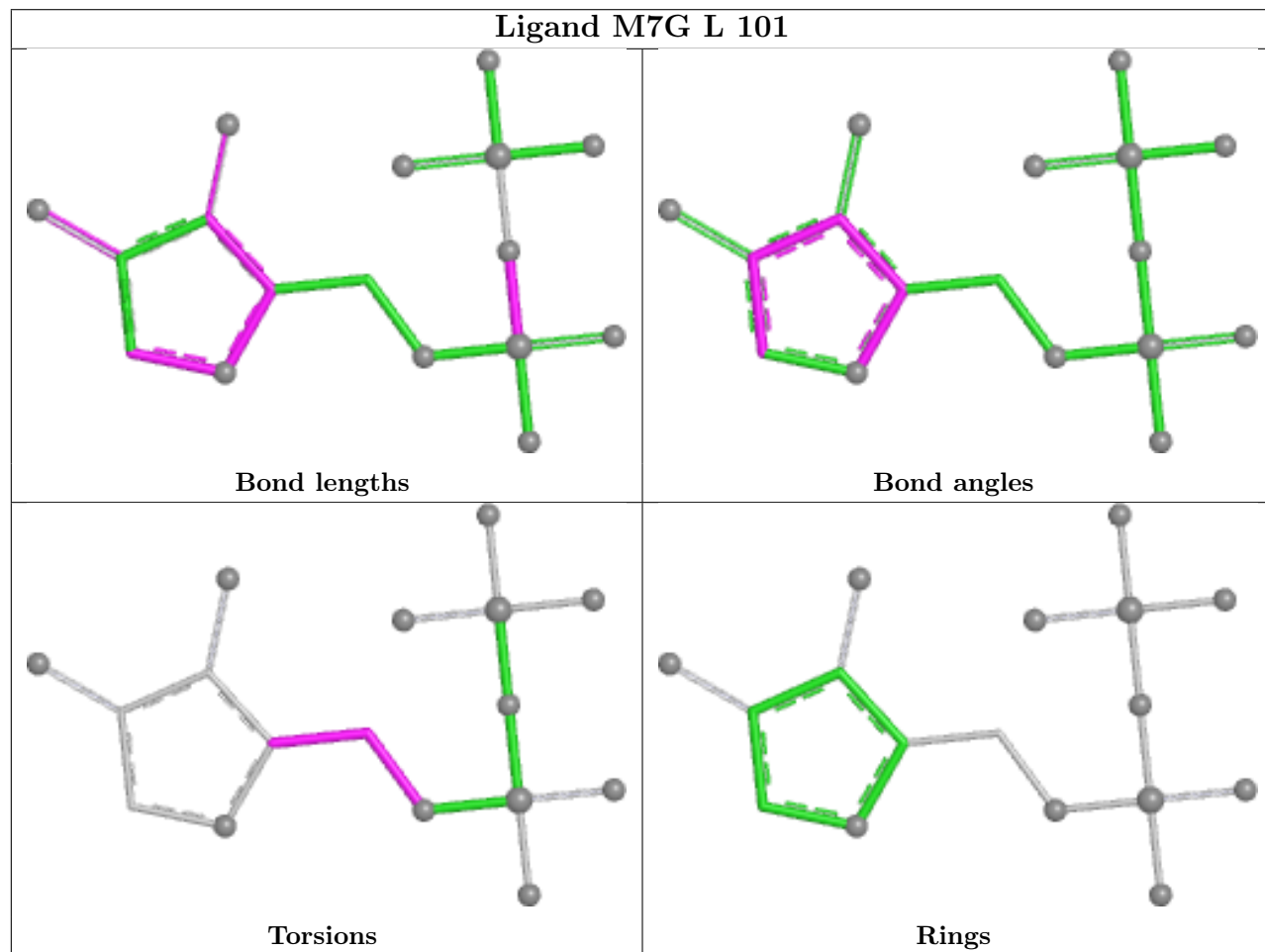
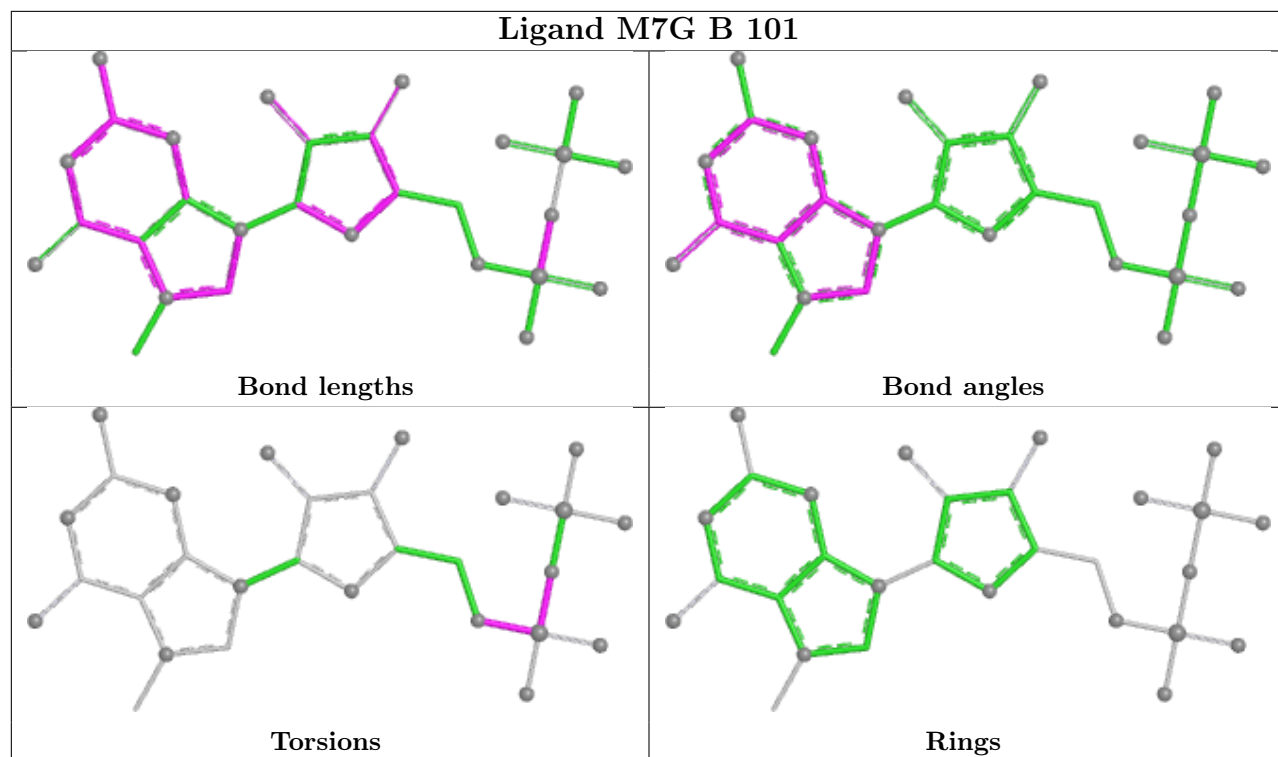
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5	D	101	M7G	C5'-O5'-PA-O2A
5	D	101	M7G	C5'-O5'-PA-O3A
5	H	101	M7G	O4'-C4'-C5'-O5'
5	H	101	M7G	C3'-C4'-C5'-O5'
5	J	101	M7G	C5'-O5'-PA-O3A
5	L	101	M7G	O4'-C4'-C5'-O5'
5	D	101	M7G	O4'-C4'-C5'-O5'
5	F	101	M7G	C4'-C5'-O5'-PA
5	L	101	M7G	C3'-C4'-C5'-O5'
5	B	101	M7G	PB-O3A-PA-O5'
5	J	101	M7G	PB-O3A-PA-O1A
5	B	101	M7G	C5'-O5'-PA-O2A
5	J	101	M7G	C5'-O5'-PA-O2A
5	F	101	M7G	PB-O3A-PA-O2A
5	B	101	M7G	PB-O3A-PA-O1A
5	B	101	M7G	PB-O3A-PA-O2A
5	F	101	M7G	PB-O3A-PA-O1A
5	H	101	M7G	PB-O3A-PA-O2A
5	H	101	M7G	C2'-C1'-N9-C4
5	L	101	M7G	C4'-C5'-O5'-PA
5	D	101	M7G	PB-O3A-PA-O2A
5	J	101	M7G	PB-O3A-PA-O2A

