



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 31, 2017 – 03:49 PM EDT

PDB ID : 3OL7  
Title : Poliovirus polymerase elongation complex with CTP  
Authors : Gong, P.; Peersen, O.B.  
Deposited on : unknown  
Resolution : 2.70 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030345  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030345

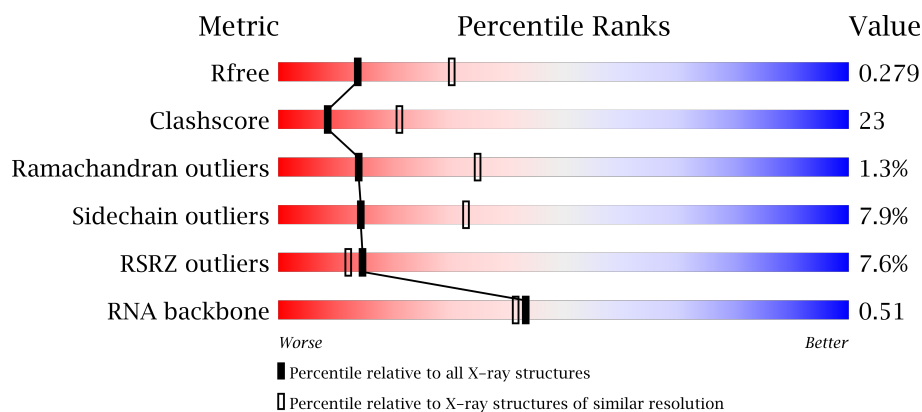
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 Å.

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





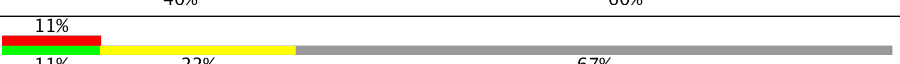
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	100719	2259 (2.70-2.70)
Clashscore	112137	2590 (2.70-2.70)
Ramachandran outliers	110173	2550 (2.70-2.70)
Sidechain outliers	110143	2550 (2.70-2.70)
RSRZ outliers	101464	2275 (2.70-2.70)
RNA backbone	2435	1011 (3.06-2.34)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	471	<div> <div>6%</div> <div>58%</div> <div>36%</div> <div>..</div> </div>
1	E	471	<div> <div>7%</div> <div>56%</div> <div>38%</div> <div>..</div> </div>
1	I	471	<div> <div>8%</div> <div>60%</div> <div>33%</div> <div>..</div> </div>
1	M	471	<div> <div>7%</div> <div>61%</div> <div>32%</div> <div>..</div> </div>

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Mol	Chain	Length	Quality of chain
2	B	26	
2	F	26	
2	J	26	
2	N	26	
3	C	15	
3	G	15	
3	K	15	
3	O	15	
4	D	9	
4	H	9	
4	L	9	
4	P	9	

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
10	GOL	I	8002	-	-	X	X
10	GOL	I	8003	-	-	X	X
10	GOL	I	8004	-	-	X	-
10	GOL	I	8006	-	-	X	-
10	GOL	J	8005	-	-	-	X
7	IPA	A	6008	-	-	-	X
7	IPA	A	6009	-	-	-	X
7	IPA	A	6011	-	-	-	X
7	IPA	E	6014	-	-	X	-
7	IPA	E	6015	-	-	-	X
7	IPA	I	6023	-	-	-	X
7	IPA	M	6007	-	-	-	X
7	IPA	M	6016	-	-	X	-
7	IPA	M	6019	-	-	X	-
8	PEG	A	7001	-	-	X	-
8	PEG	E	7002	-	-	X	-

## 2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 18525 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 Polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	461	Total	C	N	O	S	0	0	0
			3697	2370	610	695	22			
1	E	461	Total	C	N	O	S	0	0	0
			3697	2370	610	695	22			
1	I	461	Total	C	N	O	S	0	0	0
			3697	2370	610	695	22			
1	M	461	Total	C	N	O	S	0	0	0
			3697	2370	610	695	22			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	446	ASP	LEU	ENGINEERED MUTATION	UNP B3VQP5
A	462	GLY	-	EXPRESSION TAG	UNP B3VQP5
A	463	SER	-	EXPRESSION TAG	UNP B3VQP5
A	464	SER	-	EXPRESSION TAG	UNP B3VQP5
A	465	SER	-	EXPRESSION TAG	UNP B3VQP5
A	466	HIS	-	EXPRESSION TAG	UNP B3VQP5
A	467	HIS	-	EXPRESSION TAG	UNP B3VQP5
A	468	HIS	-	EXPRESSION TAG	UNP B3VQP5
A	469	HIS	-	EXPRESSION TAG	UNP B3VQP5
A	470	HIS	-	EXPRESSION TAG	UNP B3VQP5
A	471	HIS	-	EXPRESSION TAG	UNP B3VQP5
E	446	ASP	LEU	ENGINEERED MUTATION	UNP B3VQP5
E	462	GLY	-	EXPRESSION TAG	UNP B3VQP5
E	463	SER	-	EXPRESSION TAG	UNP B3VQP5
E	464	SER	-	EXPRESSION TAG	UNP B3VQP5
E	465	SER	-	EXPRESSION TAG	UNP B3VQP5
E	466	HIS	-	EXPRESSION TAG	UNP B3VQP5
E	467	HIS	-	EXPRESSION TAG	UNP B3VQP5
E	468	HIS	-	EXPRESSION TAG	UNP B3VQP5
E	469	HIS	-	EXPRESSION TAG	UNP B3VQP5
E	470	HIS	-	EXPRESSION TAG	UNP B3VQP5

