



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 15, 2023 – 10:43 PM EDT

PDB ID : 2DY4
Title : Crystal structure of RB69 GP43 in complex with DNA containing Thymine Glycol
Authors : Aller, P.; Rould, M.A.; Hogg, M.; Wallace, S.S.; Doublie, S.
Deposited on : 2006-09-06
Resolution : 2.65 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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-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

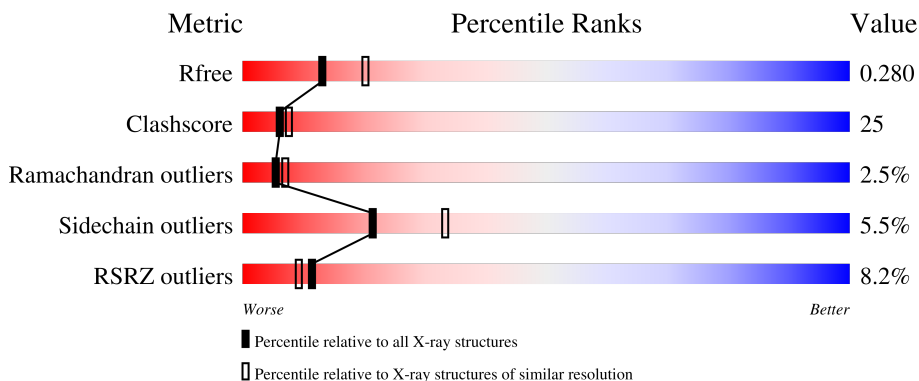
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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.



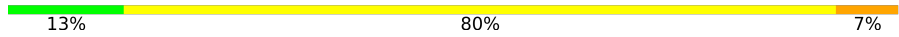
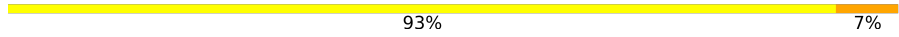
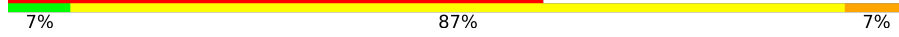



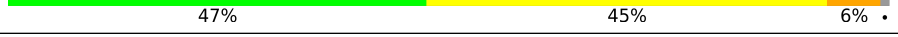
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1332 (2.68-2.64)
Clashscore	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)
RSRZ outliers	127900	1318 (2.68-2.64)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	E	18	
1	G	18	
1	I	18	
1	K	18	
2	F	15	

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Mol	Chain	Length	Quality of chain
2	H	15	 13% 80% 7%
2	J	15	 93% 7%
2	L	15	 7% 60% 87% 7%
3	A	903	 6% 59% 37% .
3	B	903	 5% 63% 32% . .
3	C	903	 4% 64% 32% .
3	D	903	 16% 47% 45% 6% .

2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 31943 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 DNA chain called 5'-D(*CP*GP*(CTG)P*GP*GP*AP*AP*TP*GP*A*CP*AP*GP*CP*CP*GP*CP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	17	Total	C	N	O	P	0	0	0
			348	165	69	99	15			
1	G	18	Total	C	N	O	P	0	0	0
			372	175	74	106	17			
1	I	18	Total	C	N	O	P	0	0	0
			372	175	74	106	17			
1	K	18	Total	C	N	O	P	0	0	0
			372	175	74	106	17			

- Molecule 2 is a DNA chain called 5'-D(*GP*CP*GP*GP*CP*TP*GP*T*CP*AP*TP*TP*CP*CP*A)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	14	Total	C	N	O	P	0	0	0
			276	133	51	80	12			
2	H	15	Total	C	N	O	P	0	0	0
			299	143	53	89	14			
2	J	15	Total	C	N	O	P	0	0	0
			299	143	53	89	14			
2	L	15	Total	C	N	O	P	0	0	0
			299	143	53	89	14			

- Molecule 3 is a protein called DNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
3	A	902	Total	C	N	O	S	Se	0	0	0
			7302	4689	1213	1367	8	25			
3	B	888	Total	C	N	O	S	Se	0	0	0
			7175	4608	1193	1341	8	25			
3	C	900	Total	C	N	O	S	Se	0	0	0
			7300	4683	1214	1370	8	25			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	N	O	S				Se
3	D	890	6923	4449	1130	1313	8	23	0	0	0

