



wwPDB X-ray Structure Validation Summary Report

Sep 5, 2014 – 01:14 AM EDT

PDB ID : 2P5O
Title : Crystal structure of RB69 GP43 in complex with DNA containing an abasic site analog
Authors : Hogg, M.; Wallace, S.S.; Doublie, S.
Deposited on : 2007-03-15
Resolution : 2.80 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

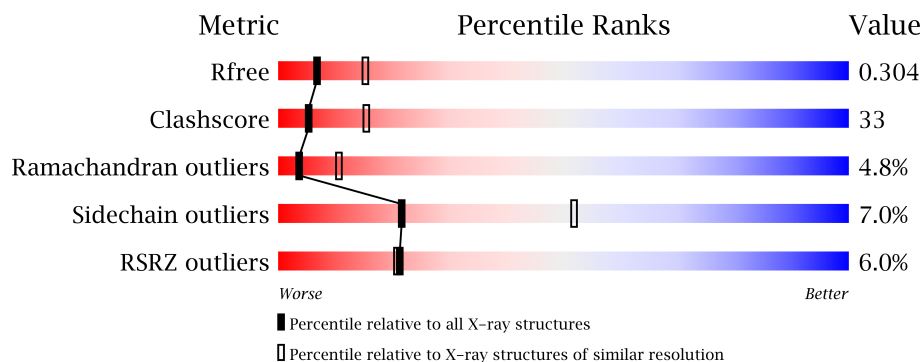
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.16 November 2013
Xtriage (Phenix) : dev-1439
EDS : stable23489
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable23489

1 Overall quality at a glance

The reported resolution of this entry is 2.80 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}	66092	1799 (2.80-2.80)
Clashscore	79885	2295 (2.80-2.80)
Ramachandran outliers	78287	2252 (2.80-2.80)
Sidechain outliers	78261	2254 (2.80-2.80)
RSRZ outliers	66119	1802 (2.80-2.80)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	E	18	
1	G	18	
1	I	18	
1	K	18	
2	F	15	
2	H	15	
2	J	15	
2	L	15	
3	A	903	
3	B	903	
3	C	903	
3	D	903	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 27752 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Template DNA.

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	13	Total	C	N	O	P	0	0	0
			264	126	51	75	12			
1	I	18	Total	C	N	O	P	0	0	0
			355	169	64	105	17			
1	K	9	Total	C	N	O	P	0	0	0
			181	86	37	50	8			

- Molecule 2 is a DNA chain called Primer DNA.

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	8	Total	C	N	O	P	0	0	0
			163	78	30	48	7			

- Molecule 3 is a protein called DNA polymerase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	A	856	Total	C	N	O	S	Se	0	0	0
			6941	4460	1154	1295	8	24			
3	B	771	Total	C	N	O	S	Se	0	0	0
			6245	4013	1034	1167	6	25			
3	C	853	Total	C	N	O	S	Se	0	0	0
			6895	4430	1143	1290	8	24			
3	D	671	Total	C	N	O	S	Se	0	0	0
			4934	3144	818	948	6	18			