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Chain	Residue	Modelled	Actual	Comment	Reference
E	471	HIS	-	EXPRESSION TAG	UNP B3VQP5
I	446	ASP	LEU	ENGINEERED MUTATION	UNP B3VQP5
I	462	GLY	-	EXPRESSION TAG	UNP B3VQP5
I	463	SER	-	EXPRESSION TAG	UNP B3VQP5
I	464	SER	-	EXPRESSION TAG	UNP B3VQP5
I	465	SER	-	EXPRESSION TAG	UNP B3VQP5
I	466	HIS	-	EXPRESSION TAG	UNP B3VQP5
I	467	HIS	-	EXPRESSION TAG	UNP B3VQP5
I	468	HIS	-	EXPRESSION TAG	UNP B3VQP5
I	469	HIS	-	EXPRESSION TAG	UNP B3VQP5
I	470	HIS	-	EXPRESSION TAG	UNP B3VQP5
I	471	HIS	-	EXPRESSION TAG	UNP B3VQP5
M	446	ASP	LEU	ENGINEERED MUTATION	UNP B3VQP5
M	462	GLY	-	EXPRESSION TAG	UNP B3VQP5
M	463	SER	-	EXPRESSION TAG	UNP B3VQP5
M	464	SER	-	EXPRESSION TAG	UNP B3VQP5
M	465	SER	-	EXPRESSION TAG	UNP B3VQP5
M	466	HIS	-	EXPRESSION TAG	UNP B3VQP5
M	467	HIS	-	EXPRESSION TAG	UNP B3VQP5
M	468	HIS	-	EXPRESSION TAG	UNP B3VQP5
M	469	HIS	-	EXPRESSION TAG	UNP B3VQP5
M	470	HIS	-	EXPRESSION TAG	UNP B3VQP5
M	471	HIS	-	EXPRESSION TAG	UNP B3VQP5

- Molecule 2 is a RNA chain called RNA (5'-R(\*AP\*AP\*GP\*UP\*CP\*UP\*CP\*CP\*AP\*GP\*GP\*UP\*CP\*UP\*CP\*UP\*CP\*GP\*UP\*CP\*CP\*GP\*GP\*AP\*AP\*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	18	Total	C	N	O	P	0	0	0
			361	159	59	125	18			
2	F	18	Total	C	N	O	P	0	0	0
			361	159	59	125	18			
2	J	16	Total	C	N	O	P	0	0	0
			337	150	56	115	16			
2	N	16	Total	C	N	O	P	0	0	0
			337	150	56	115	16			

- Molecule 3 is a RNA chain called RNA (5'-R(\*GP\*CP\*CP\*CP\*GP\*GP\*AP\*CP\*GP\*AP\*GP\*AP\*GP\*AP\*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	15	Total 323	C 145	N 65	O 99	P 14	0	0	0
3	G	15	Total 323	C 145	N 65	O 99	P 14	0	0	0
3	K	15	Total 323	C 145	N 65	O 99	P 14	0	0	0
3	O	15	Total 323	C 145	N 65	O 99	P 14	0	0	0

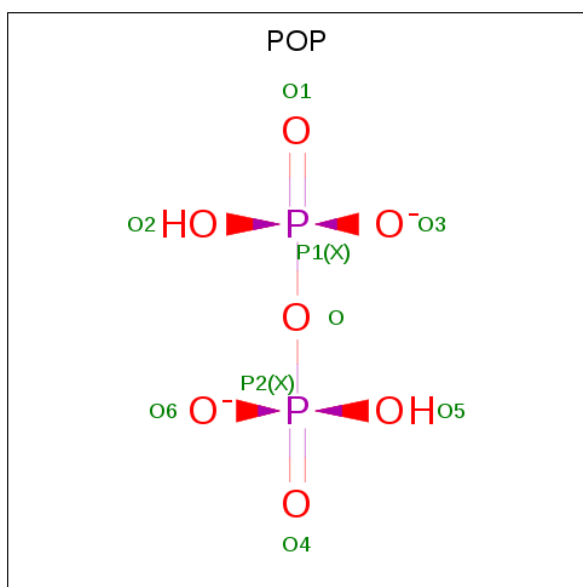
- Molecule 4 is a RNA chain called RNA (5'-R(\*GP\*GP\*GP\*AP\*GP\*AP\*UP\*GP\*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	3	Total 68	C 30	N 15	O 20	P 3	0	0	0
4	H	3	Total 68	C 30	N 15	O 20	P 3	0	0	0
4	L	4	Total 91	C 40	N 20	O 27	P 4	0	0	0
4	P	4	Total 91	C 40	N 20	O 27	P 4	0	0	0

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

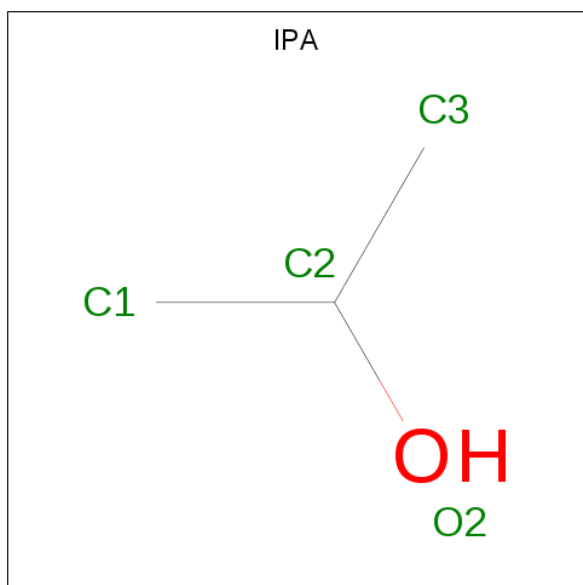
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	I	1	Total 1	Mg 1	0	0
5	A	2	Total 2	Mg 2	0	0
5	M	1	Total 1	Mg 1	0	0
5	E	2	Total 2	Mg 2	0	0

- Molecule 6 is PYROPHOSPHATE 2- (three-letter code: POP) (formula: H<sub>2</sub>O<sub>7</sub>P<sub>2</sub>).



