Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 11:22 AM GMT

PDB ID	:	3OL9
Title	:	Poliovirus polymerase elongation complex with 3'-deoxy-CTP
Authors	:	Gong, P.; Peersen, O.B.
Deposited on	:	2010-08-25
Resolution	:	2.25 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

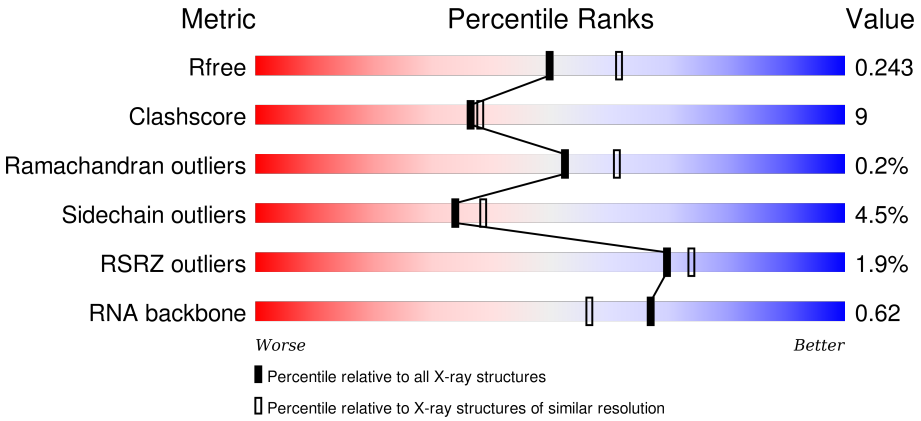
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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}	91344	1640 (2.28-2.24)
Clashscore	102246	1095 (2.26-2.26)
Ramachandran outliers	100387	1063 (2.26-2.26)
Sidechain outliers	100360	1063 (2.26-2.26)
RSRZ outliers	91569	1647 (2.28-2.24)
RNA backbone	2183	1002 (2.80-1.74)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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 <=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	2% 76% 20%
1	E	471	2% 76% 20%
1	I	471	2% 83% 14%
1	M	471	2% 83% 13%

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Mol	Chain	Length	Quality of chain
2	B	26	15% 50% 31%
2	F	26	19% 46% 31%
2	J	26	4% 35% 35% 27%
2	N	26	4% 35% 38% 27%
3	C	15	73% 27%
3	G	15	80% 20%
3	K	15	87% 13%
3	O	15	87% 13%
4	D	9	22% 11% 67%
4	H	9	11% 22% 11% 67%
4	L	9	33% 11% 56%
4	P	9	33% 11% 56%

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
6	IPA	A	6008	-	-	-	X
6	IPA	A	6009	-	-	-	X
6	IPA	A	6013	-	-	-	X
6	IPA	E	6010	-	-	X	X
6	IPA	I	6011	-	-	-	X
6	IPA	I	6027	-	-	X	-
6	IPA	M	6001	-	-	X	X
6	IPA	M	6004	-	-	X	X
6	IPA	O	6024	-	-	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 19065 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	19	Total	C	N	O	P	0	0	0
			381	168	61	133	19			
2	N	19	Total	C	N	O	P	0	0	0
			381	168	61	133	19			

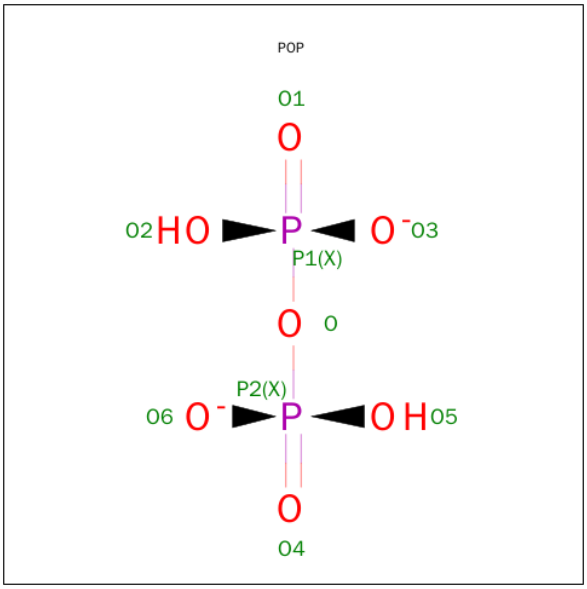
- Molecule 3 is a RNA chain called RNA (5'-R(*GP*CP*CP*CP*GP*GP*AP*CP*GP*AP*GP*AP*GP*AP*(O2C))-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	15	Total	C	N	O	P	0	0	0
			322	145	65	98	14			
3	G	15	Total	C	N	O	P	0	0	0
			322	145	65	98	14			
3	K	15	Total	C	N	O	P	0	0	0
			322	145	65	98	14			
3	O	15	Total	C	N	O	P	0	0	0
			322	145	65	98	14			

- 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	C	N	O	P	0	0	0
			68	30	15	20	3			
4	H	3	Total	C	N	O	P	0	0	0
			68	30	15	20	3			
4	L	4	Total	C	N	O	P	0	0	0
			91	40	20	27	4			
4	P	4	Total	C	N	O	P	0	0	0
			91	40	20	27	4			

- Molecule 5 is PYROPHOSPHATE 2- (three-letter code: POP) (formula: $H_2O_7P_2$).



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

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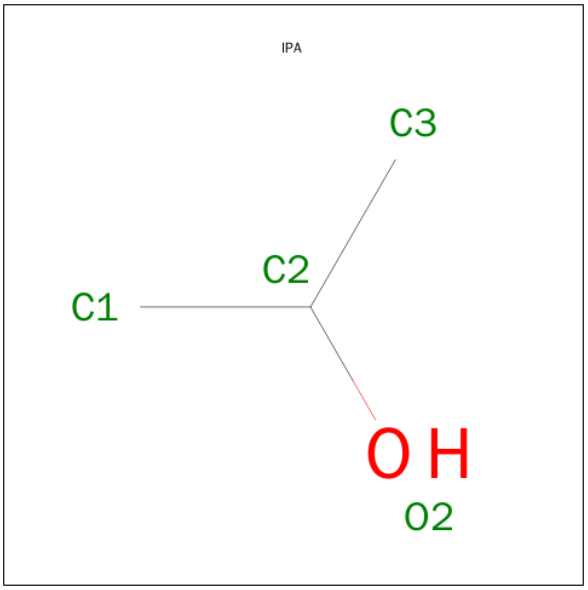
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	I	1	Total O P 9 7 2	0	0
5	M	1	Total O P 9 7 2	0	0

- Molecule 6 is ISOPROPYL ALCOHOL (three-letter code: IPA) (formula: C_3H_8O).



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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	I	1	Total C O 4 3 1	0	0
6	I	1	Total C O 4 3 1	0	0
6	M	1	Total C O 4 3 1	0	0
6	M	1	Total C O 4 3 1	0	0
6	M	1	Total C O 4 3 1	0	0
6	O	1	Total C O 4 3 1	0	0

- Molecule 7 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	212	Total O 212 212	0	0
8	B	38	Total O 38 38	0	0
8	C	22	Total O 22 22	0	0
8	D	1	Total O 1 1	0	0
8	E	214	Total O 214 214	0	0
8	F	38	Total O 38 38	0	0
8	G	25	Total O 25 25	0	0