There are 8 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
B	222	ALA	ASP	engineered mutation	UNP Q38087
B	327	ALA	ASP	engineered mutation	UNP Q38087
C	222	ALA	ASP	engineered mutation	UNP Q38087
C	327	ALA	ASP	engineered mutation	UNP Q38087
D	222	ALA	ASP	engineered mutation	UNP Q38087
D	327	ALA	ASP	engineered mutation	UNP Q38087

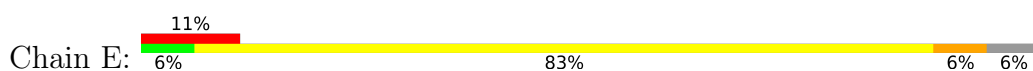
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	9	Total 9	O 9	0	0
4	F	5	Total 5	O 5	0	0
4	G	18	Total 18	O 18	0	0
4	H	9	Total 9	O 9	0	0
4	I	17	Total 17	O 17	0	0
4	J	4	Total 4	O 4	0	0
4	K	5	Total 5	O 5	0	0
4	L	2	Total 2	O 2	0	0
4	A	117	Total 117	O 117	0	0
4	B	205	Total 205	O 205	0	0
4	C	160	Total 160	O 160	0	0
4	D	55	Total 55	O 55	0	0

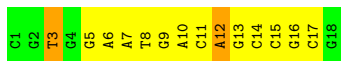
3 Residue-property plots [i](#)

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.

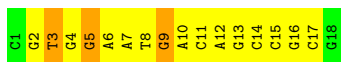
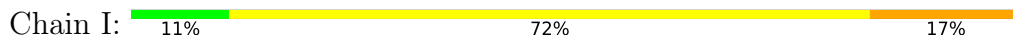
- Molecule 1: 5'-D(*CP*GP*(CTG)P*GP*GP*AP*AP*TP*GP*A*CP*AP*GP*CP*CP*GP*CP*G)-3'



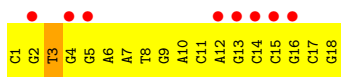
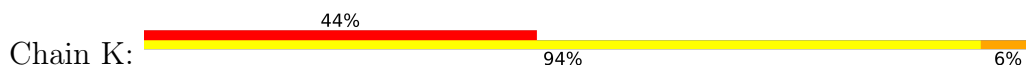
- Molecule 1: 5'-D(*CP*GP*(CTG)P*GP*GP*AP*AP*TP*GP*A*CP*AP*GP*CP*CP*GP*CP*G)-3'



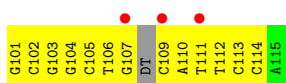
- Molecule 1: 5'-D(*CP*GP*(CTG)P*GP*GP*AP*AP*TP*GP*A*CP*AP*GP*CP*CP*GP*CP*G)-3'



- Molecule 1: 5'-D(*CP*GP*(CTG)P*GP*GP*AP*AP*TP*GP*A*CP*AP*GP*CP*CP*GP*CP*G)-3'



- Molecule 2: 5'-D(*GP*CP*GP*GP*CP*TP*GP*T*CP*AP*TP*TP*CP*CP*A)-3'




- Molecule 2: 5'-D(*GP*CP*GP*GP*CP*TP*GP*T*CP*AP*TP*TP*CP*CP*A)-3'

Chain H:  13% 80% 7%

G101
C102
G103
G104
C105
T106
G107
T108
C109
A110
T111
T112
C113
C114
A115

- Molecule 2: 5'-D(*GP*CP*GP*GP*CP*TP*GP*T*CP*AP*TP*TP*CP*CP*A)-3'

Chain J:  93% 7%

G101
C102
G103
G104
C105
T106
G107
T108
C109
A110
T111
T112
C113
C114
A115

- Molecule 2: 5'-D(*GP*CP*GP*GP*CP*TP*GP*T*CP*AP*TP*TP*CP*CP*A)-3'