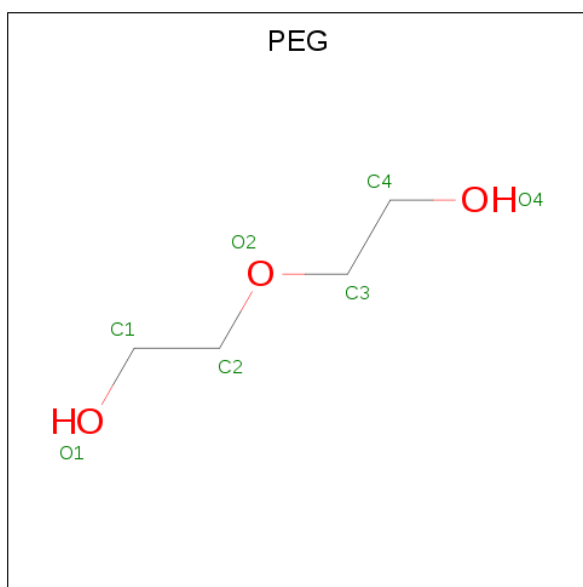
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	P	0	0
			9	7	2		
6	E	1	Total	O	P	0	0
			9	7	2		
6	K	1	Total	O	P	0	0
			9	7	2		
6	M	1	Total	O	P	0	0
			9	7	2		

- Molecule 7 is ISOPROPYL ALCOHOL (three-letter code: IPA) (formula: C<sub>3</sub>H<sub>8</sub>O).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total 4	C 3	O 1	0	0
7	A	1	Total 4	C 3	O 1	0	0
7	A	1	Total 4	C 3	O 1	0	0
7	A	1	Total 4	C 3	O 1	0	0
7	E	1	Total 4	C 3	O 1	0	0
7	E	1	Total 4	C 3	O 1	0	0
7	E	1	Total 4	C 3	O 1	0	0
7	E	1	Total 4	C 3	O 1	0	0
7	I	1	Total 4	C 3	O 1	0	0
7	I	1	Total 4	C 3	O 1	0	0
7	M	1	Total 4	C 3	O 1	0	0
7	M	1	Total 4	C 3	O 1	0	0
7	M	1	Total 4	C 3	O 1	0	0
7	N	1	Total 4	C 3	O 1	0	0
7	O	1	Total 4	C 3	O 1	0	0

- Molecule 8 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).

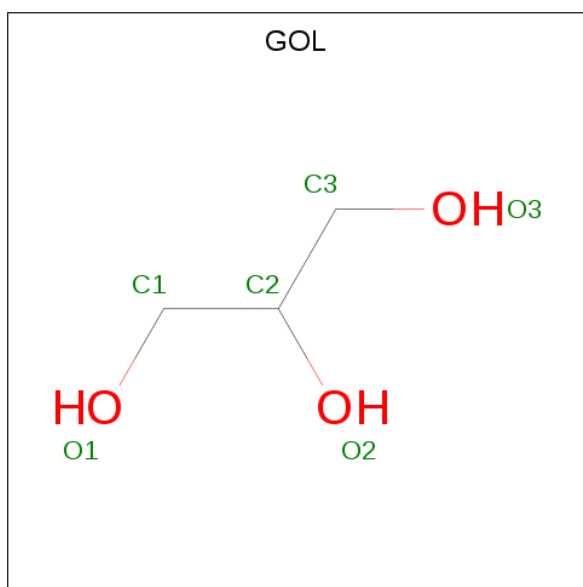


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			7	4	3		
8	E	1	Total	C	O	0	0
			7	4	3		
8	J	1	Total	C	O	0	0
			7	4	3		
8	N	1	Total	C	O	0	0
			7	4	3		

- Molecule 9 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	I	1	Total	Zn	0	0
			1	1		
9	A	1	Total	Zn	0	0
			1	1		
9	M	1	Total	Zn	0	0
			1	1		
9	E	1	Total	Zn	0	0
			1	1		

- Molecule 10 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	E	1	Total	C	O	0	0
			6	3	3		
10	I	1	Total	C	O	0	0
			6	3	3		
10	I	1	Total	C	O	0	0
			6	3	3		
10	I	1	Total	C	O	0	0
			6	3	3		
10	I	1	Total	C	O	0	0
			6	3	3		
10	J	1	Total	C	O	0	0
			6	3	3		
10	M	1	Total	C	O	0	0
			6	3	3		
10	N	1	Total	C	O	0	0
			6	3	3		

- Molecule 11 is water.

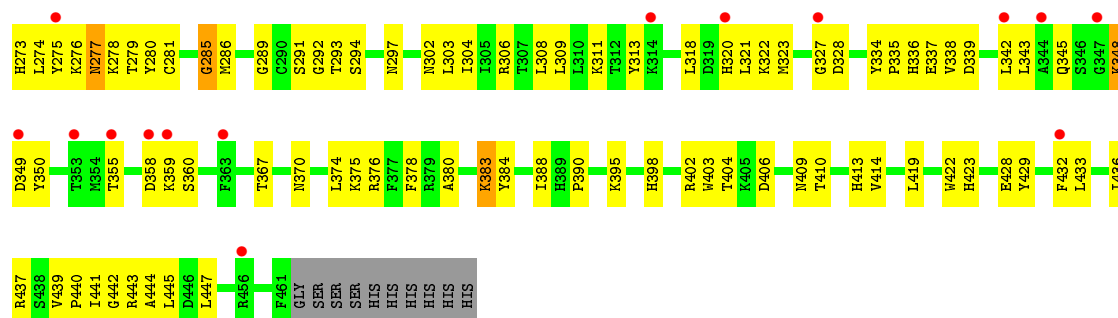
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	122	Total	O	0	0
			122	122		
11	B	19	Total	O	0	0
			19	19		
11	C	14	Total	O	0	0
			14	14		
11	D	1	Total	O	0	0
			1	1		