There are 108 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	-	MODIFIED RESIDUE	UNP Q38087
A	65	MSE	MET	MODIFIED RESIDUE	UNP Q38087
A	75	MSE	MET	MODIFIED RESIDUE	UNP Q38087
A	85	MSE	MET	MODIFIED RESIDUE	UNP Q38087
A	189	MSE	MET	MODIFIED RESIDUE	UNP Q38087
A	199	MSE	MET	MODIFIED RESIDUE	UNP Q38087
A	222	ALA	ASP	ENGINEERED	UNP Q38087
A	256	MSE	MET	MODIFIED RESIDUE	UNP Q38087
A	327	ALA	ASP	ENGINEERED	UNP Q38087
A	347	MSE	MET	MODIFIED RESIDUE	UNP Q38087
A	408	MSE	MET	MODIFIED RESIDUE	UNP Q38087
A	461	MSE	MET	MODIFIED RESIDUE	UNP Q38087
A	462	MSE	MET	MODIFIED RESIDUE	UNP Q38087
A	489	MSE	MET	MODIFIED RESIDUE	UNP Q38087
A	541	MSE	MET	MODIFIED RESIDUE	UNP Q38087
A	553	MSE	MET	MODIFIED RESIDUE	UNP Q38087
A	592	MSE	MET	MODIFIED RESIDUE	UNP Q38087
A	659	MSE	MET	MODIFIED RESIDUE	UNP Q38087
A	670	MSE	MET	MODIFIED RESIDUE	UNP Q38087
A	674	MSE	MET	MODIFIED RESIDUE	UNP Q38087
A	681	MSE	MET	MODIFIED RESIDUE	UNP Q38087
A	683	MSE	MET	MODIFIED RESIDUE	UNP Q38087
A	715	MSE	MET	MODIFIED RESIDUE	UNP Q38087
A	728	MSE	MET	MODIFIED RESIDUE	UNP Q38087
A	752	MSE	MET	MODIFIED RESIDUE	UNP Q38087
A	866	MSE	MET	MODIFIED RESIDUE	UNP Q38087
A	900	MSE	MET	MODIFIED RESIDUE	UNP Q38087
B	1	MSE	-	MODIFIED RESIDUE	UNP Q38087
B	65	MSE	MET	MODIFIED RESIDUE	UNP Q38087
B	75	MSE	MET	MODIFIED RESIDUE	UNP Q38087
B	85	MSE	MET	MODIFIED RESIDUE	UNP Q38087
B	189	MSE	MET	MODIFIED RESIDUE	UNP Q38087
B	199	MSE	MET	MODIFIED RESIDUE	UNP Q38087
B	222	ALA	ASP	ENGINEERED	UNP Q38087
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B	347	MSE	MET	MODIFIED RESIDUE	UNP Q38087
B	408	MSE	MET	MODIFIED RESIDUE	UNP Q38087
B	461	MSE	MET	MODIFIED RESIDUE	UNP Q38087
B	462	MSE	MET	MODIFIED RESIDUE	UNP Q38087
B	489	MSE	MET	MODIFIED RESIDUE	UNP Q38087
B	541	MSE	MET	MODIFIED RESIDUE	UNP Q38087

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Chain	Residue	Modelled	Actual	Comment	Reference
B	553	MSE	MET	MODIFIED RESIDUE	UNP Q38087
B	592	MSE	MET	MODIFIED RESIDUE	UNP Q38087
B	659	MSE	MET	MODIFIED RESIDUE	UNP Q38087
B	670	MSE	MET	MODIFIED RESIDUE	UNP Q38087
B	674	MSE	MET	MODIFIED RESIDUE	UNP Q38087
B	681	MSE	MET	MODIFIED RESIDUE	UNP Q38087
B	683	MSE	MET	MODIFIED RESIDUE	UNP Q38087
B	715	MSE	MET	MODIFIED RESIDUE	UNP Q38087
B	728	MSE	MET	MODIFIED RESIDUE	UNP Q38087
B	752	MSE	MET	MODIFIED RESIDUE	UNP Q38087
B	866	MSE	MET	MODIFIED RESIDUE	UNP Q38087
B	900	MSE	MET	MODIFIED RESIDUE	UNP Q38087
C	1	MSE	-	MODIFIED RESIDUE	UNP Q38087
C	65	MSE	MET	MODIFIED RESIDUE	UNP Q38087
C	75	MSE	MET	MODIFIED RESIDUE	UNP Q38087
C	85	MSE	MET	MODIFIED RESIDUE	UNP Q38087
C	189	MSE	MET	MODIFIED RESIDUE	UNP Q38087
C	199	MSE	MET	MODIFIED RESIDUE	UNP Q38087
C	222	ALA	ASP	ENGINEERED	UNP Q38087
C	256	MSE	MET	MODIFIED RESIDUE	UNP Q38087
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C	489	MSE	MET	MODIFIED RESIDUE	UNP Q38087
C	541	MSE	MET	MODIFIED RESIDUE	UNP Q38087
C	553	MSE	MET	MODIFIED RESIDUE	UNP Q38087
C	592	MSE	MET	MODIFIED RESIDUE	UNP Q38087
C	659	MSE	MET	MODIFIED RESIDUE	UNP Q38087
C	670	MSE	MET	MODIFIED RESIDUE	UNP Q38087
C	674	MSE	MET	MODIFIED RESIDUE	UNP Q38087
C	681	MSE	MET	MODIFIED RESIDUE	UNP Q38087
C	683	MSE	MET	MODIFIED RESIDUE	UNP Q38087
C	715	MSE	MET	MODIFIED RESIDUE	UNP Q38087
C	728	MSE	MET	MODIFIED RESIDUE	UNP Q38087
C	752	MSE	MET	MODIFIED RESIDUE	UNP Q38087
C	866	MSE	MET	MODIFIED RESIDUE	UNP Q38087
C	900	MSE	MET	MODIFIED RESIDUE	UNP Q38087
D	1	MSE	-	MODIFIED RESIDUE	UNP Q38087
D	65	MSE	MET	MODIFIED RESIDUE	UNP Q38087
D	75	MSE	MET	MODIFIED RESIDUE	UNP Q38087