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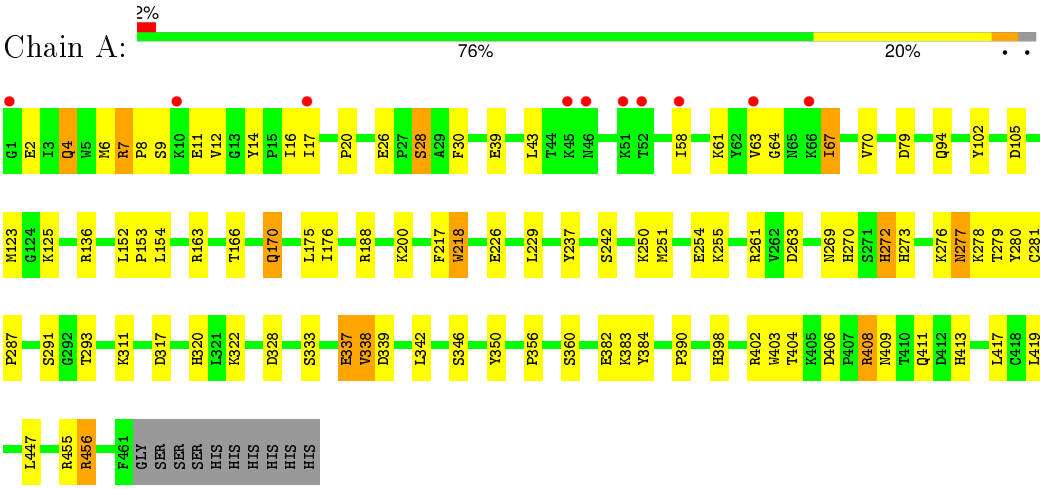
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	H	3	Total O 3 3	0	0
8	I	197	Total O 197 197	0	0
8	J	37	Total O 37 37	0	0
8	K	26	Total O 26 26	0	0
8	L	2	Total O 2 2	0	0
8	M	206	Total O 206 206	0	0
8	N	40	Total O 40 40	0	0
8	O	26	Total O 26 26	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

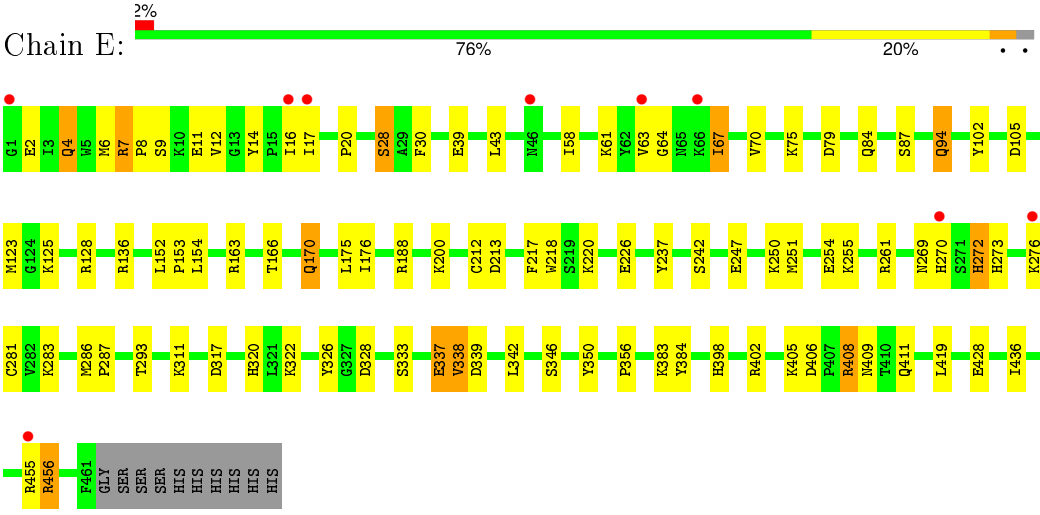
- Molecule 1: Polymerase

Chain A:



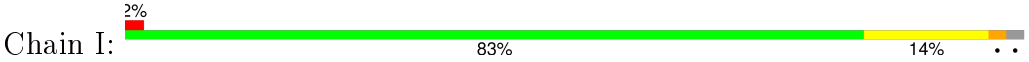
- Molecule 1: Polymerase

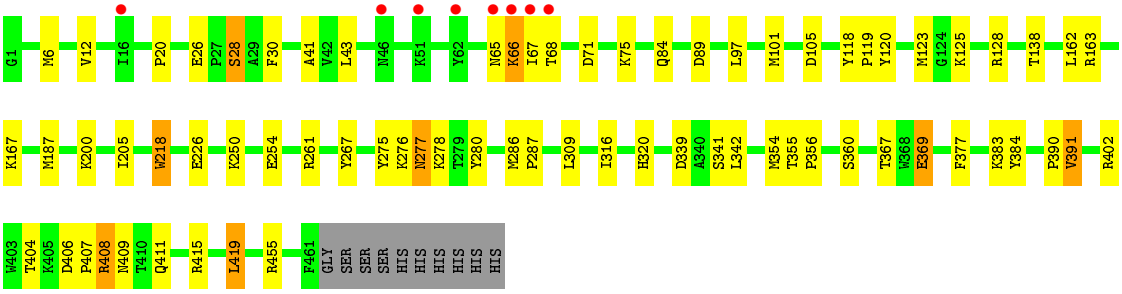
Chain E:



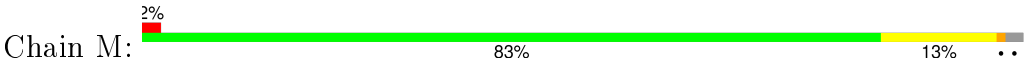
- Molecule 1: Polymerase

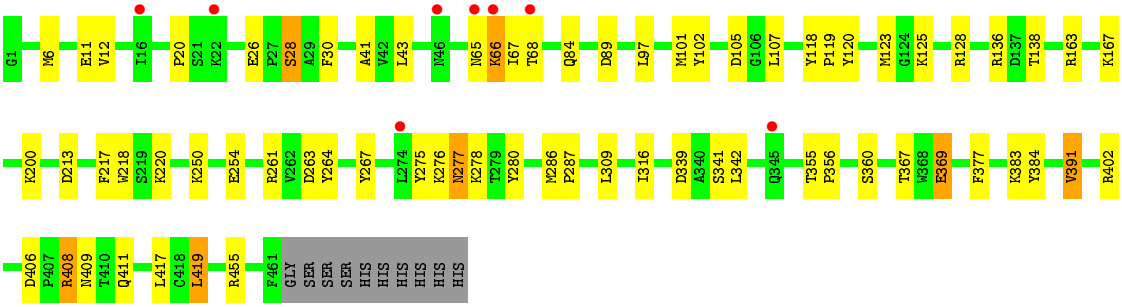
Chain I:



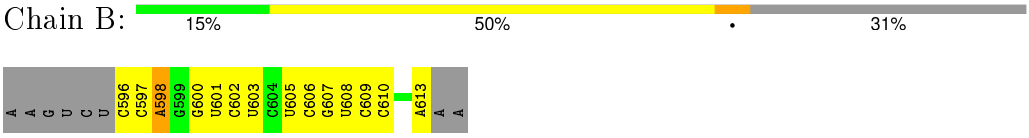


• Molecule 1: Polymerase

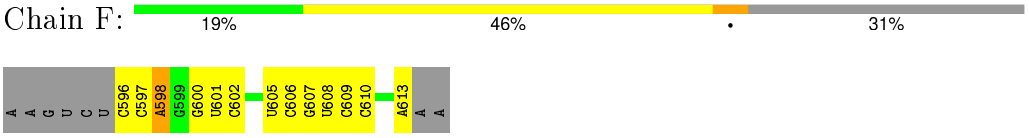




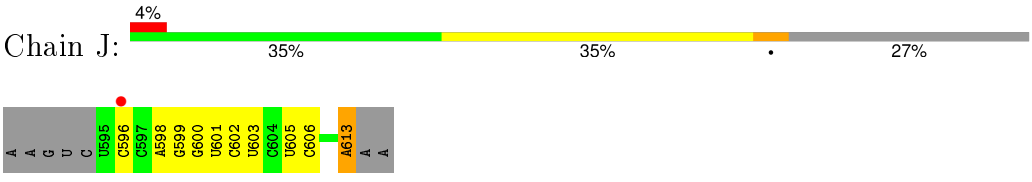
• Molecule 2: RNA (5'-R(*AP*AP*GP*UP*CP*UP*CP*CP*AP*GP*GP*UP*CP*UP*CP*UP *CP*GP*UP*CP*CP*GP*GP*AP*AP*A)-3')



• 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')

