wwPDB X-ray Structure Validation Summary Report (i)

Feb 17, 2024 – 08:25 AM EST

PDB ID	:	3RMA
Title	:	Crystal Structure of a replicative DNA polymerase bound to DNA containing Thymine Glycol
Authors	:	Aller, P.; Duclos, S.; Wallace, S.S.; Doublie, S.
Deposited on	:	2011-04-20
Resolution	:	2.84 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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

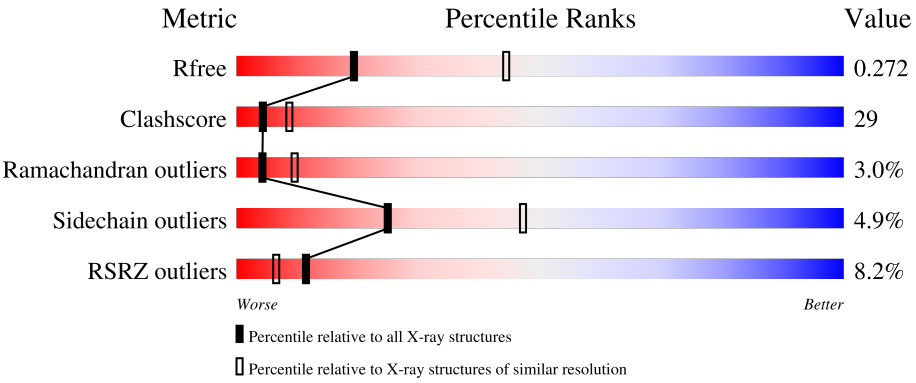
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.84 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1031 (2.86-2.82)
Clashscore	141614	1078 (2.86-2.82)
Ramachandran outliers	138981	1050 (2.86-2.82)
Sidechain outliers	138945	1051 (2.86-2.82)
RSRZ outliers	127900	1019 (2.86-2.82)

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 <=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	906	3% 60% 37%
1	B	906	14% 53% 42%
1	C	906	2% 59% 35%
1	D	906	13% 39% 52% 7%
2	E	18	22% 56% 22%

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Mol	Chain	Length	Quality of chain
2	G	18	17% 6% 67% 28%
2	I	18	39% 44% 11% 6%
2	K	18	6% 17% 50% 33%
3	F	14	29% 71%
3	H	14	7% 21% 71% 7%
3	J	14	14% 86%
3	L	14	21% 71% 7%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 31451 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 DNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	894	Total	C	N	O	S	4	0	0
			7273	4672	1207	1362	32			
1	B	897	Total	C	N	O	S	62	0	0
			7230	4645	1200	1353	32			
1	C	890	Total	C	N	O	S	8	0	0
			7227	4642	1198	1356	31			
1	D	890	Total	C	N	O	S	20	0	0
			7161	4599	1190	1341	31			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	222	ALA	ASP	engineered mutation	UNP Q38087
A	327	ALA	ASP	engineered mutation	UNP Q38087
A	904	HIS	-	expression tag	UNP Q38087
A	905	HIS	-	expression tag	UNP Q38087
A	906	HIS	-	expression tag	UNP Q38087
B	222	ALA	ASP	engineered mutation	UNP Q38087
B	327	ALA	ASP	engineered mutation	UNP Q38087
B	904	HIS	-	expression tag	UNP Q38087
B	905	HIS	-	expression tag	UNP Q38087
B	906	HIS	-	expression tag	UNP Q38087
C	222	ALA	ASP	engineered mutation	UNP Q38087
C	327	ALA	ASP	engineered mutation	UNP Q38087
C	904	HIS	-	expression tag	UNP Q38087
C	905	HIS	-	expression tag	UNP Q38087
C	906	HIS	-	expression tag	UNP Q38087
D	222	ALA	ASP	engineered mutation	UNP Q38087
D	327	ALA	ASP	engineered mutation	UNP Q38087
D	904	HIS	-	expression tag	UNP Q38087
D	905	HIS	-	expression tag	UNP Q38087
D	906	HIS	-	expression tag	UNP Q38087

