



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 01:41 AM GMT

PDB ID : 2DTU
Title : Crystal structure of the beta hairpin loop deletion variant of RB69 gp43 in complex with DNA containing an abasic site analog
Authors : Aller, P.; Hogg, M.; Konigsberg, W.; Wallace, S.S.; Doublié, S.
Deposited on : 2006-07-15
Resolution : 2.37 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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

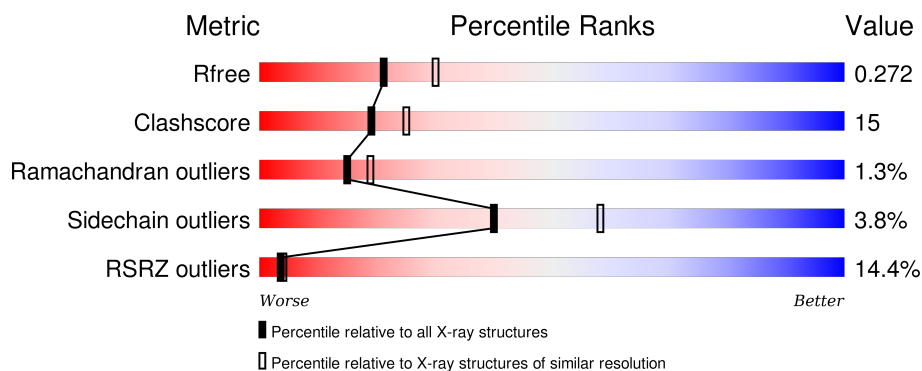
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.37 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	4019 (2.40-2.36)
Clashscore	102246	4595 (2.40-2.36)
Ramachandran outliers	100387	4520 (2.40-2.36)
Sidechain outliers	100360	4522 (2.40-2.36)
RSRZ outliers	91569	4034 (2.40-2.36)

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 $\leq 5\%$. 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	<div> <div>6%</div> <div>17%</div> <div>78%</div> <div>6%</div> </div>
1	G	18	<div> <div>6%</div> <div>28%</div> <div>56%</div> <div>11%</div> <div>6%</div> </div>
1	I	18	<div> <div>6%</div> <div>39%</div> <div>50%</div> <div>6%</div> <div>6%</div> </div>
1	K	18	<div> <div>17%</div> <div>28%</div> <div>72%</div> </div>
2	F	15	<div> <div>7%</div> <div>13%</div> <div>87%</div> </div>

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Mol	Chain	Length	Quality of chain
2	H	15	<div><div></div><div>13%</div><div>13%</div><div>80%</div><div>7%</div></div>
2	J	15	<div><div></div><div>20%</div><div>40%</div><div>27%</div><div>13%</div></div>
2	L	15	<div><div></div><div>33%</div><div>100%</div></div>
3	A	896	<div><div></div><div>7%</div><div>74%</div><div>24%</div><div>•</div></div>
3	B	896	<div><div></div><div>18%</div><div>72%</div><div>26%</div><div>•</div></div>
3	C	896	<div><div></div><div>3%</div><div>76%</div><div>21%</div><div>•</div></div>
3	D	896	<div><div></div><div>30%</div><div>57%</div><div>39%</div><div>• •</div></div>

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 32454 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*(3DR)P*CP*TP*TP*AP*TP*GP*AP*C P*AP*GP*CP*CP*GP*CP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	18	Total	C	N	O	P	0	0	0
			355	169	64	105	17			
1	G	18	Total	C	N	O	P	0	0	0
			355	169	64	105	17			
1	I	18	Total	C	N	O	P	0	0	0
			355	169	64	105	17			
1	K	18	Total	C	N	O	P	0	0	0
			355	169	64	105	17			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	15	Total	C	N	O	P	0	0	0
			308	147	60	87	14			
2	H	15	Total	C	N	O	P	0	0	0
			308	147	60	87	14			
2	J	15	Total	C	N	O	P	0	0	0
			308	147	60	87	14			
2	L	15	Total	C	N	O	P	0	0	0
			308	147	60	87	14			