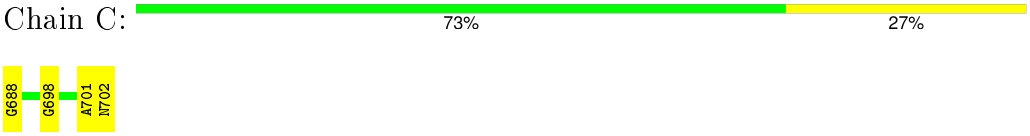


• Molecule 2: RNA (5'-R(*AP*AP*GP*UP*CP*UP*CP*CP*AP*GP*GP*UP*CP*UP*CP*UP *CP*GP*UP*CP*CP*GP*GP*AP*AP*A)-3')

Chain N:

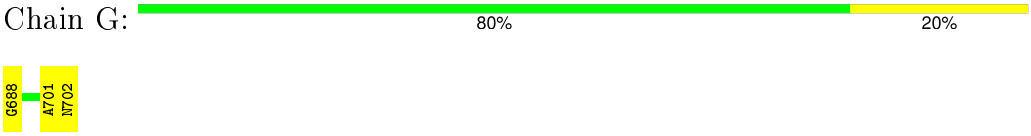
• Molecule 3: RNA (5'-R(*GP*CP*CP*CP*GP*GP*AP*CP*GP*AP*GP*AP*GP*AP*(O2C))-3')

Chain C:



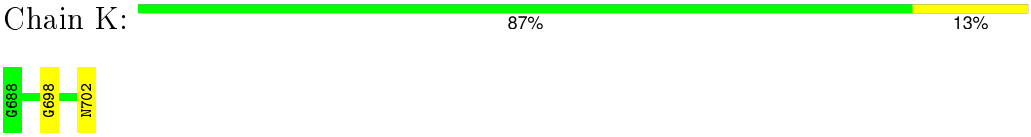
• Molecule 3: RNA (5'-R(*GP*CP*CP*CP*GP*GP*AP*CP*GP*AP*GP*AP*GP*AP*(O2C))-3')

Chain G:



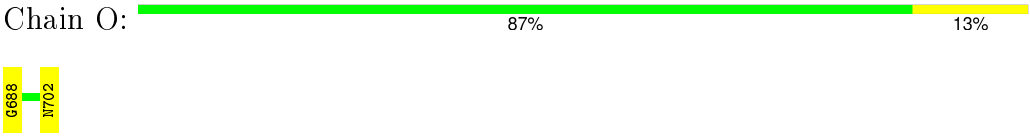
• Molecule 3: RNA (5'-R(*GP*CP*CP*CP*GP*GP*AP*CP*GP*AP*GP*AP*GP*AP*(O2C))-3')

Chain K:



• Molecule 3: RNA (5'-R(*GP*CP*CP*CP*GP*GP*AP*CP*GP*AP*GP*AP*GP*AP*(O2C))-3')

Chain O:

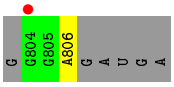


• Molecule 4: RNA (5'-R(*GP*GP*GP*AP*GP*AP*UP*GP*A)-3')

Chain D:

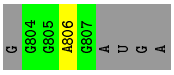
• Molecule 4: RNA (5'-R(*GP*GP*GP*AP*GP*AP*UP*GP*A)-3')

Chain H:



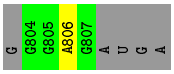
• Molecule 4: RNA (5'-R(*GP*GP*GP*AP*GP*AP*UP*GP*A)-3')

Chain L:



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

Chain P:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	60.50Å 60.55Å 192.35Å 83.69° 83.67° 77.45°	Depositor
Resolution (Å)	41.38 – 2.25 48.16 – 2.10	Depositor EDS
% Data completeness (in resolution range)	92.5 (41.38-2.25) 88.7 (48.16-2.10)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.46 (at 2.10Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, R_{free}	0.203 , 0.249 0.202 , 0.243	Depositor DCC
R_{free} test set	2027 reflections (1.78%)	DCC
Wilson B-factor (Å^2)	51.0	Xtriage
Anisotropy	0.332	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 40.3	EDS
Estimated twinning fraction	0.447 for -k,-h,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.62$, $< L^2 > = 0.48$	Xtriage
Outliers	0 of 140746 reflections	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	19065	wwPDB-VP
Average B, all atoms (Å^2)	62.0	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 48.83 % 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 8.1371e-05.The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: ZN, IPA, O2C, POP

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	0.41	0/3787	0.55	0/5122
1	E	0.41	0/3787	0.55	0/5122
1	I	0.41	0/3787	0.56	0/5122
1	M	0.41	0/3787	0.56	0/5122
2	B	0.55	0/400	0.90	0/621
2	F	0.57	0/400	0.90	0/621
2	J	0.68	1/422 (0.2%)	0.94	0/655
2	N	0.69	0/422	0.94	1/655 (0.2%)
3	C	0.57	0/340	0.92	0/530
3	G	0.55	0/340	0.88	0/530
3	K	0.58	0/340	0.90	0/530
3	O	0.58	0/340	0.89	0/530
4	D	0.30	0/76	0.59	0/117
4	H	0.27	0/76	0.58	0/117
4	L	0.25	0/102	0.52	0/158
4	P	0.24	0/102	0.54	0/158
All	All	0.45	1/18508 (0.0%)	0.63	1/25710 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	613	A	P-O5'	-5.21	1.54	1.59

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	N	613	A	O5'-P-OP1	-5.08	101.13	105.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3697	0	3658	81	0
1	E	3697	0	3658	85	0
1	I	3697	0	3658	52	0
1	M	3697	0	3658	54	0
2	B	361	0	183	18	0
2	F	361	0	183	16	0
2	J	381	0	193	8	0
2	N	381	0	193	7	0
3	C	322	0	167	7	0
3	G	322	0	167	6	0
3	K	322	0	167	5	0
3	O	322	0	167	3	0
4	D	68	0	34	0	0
4	H	68	0	34	0	0
4	L	91	0	45	0	0
4	P	91	0	45	0	0
5	A	9	0	0	0	0
5	E	9	0	0	0	0
5	I	9	0	0	2	0
5	M	9	0	0	0	0
6	A	20	0	39	5	0
6	E	12	0	23	4	0
6	I	12	0	24	7	0
6	M	12	0	24	10	0
6	O	4	0	8	0	0
7	A	1	0	0	0	0
7	E	1	0	0	0	0
7	I	1	0	0	0	0
7	M	1	0	0	0	0
8	A	212	0	0	6	0
8	B	38	0	0	0	0
8	C	22	0	0	0	0
8	D	1	0	0	0	0
8	E	214	0	0	9	0
8	F	38	0	0	0	0
8	G	25	0	0	0	0
8	H	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	I	197	0	0	6	0
8	J	37	0	0	0	0
8	K	26	0	0	0	0
8	L	2	0	0	0	0
8	M	206	0	0	5	0
8	N	40	0	0	1	0
8	O	26	0	0	0	0
All	All	19065	0	16328	322	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 9.