Chain L:  7% 60% 87% 7%

G101
C102
G103
G104
C105
T106
G107
T108
C109
A110
T111
T112
C113
C114
A115

- Molecule 3: DNA polymerase

Chain A:  6% 59% 37%

H1
K2
E3
L6
Q10
I11
G12
S13
S14
I15
E16
E17
D21
R25
E26
R27
T28
R29
E32
S36
L37
C41
D51
P56
T57
T58
M64
M65
R66
D67
W71
I72
M75
E76
E81
A82
L83
S84
R85
Q207
D86
L90
E100
I101
K102
Y103

D104
H105
T106
M112
F113
Q110
E116
P120
D121
S114
E125
P126
A129
K130
H131
P132
A135
S154
P155
Y156
G157
M158
V159
S163
L170
Q171
D176
E177
E181
M193
E194
K195
E196
L197
L198
M199
L202
G301
N203
F204
W205
Q206
K208
V211
I212
L213
W216

M217
V218
F221
A222
I223
P224
Y225
R229
Q230
L230
K231
F234
G235
E236
K240
R241
L242
H245
K251
E254
Y257
G258
S259
L262
S269
Y273
S287
D291
Y292
I293
S294
L298
M299
V300
G301
A394
F395
L303
K304
P308
K311
H317
Q318
R319

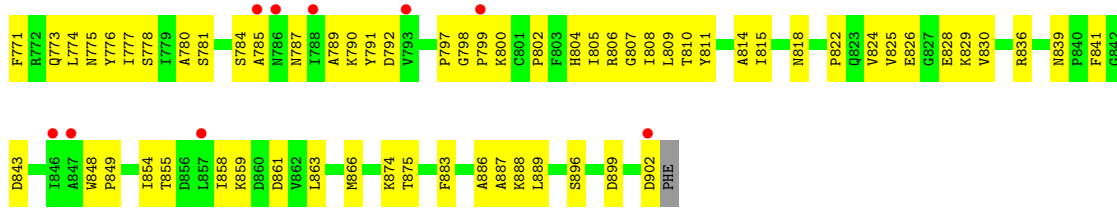
I326
R330
V331
L332
D335
R338
Q339
F340
D346
K347
Y349
L353
S357
V358
F359
S360
P361
I362
D366
R467
D468
A367
L373
Q376
M377
K378
V379
I380
P381
Q382
H386
P387
H485
K486
M489
L490
A491
G392
G393
A394
R494
M495
G496
E497
I498
I499
L400
P401
K500
A502
L503
H504
Y406

V407
M408
L508
F410
V510
D411
T413
S414
L415
I419
Q422
V423
L439
I443
S455
C456
S457
P458
D466
R467
D468
V471
P472
T476
K477
F478
N480
Q481
R482
K483
E484
H485
K486
M489
L490
A491
G392
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I498
I499
L400
P401
K500
A502
L503
H504
Y406