- Molecule 3 is a protein called DNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	896	Total	C	N	O	S	0	0	0
			7281	4678	1209	1362	32			
3	B	896	Total	C	N	O	S	0	0	0
			7235	4649	1201	1353	32			
3	C	892	Total	C	N	O	S	0	0	0
			7238	4650	1200	1357	31			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	891	Total	C	N	O	S	0	0	0
			7191	4619	1192	1349	31			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	222	ALA	ASP	ENGINEERED	UNP Q38087
A	253	GLY	ILE	ENGINEERED	UNP Q38087
A	?	-	GLU	DELETION	UNP Q38087
A	?	-	ASN	DELETION	UNP Q38087
A	?	-	MET	DELETION	UNP Q38087
A	?	-	TYR	DELETION	UNP Q38087
A	?	-	GLY	DELETION	UNP Q38087
A	?	-	SER	DELETION	UNP Q38087
A	?	-	ARG	DELETION	UNP Q38087
A	327	ALA	ASP	ENGINEERED	UNP Q38087
B	222	ALA	ASP	ENGINEERED	UNP Q38087
B	253	GLY	ILE	ENGINEERED	UNP Q38087
B	?	-	GLU	DELETION	UNP Q38087
B	?	-	ASN	DELETION	UNP Q38087
B	?	-	MET	DELETION	UNP Q38087
B	?	-	TYR	DELETION	UNP Q38087
B	?	-	GLY	DELETION	UNP Q38087
B	?	-	SER	DELETION	UNP Q38087
B	?	-	ARG	DELETION	UNP Q38087
B	327	ALA	ASP	ENGINEERED	UNP Q38087
C	222	ALA	ASP	ENGINEERED	UNP Q38087
C	253	GLY	ILE	ENGINEERED	UNP Q38087
C	?	-	GLU	DELETION	UNP Q38087
C	?	-	ASN	DELETION	UNP Q38087
C	?	-	MET	DELETION	UNP Q38087
C	?	-	TYR	DELETION	UNP Q38087
C	?	-	GLY	DELETION	UNP Q38087
C	?	-	SER	DELETION	UNP Q38087
C	?	-	ARG	DELETION	UNP Q38087
C	327	ALA	ASP	ENGINEERED	UNP Q38087
D	222	ALA	ASP	ENGINEERED	UNP Q38087
D	253	GLY	ILE	ENGINEERED	UNP Q38087
D	?	-	GLU	DELETION	UNP Q38087
D	?	-	ASN	DELETION	UNP Q38087
D	?	-	MET	DELETION	UNP Q38087
D	?	-	TYR	DELETION	UNP Q38087

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Chain	Residue	Modelled	Actual	Comment	Reference
D	?	-	GLY	DELETION	UNP Q38087
D	?	-	SER	DELETION	UNP Q38087
D	?	-	ARG	DELETION	UNP Q38087
D	327	ALA	ASP	ENGINEERED	UNP Q38087

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	251	Total 251	O 251	0	0
4	B	195	Total 195	O 195	0	0
4	C	272	Total 272	O 272	0	0
4	D	38	Total 38	O 38	0	0
4	E	9	Total 9	O 9	0	0
4	F	10	Total 10	O 10	0	0
4	G	15	Total 15	O 15	0	0
4	H	8	Total 8	O 8	0	0
4	I	31	Total 31	O 31	0	0
4	J	18	Total 18	O 18	0	0
4	K	10	Total 10	O 10	0	0

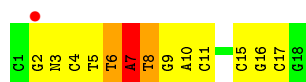
3 Residue-property plots [i](#)

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: 5'-D(*CP*GP*(3DR)P*CP*TP*TP*AP*TP*GP*AP*CP*AP*GP*CP*CP*GP*CP*G)-3'



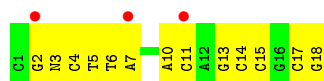
- Molecule 1: 5'-D(*CP*GP*(3DR)P*CP*TP*TP*AP*TP*GP*AP*CP*AP*GP*CP*CP*GP*CP*G)-3'



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

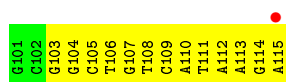


- Molecule 1: 5'-D(*CP*GP*(3DR)P*CP*TP*TP*AP*TP*GP*AP*CP*AP*GP*CP*CP*GP*CP*G)-3'



- Molecule 2: 5'-D(*GP*CP*GP*GP*CP*TP*GP*TP*CP*AP*TP*AP*AP*GP*A)-3'

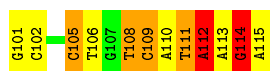
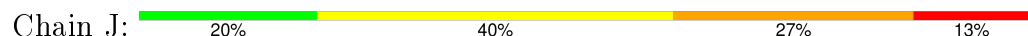