All (322) 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:M:213:ASP:H	6:M:6001:IPA:H13	1.17	1.04
6:I:6027:IPA:H11	8:I:1127:HOH:O	1.63	0.99
1:A:456:ARG:HH11	1:A:456:ARG:HG3	1.29	0.97
1:E:456:ARG:HH11	1:E:456:ARG:HG3	1.28	0.95
1:A:229:LEU:HG	6:A:6008:IPA:H31	1.50	0.94
1:A:277:ASN:HD22	1:A:278:LYS:HG3	1.37	0.88
1:E:277:ASN:HD22	1:E:278:LYS:HG3	1.37	0.88
1:E:311:LYS:HD3	1:E:346:SER:HB3	1.54	0.88
1:A:311:LYS:HD3	1:A:346:SER:HB3	1.57	0.87
1:A:9:SER:HB3	1:A:279:THR:OG1	1.76	0.85
1:E:9:SER:HB3	1:E:279:THR:OG1	1.77	0.84
1:M:213:ASP:H	6:M:6001:IPA:C1	1.91	0.81
2:J:613:A:OP1	3:O:688:G:H5'	1.82	0.80
1:E:277:ASN:ND2	1:E:278:LYS:HG3	1.98	0.79
1:A:277:ASN:ND2	1:A:278:LYS:HG3	1.98	0.78
1:M:20:PRO:HG3	2:N:598:A:C4	2.24	0.73
1:A:217:PHE:HD1	6:A:6009:IPA:H2	1.55	0.72
6:I:6027:IPA:H31	3:K:698:G:OP1	1.90	0.72
1:E:213:ASP:H	6:E:6010:IPA:H33	1.53	0.71
1:M:377:PHE:HB2	1:M:391:VAL:HG22	1.73	0.71
1:M:220:LYS:HE3	8:M:1094:HOH:O	1.91	0.70
1:M:277:ASN:ND2	1:M:278:LYS:HG3	2.07	0.70
1:I:20:PRO:HG3	2:J:598:A:C4	2.28	0.69
1:A:217:PHE:CD1	6:A:6009:IPA:H2	2.28	0.69
1:A:4:GLN:HE21	1:A:283:LYS:HD2	1.58	0.69
1:I:277:ASN:ND2	1:I:278:LYS:HG3	2.07	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:70:VAL:HG21	1:E:251:MET:CE	2.23	0.69
1:A:70:VAL:HG21	1:A:251:MET:CE	2.23	0.69
1:A:242:SER:HB3	8:A:1001:HOH:O	1.94	0.68
1:E:4:GLN:HE21	1:E:283:LYS:HD2	1.59	0.67
1:I:377:PHE:HB2	1:I:391:VAL:HG22	1.75	0.67
1:E:20:PRO:HG3	2:F:598:A:C4	2.29	0.67
1:M:383:LYS:HE3	1:M:384:TYR:CE1	2.30	0.67
1:E:217:PHE:HB2	6:E:6010:IPA:H2	1.76	0.67
1:A:20:PRO:HG3	2:B:598:A:C4	2.29	0.67
1:E:242:SER:HB3	8:E:980:HOH:O	1.95	0.66
1:M:355:THR:HB	1:M:356:PRO:HD2	1.78	0.66
1:M:217:PHE:HB2	6:M:6001:IPA:H11	1.78	0.66
1:E:212:CYS:HA	6:E:6010:IPA:H12	1.77	0.65
1:I:356:PRO:HG2	1:I:360:SER:O	1.97	0.65
1:E:16:ILE:HG12	1:E:277:ASN:HA	1.79	0.65
1:I:355:THR:HB	1:I:356:PRO:HD2	1.79	0.65
1:I:383:LYS:HE3	1:I:384:TYR:CE1	2.31	0.65
1:M:356:PRO:HG2	1:M:360:SER:O	1.98	0.64
1:A:16:ILE:HG12	1:A:277:ASN:HA	1.80	0.64
1:M:128:ARG:HG3	8:M:511:HOH:O	1.98	0.64
1:A:456:ARG:HH11	1:A:456:ARG:CG	2.06	0.64
1:E:356:PRO:HD2	8:E:745:HOH:O	1.96	0.64
1:I:277:ASN:HD22	1:I:278:LYS:HG3	1.63	0.63
1:M:277:ASN:HD22	1:M:278:LYS:HG3	1.63	0.63
1:E:8:PRO:O	1:E:11:GLU:HG2	1.98	0.63
1:A:8:PRO:O	1:A:11:GLU:HG2	1.98	0.62
1:M:213:ASP:N	6:M:6001:IPA:H13	2.02	0.62
1:M:28:SER:HB3	1:M:30:PHE:H	1.64	0.62
1:M:267:TYR:CB	6:M:6004:IPA:H33	2.30	0.62
1:I:28:SER:HB3	1:I:30:PHE:H	1.64	0.61
1:E:456:ARG:HH11	1:E:456:ARG:CG	2.06	0.61
1:A:166:THR:O	1:A:170:GLN:HB2	2.01	0.60
1:M:41:ALA:HB2	1:M:163:ARG:CG	2.32	0.60
1:I:12:VAL:HG12	1:I:12:VAL:O	2.01	0.60
1:E:166:THR:O	1:E:170:GLN:HB2	2.01	0.60
1:A:12:VAL:O	1:A:12:VAL:HG12	2.02	0.59
1:M:11:GLU:HG2	8:M:1055:HOH:O	2.03	0.59
1:M:12:VAL:HG12	1:M:12:VAL:O	2.02	0.59
1:I:41:ALA:HB2	1:I:163:ARG:CG	2.33	0.58
1:M:264:TYR:CD1	6:M:6004:IPA:H32	2.38	0.58
1:E:217:PHE:CD1	6:E:6010:IPA:H11	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:404:THR:HA	6:A:6029:IPA:H32	1.86	0.58
1:M:65:ASN:O	1:M:66:LYS:HB2	2.03	0.57
1:E:12:VAL:HG12	1:E:12:VAL:O	2.04	0.57
1:A:411:GLN:HB3	8:A:1032:HOH:O	2.02	0.57
1:I:65:ASN:O	1:I:66:LYS:HB2	2.04	0.57
1:E:419:LEU:HD11	2:F:606:C:H4'	1.87	0.57
1:E:406:ASP:OD1	1:E:408:ARG:HG3	2.05	0.57
2:J:600:G:O2'	2:J:601:U:H5'	2.04	0.57
1:E:28:SER:HB3	1:E:30:PHE:H	1.70	0.56
1:A:419:LEU:HD11	2:B:606:C:H4'	1.88	0.56
1:M:41:ALA:HB2	1:M:163:ARG:HG3	1.87	0.56
1:I:41:ALA:HB2	1:I:163:ARG:HG3	1.88	0.56
6:I:6027:IPA:C3	3:K:698:G:OP1	2.54	0.56
2:N:600:G:O2'	2:N:601:U:H5'	2.05	0.56
1:E:152:LEU:HB3	1:E:153:PRO:HD2	1.87	0.55
1:I:128:ARG:HG3	8:I:676:HOH:O	2.06	0.55
1:A:28:SER:HB3	1:A:30:PHE:H	1.71	0.55
1:I:119:PRO:O	1:I:123:MET:HG3	2.06	0.55
1:A:70:VAL:HG21	1:A:251:MET:HE1	1.89	0.55
1:I:309:LEU:HB3	1:I:316:ILE:HD13	1.89	0.55
1:A:6:MET:O	1:A:7:ARG:HB3	2.06	0.55
1:A:406:ASP:OD1	1:A:408:ARG:HG3	2.07	0.55
1:A:79:ASP:OD1	1:A:255:LYS:HE2	2.08	0.54
2:B:600:G:O2'	2:B:601:U:H5'	2.07	0.54
1:M:20:PRO:HG3	2:N:598:A:C5	2.43	0.54
1:M:309:LEU:HB3	1:M:316:ILE:HD13	1.89	0.54
1:E:128:ARG:HG3	8:E:963:HOH:O	2.08	0.54
1:E:61:LYS:O	1:E:63:VAL:HG13	2.08	0.54
1:E:6:MET:O	1:E:7:ARG:HB3	2.07	0.54
1:A:152:LEU:HB3	1:A:153:PRO:HD2	1.88	0.54
1:M:119:PRO:O	1:M:123:MET:HG3	2.08	0.53
1:E:436:ILE:HG21	1:E:447:LEU:HD11	1.90	0.53
1:E:247:GLU:HG3	8:E:1167:HOH:O	2.09	0.53
1:A:436:ILE:HG21	1:A:447:LEU:HD11	1.91	0.53
1:E:79:ASP:OD1	1:E:255:LYS:HE2	2.09	0.53
1:I:404:THR:HA	6:I:6027:IPA:H32	1.91	0.53
2:F:600:G:O2'	2:F:601:U:H5'	2.09	0.53
2:B:596:C:H2'	2:B:597:C:H6	1.74	0.52
2:F:596:C:H2'	2:F:597:C:H6	1.74	0.52
1:M:105:ASP:OD2	1:M:200:LYS:HE2	2.10	0.52
1:E:339:ASP:HB3	1:E:342:LEU:HD12	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:339:ASP:HB3	1:A:342:LEU:HD12	1.90	0.52