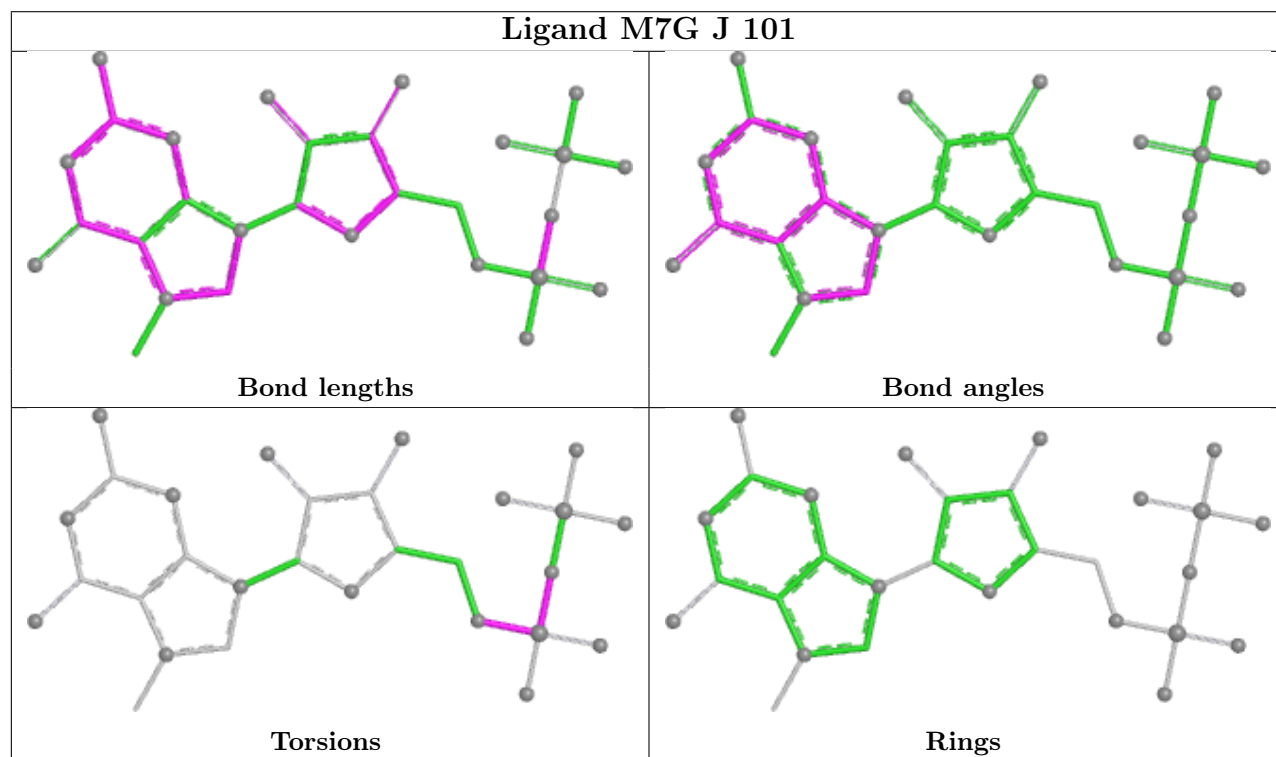
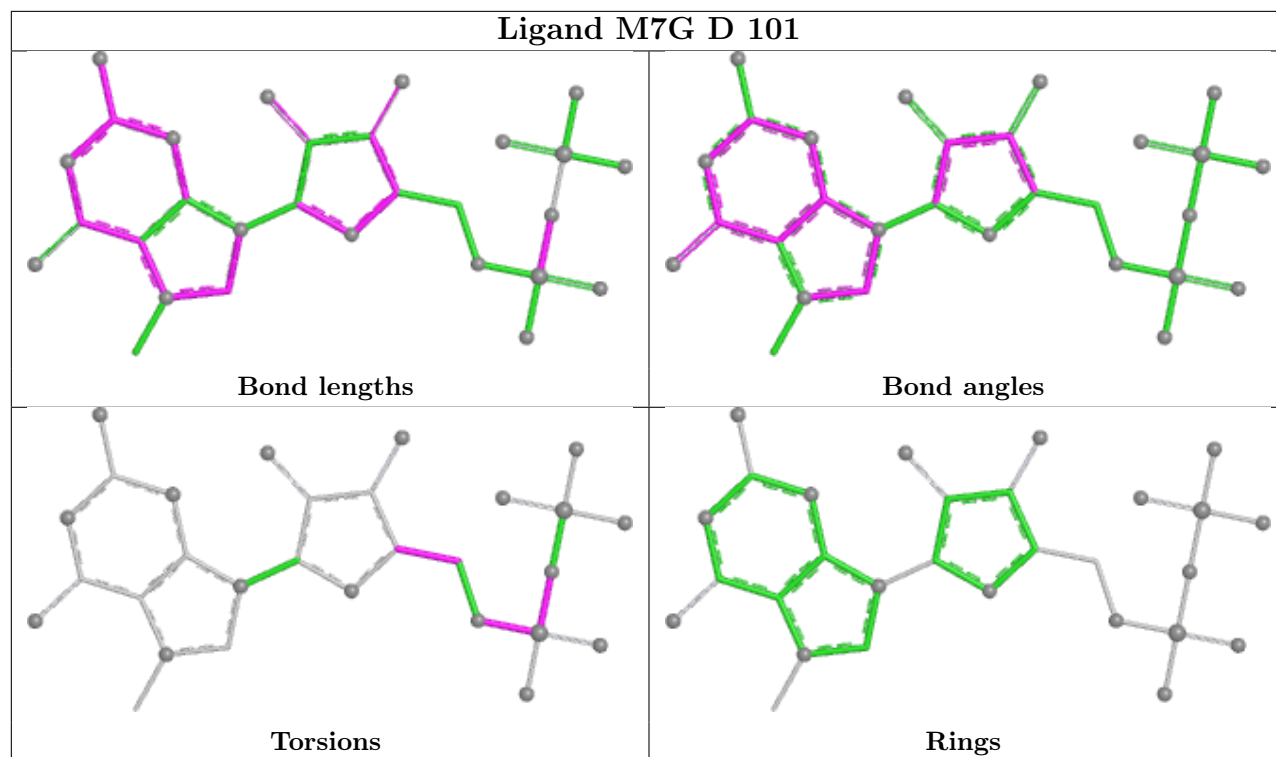
There are no ring outliers.