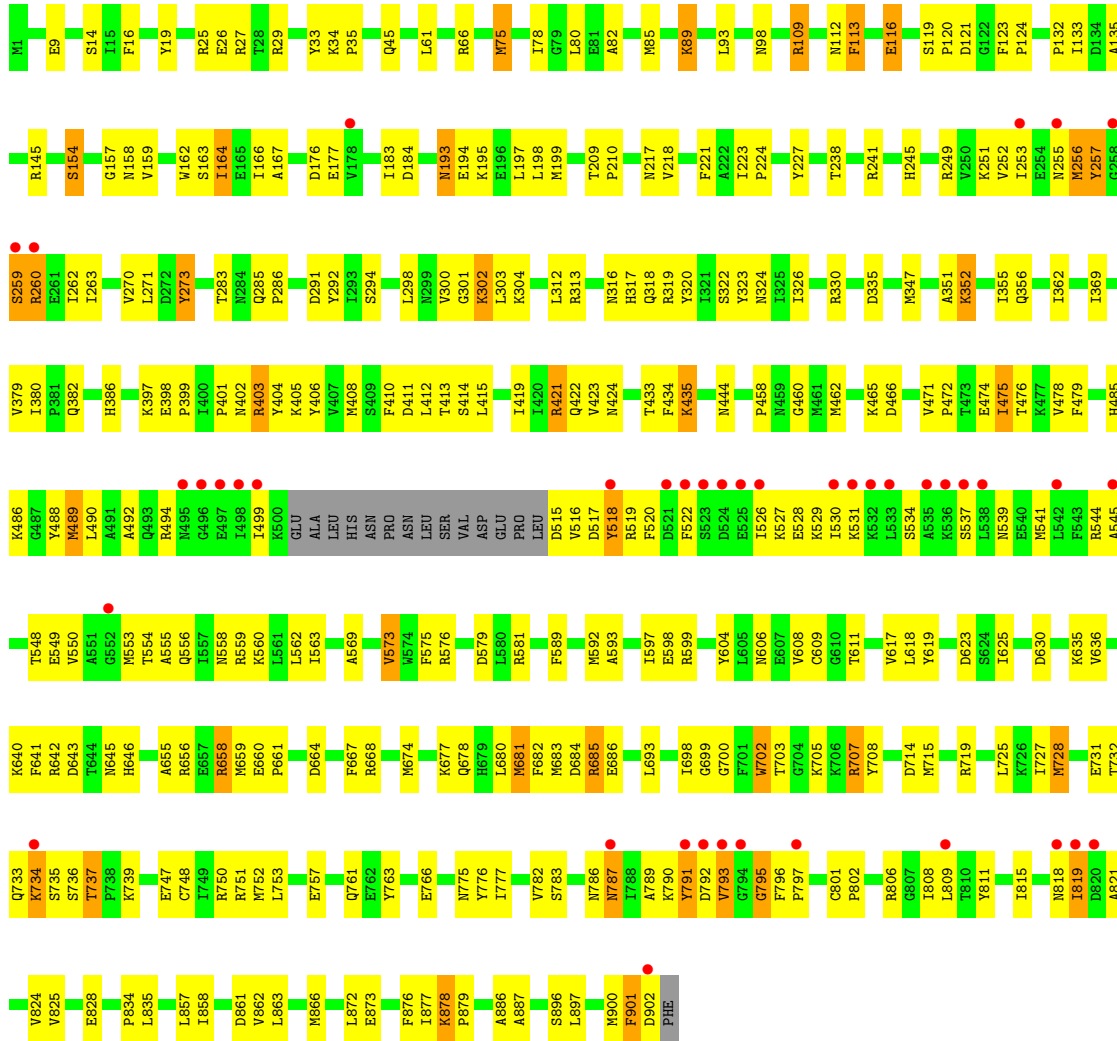
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V510
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T512
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L514
D515
V516
D517
R519
F520
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S523
I526
K527
E528
K529
G620
D621
T622
K532
L533
S534
A535
K536
S537
L538
M539
E540
M541
L542
T548
G552
M553
H554
T554
A555
Q556
I557
R558
M559
K560
L561
L562
I563
L570
G571
I572
M573
Y578
T587

M592
A593
L594
M683
Q595
W596
I597
M602
M606
E607
T611
E612
G613
E614
A615
F616
V617
L618
Y619
A709
L710
D621
T622
I625
A629
K631
L632
I633
V636
K640
F641
R642
H646
K653
F654
A655
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A662
I663
M674
M675
M676
A677
K679
E770

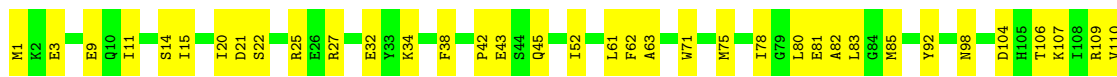
L680
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M683
D684
R685
I688
A689
G690
P691
G699
G700
F701
W702
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R707
Y708
A709
L710
W711
V712
M715
E716
G717
K724
L725
K726
I727
M728
G729
L730
E731
T732
Q733
K734
S735
S736
T737
F738
K739
Q742
M659
E747
L753
E757
E758
E762
K769
E770