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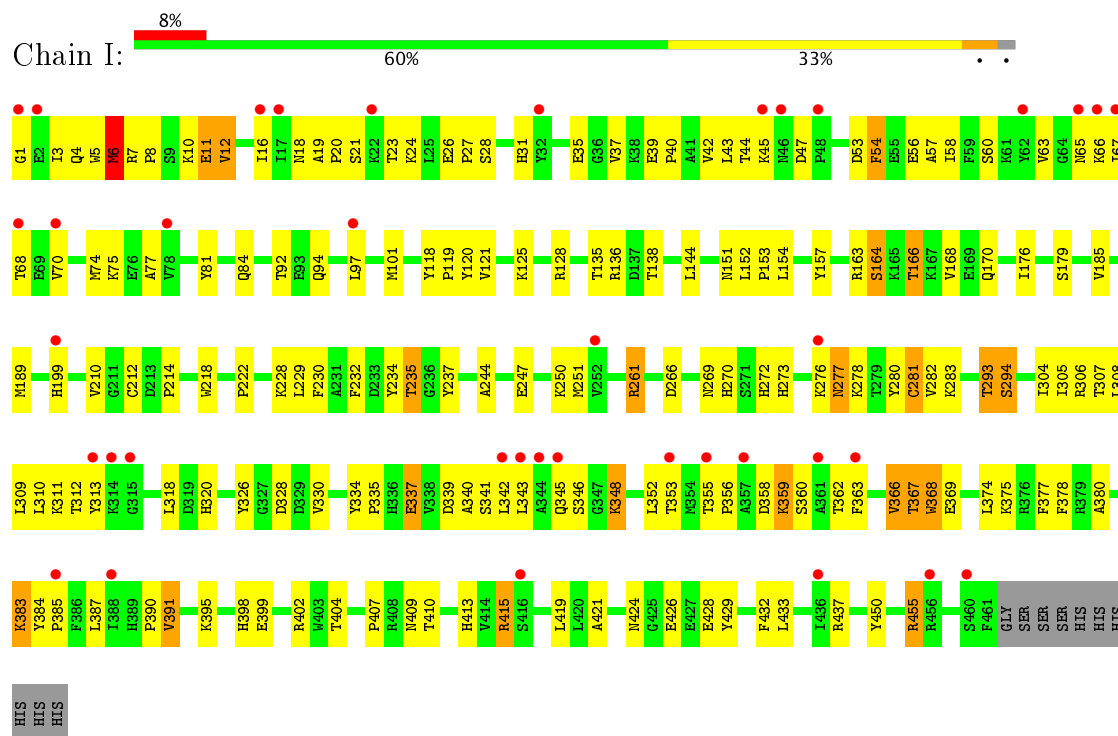
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	E	100	Total 100	O 100	0	0
11	F	25	Total 25	O 25	0	0
11	G	9	Total 9	O 9	0	0
11	H	1	Total 1	O 1	0	0
11	I	95	Total 95	O 95	0	0
11	J	19	Total 19	O 19	0	0
11	K	11	Total 11	O 11	0	0
11	M	105	Total 105	O 105	0	0
11	N	21	Total 21	O 21	0	0
11	O	7	Total 7	O 7	0	0