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Chain	Residue	Modelled	Actual	Comment	Reference
D	85	MSE	MET	MODIFIED RESIDUE	UNP Q38087
D	189	MSE	MET	MODIFIED RESIDUE	UNP Q38087
D	199	MSE	MET	MODIFIED RESIDUE	UNP Q38087
D	222	ALA	ASP	ENGINEERED	UNP Q38087
D	256	MSE	MET	MODIFIED RESIDUE	UNP Q38087
D	327	ALA	ASP	ENGINEERED	UNP Q38087
D	347	MSE	MET	MODIFIED RESIDUE	UNP Q38087
D	408	MSE	MET	MODIFIED RESIDUE	UNP Q38087
D	461	MSE	MET	MODIFIED RESIDUE	UNP Q38087
D	462	MSE	MET	MODIFIED RESIDUE	UNP Q38087
D	489	MSE	MET	MODIFIED RESIDUE	UNP Q38087
D	541	MSE	MET	MODIFIED RESIDUE	UNP Q38087
D	553	MSE	MET	MODIFIED RESIDUE	UNP Q38087
D	592	MSE	MET	MODIFIED RESIDUE	UNP Q38087
D	659	MSE	MET	MODIFIED RESIDUE	UNP Q38087
D	670	MSE	MET	MODIFIED RESIDUE	UNP Q38087
D	674	MSE	MET	MODIFIED RESIDUE	UNP Q38087
D	681	MSE	MET	MODIFIED RESIDUE	UNP Q38087
D	683	MSE	MET	MODIFIED RESIDUE	UNP Q38087
D	715	MSE	MET	MODIFIED RESIDUE	UNP Q38087
D	728	MSE	MET	MODIFIED RESIDUE	UNP Q38087
D	752	MSE	MET	MODIFIED RESIDUE	UNP Q38087
D	866	MSE	MET	MODIFIED RESIDUE	UNP Q38087
D	900	MSE	MET	MODIFIED RESIDUE	UNP Q38087

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	E	3	Total O 3 3	0	0
4	F	5	Total O 5 5	0	0
4	G	7	Total O 7 7	0	0
4	H	2	Total O 2 2	0	0
4	I	17	Total O 17 17	0	0
4	J	9	Total O 9 9	0	0
4	K	8	Total O 8 8	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	L	6	Total 6	O 6	0	0
4	A	139	Total 139	O 139	0	0
4	B	106	Total 106	O 106	0	0
4	C	147	Total 147	O 147	0	0
4	D	46	Total 46	O 46	0	0

3 Residue-property plots

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.

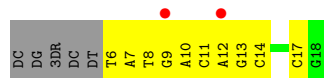
- Molecule 1: Template DNA

Chain E: 



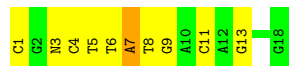
- Molecule 1: Template DNA

Chain G: 



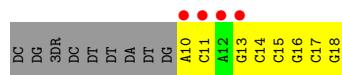
- Molecule 1: Template DNA

Chain I: 



- Molecule 1: Template DNA

Chain K: 



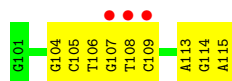
- Molecule 2: Primer DNA

Chain F: 



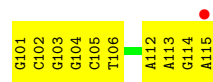
- Molecule 2: Primer DNA

Chain H: 