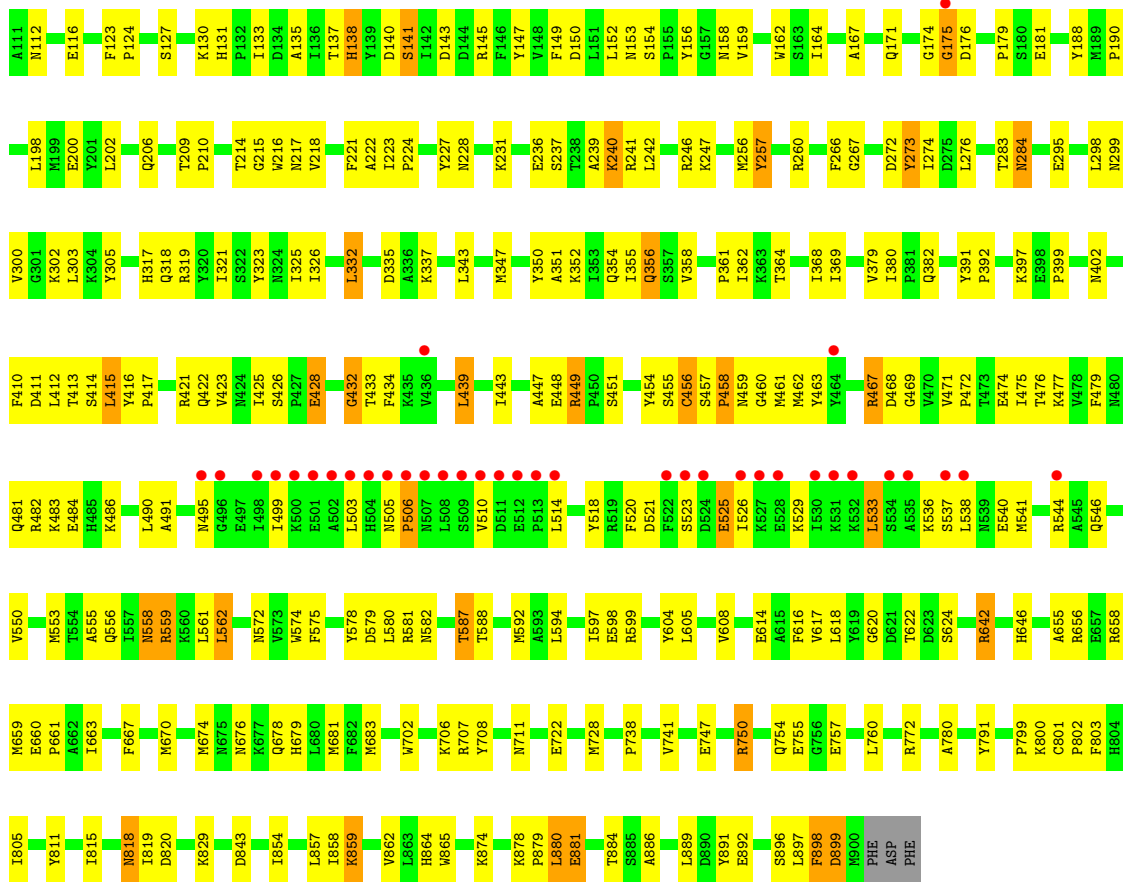


• Molecule 3: DNA polymerase

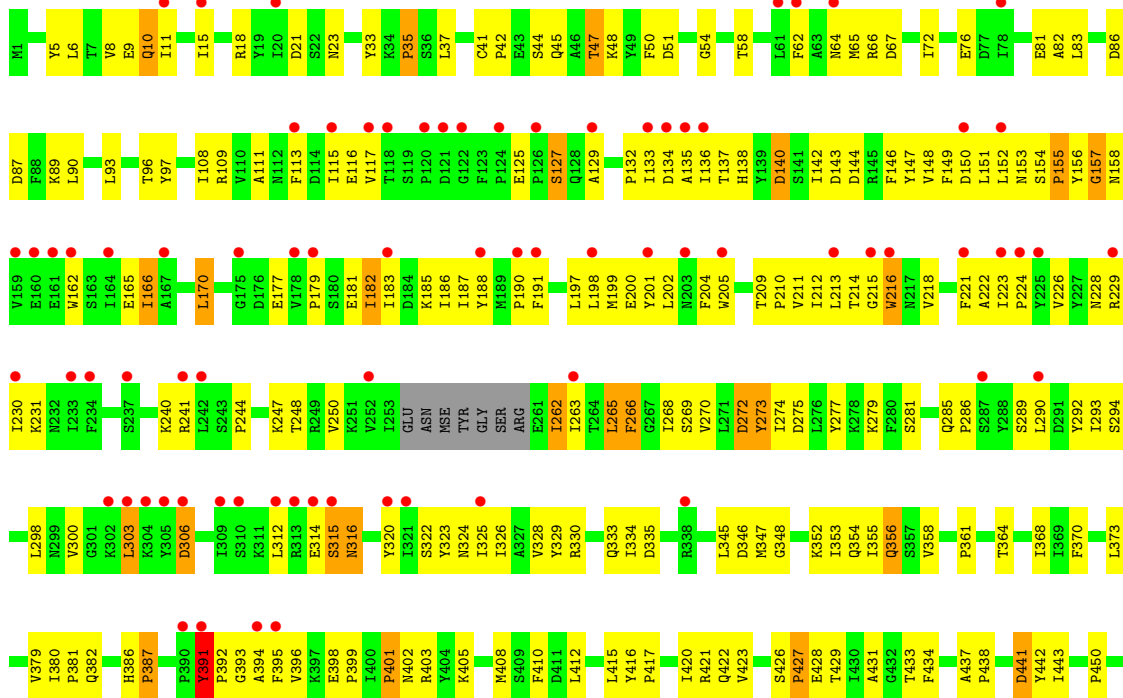


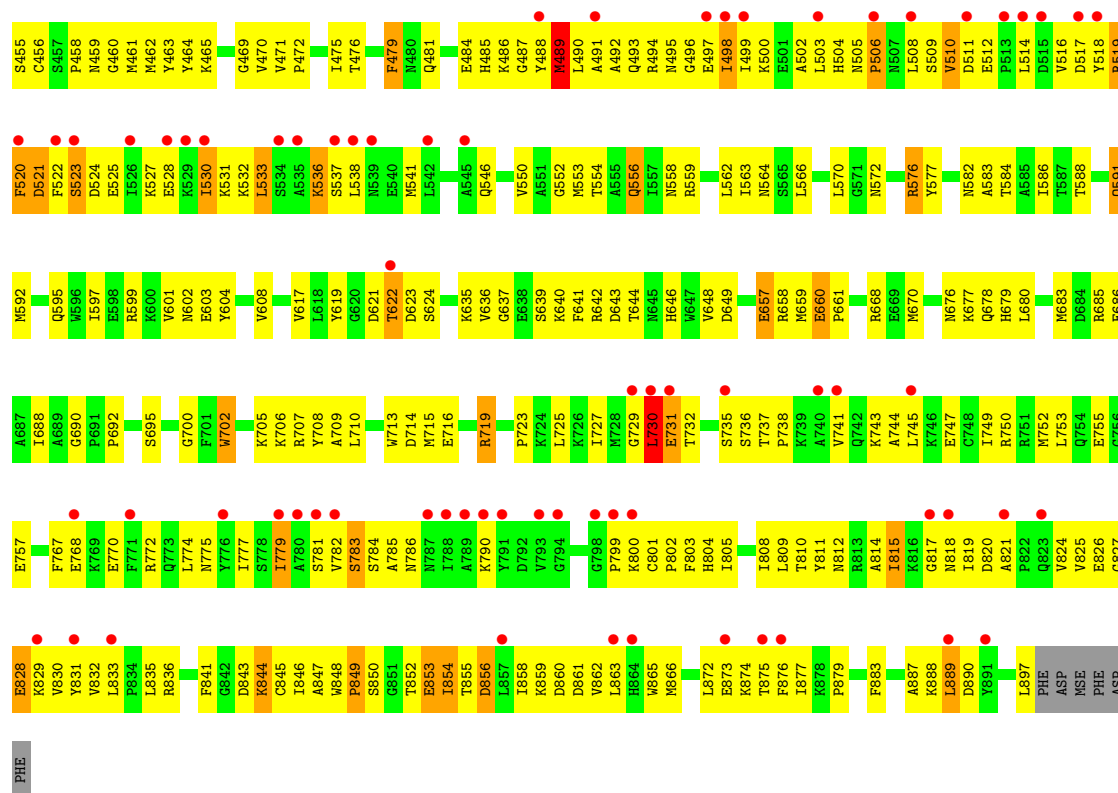
• Molecule 3: DNA polymerase





• Molecule 3: DNA polymerase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	132.61Å 122.63Å 168.69Å 90.00° 96.31° 90.00°	Depositor
Resolution (Å)	50.00 – 2.65 49.49 – 2.60	Depositor EDS
% Data completeness (in resolution range)	88.3 (50.00-2.65) 93.6 (49.49-2.60)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.54 (at 2.61Å)	Xtrriage
Refinement program	CNS	Depositor
R, R_{free}	0.229 , 0.281 0.229 , 0.280	Depositor DCC
R_{free} test set	28873 reflections (9.49%)	wwPDB-VP
Wilson B-factor (Å ²)	47.3	Xtrriage
Anisotropy	0.252	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 56.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	31943	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.13% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	E	0.41	0/365	1.28	0/558
1	G	0.52	0/393	1.33	1/603 (0.2%)
1	I	0.60	0/393	1.31	2/603 (0.3%)