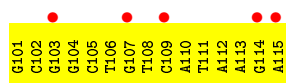
- Molecule 2: 5'-D(*GP*CP*GP*GP*CP*TP*GP*TP*CP*AP*TP*AP*AP*GP*A)-3'



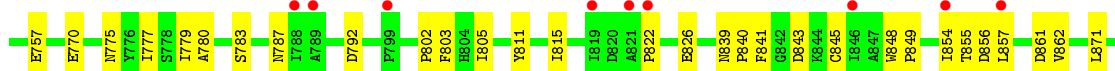
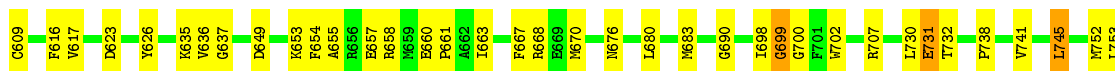
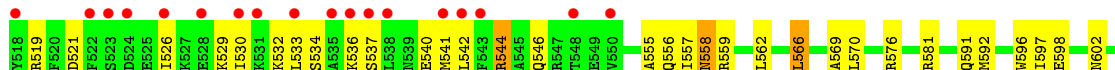
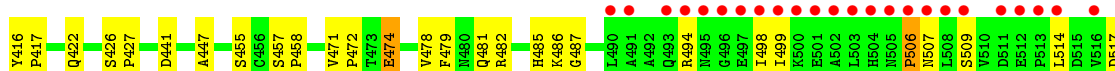
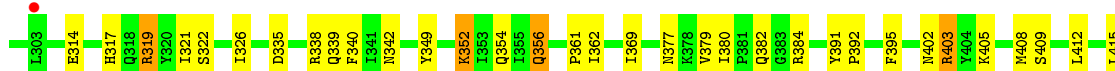
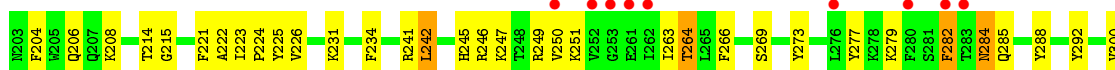
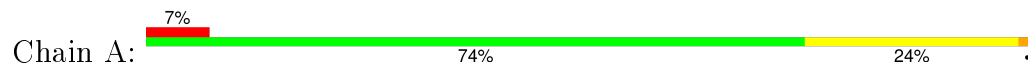
- Molecule 2: 5'-D(*GP*CP*GP*GP*CP*TP*GP*TP*CP*AP*TP*AP*AP*GP*A)-3'



- Molecule 2: 5'-D(*GP*CP*GP*GP*CP*TP*GP*TP*CP*AP*TP*AP*AP*GP*A)-3'