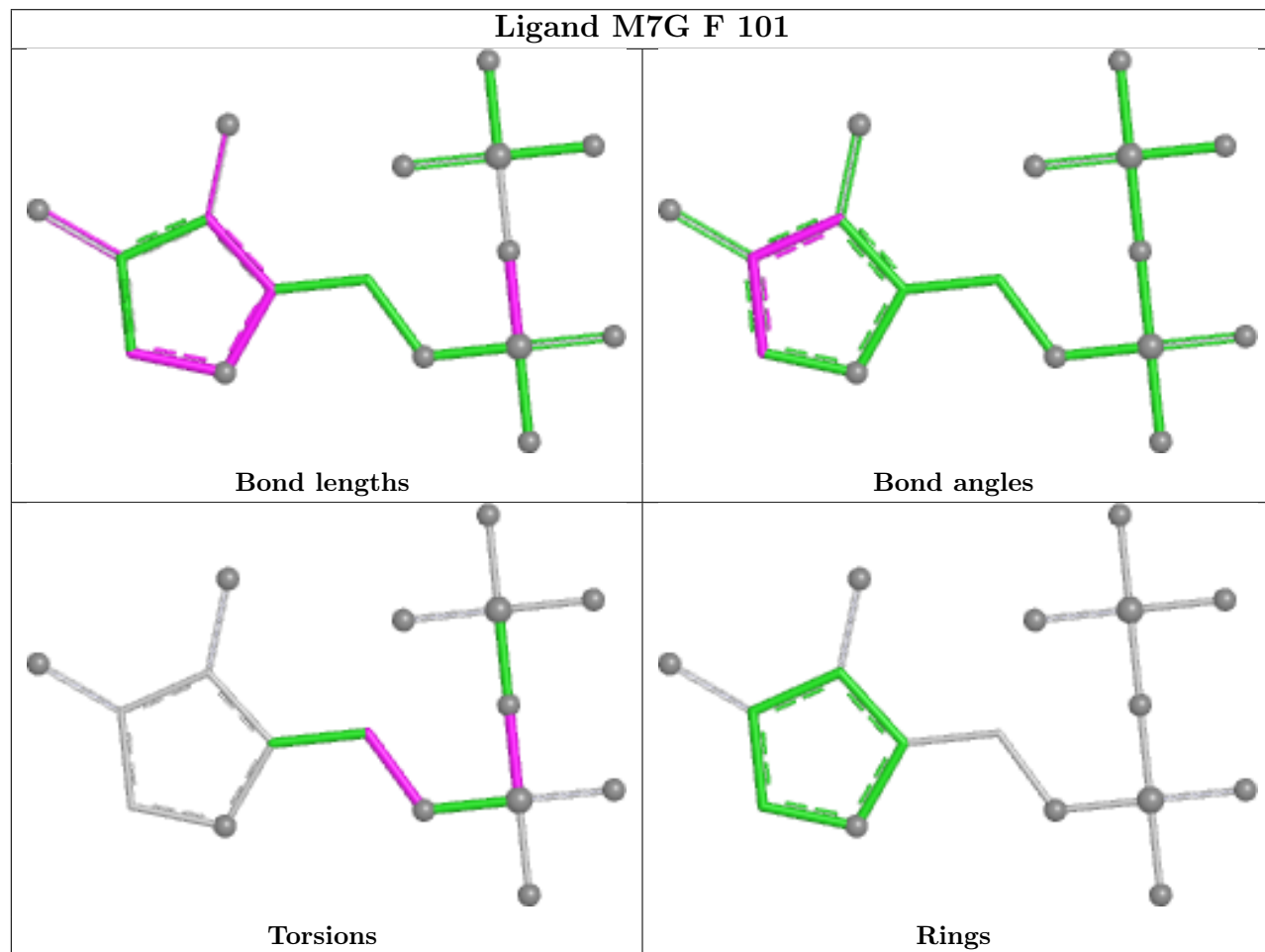
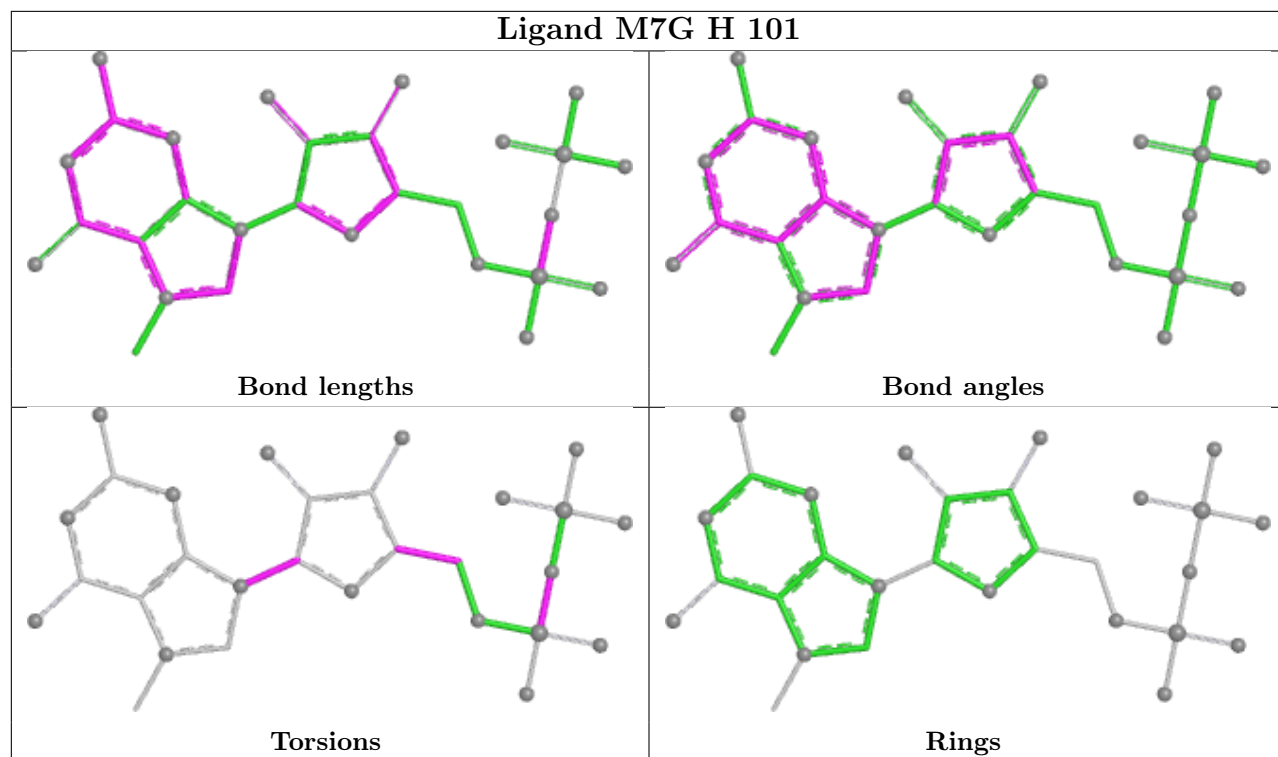
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	J	101	M7G	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	650/695 (93%)	0.24	7 (1%) 78 61	16, 52, 88, 122	0
1	C	648/695 (93%)	0.34	22 (3%) 48 32	16, 53, 97, 135	0
1	E	641/695 (92%)	0.49	22 (3%) 48 32	20, 60, 97, 108	0
1	G	647/695 (93%)	0.26	10 (1%) 72 53	22, 53, 87, 106	1 (0%)
1	I	647/695 (93%)	0.43	12 (1%) 66 48	19, 57, 96, 121	0
1	K	644/695 (92%)	0.34	13 (2%) 65 46	21, 57, 97, 123	0
2	B	24/24 (100%)	-0.19	0 100 100	32, 43, 122, 140	0
2	D	24/24 (100%)	-0.34	0 100 100	20, 39, 117, 133	0
2	F	24/24 (100%)	-0.19	0 100 100	34, 51, 111, 118	0
2	H	24/24 (100%)	-0.15	0 100 100	30, 43, 121, 124	0
2	J	24/24 (100%)	-0.20	0 100 100	29, 42, 118, 131	0
2	L	24/24 (100%)	-0.29	0 100 100	33, 45, 114, 132	0
All	All	4021/4314 (93%)	0.33	86 (2%) 63 44	16, 55, 96, 140	1 (0%)