1	K	0.73	0/393	1.31	0/603
2	F	0.41	0/307	1.24	0/468
2	H	0.57	0/333	1.37	1/510 (0.2%)
2	J	0.54	0/333	1.30	1/510 (0.2%)
2	L	0.79	0/333	1.27	1/510 (0.2%)
3	A	0.39	0/7457	0.57	0/10050
3	B	0.42	0/7326	0.62	1/9873 (0.0%)
3	C	0.41	0/7454	0.59	1/10045 (0.0%)
3	D	0.30	0/7072	0.50	0/9590
All	All	0.41	0/32159	0.68	8/43923 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	G	1	0
2	H	0	1
All	All	1	1

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	255	ASN	N-CA-C	-5.75	95.47	111.00
1	G	12	DA	C4'-C3'-O3'	5.52	123.50	109.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	110	DA	C4'-C3'-C2'	5.47	108.03	103.10
2	J	113	DC	C4'-C3'-C2'	5.39	107.95	103.10
3	C	750	ARG	NE-CZ-NH2	-5.35	117.62	120.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	G	12	DA	C3'

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	115	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	E	348	0	195	40	0
1	G	372	0	204	26	0
1	I	372	0	204	39	0
1	K	372	0	204	38	0
2	F	276	0	155	22	0
2	H	299	0	165	22	0
2	J	299	0	165	28	0
2	L	299	0	165	26	0
3	A	7302	0	7141	309	0
3	B	7175	0	6995	306	0