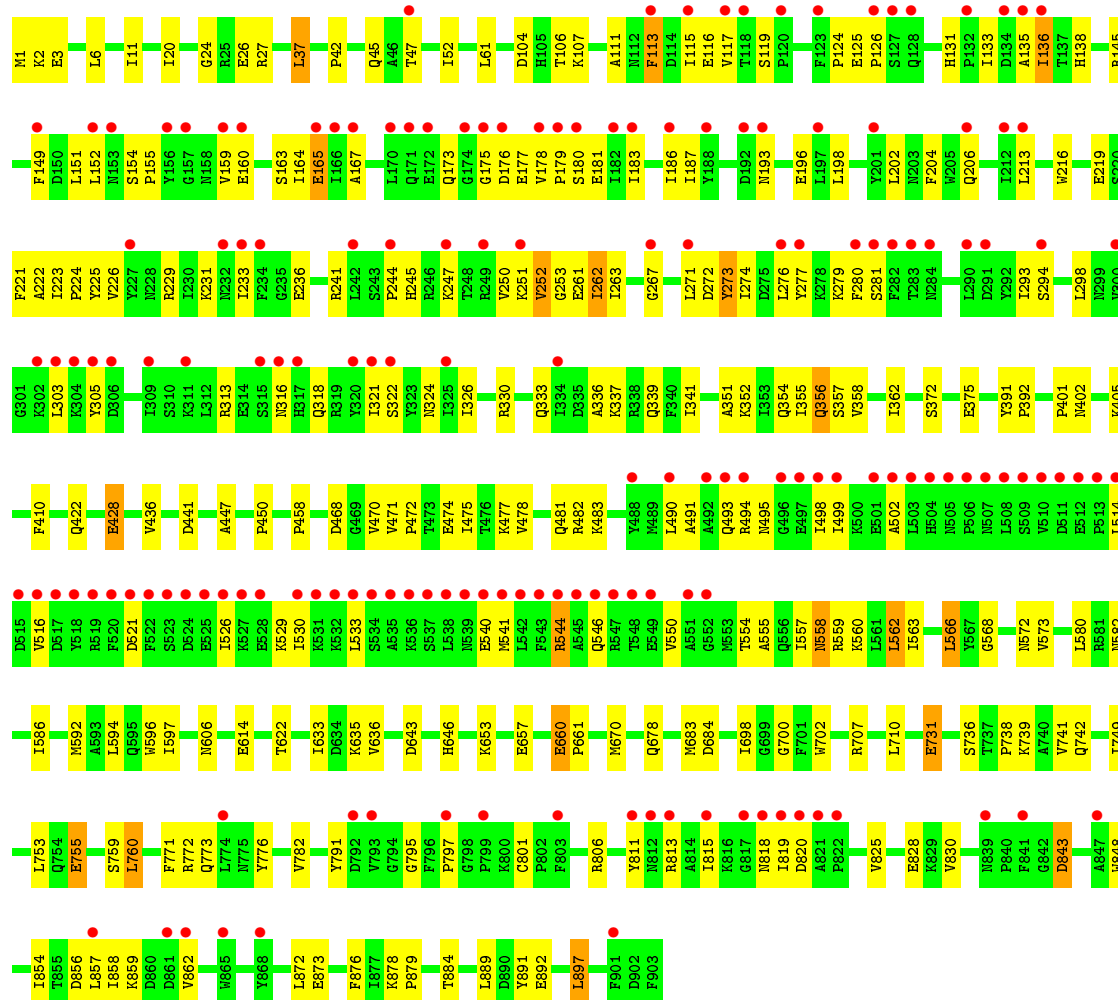


- Molecule 3: DNA polymerase

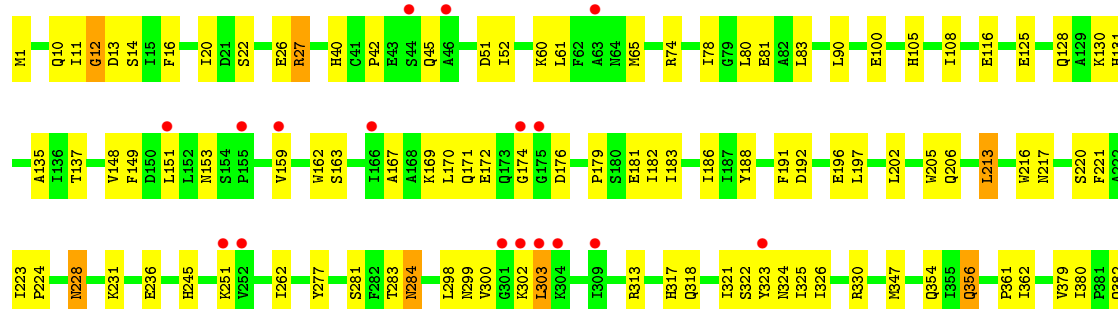
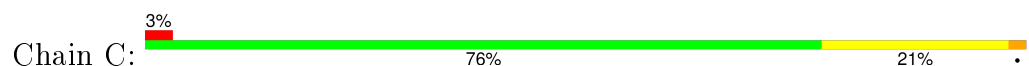