- Molecule 2 is a DNA chain called DNA (5'-D(*CP*GP*AP*(CTG)*GP*AP*AP*TP*GP*AP*CP*AP*GP*CP*CP*GP*CP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	14	Total	C	N	O	P	0	0	0
			287	136	59	79	13			
2	G	13	Total	C	N	O	P	0	0	0
			265	126	54	73	12			
2	I	17	Total	C	N	O	P	0	0	0
			352	166	71	99	16			
2	K	12	Total	C	N	O	P	0	0	0
			244	116	49	68	11			

- Molecule 3 is a DNA chain called DNA (5'-D(*GP*CP*GP*GP*CP*TP*GP*TP*CP*AP*TP*TP*CP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	14	Total	C	N	O	P	0	0	0
			282	136	50	83	13			
3	H	13	Total	C	N	O	P	0	0	0
			262	126	45	79	12			
3	J	14	Total	C	N	O	P	0	0	0
			282	136	50	83	13			
3	L	13	Total	C	N	O	P	0	0	0
			262	126	45	79	12			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	114	Total	O	0	0
			114	114		
4	B	61	Total	O	0	0
			61	61		
4	C	99	Total	O	0	0
			99	99		
4	D	16	Total	O	0	0
			16	16		
4	E	5	Total	O	0	0
			5	5		
4	F	2	Total	O	0	0
			2	2		
4	G	4	Total	O	0	0
			4	4		
4	H	4	Total	O	0	0
			4	4		

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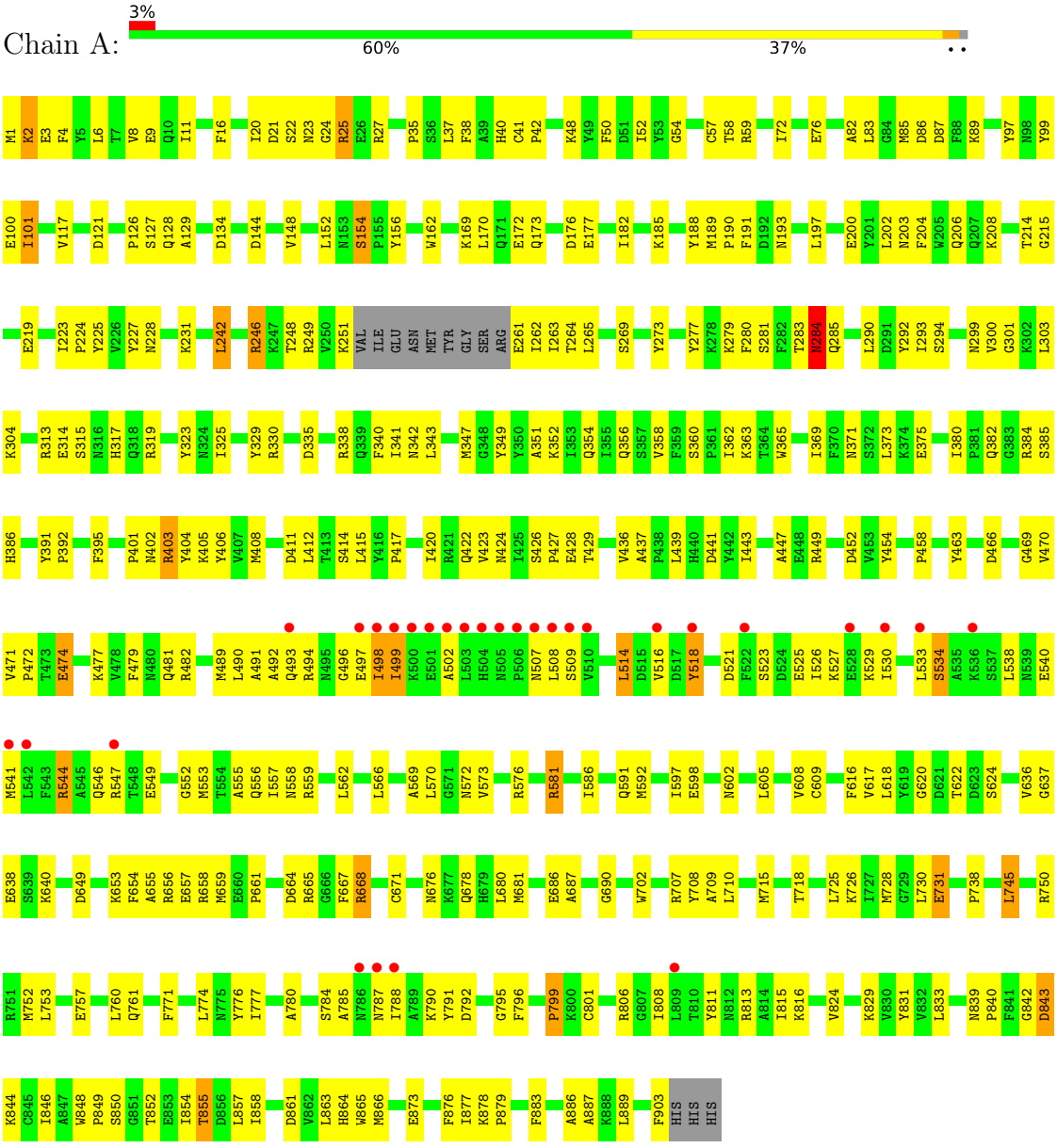
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	I	7	Total O 7 7	0	0
4	J	6	Total O 6 6	0	0
4	K	6	Total O 6 6	0	0