3	C	7300	0	7144	254	0
3	D	6923	0	6512	420	0
4	A	117	0	0	28	0
4	B	205	0	0	17	0
4	C	160	0	0	14	0
4	D	55	0	0	25	0
4	E	9	0	0	2	0
4	F	5	0	0	1	0
4	G	18	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	9	0	0	2	0
4	I	17	0	0	3	0
4	J	4	0	0	0	0
4	K	5	0	0	1	0
4	L	2	0	0	0	0
All	All	31943	0	29249	1491	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 25.

The worst 5 of 1491 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:14:DC:H2''	1:I:15:DC:H5''	1.21	1.17
2:J:111:DT:H2''	2:J:112:DT:H5'	1.16	1.13
3:B:164:ILE:HD12	3:B:164:ILE:H	1.13	1.09
2:L:104:DG:H2''	2:L:105:DC:H5''	1.32	1.07
1:G:11:DC:H2''	1:G:12:DA:H5''	1.34	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	
3	A	900/903 (100%)	804 (89%)	84 (9%)	12 (1%)	12	18
3	B	884/903 (98%)	802 (91%)	70 (8%)	12 (1%)	11	16
3	C	898/903 (99%)	830 (92%)	56 (6%)	12 (1%)	12	18
3	D	886/903 (98%)	701 (79%)	131 (15%)	54 (6%)	1	1
All	All	3568/3612 (99%)	3137 (88%)	341 (10%)	90 (2%)	5	7

5 of 90 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	519	ARG
3	A	611	THR
3	A	621	ASP
3	B	177	GLU
3	C	256	MSE