1:I:20:PRO:HG3	2:J:598:A:C5	2.45	0.52
2:B:605:U:H2'	2:B:606:C:C6	2.45	0.52
3:C:702:O2C:H6	3:C:702:O2C:H5'2	1.91	0.52
1:A:28:SER:HB2	1:A:402:ARG:C	2.30	0.52
3:G:702:O2C:H6	3:G:702:O2C:H5'2	1.91	0.52
1:I:105:ASP:OD2	1:I:200:LYS:HE2	2.10	0.52
1:A:61:LYS:O	1:A:63:VAL:HG13	2.09	0.52
5:I:5002:POP:O3	3:K:702:O2C:H5'1	2.10	0.52
1:I:411:GLN:HB3	8:I:722:HOH:O	2.09	0.52
3:C:701:A:H2'	3:C:702:O2C:O4'	2.10	0.51
1:E:270:HIS:NE2	1:E:272:HIS:HE1	2.08	0.51
3:G:701:A:H2'	3:G:702:O2C:O4'	2.11	0.51
1:A:17:ILE:O	1:A:276:LYS:HA	2.10	0.51
2:F:605:U:H2'	2:F:606:C:C6	2.45	0.51
1:E:411:GLN:HB3	8:E:1183:HOH:O	2.10	0.51
1:E:220:LYS:HD2	8:E:1165:HOH:O	2.11	0.50
1:E:2:GLU:HG3	1:E:64:GLY:HA2	1.93	0.50
1:E:70:VAL:HG21	1:E:251:MET:HE1	1.94	0.50
1:E:17:ILE:O	1:E:276:LYS:HA	2.11	0.50
1:M:411:GLN:HB3	8:M:909:HOH:O	2.11	0.50
1:E:70:VAL:HG21	1:E:251:MET:HE3	1.94	0.50
1:A:403:TRP:O	6:A:6029:IPA:H13	2.12	0.50
1:I:406:ASP:OD1	1:I:408:ARG:HG3	2.12	0.50
1:I:277:ASN:HD22	1:I:278:LYS:CG	2.25	0.50
1:A:277:ASN:HD22	1:A:277:ASN:C	2.15	0.49
6:M:6004:IPA:H11	8:M:807:HOH:O	2.12	0.49
1:E:28:SER:HB2	1:E:402:ARG:C	2.33	0.49
1:M:41:ALA:HB2	1:M:163:ARG:HG2	1.95	0.49
1:M:406:ASP:OD1	1:M:408:ARG:HG3	2.12	0.49
3:G:688:G:H8	3:G:688:G:HO5'	1.58	0.49
2:B:597:C:C2'	2:B:598:A:H5'	2.42	0.49
1:A:2:GLU:HG3	1:A:64:GLY:HA2	1.93	0.49
1:E:277:ASN:C	1:E:277:ASN:HD22	2.16	0.49
2:F:597:C:C2'	2:F:598:A:H5'	2.42	0.49
1:A:270:HIS:NE2	1:A:272:HIS:HE1	2.09	0.49
3:K:702:O2C:H6	3:K:702:O2C:H5'2	1.95	0.49
1:E:226:GLU:HG2	1:E:322:LYS:HG2	1.94	0.48
1:E:120:TYR:HA	1:E:123:MET:HE2	1.95	0.48
3:C:688:G:HO5'	3:C:688:G:H8	1.59	0.48
1:M:277:ASN:HD22	1:M:278:LYS:CG	2.25	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:TYR:HA	1:A:123:MET:HE2	1.94	0.48
1:E:120:TYR:HB3	1:E:125:LYS:HB3	1.96	0.48
1:A:287:PRO:O	1:A:293:THR:HG21	2.14	0.48
1:A:338:VAL:HG13	8:A:679:HOH:O	2.13	0.47
1:I:162:LEU:HD11	8:I:1127:HOH:O	2.13	0.47
1:E:287:PRO:O	1:E:293:THR:HG21	2.14	0.47
1:I:41:ALA:HB2	1:I:163:ARG:HG2	1.95	0.47
1:I:339:ASP:HB3	1:I:342:LEU:HD12	1.96	0.47
1:M:339:ASP:HB3	1:M:342:LEU:HD12	1.97	0.47
1:E:456:ARG:NH1	1:E:456:ARG:HG3	2.10	0.47
1:A:237:TYR:CD2	1:A:328:ASP:HB3	2.49	0.47
1:I:406:ASP:HB3	1:I:409:ASN:ND2	2.30	0.47
2:J:602:C:H2'	2:J:603:U:C6	2.49	0.47
1:E:338:VAL:HG13	8:E:575:HOH:O	2.14	0.47
1:M:419:LEU:HD11	2:N:606:C:H4'	1.96	0.47
3:O:702:O2C:H5'2	3:O:702:O2C:H6	1.96	0.47
2:F:609:C:C2'	2:F:610:C:H5'	2.45	0.47
1:A:398:HIS:O	1:A:402:ARG:HG3	2.15	0.47
2:F:607:G:H2'	2:F:608:U:C6	2.50	0.47
1:A:226:GLU:HG2	1:A:322:LYS:HG2	1.96	0.47
1:A:337:GLU:O	1:A:337:GLU:HG3	2.15	0.47
1:M:250:LYS:O	1:M:254:GLU:HG3	2.16	0.47
1:E:383:LYS:HB3	1:E:384:TYR:CD1	2.50	0.47
1:M:339:ASP:OD1	1:M:341:SER:OG	2.27	0.46
1:A:322:LYS:HB2	1:A:333:SER:OG	2.15	0.46
1:M:383:LYS:HE3	1:M:384:TYR:HE1	1.79	0.46
1:I:267:TYR:CB	6:I:6011:IPA:H11	2.46	0.46
1:E:337:GLU:HG3	1:E:337:GLU:O	2.16	0.46
1:A:70:VAL:HG21	1:A:251:MET:HE3	1.98	0.46
1:I:187:MET:HG2	6:I:6011:IPA:H33	1.96	0.46
1:I:97:LEU:O	1:I:101:MET:HG3	2.15	0.46
1:A:120:TYR:HB3	1:A:125:LYS:HB3	1.98	0.46
1:I:419:LEU:HD11	2:J:606:C:H4'	1.98	0.46
1:A:176:ILE:HA	8:A:1023:HOH:O	2.15	0.46
1:A:383:LYS:HB3	1:A:384:TYR:CD1	2.51	0.46
2:B:607:G:H2'	2:B:608:U:C6	2.51	0.46
1:M:406:ASP:HB3	1:M:409:ASN:ND2	2.31	0.46
3:C:688:G:H4'	2:F:613:A:OP1	2.16	0.46
1:M:6:MET:HG3	1:M:280:TYR:HB3	1.97	0.46
1:E:250:LYS:O	1:E:254:GLU:HG3	2.16	0.46
1:M:217:PHE:HB2	6:M:6001:IPA:C1	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:398:HIS:O	1:E:402:ARG:HG3	2.15	0.46
2:F:596:C:H2'	2:F:597:C:C6	2.51	0.45
1:E:118:TYR:CD2	1:E:153:PRO:HD2	2.51	0.45
1:M:107:LEU:HD12	8:N:1066:HOH:O	2.16	0.45
1:I:415:ARG:HD2	8:I:1141:HOH:O	2.15	0.45
1:I:66:LYS:O	1:I:68:THR:HG23	2.17	0.45
1:I:339:ASP:OD1	1:I:341:SER:OG	2.31	0.45
2:N:605:U:H2'	2:N:606:C:C6	2.51	0.45
1:I:250:LYS:O	1:I:254:GLU:HG3	2.16	0.45
1:A:105:ASP:OD2	1:A:200:LYS:HE2	2.17	0.45
2:B:609:C:C2'	2:B:610:C:H5'	2.46	0.45
2:B:596:C:H2'	2:B:597:C:C6	2.52	0.45
2:N:598:A:H3'	2:N:599:G:C8	2.52	0.45
2:N:602:C:H2'	2:N:603:U:C6	2.52	0.45
1:E:317:ASP:OD2	1:E:320:HIS:HD2	1.99	0.45
2:J:605:U:H2'	2:J:606:C:C6	2.52	0.45
1:E:237:TYR:CD2	1:E:328:ASP:HB3	2.52	0.45
1:A:317:ASP:OD2	1:A:320:HIS:HD2	2.00	0.45
1:E:322:LYS:HB2	1:E:333:SER:OG	2.17	0.45
3:C:688:G:H5'	2:F:613:A:OP1	2.16	0.45
1:M:28:SER:HB2	1:M:402:ARG:C	2.37	0.45
2:J:598:A:H3'	2:J:599:G:C8	2.52	0.44
1:A:9:SER:HB2	1:A:14:TYR:HB2	1.99	0.44
1:E:176:ILE:HG21	2:F:600:G:C8	2.52	0.44
1:A:2:GLU:CG	1:A:64:GLY:HA2	2.47	0.44
1:M:97:LEU:HD23	1:M:138:THR:HB	1.99	0.44
1:A:356:PRO:HD2	8:A:767:HOH:O	2.16	0.44
1:E:9:SER:HB2	1:E:14:TYR:HB2	1.99	0.44
1:E:2:GLU:CG	1:E:64:GLY:HA2	2.47	0.44