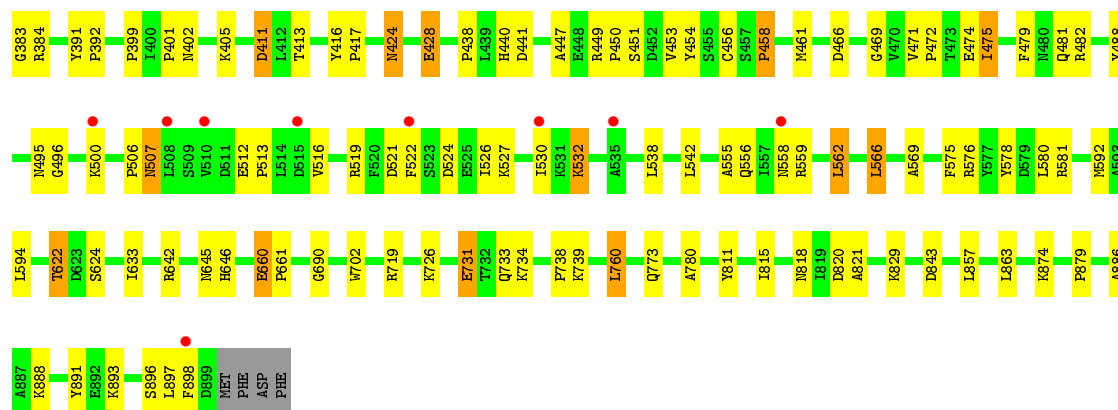


• Molecule 3: DNA polymerase

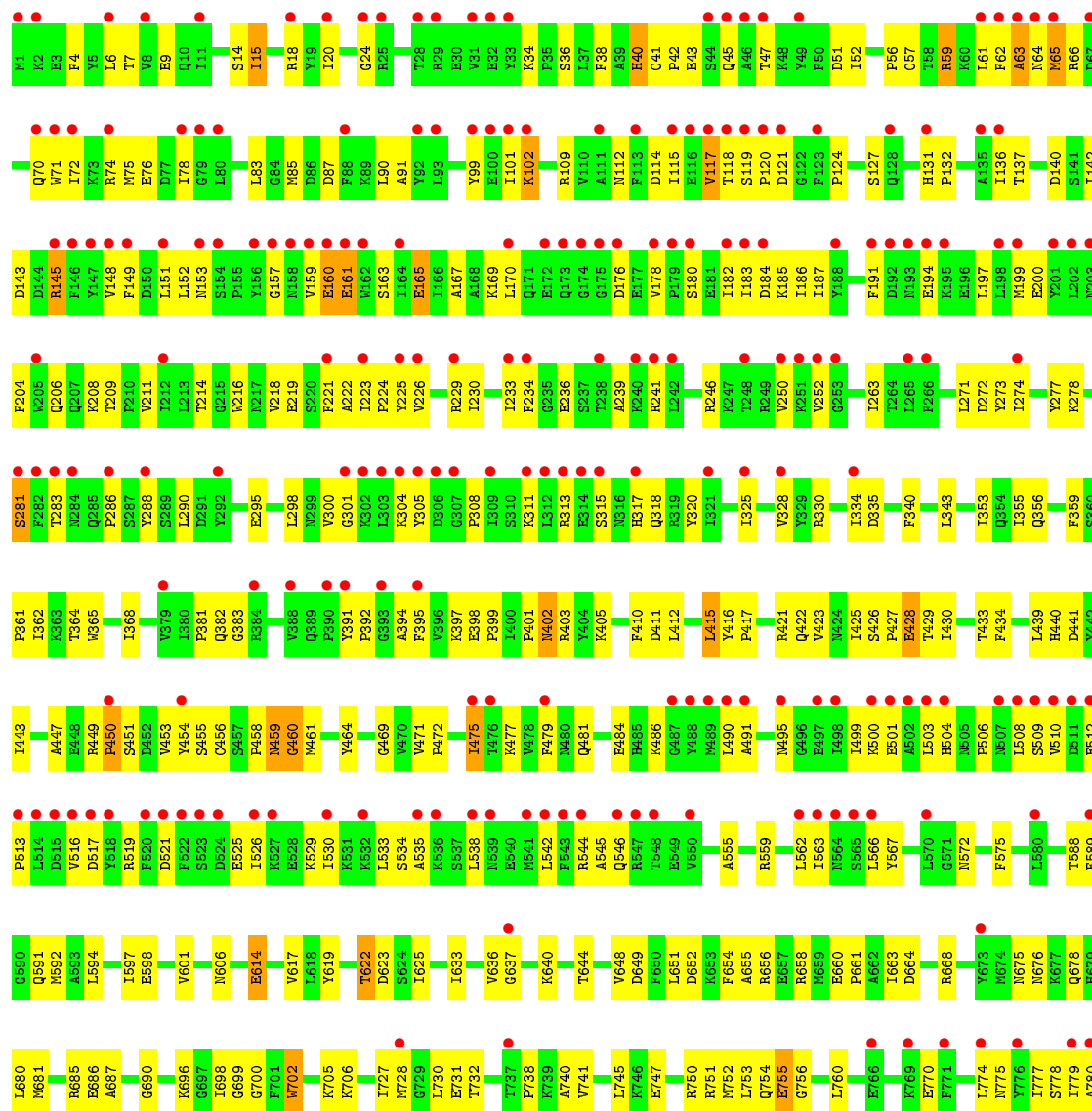


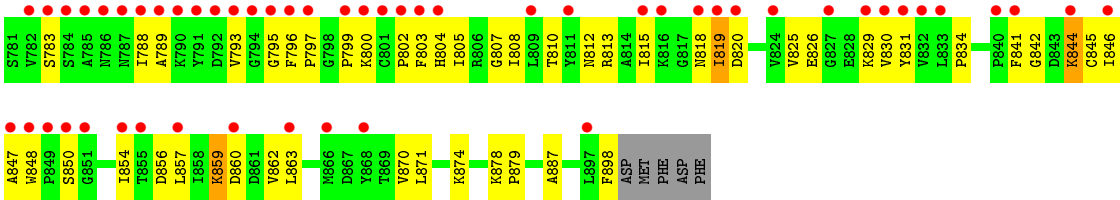
• Molecule 3: DNA polymerase





● 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	133.07Å 123.06Å 164.56Å 90.00° 96.78° 90.00°	Depositor
Resolution (Å)	50.00 – 2.37 48.64 – 2.38	Depositor EDS
% Data completeness (in resolution range)	89.4 (50.00-2.37) 94.2 (48.64-2.38)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.92 (at 2.37Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.223 , 0.268 0.227 , 0.272	Depositor DCC
R_{free} test set	18819 reflections (9.45%)	DCC
Wilson B-factor (Å ²)	47.7	Xtriage
Anisotropy	0.216	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 53.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 396029 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	32454	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 2.44% 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, 0.375 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: 3DR

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	0.49	0/384	1.35	1/588 (0.2%)
1	G	0.55	0/384	1.44	5/588 (0.9%)
1	I	0.63	0/384	1.42	5/588 (0.9%)
1	K	0.40	0/384	1.26	0/588
2	F	0.42	0/346	1.28	0/533
2	H	0.50	0/346	1.29	1/533 (0.2%)
2	J	0.68	0/346	1.40	6/533 (1.1%)