3 Residue-property plots (i)

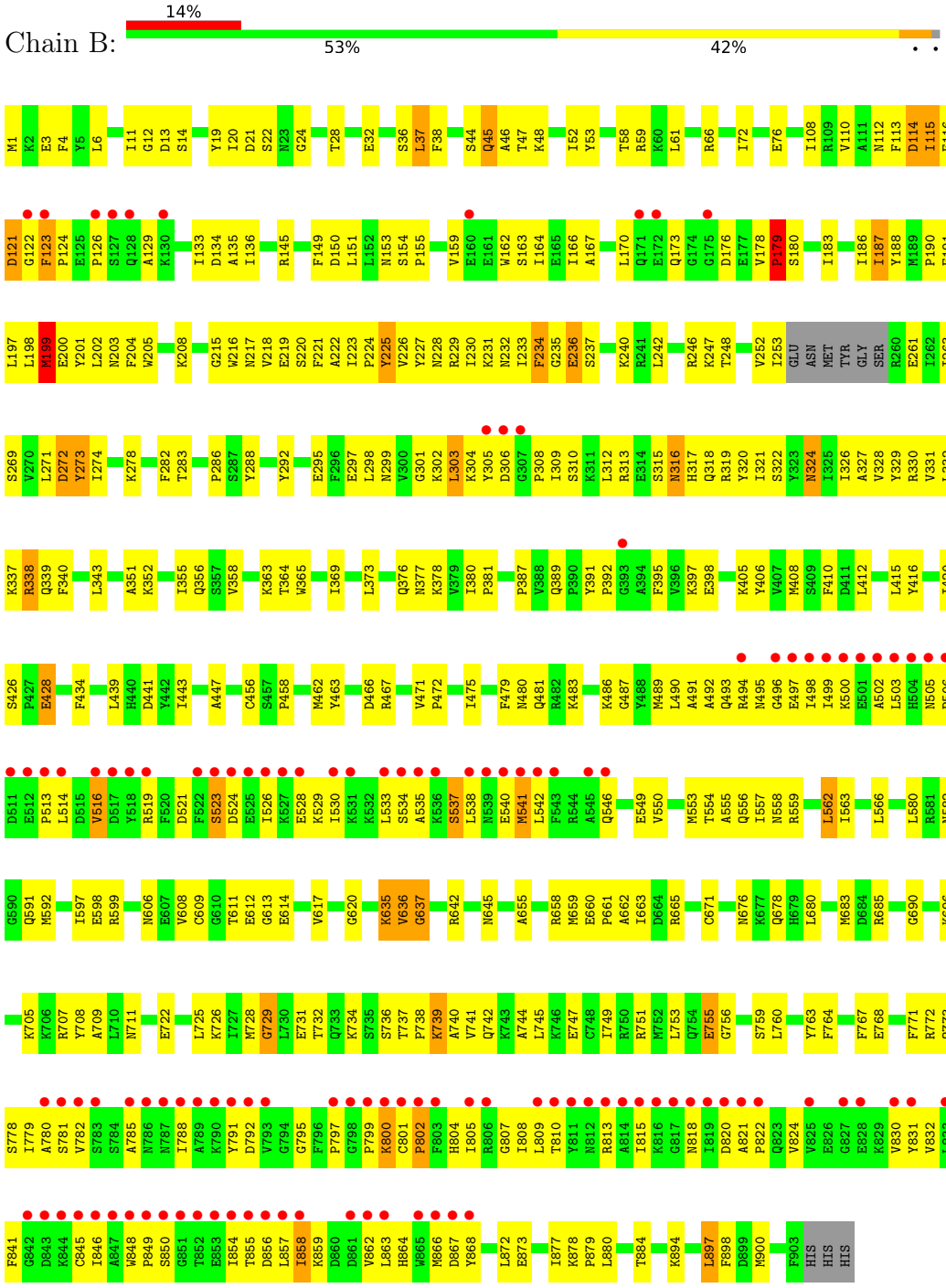
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: DNA polymerase