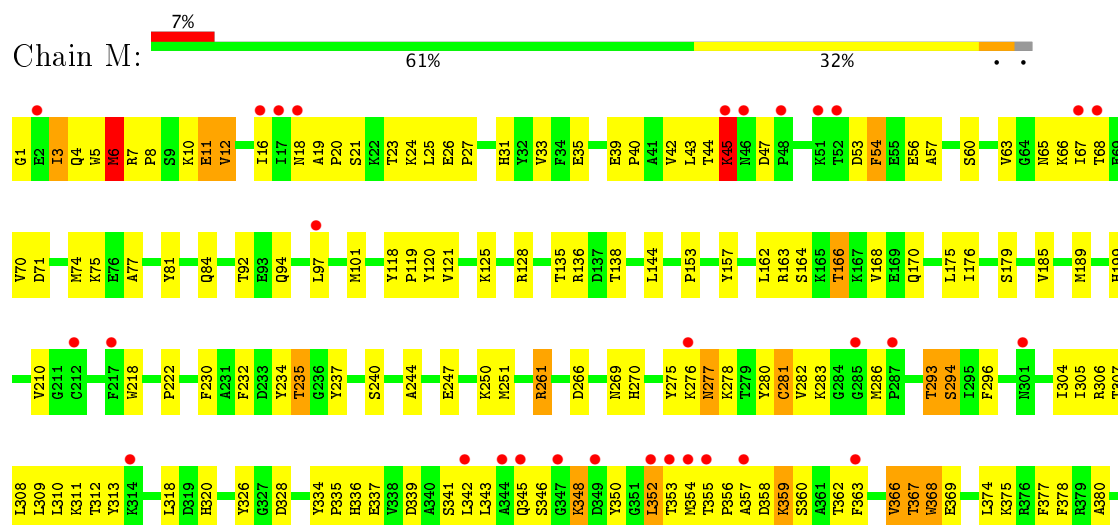


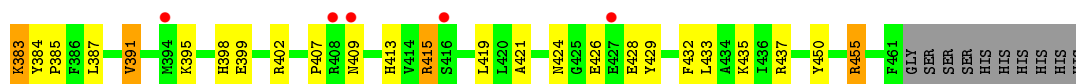


• Molecule 1: Polymerase

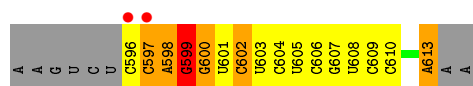


• Molecule 1: Polymerase

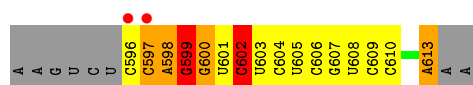




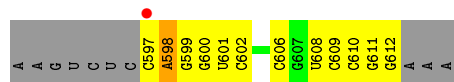
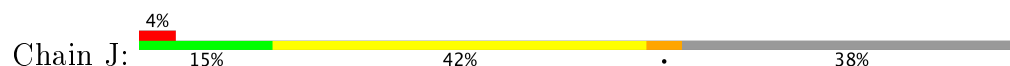
- Molecule 2: RNA (5'-R(\*AP\*AP\*GP\*UP\*CP\*UP\*CP\*CP\*AP\*GP\*GP\*UP\*CP\*UP\*CP\*UP\*CP\*GP\*UP\*CP\*CP\*GP\*GP\*AP\*AP\*A)-3')



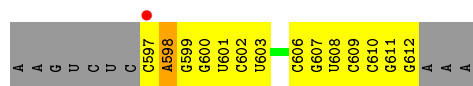
- Molecule 2: RNA (5'-R(\*AP\*AP\*GP\*UP\*CP\*UP\*CP\*CP\*AP\*GP\*GP\*UP\*CP\*UP\*CP\*UP\*CP\*GP\*UP\*CP\*CP\*GP\*GP\*AP\*AP\*A)-3')



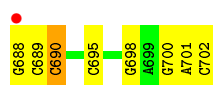
- Molecule 2: RNA (5'-R(\*AP\*AP\*GP\*UP\*CP\*UP\*CP\*CP\*AP\*GP\*GP\*UP\*CP\*UP\*CP\*UP\*CP\*GP\*UP\*CP\*CP\*GP\*GP\*AP\*AP\*A)-3')



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

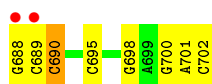


- Molecule 3: RNA (5'-R(\*GP\*CP\*CP\*CP\*GP\*GP\*AP\*CP\*GP\*AP\*GP\*AP\*GP\*AP\*C)-3')

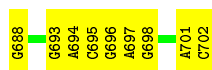


- Molecule 3: RNA (5'-R(\*GP\*CP\*CP\*CP\*GP\*GP\*AP\*CP\*GP\*AP\*GP\*AP\*GP\*AP\*C)-3')

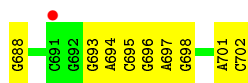




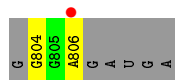
- Molecule 3: RNA (5'-R(\*GP\*CP\*CP\*CP\*GP\*GP\*AP\*CP\*GP\*AP\*GP\*AP\*GP\*AP\*C)-3')



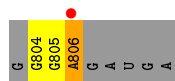
- Molecule 3: RNA (5'-R(\*GP\*CP\*CP\*CP\*GP\*GP\*AP\*CP\*GP\*AP\*GP\*AP\*GP\*AP\*C)-3')



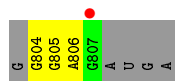
- Molecule 4: RNA (5'-R(\*GP\*GP\*GP\*AP\*GP\*AP\*UP\*GP\*A)-3')



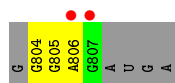
- Molecule 4: RNA (5'-R(\*GP\*GP\*GP\*AP\*GP\*AP\*UP\*GP\*A)-3')



- Molecule 4: RNA (5'-R(\*GP\*GP\*GP\*AP\*GP\*AP\*UP\*GP\*A)-3')



- Molecule 4: RNA (5'-R(\*GP\*GP\*GP\*AP\*GP\*AP\*UP\*GP\*A)-3')



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	60.72Å 60.77Å 192.97Å 83.01° 82.93° 77.12°	Depositor
Resolution (Å)	48.08 – 2.70 48.09 – 2.40	Depositor EDS
% Data completeness (in resolution range)	97.5 (48.08-2.70) 94.6 (48.09-2.40)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.37 (at 2.39Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4 _486)	Depositor
R, $R_{free}$	0.226 , 0.290 0.215 , 0.279	Depositor DCC
$R_{free}$ test set	3576 reflections (5.03%)	DCC
Wilson B-factor (Å <sup>2</sup> )	60.8	Xtriage
Anisotropy	0.445	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	(Not available) , (Not available)	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.61$ , $\langle L^2 \rangle = 0.46$	Xtriage
Estimated twinning fraction	0.448 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	18525	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 43.74 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.6883e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>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 ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, ZN, IPA, MG, POP, PEG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.45	0/3787	0.60	0/5122
1	E	0.45	0/3787	0.60	0/5122
1	I	0.43	0/3787	0.62	0/5122
1	M	0.44	0/3787	0.62	1/5122 (0.0%)
2	B	0.79	2/400 (0.5%)	1.21	2/621 (0.3%)
2	F	0.79	2/400 (0.5%)	1.20	3/621 (0.5%)
2	J	0.62	0/374	1.01	0/580
2	N	0.63	0/374	1.01	0/580
3	C	0.66	0/362	1.19	0/564
3	G	0.68	0/362	1.15	0/564
3	K	0.64	0/362	1.01	0/564
3	O	0.66	0/362	0.99	0/564
4	D	0.28	0/76	0.54	0/117
4	H	0.31	0/76	0.54	0/117
4	L	0.29	0/102	0.62	0/158
4	P	0.32	0/102	0.63	0/158
All	All	0.49	4/18500 (0.0%)	0.73	6/25696 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	613	A	P-OP1	6.71	1.60	1.49
2	F	613	A	P-OP1	6.70	1.60	1.49
2	F	613	A	P-OP2	6.36	1.59	1.49
2	B	613	A	P-OP2	6.31	1.59	1.49