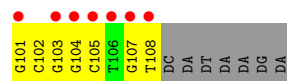
- Molecule 2: Primer DNA

Chain J:



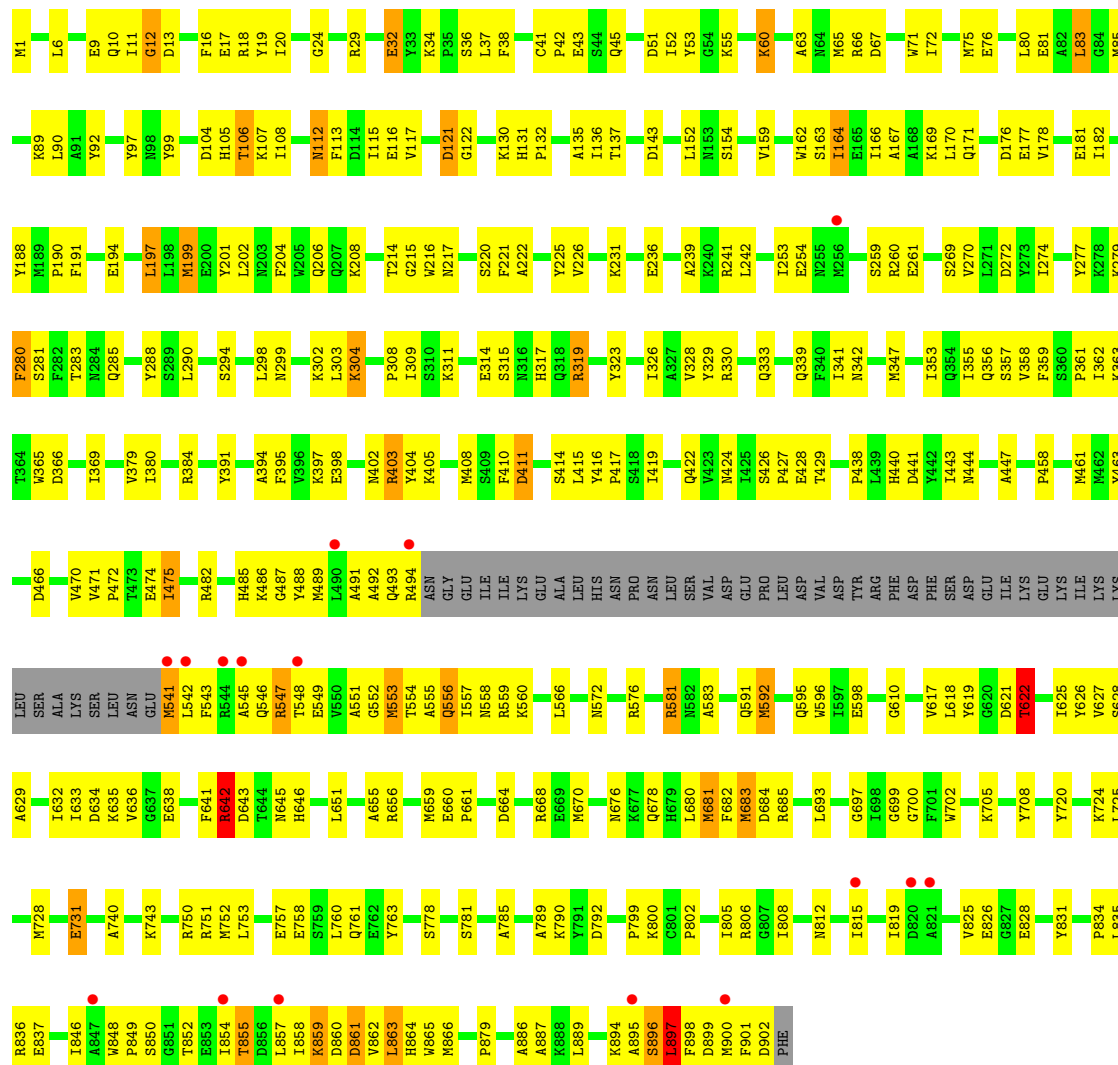
- Molecule 2: Primer DNA

Chain L:



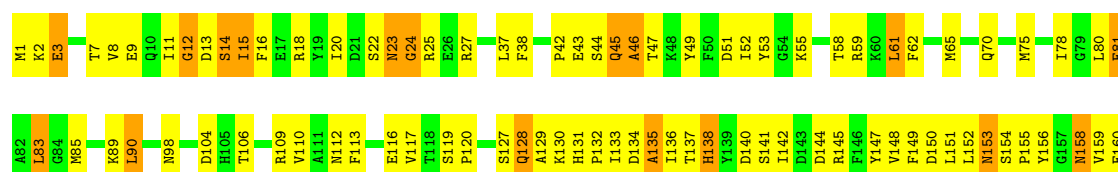
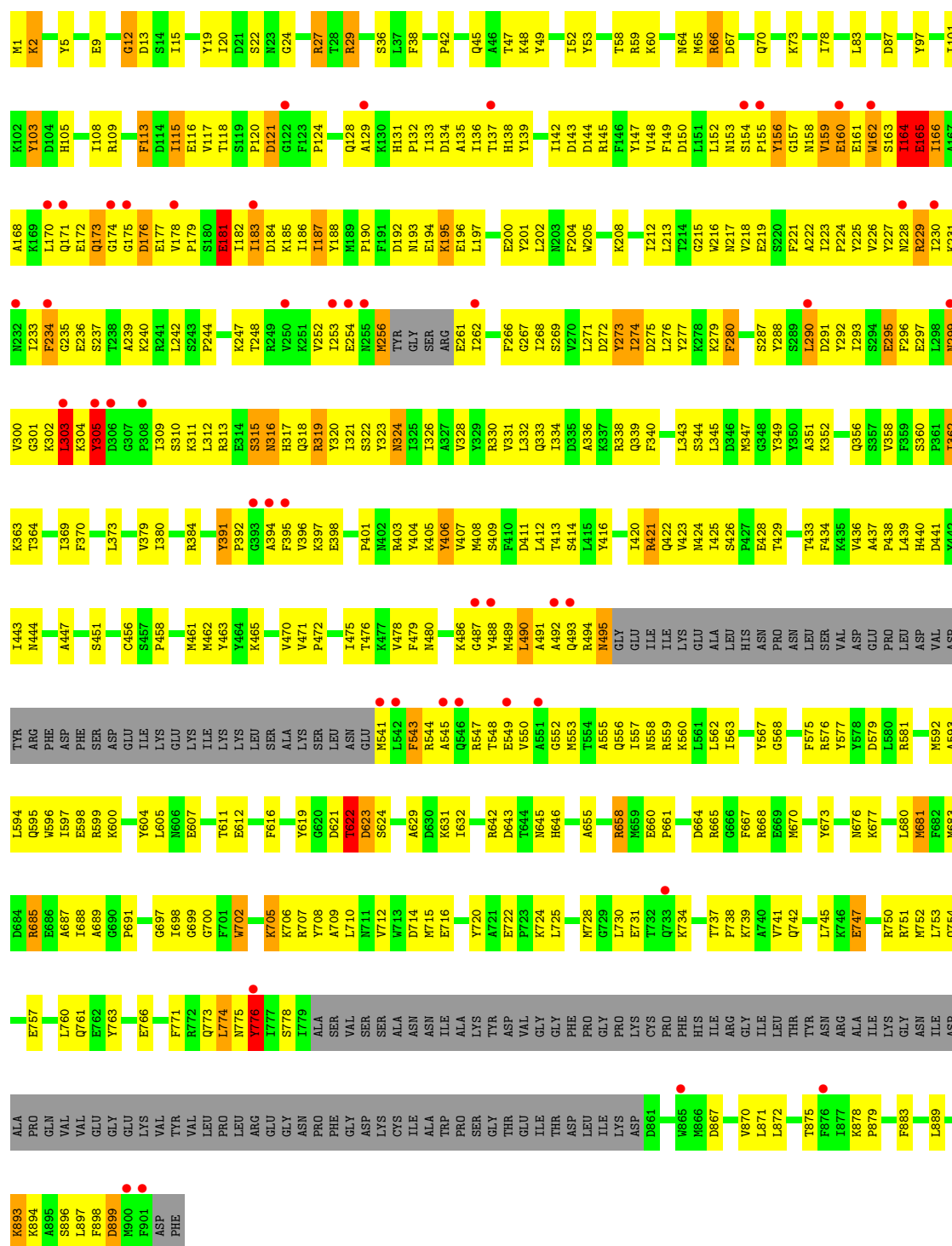
- Molecule 3: DNA polymerase