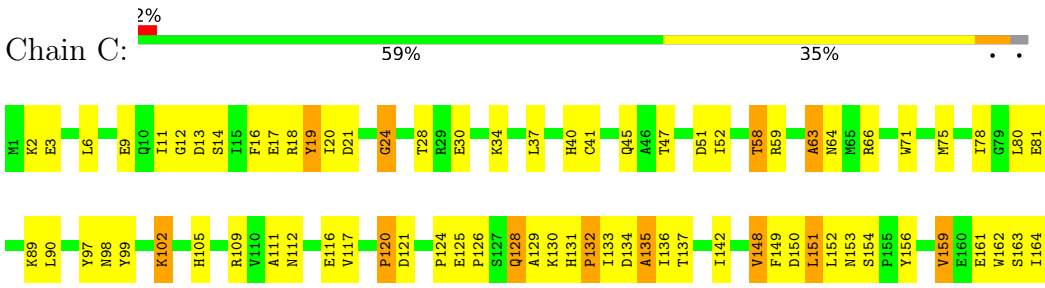
• Molecule 1: DNA polymerase

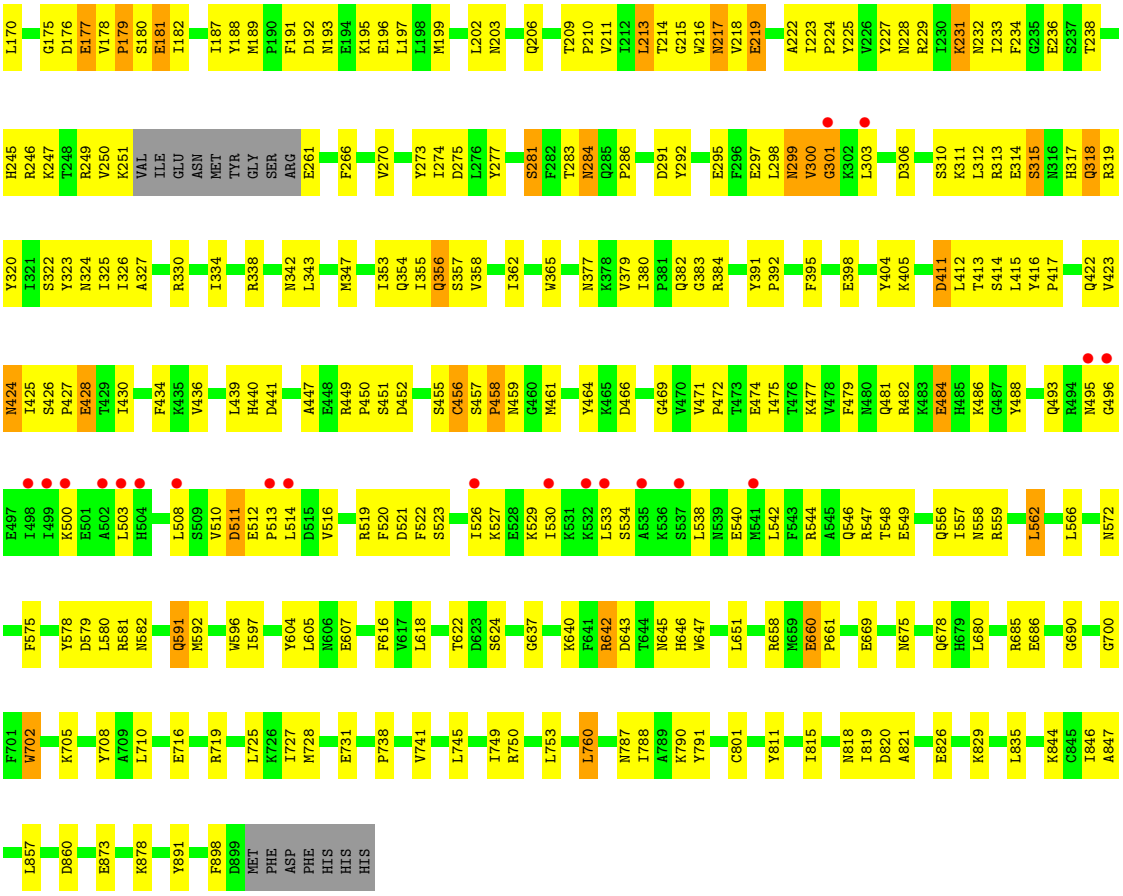
Chain B:



• Molecule 1: DNA polymerase

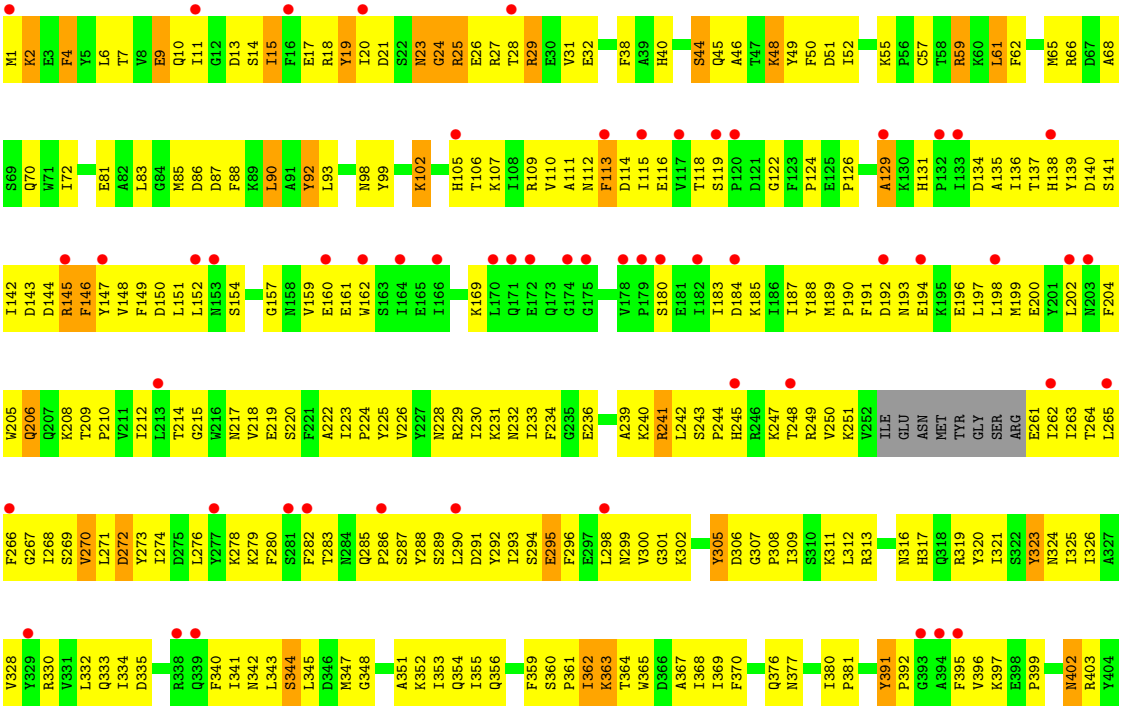
Chain C:

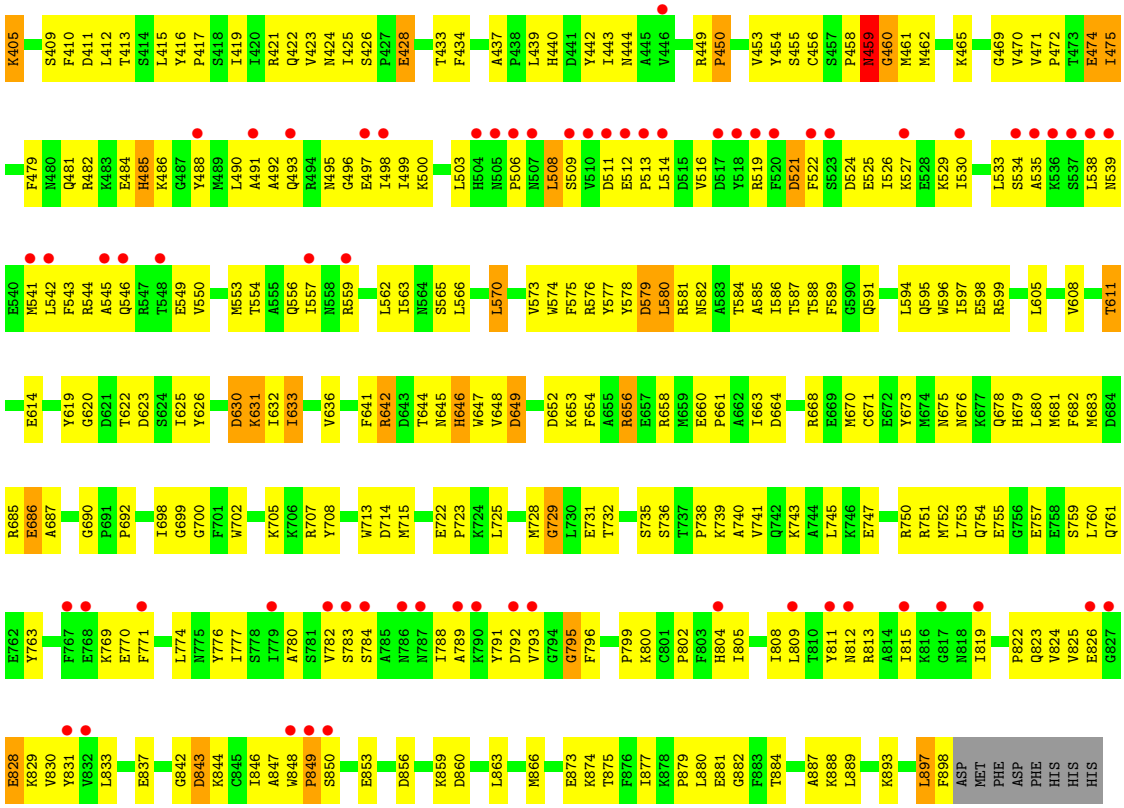




• Molecule 1: DNA polymerase

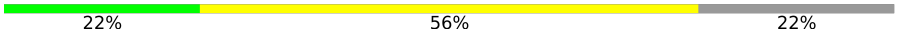
Chain D:

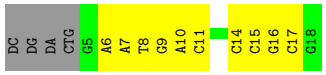




• Molecule 2: DNA (5'-D(*CP*GP*AP*(CTG)*GP*AP*AP*TP*GP*AP*CP*AP*GP*CP*CP*GP*CP*G)-3')

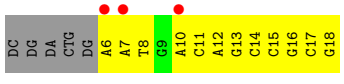
Chain E:





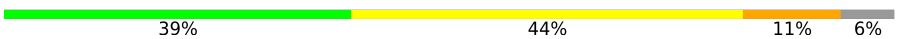
• Molecule 2: DNA (5'-D(*CP*GP*AP*(CTG)*GP*AP*AP*TP*GP*AP*CP*AP*GP*CP*CP*GP*CP*G)-3')

Chain G:



• Molecule 2: DNA (5'-D(*CP*GP*AP*(CTG)*GP*AP*AP*TP*GP*AP*CP*AP*GP*CP*CP*GP*CP*G)-3')

Chain I:

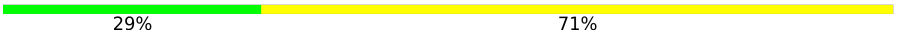


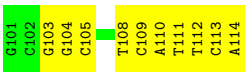
• Molecule 2: DNA (5'-D(*CP*GP*AP*(CTG)*GP*AP*AP*TP*GP*AP*CP*AP*GP*CP*CP*GP*CP*G)-3')

Chain K:

• Molecule 3: DNA (5’-D(*GP*CP*GP*GP*CP*TP*GP*TP*CP*AP*TP*TP*CP*A)-3’)

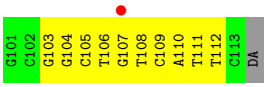
Chain F:





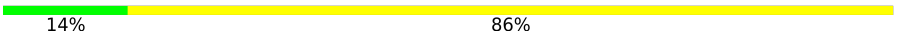
• Molecule 3: DNA (5’-D(*GP*CP*GP*GP*CP*TP*GP*TP*CP*AP*TP*TP*CP*A)-3’)

Chain H:



• Molecule 3: DNA (5’-D(*GP*CP*GP*GP*CP*TP*GP*TP*CP*AP*TP*TP*CP*A)-3’)

Chain J:



• Molecule 3: DNA (5’-D(*GP*CP*GP*GP*CP*TP*GP*TP*CP*AP*TP*TP*CP*A)-3’)

Chain L:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	132.70Å 123.00Å 163.94Å 90.00° 96.08° 90.00°	Depositor
Resolution (Å)	50.00 – 2.84 49.09 – 2.84	Depositor EDS
% Data completeness (in resolution range)	94.6 (50.00-2.84) 98.2 (49.09-2.84)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.54 (at 2.86Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.215 , 0.275 0.214 , 0.272	Depositor DCC
R_{free} test set	23396 reflections (9.62%)	wwPDB-VP
Wilson B-factor (Å^2)	51.9	Xtriage
Anisotropy	0.250	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 62.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	31451	wwPDB-VP
Average B, all atoms (Å^2)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.45% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: CTG

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	0/7452	0.65	0/10078
1	B	0.38	0/7405	0.60	0/10021
1	C	0.42	0/7404	0.63	0/10015
1	D	0.32	0/7337	0.55	0/9939
2	E	0.34	0/323	0.68	0/497
2	G	0.33	0/298	0.70	0/458
2	I	0.55	0/371	0.74	0/569
2	K	0.31	0/274	0.66	0/421
3	F	0.29	0/315	0.69	0/484
3	H	0.25	0/292	0.65	0/449
3	J	0.48	0/315	0.73	0/484
3	L	0.28	0/292	0.65	0/449
All	All	0.39	0/32078	0.62	0/43864

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
2	I	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	I	7	DA	Sidechain

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	7273	0	7125	292	0
1	B	7230	0	7057	418	0
1	C	7227	0	7083	327	0
1	D	7161	0	6961	604	0
2	E	287	0	157	17	0
2	G	265	0	146	22	0
2	I	352	0	193	11	0
2	K	244	0	135	16	0
3	F	282	0	158	19	0
3	H	262	0	149	22	0
3	J	282	0	158	20	0
3	L	262	0	149	17	0
4	A	114	0	0	6	0
4	B	61	0	0	3	0
4	C	99	0	0	3	0
4	D	16	0	0	3	0
4	E	5	0	0	2	0
4	F	2	0	0	0	0
4	G	4	0	0	0	0
4	H	4	0	0	1	0
4	I	7	0	0	1	0
4	J	6	0	0	0	0
4	K	6	0	0	1	0
All	All	31451	0	29471	1758	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 29.