2	L	0.38	0/346	1.21	0/533
3	A	0.42	0/7461	0.57	0/10092
3	B	0.38	0/7414	0.53	0/10036
3	C	0.41	0/7416	0.57	0/10032
3	D	0.29	0/7369	0.45	0/9980
All	All	0.39	0/32580	0.66	18/44624 (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	E	0	1
1	G	0	1
1	I	0	1
2	J	0	2
All	All	0	5

There are no bond length outliers.

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	6	DT	C4'-C3'-C2'	6.36	108.82	103.10
1	G	7	DA	C4'-C3'-O3'	5.95	124.58	109.70
1	E	7	DA	C4'-C3'-C2'	5.75	108.28	103.10
2	J	109	DC	O4'-C1'-C2'	5.64	110.42	105.90
1	I	7	DA	C4'-C3'-C2'	5.50	108.05	103.10

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	7	DA	Sidechain
1	G	7	DA	Sidechain
1	I	7	DA	Sidechain
2	J	112	DA	Sidechain
2	J	114	DG	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	355	0	200	17	0
1	G	355	0	200	16	0
1	I	355	0	200	10	0
1	K	355	0	200	18	0
2	F	308	0	170	17	0
2	H	308	0	170	20	0
2	J	308	0	170	21	0
2	L	308	0	170	17	0
3	A	7281	0	7136	177	0
3	B	7235	0	7052	190	0
3	C	7238	0	7101	151	0
3	D	7191	0	7005	289	0
4	A	251	0	0	18	0
4	B	195	0	0	19	0
4	C	272	0	0	18	0
4	D	38	0	0	9	0
4	E	9	0	0	0	0
4	F	10	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	G	15	0	0	1	0
4	H	8	0	0	3	0
4	I	31	0	0	1	0
4	J	18	0	0	5	0
4	K	10	0	0	4	0
All	All	32454	0	29774	930	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 15.