1:I:267:TYR:HB2	6:I:6011:IPA:H11	2.00	0.44
1:I:6:MET:HG3	1:I:280:TYR:HB3	1.98	0.44
5:I:5002:POP:P1	3:K:702:O2C:H5'1	2.58	0.44
2:B:613:A:OP1	3:G:688:G:H5'	2.18	0.44
1:I:97:LEU:HD23	1:I:138:THR:HB	1.98	0.44
1:A:4:GLN:NE2	1:A:283:LYS:HD2	2.30	0.44
1:M:66:LYS:O	1:M:68:THR:HG23	2.18	0.44
1:E:406:ASP:HB3	1:E:409:ASN:ND2	2.32	0.44
3:G:688:G:O5'	3:G:688:G:H8	2.01	0.44
1:M:267:TYR:CD2	6:M:6004:IPA:H33	2.53	0.43
1:A:119:PRO:O	1:A:123:MET:HG3	2.18	0.43
1:E:188:ARG:HD2	2:F:602:C:OP1	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:ARG:O	1:A:8:PRO:C	2.57	0.43
1:E:20:PRO:HG3	2:F:598:A:N3	2.34	0.43
1:I:118:TYR:CD1	1:I:119:PRO:HA	2.52	0.43
1:I:367:THR:C	1:I:369:GLU:H	2.22	0.43
1:M:367:THR:C	1:M:369:GLU:H	2.22	0.43
1:A:176:ILE:HG21	2:B:600:G:C8	2.53	0.43
2:B:613:A:OP1	3:G:688:G:H4'	2.18	0.43
3:C:688:G:O5'	3:C:688:G:H8	2.02	0.43
1:A:250:LYS:O	1:A:254:GLU:HG3	2.18	0.43
1:A:406:ASP:HB3	1:A:409:ASN:ND2	2.34	0.43
1:A:286:MET:HA	1:A:287:PRO:HD3	1.86	0.43
1:E:102:TYR:CE1	1:E:136:ARG:HA	2.54	0.43
1:M:118:TYR:CD1	1:M:119:PRO:HA	2.53	0.43
1:E:405:LYS:HD2	8:E:1178:HOH:O	2.18	0.43
1:E:286:MET:HA	1:E:287:PRO:HD3	1.84	0.43
1:E:4:GLN:NE2	1:E:283:LYS:HD2	2.30	0.42
1:M:267:TYR:HB2	6:M:6004:IPA:H33	2.01	0.42
1:M:163:ARG:NH2	1:M:167:LYS:HD2	2.34	0.42
2:F:609:C:O2'	2:F:610:C:H5'	2.20	0.42
1:A:218:TRP:CD1	1:A:390:PRO:HA	2.53	0.42
1:M:65:ASN:O	1:M:66:LYS:CB	2.67	0.42
1:E:67:ILE:HD13	1:E:350:TYR:HD1	1.85	0.42
1:I:28:SER:HB2	1:I:402:ARG:C	2.39	0.42
1:I:286:MET:HA	1:I:287:PRO:HD3	1.86	0.42
1:I:12:VAL:CG1	1:I:12:VAL:O	2.68	0.42
1:E:105:ASP:OD2	1:E:200:LYS:HE2	2.19	0.42
1:E:7:ARG:O	1:E:8:PRO:C	2.57	0.42
1:E:447:LEU:HA	1:E:448:PRO:HD3	1.87	0.42
2:B:602:C:H2'	2:B:603:U:C6	2.54	0.42
1:A:263:ASP:HB2	8:A:763:HOH:O	2.18	0.42
1:E:270:HIS:ND1	1:E:283:LYS:HG2	2.34	0.42
1:E:6:MET:O	1:E:7:ARG:CB	2.68	0.42
1:E:409:ASN:ND2	8:E:541:HOH:O	2.38	0.42
1:E:94:GLN:HB3	1:E:94:GLN:HE21	1.55	0.42
1:E:119:PRO:O	1:E:123:MET:HG3	2.20	0.42
1:M:97:LEU:O	1:M:101:MET:HG3	2.20	0.42
1:M:102:TYR:CE1	1:M:136:ARG:HA	2.55	0.42
2:B:609:C:O2'	2:B:610:C:H5'	2.20	0.41
1:A:188:ARG:HD2	2:B:602:C:OP1	2.20	0.41
1:A:2:GLU:CD	1:A:64:GLY:HA2	2.41	0.41
1:A:226:GLU:HG2	1:A:322:LYS:CG	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:275:TYR:O	1:I:276:LYS:HB2	2.19	0.41
1:I:407:PRO:HD2	8:I:1139:HOH:O	2.20	0.41
1:E:436:ILE:O	1:E:442:GLY:HA3	2.20	0.41
1:I:226:GLU:HG3	1:I:320:HIS:O	2.21	0.41
1:M:275:TYR:O	1:M:276:LYS:HB2	2.20	0.41
1:E:67:ILE:HG13	1:E:242:SER:OG	2.20	0.41
1:A:270:HIS:ND1	1:A:283:LYS:HG2	2.35	0.41
2:B:597:C:H2'	2:B:598:A:H5'	2.03	0.41
2:B:596:C:H2'	2:B:597:C:O4'	2.20	0.41
1:M:356:PRO:HB2	1:M:360:SER:HB2	2.02	0.41
1:E:226:GLU:HG2	1:E:322:LYS:CG	2.50	0.41
1:M:120:TYR:HB3	1:M:125:LYS:HB3	2.02	0.41
1:I:71:ASP:O	1:I:75:LYS:HG3	2.20	0.41
1:E:311:LYS:HD2	1:E:350:TYR:HE2	1.86	0.41
1:A:67:ILE:HD13	1:A:350:TYR:HD1	1.85	0.41
1:I:383:LYS:HE3	1:I:384:TYR:HE1	1.82	0.41
1:A:417:LEU:HD23	1:A:417:LEU:HA	1.84	0.41
1:A:413:HIS:CD2	3:C:698:G:H4'	2.56	0.41
1:A:67:ILE:HG13	1:A:242:SER:OG	2.20	0.41
1:A:20:PRO:HG3	2:B:598:A:N3	2.35	0.41
1:E:58:ILE:HD12	1:E:175:LEU:HD21	2.02	0.41
1:E:456:ARG:CG	1:E:456:ARG:NH1	2.74	0.41
1:E:226:GLU:HG3	1:E:320:HIS:O	2.21	0.41
1:A:456:ARG:HG3	1:A:456:ARG:NH1	2.10	0.41
1:E:270:HIS:CE1	1:E:283:LYS:HE3	2.56	0.41
1:A:26:GLU:HG2	1:A:404:THR:O	2.21	0.41
1:E:2:GLU:CD	1:E:64:GLY:HA2	2.41	0.41
1:M:417:LEU:HA	1:M:417:LEU:HD23	1.91	0.41
2:F:596:C:H2'	2:F:597:C:O4'	2.20	0.41
1:I:356:PRO:HB2	1:I:360:SER:HB2	2.03	0.41
1:A:154:LEU:O	1:A:273:HIS:HA	2.21	0.41
1:A:436:ILE:O	1:A:442:GLY:HA3	2.20	0.41
1:A:102:TYR:CE1	1:A:136:ARG:HA	2.56	0.41
3:O:688:G:H8	3:O:688:G:HO5'	1.69	0.40
1:I:163:ARG:NH2	1:I:167:LYS:HD2	2.36	0.40
1:A:118:TYR:CD2	1:A:153:PRO:HD2	2.56	0.40
1:A:273:HIS:HB2	1:A:280:TYR:CE2	2.56	0.40
1:A:118:TYR:CD1	1:A:119:PRO:HA	2.56	0.40
1:M:286:MET:HA	1:M:287:PRO:HD3	1.86	0.40
1:E:84:GLN:O	1:E:87:SER:OG	2.33	0.40
1:I:205:ILE:HD13	1:I:205:ILE:N	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:354:MET:HE2	1:I:354:MET:HB3	2.00	0.40
1:I:218:TRP:CD1	1:I:390:PRO:HA	2.56	0.40
1:I:120:TYR:HB3	1:I:125:LYS:HB3	2.02	0.40
1:E:6:MET:HG2	1:E:280:TYR:HB3	2.02	0.40
1:E:70:VAL:HG12	1:E:75:LYS:HG3	2.04	0.40
1:A:6:MET:HG2	1:A:280:TYR:HB3	2.03	0.40
1:A:356:PRO:HB2	1:A:360:SER:HB2	2.04	0.40
1:E:154:LEU:O	1:E:273:HIS:HA	2.21	0.40
1:A:58:ILE:HD12	1:A:175:LEU:HD21	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	459/471 (98%)	444 (97%)	14 (3%)	1 (0%)	52	61
1	E	459/471 (98%)	443 (96%)	15 (3%)	1 (0%)	52	61
1	I	459/471 (98%)	444 (97%)	14 (3%)	1 (0%)	52	61
1	M	459/471 (98%)	443 (96%)	15 (3%)	1 (0%)	52	61
All	All	1836/1884 (98%)	1774 (97%)	58 (3%)	4 (0%)	52	61