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	599	G	C4-N9-C1'	5.72	133.94	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	599	G	C4-N9-C1'	5.66	133.86	126.50
2	B	597	C	C2-N1-C1'	5.48	124.83	118.80
2	F	597	C	C2-N1-C1'	5.41	124.76	118.80
1	M	45	LYS	CD-CE-NZ	5.25	123.77	111.70

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	3697	0	3659	161	0
1	E	3697	0	3659	177	0
1	I	3697	0	3658	177	0
1	M	3697	0	3658	167	0
2	B	361	0	183	34	0
2	F	361	0	183	33	0
2	J	337	0	173	17	0
2	N	337	0	173	19	0
3	C	323	0	167	10	0
3	G	323	0	167	9	0
3	K	323	0	167	9	0
3	O	323	0	167	10	0
4	D	68	0	34	3	0
4	H	68	0	34	2	0
4	L	91	0	45	2	0
4	P	91	0	45	2	0
5	A	2	0	0	0	0
5	E	2	0	0	0	0
5	I	1	0	0	0	0
5	M	1	0	0	0	0
6	A	9	0	0	0	0
6	E	9	0	0	0	0
6	K	9	0	0	0	0
6	M	9	0	0	0	0
7	A	16	0	32	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	E	16	0	32	16	0
7	I	8	0	16	2	0
7	M	12	0	24	9	0
7	N	4	0	8	2	0
7	O	4	0	8	0	0
8	A	7	0	10	7	0
8	E	7	0	10	9	0
8	J	7	0	10	0	0
8	N	7	0	10	1	0
9	A	1	0	0	0	0
9	E	1	0	0	0	0
9	I	1	0	0	0	0
9	M	1	0	0	0	0
10	E	6	0	8	0	0
10	I	24	0	32	27	0
10	J	6	0	8	3	0
10	M	6	0	8	2	0
10	N	6	0	8	3	0
11	A	122	0	0	12	0
11	B	19	0	0	1	0
11	C	14	0	0	0	0
11	D	1	0	0	0	0
11	E	100	0	0	6	0
11	F	25	0	0	2	0
11	G	9	0	0	0	0
11	H	1	0	0	1	0
11	I	95	0	0	6	0
11	J	19	0	0	2	0
11	K	11	0	0	0	0
11	M	105	0	0	16	0
11	N	21	0	0	2	0
11	O	7	0	0	1	0
All	All	18525	0	16396	783	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 23.

The worst 5 of 783 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:E:404:THR:HB	8:E:7002:PEG:H32	1.35	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:N:6020:IPA:H31	8:N:7004:PEG:H42	1.33	1.06
1:A:410:THR:HA	8:A:7001:PEG:H41	1.35	1.05
1:I:337:GLU:HG2	10:I:8003:GOL:H31	1.41	1.02
1:A:404:THR:HB	8:A:7001:PEG:H32	1.38	1.01

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	459/471 (98%)	426 (93%)	29 (6%)	4 (1%)	20	46
1	E	459/471 (98%)	425 (93%)	30 (6%)	4 (1%)	20	46
1	I	459/471 (98%)	400 (87%)	51 (11%)	8 (2%)	11	27
1	M	459/471 (98%)	396 (86%)	56 (12%)	7 (2%)	12	30
All	All	1836/1884 (98%)	1647 (90%)	166 (9%)	23 (1%)	14	35

5 of 23 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	66	LYS
1	E	66	LYS
1	I	6	MET
1	I	12	VAL
1	M	6	MET

### 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	403/412 (98%)	372 (92%)	31 (8%)	15	34
1	E	403/412 (98%)	372 (92%)	31 (8%)	15	34
1	I	403/412 (98%)	370 (92%)	33 (8%)	13	30
1	M	403/412 (98%)	370 (92%)	33 (8%)	13	30
All	All	1612/1648 (98%)	1484 (92%)	128 (8%)	14	33

5 of 128 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	338	VAL
1	I	68	THR
1	M	348	LYS
1	E	376	ARG
1	I	26	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
1	I	4	GLN
1	I	277	ASN
1	M	398	HIS
1	I	170	GLN
1	I	269	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	16/26 (61%)	4 (25%)	1 (6%)
2	F	16/26 (61%)	4 (25%)	1 (6%)
2	J	15/26 (57%)	2 (13%)	1 (6%)
2	N	15/26 (57%)	2 (13%)	1 (6%)
3	C	14/15 (93%)	2 (14%)	0
3	G	14/15 (93%)	2 (14%)	0
3	K	14/15 (93%)	0	0
3	O	14/15 (93%)	0	0
4	D	2/9 (22%)	1 (50%)	0
4	H	2/9 (22%)	1 (50%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
4	L	3/9 (33%)	1 (33%)	0
4	P	3/9 (33%)	1 (33%)	0
All	All	128/200 (64%)	20 (15%)	4 (3%)

5 of 20 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	598	A
2	B	599	G
2	B	600	G
2	B	602	C
3	C	690	C

All (4) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	B	599	G
2	F	599	G
2	J	598	A
2	N	598	A