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	
3	A	785/775 (101%)	739 (94%)	46 (6%)	19	30
3	B	767/775 (99%)	722 (94%)	45 (6%)	19	30
3	C	786/775 (101%)	744 (95%)	42 (5%)	22	35
3	D	711/775 (92%)	675 (95%)	36 (5%)	24	37
All	All	3049/3100 (98%)	2880 (94%)	169 (6%)	21	33

5 of 169 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	561	LEU
3	D	306	ASP
3	C	618	LEU
3	C	881	GLU
3	D	498	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 92 such sidechains are listed below:

Mol	Chain	Res	Type
3	C	285	GLN
3	C	864	HIS
3	C	481	GLN
3	C	675	ASN
3	D	228	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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
1	CTG	G	3	1,2	19,23,24	0.86	1 (5%)	21,35,38	1.03	1 (4%)
1	CTG	K	3	1	19,23,24	1.01	1 (5%)	21,35,38	1.04	2 (9%)
1	CTG	I	3	1,2	19,23,24	0.88	1 (5%)	21,35,38	1.09	2 (9%)
1	CTG	E	3	1,2	19,23,24	0.74	0	21,35,38	1.03	2 (9%)

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
1	CTG	G	3	1,2	-	0/7/45/46	0/2/2/2
1	CTG	K	3	1	-	0/7/45/46	0/2/2/2
1	CTG	I	3	1,2	-	2/7/45/46	0/2/2/2
1	CTG	E	3	1,2	-	2/7/45/46	0/2/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	3	CTG	C5-C4	2.82	1.55	1.52
1	I	3	CTG	C1'-N1	2.41	1.48	1.45
1	G	3	CTG	C1'-N1	2.04	1.48	1.45

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	3	CTG	O3'-C3'-C2'	2.77	120.79	110.90
1	E	3	CTG	O3'-C3'-C2'	2.52	119.92	110.90
1	G	3	CTG	N3-C2-N1	-2.40	114.20	116.69
1	K	3	CTG	N3-C2-N1	-2.32	114.28	116.69
1	K	3	CTG	O3'-C3'-C2'	2.25	118.95	110.90

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	E	3	CTG	O4'-C4'-C5'-O5'
1	E	3	CTG	C3'-C4'-C5'-O5'
1	I	3	CTG	O4'-C4'-C5'-O5'
1	I	3	CTG	C3'-C4'-C5'-O5'

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	G	3	CTG	1	0
1	K	3	CTG	3	0
1	I	3	CTG	1	0
1	E	3	CTG	2	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	E	16/18 (88%)	0.73	2 (12%) 3 2	87, 109, 126, 131	0
1	G	17/18 (94%)	-0.26	0 100 100	34, 47, 76, 79	0
1	I	17/18 (94%)	-0.06	0 100 100	35, 50, 84, 91	0
1	K	17/18 (94%)	1.92	8 (47%) 0 0	65, 80, 81, 81	0
2	F	14/15 (93%)	1.08	3 (21%) 0 1	106, 125, 133, 135	0
2	H	15/15 (100%)	-0.36	0 100 100	36, 49, 100, 100	0
2	J	15/15 (100%)	-0.09	0 100 100	33, 65, 112, 113	0
2	L	15/15 (100%)	2.30	9 (60%) 0 0	78, 80, 82, 82	0
3	A	877/903 (97%)	0.20	51 (5%) 23 19	23, 51, 125, 141	0
3	B	863/903 (95%)	0.04	41 (4%) 30 27	16, 44, 116, 139	0
3	C	875/903 (96%)	0.07	36 (4%) 37 33	17, 47, 114, 142	0
3	D	867/903 (96%)	0.90	145 (16%) 1 1	54, 102, 140, 153	0
All	All	3608/3744 (96%)	0.32	295 (8%) 11 9	16, 58, 131, 153	0

The worst 5 of 295 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	503	LEU	9.4
3	C	503	LEU	9.2
3	D	309	ILE	9.1
3	D	498	ILE	8.8
3	D	135	ALA	8.7

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. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	CTG	K	3	22/23	0.81	0.42	75,79,85,88	0
1	CTG	E	3	22/23	0.82	0.23	110,111,113,114	0
1	CTG	I	3	22/23	0.96	0.17	58,61,62,63	0
1	CTG	G	3	22/23	0.98	0.13	32,41,42,43	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.