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	I	66	LYS
1	M	66	LYS
1	A	7	ARG
1	E	7	ARG

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%)	382 (95%)	21 (5%)	29	31
1	E	403/412 (98%)	381 (94%)	22 (6%)	27	27
1	I	403/412 (98%)	389 (96%)	14 (4%)	43	53
1	M	403/412 (98%)	388 (96%)	15 (4%)	41	50
All	All	1612/1648 (98%)	1540 (96%)	72 (4%)	34	38

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	28	SER
1	A	39	GLU
1	A	43	LEU
1	A	67	ILE
1	A	94	GLN
1	A	163	ARG
1	A	170	GLN
1	A	218	TRP
1	A	261	ARG
1	A	269	ASN
1	A	272	HIS
1	A	277	ASN
1	A	281	CYS
1	A	291	SER
1	A	337	GLU
1	A	338	VAL
1	A	382	GLU
1	A	408	ARG
1	A	455	ARG
1	A	456	ARG
1	E	4	GLN
1	E	28	SER
1	E	39	GLU

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Mol	Chain	Res	Type
1	E	43	LEU
1	E	67	ILE
1	E	94	GLN
1	E	163	ARG
1	E	170	GLN
1	E	218	TRP
1	E	261	ARG
1	E	269	ASN
1	E	272	HIS
1	E	277	ASN
1	E	280	TYR
1	E	281	CYS
1	E	326	TYR
1	E	337	GLU
1	E	338	VAL
1	E	408	ARG
1	E	428	GLU
1	E	455	ARG
1	E	456	ARG
1	I	26	GLU
1	I	28	SER
1	I	43	LEU
1	I	67	ILE
1	I	84	GLN
1	I	89	ASP
1	I	218	TRP
1	I	261	ARG
1	I	277	ASN
1	I	369	GLU
1	I	391	VAL
1	I	408	ARG
1	I	419	LEU
1	I	455	ARG
1	M	26	GLU
1	M	28	SER
1	M	43	LEU
1	M	67	ILE
1	M	84	GLN
1	M	89	ASP
1	M	218	TRP
1	M	261	ARG
1	M	263	ASP

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Mol	Chain	Res	Type
1	M	277	ASN
1	M	369	GLU
1	M	391	VAL
1	M	408	ARG
1	M	419	LEU
1	M	455	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	GLN
1	A	170	GLN
1	A	269	ASN
1	A	272	HIS
1	A	277	ASN
1	A	320	HIS
1	A	409	ASN
1	E	94	GLN
1	E	170	GLN
1	E	269	ASN
1	E	272	HIS
1	E	277	ASN
1	E	320	HIS
1	E	398	HIS
1	E	409	ASN
1	I	269	ASN
1	I	277	ASN
1	I	409	ASN
1	M	269	ASN
1	M	277	ASN
1	M	320	HIS
1	M	409	ASN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	16/26 (61%)	1 (6%)	0
2	F	16/26 (61%)	1 (6%)	0
2	J	17/26 (65%)	1 (5%)	0
2	N	17/26 (65%)	1 (5%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	C	13/15 (86%)	0	0
3	G	13/15 (86%)	0	0
3	K	13/15 (86%)	0	0
3	O	13/15 (86%)	0	0
4	D	2/9 (22%)	1 (50%)	0
4	H	2/9 (22%)	1 (50%)	0
4	L	3/9 (33%)	1 (33%)	0
4	P	3/9 (33%)	1 (33%)	0
All	All	128/200 (64%)	8 (6%)	0

All (8) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	598	A
4	D	806	A
2	F	598	A
4	H	806	A
2	J	596	C
4	L	806	A
2	N	596	C
4	P	806	A

There are no RNA pucker outliers to report.

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	O2C	C	702	3,2	12,20,21	0.50	0	12,28,31	1.45	3 (25%)
3	O2C	G	702	3,2	12,20,21	0.50	0	12,28,31	1.33	3 (25%)
3	O2C	K	702	3,2	12,20,21	0.46	0	12,28,31	1.25	1 (8%)
3	O2C	O	702	3,2	12,20,21	0.52	0	12,28,31	1.27	1 (8%)

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
3	O2C	C	702	3,2	-	0/3/21/22	0/2/2/2
3	O2C	G	702	3,2	-	0/3/21/22	0/2/2/2
3	O2C	K	702	3,2	-	0/3/21/22	0/2/2/2
3	O2C	O	702	3,2	-	0/3/21/22	0/2/2/2

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	G	702	O2C	O4'-C1'-N1	2.03	112.35	108.08
3	G	702	O2C	O4'-C4'-C3'	2.23	108.09	105.04
3	C	702	O2C	O4'-C4'-C3'	2.29	108.17	105.04
3	O	702	O2C	C2-N3-C4	2.41	119.01	115.61
3	C	702	O2C	O4'-C1'-N1	2.46	113.28	108.08
3	K	702	O2C	C2-N3-C4	2.49	119.12	115.61
3	G	702	O2C	C2-N3-C4	2.62	119.30	115.61
3	C	702	O2C	C2-N3-C4	2.94	119.77	115.61