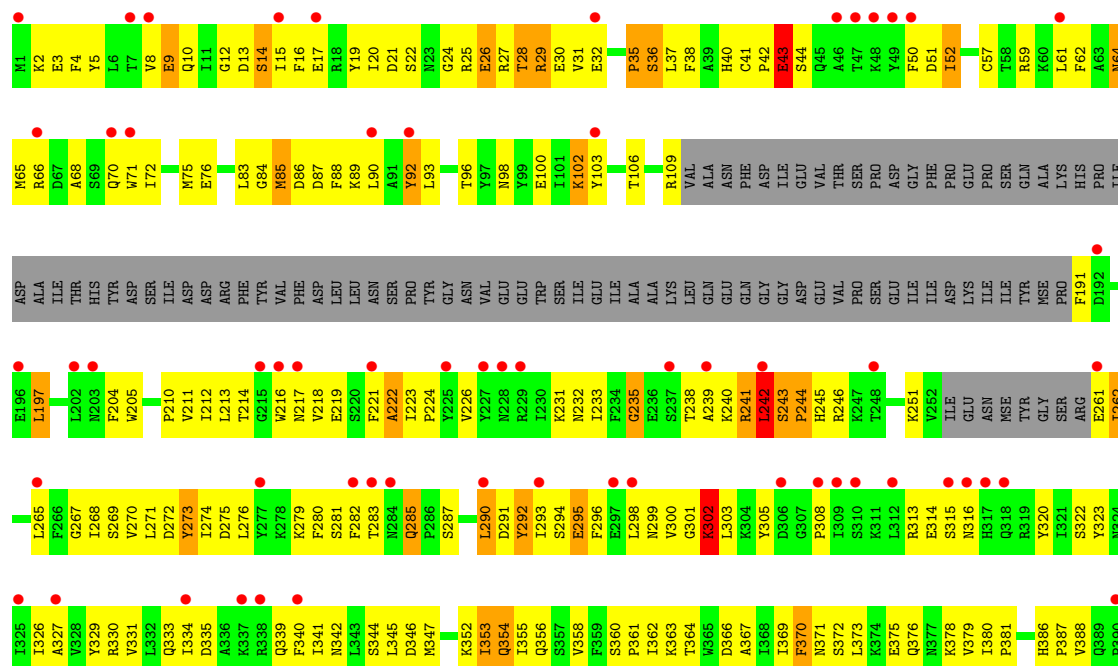
Chain A:

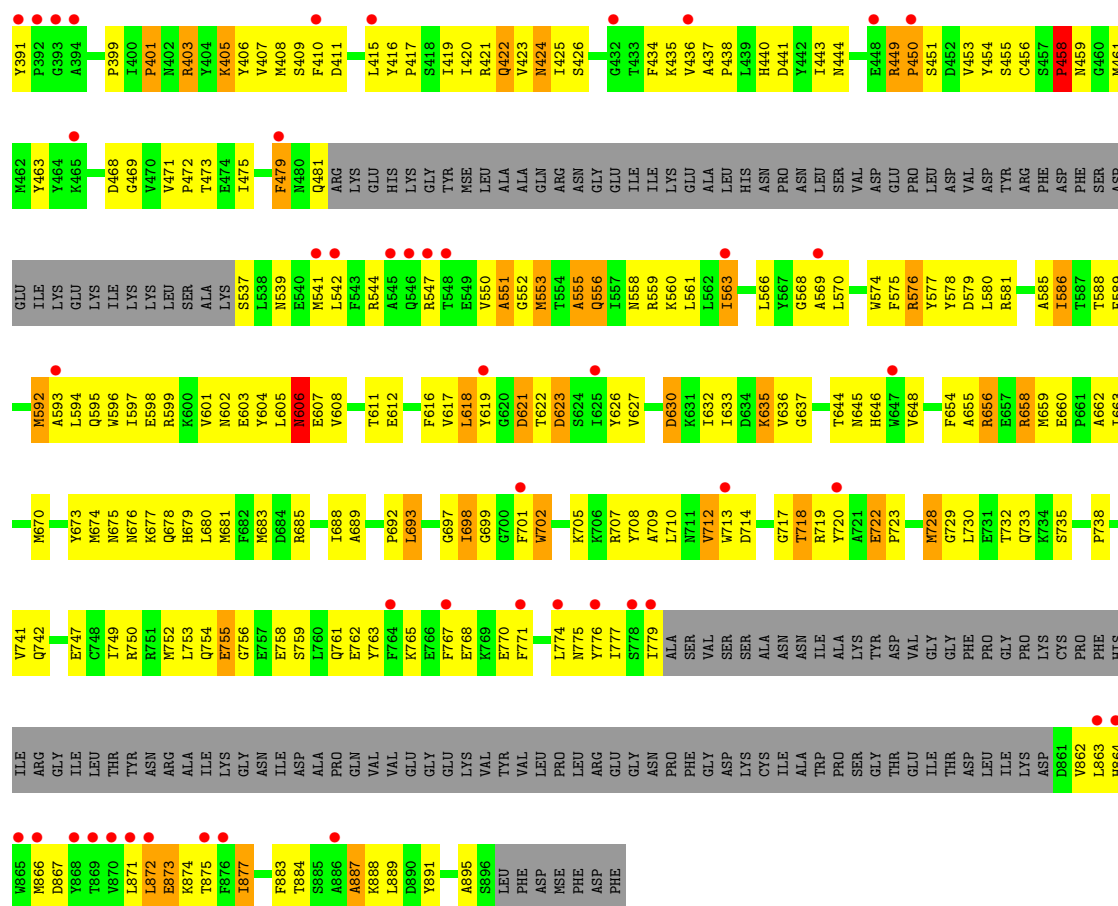


- Molecule 3: DNA polymerase

Chain B:







4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	133.02Å 123.21Å 165.62Å 90.00° 95.82° 90.00°	Depositor
Resolution (Å)	44.00 – 2.80 44.11 – 2.80	Depositor EDS
% Data completeness (in resolution range)	90.9 (44.00-2.80) 95.8 (44.11-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.39 (at 2.81Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.245 , 0.290 0.263 , 0.304	Depositor DCC
R_{free} test set	12094 reflections (10.70%)	DCC
Wilson B-factor (Å ²)	49.8	Xtriage
Anisotropy	0.156	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 34.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 252506 reflections	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	27752	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.47% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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	0.36	0/384	0.68	0/588
1	G	0.40	0/296	0.91	1/455 (0.2%)
1	I	0.55	0/384	0.78	0/588
1	K	0.37	0/203	0.66	0/311
2	F	0.31	0/346	0.67	0/533
2	H	0.33	0/346	0.68	0/533
2	J	0.43	0/346	0.73	0/533
2	L	0.26	0/182	0.63	0/280
3	A	0.49	0/7090	0.69	0/9555
3	B	0.42	0/6376	0.63	0/8593
3	C	0.46	0/7045	0.66	0/9502
3	D	0.33	0/5028	0.55	0/6831
All	All	0.43	0/28026	0.65	1/38302 (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	0	1
1	I	0	1
3	B	0	1
All	All	0	3

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	6	DT	C6-C5-C7	-5.18	119.79	122.90

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	B	273	TYR	Sidechain
1	G	17	DC	Sidechain
1	I	7	DA	Sidechain

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	355	0	200	18	0
1	G	264	0	147	12	0
1	I	355	0	200	13	0
1	K	181	0	101	15	0
2	F	308	0	170	20	0
2	H	308	0	170	18	0
2	J	308	0	170	13	0
2	L	163	0	92	24	0
3	A	6941	0	6787	309	0
3	B	6245	0	6024	495	0
3	C	6895	0	6710	380	0
3	D	4934	0	4297	420	0
4	A	139	0	0	18	0
4	B	106	0	0	24	0
4	C	147	0	0	16	0
4	D	46	0	0	9	0
4	E	3	0	0	1	0
4	F	5	0	0	0	0
4	G	7	0	0	0	0
4	H	2	0	0	0	0
4	I	17	0	0	0	0
4	J	9	0	0	0	0
4	K	8	0	0	1	0
4	L	6	0	0	2	0
All	All	27752	0	25068	1711	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 33.