The worst 5 of 930 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)
3:A:85:MET:HE2	3:A:87:ASP:H	1.18	1.03
3:A:395:PHE:HB2	3:A:591:GLN:HG3	1.43	1.01
1:G:6:DT:H2'	1:G:7:DA:H5''	1.40	1.00
1:G:6:DT:C2'	1:G:7:DA:H5''	1.91	1.00
2:J:108:DT:H2''	2:J:109:DC:H5''	1.46	0.97

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	894/896 (100%)	838 (94%)	51 (6%)	5 (1%)	30	40
3	B	894/896 (100%)	815 (91%)	69 (8%)	10 (1%)	17	23
3	C	890/896 (99%)	841 (94%)	45 (5%)	4 (0%)	39	53
3	D	889/896 (99%)	746 (84%)	116 (13%)	27 (3%)	5	4
All	All	3567/3584 (100%)	3240 (91%)	281 (8%)	46 (1%)	15	19

5 of 46 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	D	65	MET
3	D	117	VAL
3	D	304	LYS
3	D	450	PRO
3	D	819	ILE

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	A	785/793 (99%)	756 (96%)	29 (4%)	41	60
3	B	774/793 (98%)	750 (97%)	24 (3%)	47	67
3	C	781/793 (98%)	741 (95%)	40 (5%)	29	44
3	D	770/793 (97%)	746 (97%)	24 (3%)	47	67
All	All	3110/3172 (98%)	2993 (96%)	117 (4%)	40	58

5 of 117 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	B	897	LEU
3	C	384	ARG
3	D	479	PHE
3	C	27	ARG
3	C	213	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 95 such sidechains are listed below:

Mol	Chain	Res	Type
3	B	818	ASN
3	C	324	ASN
3	D	546	GLN
3	C	173	GLN
3	C	245	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	3DR	E	3	1	7,11,12	0.45	0	8,14,17	1.63	1 (12%)
1	3DR	G	3	1	7,11,12	0.47	0	8,14,17	1.84	1 (12%)
1	3DR	I	3	1	7,11,12	0.44	0	8,14,17	1.71	1 (12%)
1	3DR	K	3	1	7,11,12	0.47	0	8,14,17	1.61	1 (12%)

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	3DR	E	3	1	-	0/3/15/16	0/1/1/1
1	3DR	G	3	1	-	0/3/15/16	0/1/1/1
1	3DR	I	3	1	-	0/3/15/16	0/1/1/1
1	3DR	K	3	1	-	0/3/15/16	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	3	3DR	O3'-C3'-C2'	3.62	119.98	111.71
1	K	3	3DR	O3'-C3'-C2'	3.62	120.00	111.71
1	I	3	3DR	O3'-C3'-C2'	3.88	120.58	111.71
1	G	3	3DR	O3'-C3'-C2'	4.17	121.23	111.71

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 5 short contacts:

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

5.5 Carbohydrates [i](#)

There are no carbohydrates 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	17/18 (94%)	0.28	1 (5%) 26 30	54, 75, 126, 146	0
1	G	17/18 (94%)	0.20	1 (5%) 26 30	45, 57, 133, 148	0
1	I	17/18 (94%)	0.14	1 (5%) 26 30	35, 42, 101, 115	0
1	K	17/18 (94%)	1.24	3 (17%) 2 2	45, 123, 161, 169	0
2	F	15/15 (100%)	0.66	1 (6%) 21 24	68, 99, 128, 141	0
2	H	15/15 (100%)	0.44	2 (13%) 4 5	56, 71, 126, 153	0
2	J	15/15 (100%)	0.14	0 100 100	38, 57, 91, 96	0
2	L	15/15 (100%)	1.57	5 (33%) 0 0	126, 131, 153, 157	0
3	A	896/896 (100%)	0.54	61 (6%) 20 23	30, 47, 125, 149	0
3	B	896/896 (100%)	1.09	165 (18%) 2 2	28, 62, 154, 165	0
3	C	892/896 (99%)	0.43	26 (2%) 55 58	23, 48, 83, 106	0
3	D	891/896 (99%)	1.60	268 (30%) 1 0	53, 117, 153, 160	0
All	All	3703/3716 (99%)	0.91	534 (14%) 3 4	23, 62, 148, 169	0

The worst 5 of 534 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	B	516	VAL	13.7
3	A	530	ILE	13.5
3	D	514	LEU	13.0
3	B	508	LEU	11.5
3	D	117	VAL	11.2

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, 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
1	3DR	E	3	11/12	0.75	0.35	-	138,143,147,147	0
1	3DR	K	3	11/12	0.72	0.38	-	165,167,169,169	0
1	3DR	I	3	11/12	0.81	0.19	-	102,105,111,112	0
1	3DR	G	3	11/12	0.76	0.27	-	132,137,146,147	0

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.