All (86) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	473	TYR	4.7
1	I	476	ALA	3.5
1	C	483	GLU	3.4
1	C	541	TYR	3.4
1	G	493	LEU	3.3
1	C	479	MET	3.2
1	E	535	CYS	3.2
1	E	823	VAL	3.1
1	I	906	SER	3.1
1	E	834	LEU	3.1
1	E	579	PHE	3.0

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Mol	Chain	Res	Type	RSRZ
1	I	579	PHE	3.0
1	I	518	LYS	3.0
1	G	489	ILE	2.9
1	C	520	CYS	2.9
1	C	471	PHE	2.9
1	E	606	ASN	2.8
1	G	922	GLU	2.8
1	A	782	HIS	2.7
1	A	240	PRO	2.7
1	E	505	GLY	2.7
1	E	512	TRP	2.7
1	G	868	ASN	2.7
1	G	491	LYS	2.7
1	E	515	THR	2.6
1	E	504	PHE	2.6
1	I	240	PRO	2.6
1	C	545	LEU	2.6
1	C	606	ASN	2.6
1	K	493	LEU	2.5
1	G	492	ASP	2.5
1	C	474	ILE	2.5
1	I	799	PRO	2.5
1	E	896	ASP	2.5
1	K	575	ARG	2.5
1	C	469	ASP	2.4
1	C	240	PRO	2.4
1	G	240	PRO	2.4
1	K	522	VAL	2.4
1	C	493	LEU	2.4
1	C	482	THR	2.4
1	E	797	PRO	2.4
1	A	578	GLY	2.4
1	G	490	CYS	2.4
1	E	489	ILE	2.4
1	E	922	GLU	2.4
1	E	510	GLU	2.4
1	E	551	ALA	2.3
1	K	492	ASP	2.3
1	E	509	TYR	2.3
1	K	501	ASN	2.3
1	K	899	THR	2.3
1	K	823	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	523	PHE	2.2
1	I	468	SER	2.2
1	A	491	LYS	2.2
1	K	852	GLN	2.2
1	K	661	LEU	2.2
1	K	800	VAL	2.2
1	I	595	GLN	2.2
1	E	491	LYS	2.2
1	C	604	PRO	2.1
1	E	882	PHE	2.1
1	G	278	CYS	2.1
1	E	881	THR	2.1
1	I	521	MET	2.1
1	C	477	GLN	2.1
1	C	464	GLU	2.1
1	C	922	GLU	2.1
1	K	607	GLU	2.1
1	I	471	PHE	2.1
1	E	481	ASP	2.1
1	I	872	ASP	2.1
1	A	490	CYS	2.1
1	C	595	GLN	2.1
1	K	555	SER	2.0
1	A	486	ALA	2.0
1	I	903	THR	2.0
1	K	829	CYS	2.0
1	C	505	GLY	2.0
1	C	607	GLU	2.0
1	C	795	GLU	2.0
1	C	643	LEU	2.0
1	G	521	MET	2.0
1	A	241	PHE	2.0
1	E	863	PHE	2.0