The worst 5 of 1711 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:L:107:DG:C2'	2:L:108:DT:H71	1.77	1.14
1:G:12:DA:H2''	1:G:13:DG:H5'	1.30	1.14
3:D:14:SER:HA	3:D:32:GLU:HA	1.32	1.11
3:B:164:ILE:HD12	3:B:164:ILE:H	1.10	1.10
1:E:16:DG:H2''	1:E:17:DC:H5'	1.27	1.09

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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	852/903 (94%)	760 (89%)	76 (9%)	16 (2%)	12	37
3	B	763/903 (84%)	621 (81%)	110 (14%)	32 (4%)	4	13
3	C	849/903 (94%)	745 (88%)	74 (9%)	30 (4%)	6	18
3	D	661/903 (73%)	433 (66%)	155 (23%)	73 (11%)	1	1
All	All	3125/3612 (86%)	2559 (82%)	415 (13%)	151 (5%)	4	10

5 of 151 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	12	GLY
3	A	542	LEU
3	A	859	LYS
3	A	894	LYS
3	B	164	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	745/775 (96%)	701 (94%)	44 (6%)	28	62
3	B	663/775 (86%)	613 (92%)	50 (8%)	19	47
3	C	737/775 (95%)	689 (94%)	48 (6%)	24	57
3	D	453/775 (58%)	413 (91%)	40 (9%)	14	38
All	All	2598/3100 (84%)	2416 (93%)	182 (7%)	21	52

5 of 182 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	B	623	ASP
3	C	83	LEU
3	D	556	GLN
3	B	645	ASN
3	B	893	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 66 such sidechains are listed below:

Mol	Chain	Res	Type
3	B	556	GLN
3	C	112	ASN
3	D	333	GLN
3	B	676	ASN
3	C	10	GLN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

2 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	9,11,12	0.71	0	11,14,17	0.65	0
1	3DR	I	3	1	9,11,12	0.80	0	11,14,17	0.67	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
1	3DR	E	3	1	-	0/4/15/16	0/1/1/1
1	3DR	I	3	1	-	0/4/15/16	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.5 Carbohydrates ⓘ

There are no carbohydrates 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, 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	18/18 (100%)	0.44	0 100 100	57, 101, 126, 134	0
1	G	13/18 (72%)	1.14	2 (15%) 3 2	48, 103, 143, 144	0
1	I	18/18 (100%)	-0.20	0 100 100	27, 43, 112, 123	0
1	K	9/18 (50%)	1.41	4 (44%) 1 0	38, 140, 155, 159	0
2	F	15/15 (100%)	0.49	1 (6%) 17 16	77, 104, 136, 140	0
2	H	15/15 (100%)	1.18	3 (20%) 2 1	75, 118, 131, 139	0
2	J	15/15 (100%)	0.08	1 (6%) 17 16	28, 57, 97, 114	0
2	L	8/15 (53%)	2.44	7 (87%) 0 0	144, 148, 149, 149	0
3	A	856/903 (94%)	-0.04	16 (1%) 64 64	16, 40, 83, 138	0
3	B	771/903 (85%)	0.31	47 (6%) 21 20	19, 56, 112, 144	0
3	C	853/903 (94%)	0.01	10 (1%) 75 76	18, 46, 86, 120	0
3	D	671/903 (74%)	0.90	106 (15%) 3 2	70, 102, 134, 142	0
All	All	3262/3744 (87%)	0.27	197 (6%) 21 21	16, 56, 123, 159	0

The worst 5 of 197 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	216	TRP	7.1
3	D	394	ALA	6.6
3	D	309	ILE	6.3
3	D	450	PRO	6.0
3	D	771	PHE	5.4

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. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
1	3DR	E	3	11/12	0.36	2.63	117,125,130,133	0
1	3DR	I	3	11/12	0.25	0.55	101,102,103,103	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.