## 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 41 ligands modelled in this entry, 10 are monoatomic - leaving 31 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
6	POP	A	5004	5	8,8,8	0.83	0	8,13,13	0.65	0
7	IPA	A	6008	-	3,3,3	0.57	0	3,3,3	0.24	0
7	IPA	A	6009	-	3,3,3	0.63	0	3,3,3	0.19	0
7	IPA	A	6011	-	3,3,3	0.61	0	3,3,3	0.21	0
7	IPA	A	6025	-	3,3,3	0.58	0	3,3,3	0.24	0
8	PEG	A	7001	-	6,6,6	0.49	0	5,5,5	0.53	0
6	POP	E	5003	5	8,8,8	1.04	1 (12%)	8,13,13	0.59	0
7	IPA	E	6010	-	3,3,3	0.55	0	3,3,3	0.34	0
7	IPA	E	6013	-	3,3,3	0.59	0	3,3,3	0.19	0
7	IPA	E	6014	-	3,3,3	0.40	0	3,3,3	0.75	0
7	IPA	E	6015	-	3,3,3	0.61	0	3,3,3	0.33	0
8	PEG	E	7002	-	6,6,6	0.46	0	5,5,5	0.34	0
10	GOL	E	8008	-	5,5,5	0.35	0	5,5,5	0.36	0
7	IPA	I	6012	-	3,3,3	0.58	0	3,3,3	0.31	0
7	IPA	I	6023	-	3,3,3	0.55	0	3,3,3	0.34	0
10	GOL	I	8002	-	5,5,5	0.25	0	5,5,5	0.53	0
10	GOL	I	8003	-	5,5,5	0.42	0	5,5,5	0.41	0
10	GOL	I	8004	-	5,5,5	0.44	0	5,5,5	0.34	0
10	GOL	I	8006	-	5,5,5	0.34	0	5,5,5	0.54	0
8	PEG	J	7003	-	6,6,6	0.64	0	5,5,5	0.24	0
10	GOL	J	8005	-	5,5,5	0.47	0	5,5,5	0.60	0
6	POP	K	5002	5	8,8,8	0.67	0	8,13,13	0.44	0
6	POP	M	5001	5	8,8,8	0.81	0	8,13,13	0.33	0
7	IPA	M	6007	-	3,3,3	0.60	0	3,3,3	0.25	0
7	IPA	M	6016	-	3,3,3	0.60	0	3,3,3	0.30	0
7	IPA	M	6019	-	3,3,3	0.55	0	3,3,3	0.30	0
10	GOL	M	8009	-	5,5,5	0.37	0	5,5,5	0.57	0
7	IPA	N	6020	-	3,3,3	0.62	0	3,3,3	0.16	0
8	PEG	N	7004	-	6,6,6	0.57	0	5,5,5	0.30	0
10	GOL	N	8010	-	5,5,5	0.35	0	5,5,5	0.26	0
7	IPA	O	6021	-	3,3,3	0.64	0	3,3,3	0.13	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
6	POP	A	5004	5	-	0/6/6/6	0/0/0/0
7	IPA	A	6008	-	-	0/0/0/0	0/0/0/0
7	IPA	A	6009	-	-	0/0/0/0	0/0/0/0
7	IPA	A	6011	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	IPA	A	6025	-	-	0/0/0/0	0/0/0/0
8	PEG	A	7001	-	-	0/4/4/4	0/0/0/0
6	POP	E	5003	5	-	0/6/6/6	0/0/0/0
7	IPA	E	6010	-	-	0/0/0/0	0/0/0/0
7	IPA	E	6013	-	-	0/0/0/0	0/0/0/0
7	IPA	E	6014	-	-	0/0/0/0	0/0/0/0
7	IPA	E	6015	-	-	0/0/0/0	0/0/0/0
8	PEG	E	7002	-	-	0/4/4/4	0/0/0/0
10	GOL	E	8008	-	-	0/4/4/4	0/0/0/0
7	IPA	I	6012	-	-	0/0/0/0	0/0/0/0
7	IPA	I	6023	-	-	0/0/0/0	0/0/0/0
10	GOL	I	8002	-	-	0/4/4/4	0/0/0/0
10	GOL	I	8003	-	-	0/4/4/4	0/0/0/0
10	GOL	I	8004	-	-	0/4/4/4	0/0/0/0
10	GOL	I	8006	-	-	0/4/4/4	0/0/0/0
8	PEG	J	7003	-	-	0/4/4/4	0/0/0/0
10	GOL	J	8005	-	-	0/4/4/4	0/0/0/0
6	POP	K	5002	5	-	0/6/6/6	0/0/0/0
6	POP	M	5001	5	-	0/6/6/6	0/0/0/0
7	IPA	M	6007	-	-	0/0/0/0	0/0/0/0
7	IPA	M	6016	-	-	0/0/0/0	0/0/0/0
7	IPA	M	6019	-	-	0/0/0/0	0/0/0/0
10	GOL	M	8009	-	-	0/4/4/4	0/0/0/0
7	IPA	N	6020	-	-	0/0/0/0	0/0/0/0
8	PEG	N	7004	-	-	0/4/4/4	0/0/0/0
10	GOL	N	8010	-	-	0/4/4/4	0/0/0/0
7	IPA	O	6021	-	-	0/0/0/0	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	E	5003	POP	P1-O	2.11	1.63	1.60

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

21 monomers are involved in 84 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	6009	IPA	1	0
7	A	6011	IPA	2	0
7	A	6025	IPA	1	0
8	A	7001	PEG	7	0
7	E	6010	IPA	3	0
7	E	6013	IPA	1	0
7	E	6014	IPA	10	0
7	E	6015	IPA	2	0
8	E	7002	PEG	9	0
7	I	6023	IPA	2	0
10	I	8002	GOL	8	0
10	I	8003	GOL	5	0
10	I	8004	GOL	4	0
10	I	8006	GOL	10	0
10	J	8005	GOL	3	0
7	M	6016	IPA	4	0
7	M	6019	IPA	5	0
10	M	8009	GOL	2	0
7	N	6020	IPA	2	0
8	N	7004	PEG	1	0
10	N	8010	GOL	3	0