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	702	O2C	2	0
3	G	702	O2C	2	0
3	K	702	O2C	3	0
3	O	702	O2C	1	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 23 ligands modelled in this entry, 4 are monoatomic - leaving 19 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	POP	A	5004	-	8,8,8	0.63	0	13,13,13	1.24	1 (7%)
6	IPA	A	6008	-	3,3,3	0.54	0	3,3,3	0.40	0
6	IPA	A	6009	-	3,3,3	0.66	0	3,3,3	0.24	0
6	IPA	A	6013	-	3,3,3	0.58	0	3,3,3	0.23	0
6	IPA	A	6029	-	3,3,3	0.55	0	3,3,3	0.35	0
6	IPA	A	6032	7	3,3,3	0.56	0	3,3,3	0.35	0
5	POP	E	5003	-	8,8,8	0.61	0	13,13,13	1.29	1 (7%)
6	IPA	E	6010	-	3,3,3	0.46	0	3,3,3	0.46	0
6	IPA	E	6014	-	3,3,3	0.59	0	3,3,3	0.24	0
6	IPA	E	6030	7	3,3,3	0.57	0	3,3,3	0.35	0
5	POP	I	5002	-	8,8,8	0.69	0	13,13,13	1.09	1 (7%)
6	IPA	I	6006	-	3,3,3	0.55	0	3,3,3	0.37	0
6	IPA	I	6011	-	3,3,3	0.54	0	3,3,3	0.43	0
6	IPA	I	6027	-	3,3,3	0.47	0	3,3,3	0.48	0
5	POP	M	5001	-	8,8,8	0.54	0	13,13,13	1.19	1 (7%)
6	IPA	M	6001	-	3,3,3	0.48	0	3,3,3	0.65	0
6	IPA	M	6004	-	3,3,3	0.45	0	3,3,3	0.54	0
6	IPA	M	6023	-	3,3,3	0.56	0	3,3,3	0.29	0
6	IPA	O	6024	-	3,3,3	0.64	0	3,3,3	0.17	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
5	POP	A	5004	-	-	0/6/6/6	0/0/0/0
6	IPA	A	6008	-	-	0/0/0/0	0/0/0/0
6	IPA	A	6009	-	-	0/0/0/0	0/0/0/0
6	IPA	A	6013	-	-	0/0/0/0	0/0/0/0
6	IPA	A	6029	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	IPA	A	6032	7	-	0/0/0/0	0/0/0/0
5	POP	E	5003	-	-	0/6/6/6	0/0/0/0
6	IPA	E	6010	-	-	0/0/0/0	0/0/0/0
6	IPA	E	6014	-	-	0/0/0/0	0/0/0/0
6	IPA	E	6030	7	-	0/0/0/0	0/0/0/0
5	POP	I	5002	-	-	0/6/6/6	0/0/0/0
6	IPA	I	6006	-	-	0/0/0/0	0/0/0/0
6	IPA	I	6011	-	-	0/0/0/0	0/0/0/0
6	IPA	I	6027	-	-	0/0/0/0	0/0/0/0
5	POP	M	5001	-	-	0/6/6/6	0/0/0/0
6	IPA	M	6001	-	-	0/0/0/0	0/0/0/0
6	IPA	M	6004	-	-	0/0/0/0	0/0/0/0
6	IPA	M	6023	-	-	0/0/0/0	0/0/0/0
6	IPA	O	6024	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	E	5003	POP	P2-O-P1	-3.58	122.68	132.73
5	M	5001	POP	P2-O-P1	-3.26	123.57	132.73
5	A	5004	POP	P2-O-P1	-3.02	124.25	132.73
5	I	5002	POP	P2-O-P1	-2.68	125.21	132.73

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	6008	IPA	1	0
6	A	6009	IPA	2	0
6	A	6029	IPA	2	0
6	E	6010	IPA	4	0
5	I	5002	POP	2	0
6	I	6011	IPA	3	0
6	I	6027	IPA	4	0
6	M	6001	IPA	5	0
6	M	6004	IPA	5	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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^{th} 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	461/471 (97%)	-0.12	10 (2%) 65 70	34, 54, 94, 124	0
1	E	461/471 (97%)	-0.13	9 (1%) 68 72	33, 54, 94, 124	0
1	I	461/471 (97%)	-0.18	8 (1%) 73 77	33, 54, 90, 112	0
1	M	461/471 (97%)	-0.18	8 (1%) 73 77	33, 54, 90, 112	0
2	B	18/26 (69%)	-0.33	0 100 100	41, 66, 143, 158	0
2	F	18/26 (69%)	-0.45	0 100 100	41, 65, 143, 158	0
2	J	19/26 (73%)	-0.20	1 (5%) 30 33	40, 65, 148, 152	0
2	N	19/26 (73%)	-0.18	1 (5%) 30 33	39, 64, 148, 152	0
3	C	14/15 (93%)	-0.54	0 100 100	46, 61, 128, 130	0
3	G	14/15 (93%)	-0.60	0 100 100	46, 61, 128, 130	0
3	K	14/15 (93%)	-0.49	0 100 100	42, 57, 123, 129	0
3	O	14/15 (93%)	-0.59	0 100 100	42, 58, 123, 129	0
4	D	3/9 (33%)	0.52	0 100 100	120, 120, 123, 126	0
4	H	3/9 (33%)	0.97	1 (33%) 0 0	120, 120, 123, 126	0
4	L	4/9 (44%)	-0.06	0 100 100	106, 107, 113, 139	0
4	P	4/9 (44%)	0.04	0 100 100	106, 107, 113, 139	0
All	All	1988/2084 (95%)	-0.17	38 (1%) 70 74	33, 54, 98, 158	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	46	ASN	6.2
1	A	17	ILE	5.3
1	M	65	ASN	5.1
1	I	16	ILE	5.1
1	A	46	ASN	4.8

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Mol	Chain	Res	Type	RSRZ
1	M	16	ILE	4.3
1	E	17	ILE	4.2
1	E	66	LYS	4.1
1	I	65	ASN	4.1
1	A	63	VAL	3.8
1	E	63	VAL	3.3
1	M	66	LYS	3.1
1	E	1	GLY	3.0
1	M	68	THR	3.0
1	M	46	ASN	2.9
1	A	45	LYS	2.9
1	A	1	GLY	2.9
1	A	52	THR	2.8
1	A	66	LYS	2.7
1	I	51	LYS	2.6
1	A	51	LYS	2.6
1	I	67	ILE	2.5
1	E	455	ARG	2.5
1	I	62	TYR	2.5
1	I	68	THR	2.4
1	E	276	LYS	2.3
1	A	10	LYS	2.3
1	A	58	ILE	2.3
1	E	270	HIS	2.3
4	H	804	G	2.3
1	M	345	GLN	2.2
1	I	66	LYS	2.2
2	J	596	C	2.2
1	M	274	LEU	2.1
1	E	16	ILE	2.1
1	I	46	ASN	2.1
1	M	22	LYS	2.1
2	N	596	C	2.1

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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^{th} 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^2)	Q<0.9
3	O2C	C	702	19/20	0.95	0.11	-	50,62,97,101	0
3	O2C	K	702	19/20	0.93	0.12	-	47,55,87,101	0
3	O2C	G	702	19/20	0.95	0.14	-	50,61,95,100	0
3	O2C	O	702	19/20	0.93	0.14	-	48,55,85,101	0

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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, 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	LLDF	B-factors(Å^2)	Q<0.9
6	IPA	E	6010	4/4	0.92	0.32	9.00	49,50,64,76	0
6	IPA	A	6013	4/4	0.96	0.28	8.93	51,67,71,76	0
6	IPA	A	6009	4/4	0.92	0.33	6.81	35,44,75,80	0
6	IPA	I	6011	4/4	0.96	0.24	5.90	61,63,68,81	0
6	IPA	M	6004	4/4	0.96	0.19	4.66	61,65,69,69	0
6	IPA	A	6008	4/4	0.88	0.21	3.28	73,79,82,87	0
6	IPA	O	6024	4/4	0.87	0.17	2.80	62,70,73,74	0
6	IPA	M	6001	4/4	0.94	0.19	2.51	29,65,81,83	0
6	IPA	E	6014	4/4	0.94	0.20	1.92	52,62,66,68	0
6	IPA	A	6029	4/4	0.90	0.14	1.30	47,56,66,80	0
6	IPA	I	6027	4/4	0.91	0.12	0.31	51,66,71,79	0
6	IPA	I	6006	4/4	0.96	0.12	-0.31	61,70,71,75	0
7	ZN	E	2002	1/1	0.89	0.89	-	115,115,115,115	1
7	ZN	I	2003	1/1	0.79	0.13	-	107,107,107,107	1
6	IPA	E	6030	4/4	0.90	0.17	-	72,73,74,77	0
5	POP	A	5004	9/9	0.89	0.11	-	57,113,121,121	9
5	POP	I	5002	9/9	0.78	0.19	-	56,95,119,129	9
6	IPA	M	6023	4/4	0.90	0.23	-	63,66,73,75	0
7	ZN	A	2001	1/1	0.90	0.45	-	110,110,110,110	1
5	POP	E	5003	9/9	0.90	0.10	-	64,112,120,122	9
6	IPA	A	6032	4/4	0.87	0.18	-	68,70,72,73	0
5	POP	M	5001	9/9	0.87	0.14	-	74,92,114,141	9
7	ZN	M	2004	1/1	0.30	0.14	-	109,109,109,109	1

6.5 Other polymers (i)

There are no such residues in this entry.