The worst 5 of 1758 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2:LYS:H	1:A:2:LYS:HD2	1.13	1.10
1:D:422:GLN:HE22	1:D:681:MET:HG2	1.15	1.09
1:D:481:GLN:HB3	1:D:559:ARG:HE	1.14	1.07
1:D:85:MET:HE2	1:D:87:ASP:H	1.19	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:16:DG:H2"	2:K:17:DC:H5"	1.37	1.05

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	890/906 (98%)	804 (90%)	74 (8%)	12 (1%)	12 26
1	B	893/906 (99%)	759 (85%)	107 (12%)	27 (3%)	4 9
1	C	886/906 (98%)	769 (87%)	94 (11%)	23 (3%)	5 12
1	D	886/906 (98%)	681 (77%)	162 (18%)	43 (5%)	2 3
All	All	3555/3624 (98%)	3013 (85%)	437 (12%)	105 (3%)	4 9

5 of 105 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	514	LEU
1	A	534	SER
1	B	121	ASP
1	B	236	GLU
1	B	306	ASP

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	785/803 (98%)	751 (96%)	34 (4%)	29	54
1	B	774/803 (96%)	737 (95%)	37 (5%)	25	49
1	C	780/803 (97%)	740 (95%)	40 (5%)	24	45
1	D	764/803 (95%)	722 (94%)	42 (6%)	21	41
All	All	3103/3212 (97%)	2950 (95%)	153 (5%)	25	47

5 of 153 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	25	ARG
1	D	557	ILE
1	D	86	ASP
1	D	272	ASP
1	D	755	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 97 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	424	ASN
1	D	45	GLN
1	C	481	GLN
1	C	591	GLN
1	D	207	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	$\#\|Z\|>2$
2	CTG	I	4	3,2	19,23,24	0.97	2 (10%)	21,35,38	0.59	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
2	CTG	I	4	3,2	-	4/7/45/46	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	4	CTG	C5-C4	2.91	1.55	1.52
2	I	4	CTG	C1'-N1	2.10	1.48	1.45

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	I	4	CTG	N3-C2-N1	-2.25	114.36	116.69

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	I	4	CTG	O4'-C1'-N1-C6
2	I	4	CTG	C2'-C1'-N1-C6
2	I	4	CTG	C2'-C1'-N1-C2
2	I	4	CTG	O4'-C1'-N1-C2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	I	4	CTG	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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	894/906 (98%)	-0.03	29 (3%) 47 41	21, 41, 114, 141	1 (0%)
1	B	897/906 (99%)	0.72	129 (14%) 2 1	26, 63, 157, 177	13 (1%)
1	C	890/906 (98%)	0.06	20 (2%) 62 57	19, 49, 103, 130	2 (0%)
1	D	890/906 (98%)	0.76	120 (13%) 3 2	62, 103, 147, 163	5 (0%)
2	E	14/18 (77%)	0.41	0 100 100	69, 87, 126, 130	0
2	G	13/18 (72%)	1.61	3 (23%) 0 0	59, 143, 168, 169	0
2	I	16/18 (88%)	-0.24	0 100 100	33, 45, 113, 113	0
2	K	12/18 (66%)	0.62	1 (8%) 11 6	41, 116, 144, 150	0
3	F	14/14 (100%)	0.12	0 100 100	87, 103, 120, 132	0
3	H	13/14 (92%)	1.06	1 (7%) 13 8	137, 149, 163, 168	0
3	J	14/14 (100%)	-0.18	0 100 100	35, 61, 89, 93	0
3	L	13/14 (92%)	0.77	0 100 100	119, 128, 134, 138	0
All	All	3680/3752 (98%)	0.38	303 (8%) 11 6	19, 63, 144, 177	21 (0%)

The worst 5 of 303 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	821	ALA	11.8
1	B	507	ASN	11.6
1	B	847	ALA	11.4
1	B	785	ALA	10.6
1	B	862	VAL	10.5

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

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, 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	B-factors(Å^2)	Q<0.9
2	CTG	I	4	22/23	0.78	0.19	114,118,119,119	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.