## 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, 95<sup>th</sup> 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(Å²)	Q<0.9
1	A	461/471 (97%)	0.17	30 (6%)	20	17	33, 57, 94, 113	0
1	E	461/471 (97%)	0.12	32 (6%)	18	16	32, 57, 93, 113	0
1	I	461/471 (97%)	0.29	38 (8%)	12	10	33, 63, 114, 165	0
1	M	461/471 (97%)	0.25	35 (7%)	15	12	33, 64, 114, 166	0
2	B	18/26 (69%)	0.00	2 (11%)	6	5	43, 63, 155, 214	0
2	F	18/26 (69%)	0.16	2 (11%)	6	5	42, 63, 154, 214	0
2	J	16/26 (61%)	-0.30	1 (6%)	21	19	45, 75, 149, 160	0
2	N	16/26 (61%)	-0.17	1 (6%)	21	19	45, 76, 150, 160	0
3	C	15/15 (100%)	0.06	1 (6%)	19	16	46, 63, 121, 129	0
3	G	15/15 (100%)	0.14	2 (13%)	4	3	46, 63, 122, 131	0
3	K	15/15 (100%)	-0.37	0	100	100	51, 69, 140, 148	0
3	O	15/15 (100%)	-0.20	1 (6%)	19	16	52, 70, 142, 150	0
4	D	3/9 (33%)	1.16	1 (33%)	0	0	142, 142, 147, 150	0
4	H	3/9 (33%)	1.41	1 (33%)	0	0	142, 142, 147, 150	0
4	L	4/9 (44%)	1.45	1 (25%)	1	0	124, 130, 130, 159	0
4	P	4/9 (44%)	1.38	2 (50%)	0	0	125, 130, 130, 159	0
All	All	1986/2084 (95%)	0.20	150 (7%)	15	12	32, 60, 113, 214	0

The worst 5 of 150 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	M	342	LEU	11.1
1	A	46	ASN	10.7
1	I	46	ASN	9.8
1	I	344	ALA	9.4
1	I	342	LEU	8.7

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
10	GOL	J	8005	6/6	0.94	0.39	5.96	52,55,71,73	0
7	IPA	M	6007	4/4	0.90	0.42	5.10	86,96,100,101	0
10	GOL	I	8003	6/6	0.70	0.32	4.02	94,114,116,117	0
7	IPA	E	6015	4/4	0.73	0.31	3.40	71,72,73,78	0
7	IPA	I	6023	4/4	0.74	0.49	3.17	75,81,84,91	0
7	IPA	A	6009	4/4	0.89	0.32	2.48	52,72,73,78	0
10	GOL	I	8002	6/6	0.65	0.26	2.39	82,122,129,131	0
7	IPA	A	6011	4/4	0.62	0.37	2.13	72,85,88,93	0
7	IPA	A	6008	4/4	0.86	0.31	2.02	78,82,93,99	0
6	POP	E	5003	9/9	0.90	0.22	1.26	36,57,112,122	9
6	POP	M	5001	9/9	0.90	0.23	1.20	65,99,115,133	9
7	IPA	I	6012	4/4	0.77	0.30	0.85	89,102,107,110	0
7	IPA	E	6010	4/4	0.83	0.24	0.62	60,71,76,77	0
10	GOL	N	8010	6/6	0.91	0.20	0.41	56,64,66,87	0
7	IPA	E	6013	4/4	0.78	0.22	0.31	100,104,112,117	0
8	PEG	E	7002	7/7	0.85	0.18	0.19	61,67,96,99	0
6	POP	A	5004	9/9	0.89	0.19	0.12	46,76,111,112	9
8	PEG	A	7001	7/7	0.90	0.13	0.04	58,73,84,89	0
7	IPA	E	6014	4/4	0.91	0.24	-0.05	57,61,67,76	0
7	IPA	M	6016	4/4	0.83	0.20	-0.14	63,84,90,94	0
5	MG	E	3003	1/1	0.97	0.16	-0.24	59,59,59,59	0
5	MG	A	3005	1/1	0.97	0.15	-0.27	60,60,60,60	0
10	GOL	I	8004	6/6	0.82	0.19	-0.35	77,106,109,117	0
6	POP	K	5002	9/9	0.91	0.14	-0.40	62,94,108,117	9
10	GOL	M	8009	6/6	0.78	0.15	-0.47	75,82,101,108	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
7	IPA	M	6019	4/4	0.89	0.16	-0.77	68,94,98,105	0
10	GOL	I	8006	6/6	0.83	0.14	-0.81	94,98,108,120	0
9	ZN	I	2003	1/1	0.98	0.11	-0.83	78,78,78,78	1
5	MG	I	3004	1/1	0.85	0.12	-1.19	83,83,83,83	0
5	MG	M	3001	1/1	0.92	0.08	-2.08	74,74,74,74	0
9	ZN	M	2004	1/1	0.95	0.05	-2.48	76,76,76,76	1
10	GOL	E	8008	6/6	0.73	0.15	-	81,97,104,105	0
9	ZN	A	2001	1/1	0.27	0.40	-	114,114,114,114	1
7	IPA	N	6020	4/4	0.45	0.27	-	92,101,106,108	0
8	PEG	J	7003	7/7	0.85	0.21	-	71,79,103,103	0
9	ZN	E	2002	1/1	0.48	0.21	-	111,111,111,111	1
5	MG	A	3006	1/1	0.91	0.34	-	81,81,81,81	0
7	IPA	O	6021	4/4	0.81	0.23	-	75,82,87,99	0
5	MG	E	3002	1/1	0.82	0.29	-	83,83,83,83	0
8	PEG	N	7004	7/7	0.81	0.21	-	79,88,98,104	0
7	IPA	A	6025	4/4	0.69	0.19	-	88,91,105,115	0

## 6.5 Other polymers

There are no such residues in this entry.