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

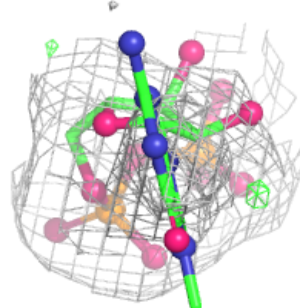
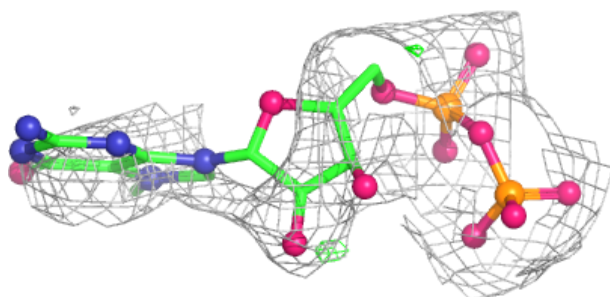
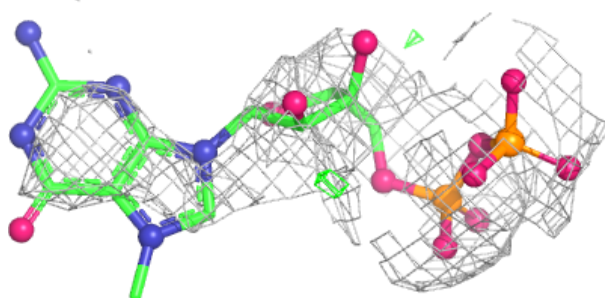
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	E	1002	1/1	0.85	0.12	46,46,46,46	0
4	MG	I	1002	1/1	0.85	0.09	47,47,47,47	0
5	M7G	J	101	29/29	0.88	0.15	43,107,137,143	0
5	M7G	H	101	29/29	0.89	0.14	46,93,124,131	0
5	M7G	D	101	29/29	0.89	0.12	42,99,123,127	0
5	M7G	B	101	29/29	0.90	0.15	48,112,135,137	0
4	MG	G	1002	1/1	0.90	0.09	27,27,27,27	0
5	M7G	L	101	17/29	0.90	0.12	39,67,94,100	0
5	M7G	F	101	17/29	0.91	0.10	64,88,103,109	0
4	MG	K	1002	1/1	0.91	0.09	18,18,18,18	0
4	MG	A	1002	1/1	0.94	0.07	28,28,28,28	0
3	ZN	C	1001	1/1	0.97	0.04	50,50,50,50	0
3	ZN	A	1001	1/1	0.98	0.04	46,46,46,46	0
4	MG	C	1002	1/1	0.98	0.12	21,21,21,21	0
3	ZN	E	1001	1/1	0.98	0.04	73,73,73,73	0
3	ZN	G	1001	1/1	0.99	0.14	96,96,96,96	0
3	ZN	I	1001	1/1	0.99	0.05	44,44,44,44	0
3	ZN	K	1001	1/1	0.99	0.05	69,69,69,69	0

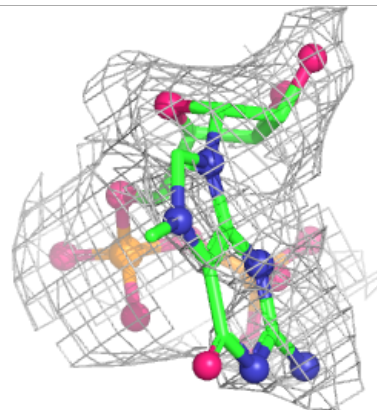
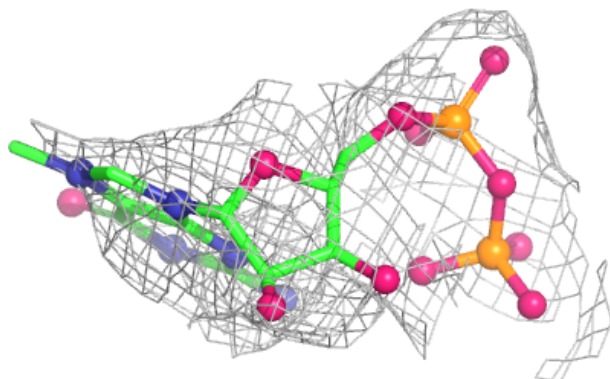
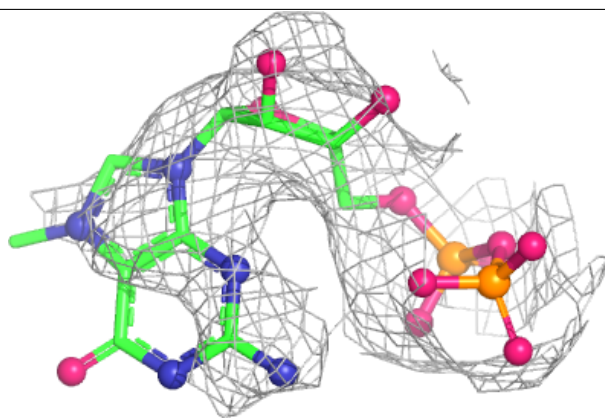
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around M7G J 101:

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

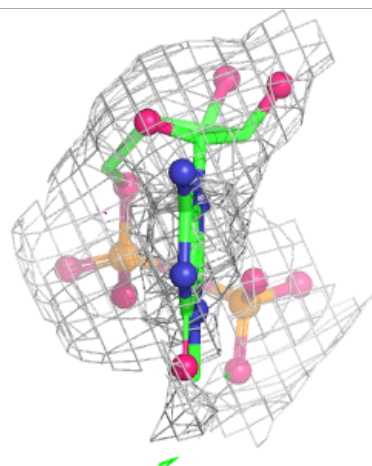
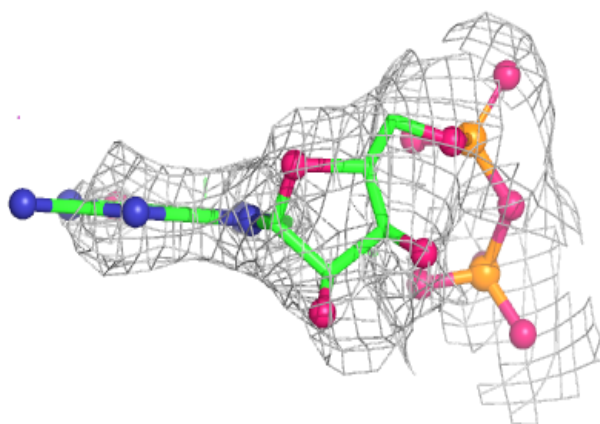
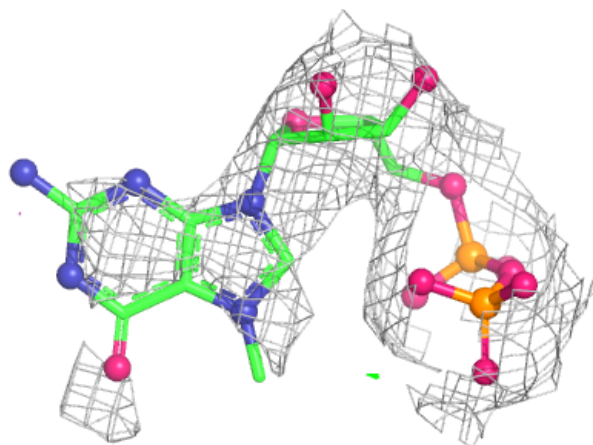
**Electron density around M7G H 101:**

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



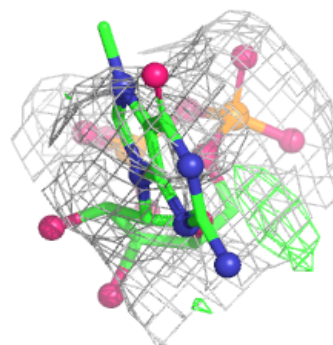
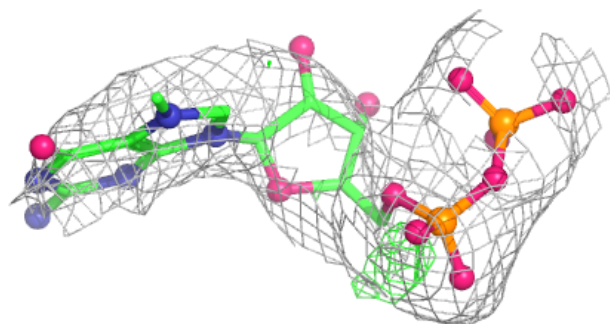
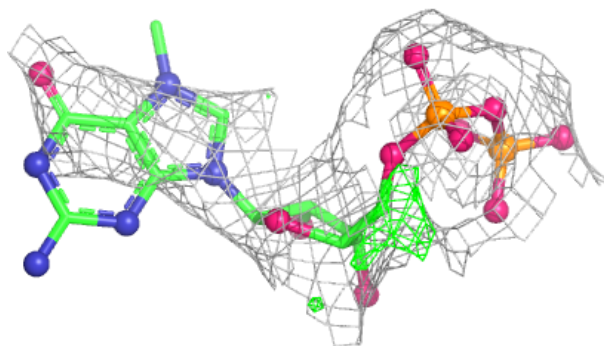
Electron density around M7G D 101:

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

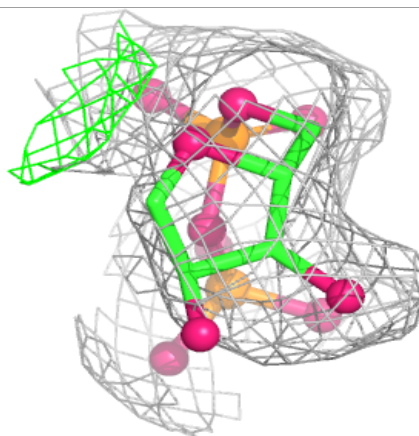
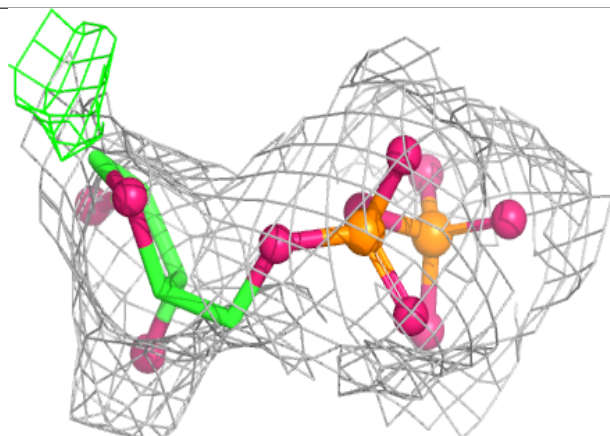
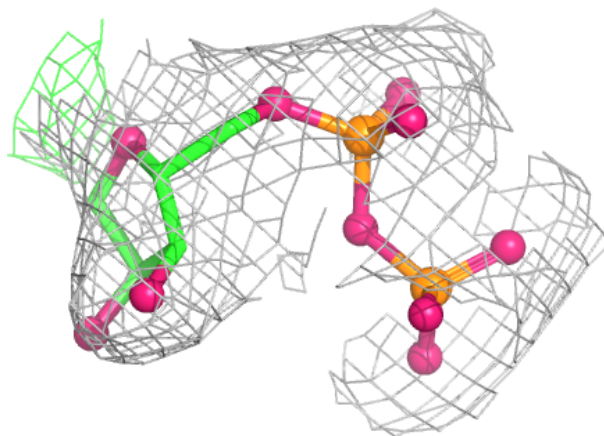


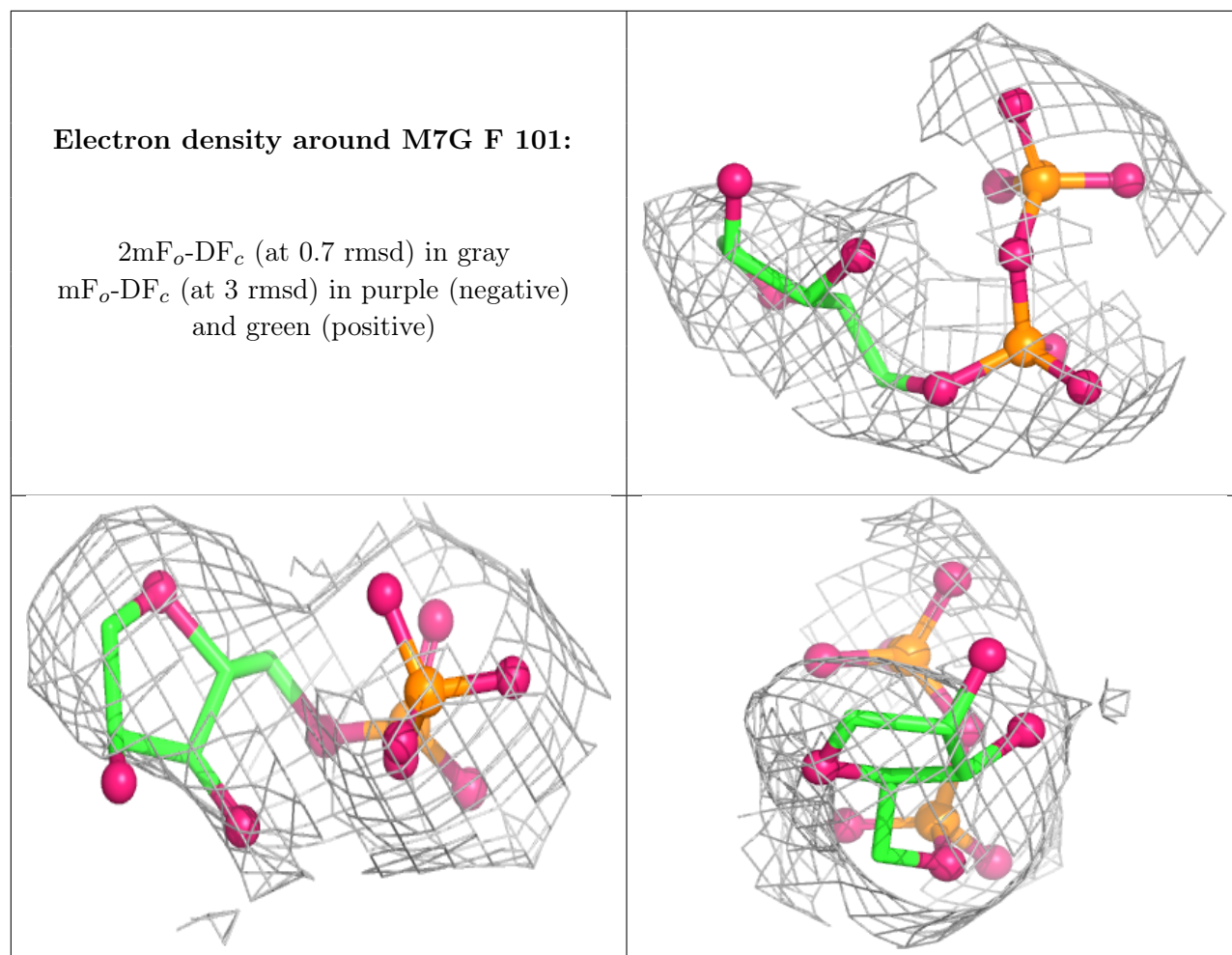
Electron density around M7G B 101:

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

**Electron density around M7G L 101:**

$2mF_o-DF_c$ (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.