wwPDB X-ray Structure Validation Summary Report (i)

Oct 16, 2023 – 06:40 PM EDT

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.; Doublie, 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
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:

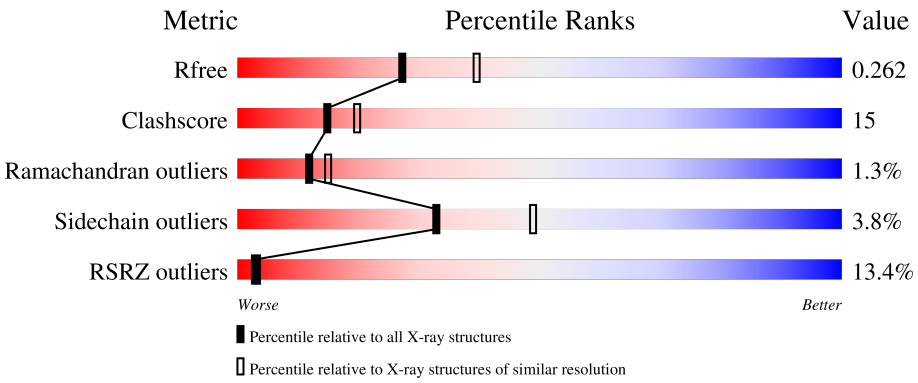
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 2.37 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}	130704	5509 (2.40-2.36)
Clashscore	141614	6082 (2.40-2.36)
Ramachandran outliers	138981	5973 (2.40-2.36)
Sidechain outliers	138945	5975 (2.40-2.36)
RSRZ outliers	127900	5397 (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 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	E	18	6%; 11%, 83%, 6%
1	G	18	6%; 28%, 50%, 17%, 6%
1	I	18	6%; 39%, 44%, 11%, 6%
1	K	18	17%; 28%, 67%, 6%
2	F	15	7%; 13%, 87%

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Mol	Chain	Length	Quality of chain
2	H	15	13% 13% 80% 7%
2	J	15	20% 40% 27% 13%
2	L	15	27% 100%
3	A	896	6% 74% 24%
3	B	896	17% 72% 26%
3	C	896	3% 76% 21%
3	D	896	28% 57% 39%

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*CP*AP*GP*CP*CP*GP*CP*G)-3'.

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

- 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
			Total	C	N	O	P			
2	F	15	308	147	60	87	14	0	0	0
2	H	15	308	147	60	87	14	0	0	0
2	J	15	308	147	60	87	14	0	0	0
2	L	15	308	147	60	87	14	0	0	0

- Molecule 3 is a protein called DNA polymerase.

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

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

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	222	ALA	ASP	engineered mutation	UNP Q38087
A	253	GLY	ILE	engineered mutation	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 mutation	UNP Q38087
B	222	ALA	ASP	engineered mutation	UNP Q38087
B	253	GLY	ILE	engineered mutation	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 mutation	UNP Q38087
C	222	ALA	ASP	engineered mutation	UNP Q38087
C	253	GLY	ILE	engineered mutation	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 mutation	UNP Q38087
D	222	ALA	ASP	engineered mutation	UNP Q38087
D	253	GLY	ILE	engineered mutation	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 mutation	UNP Q38087

- Molecule 4 is water.

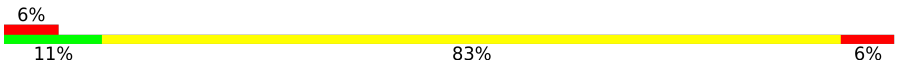
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	E	9	Total O 9 9	0	0
4	F	10	Total O 10 10	0	0
4	G	15	Total O 15 15	0	0
4	H	8	Total O 8 8	0	0
4	I	31	Total O 31 31	0	0
4	J	18	Total O 18 18	0	0
4	K	10	Total O 10 10	0	0
4	A	251	Total O 251 251	0	0
4	B	195	Total O 195 195	0	0
4	C	272	Total O 272 272	0	0
4	D	38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

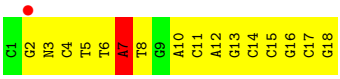
3 Residue-property plots (i)

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

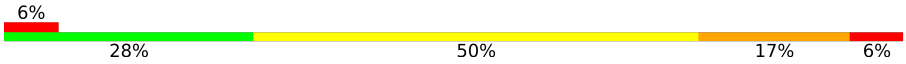
Chain E:

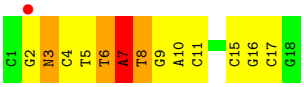




• Molecule 1: 5'-D(*CP*GP*(3DR)P*CP*TP*TP*AP*TP*GP*AP*CP*AP*GP*CP*CP*GP*CP*G)-3'

Chain G:



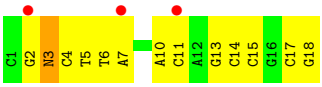


• Molecule 1: 5'-D(*CP*GP*(3DR)P*CP*TP*TP*AP*TP*GP*AP*CP*AP*GP*CP*CP*GP*CP*G)-3'

Chain I:

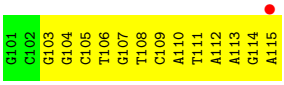
• Molecule 1: 5'-D(*CP*GP*(3DR)P*CP*TP*TP*AP*TP*GP*AP*CP*AP*GP*CP*CP*GP*CP*G)-3'

Chain K:



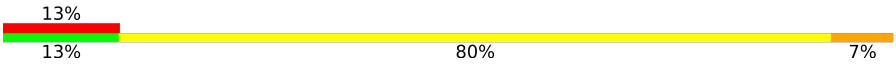
• Molecule 2: 5'-D(*GP*CP*GP*GP*CP*TP*GP*TP*CP*AP*TP*AP*AP*GP*A)-3'

Chain F:



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

Chain H:

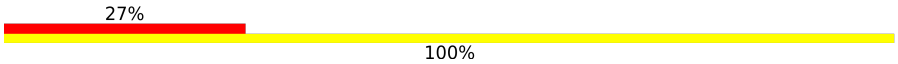


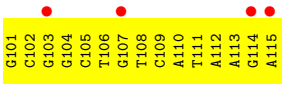
• Molecule 2: 5'-D(*GP*CP*GP*GP*CP*TP*GP*TP*CP*AP*TP*AP*AP*GP*A)-3'

Chain J:

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

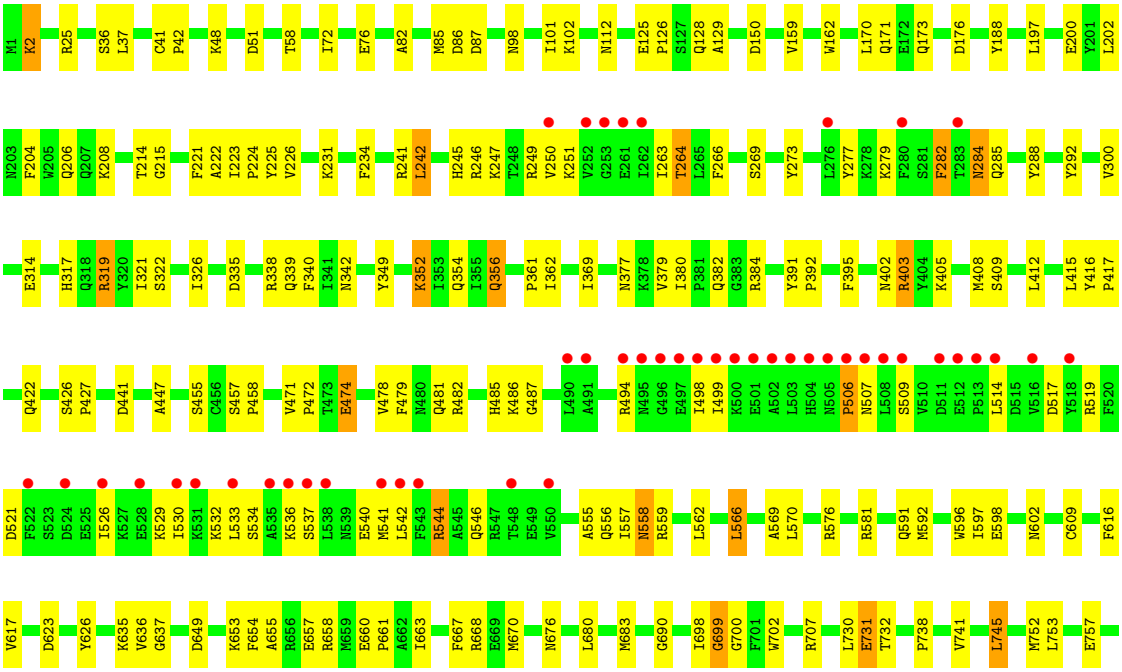
Chain L:





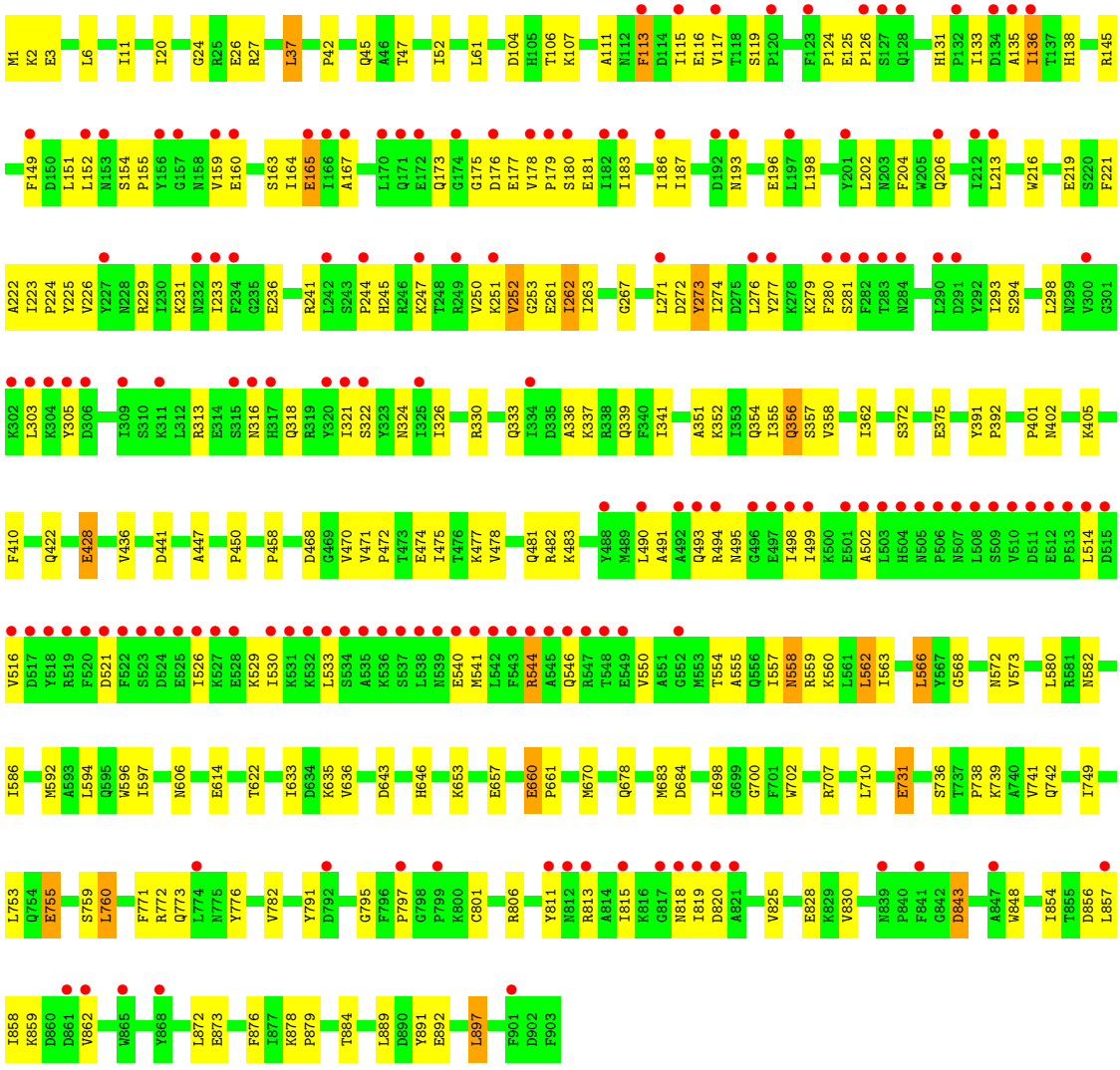
• Molecule 3: DNA polymerase

Chain A:



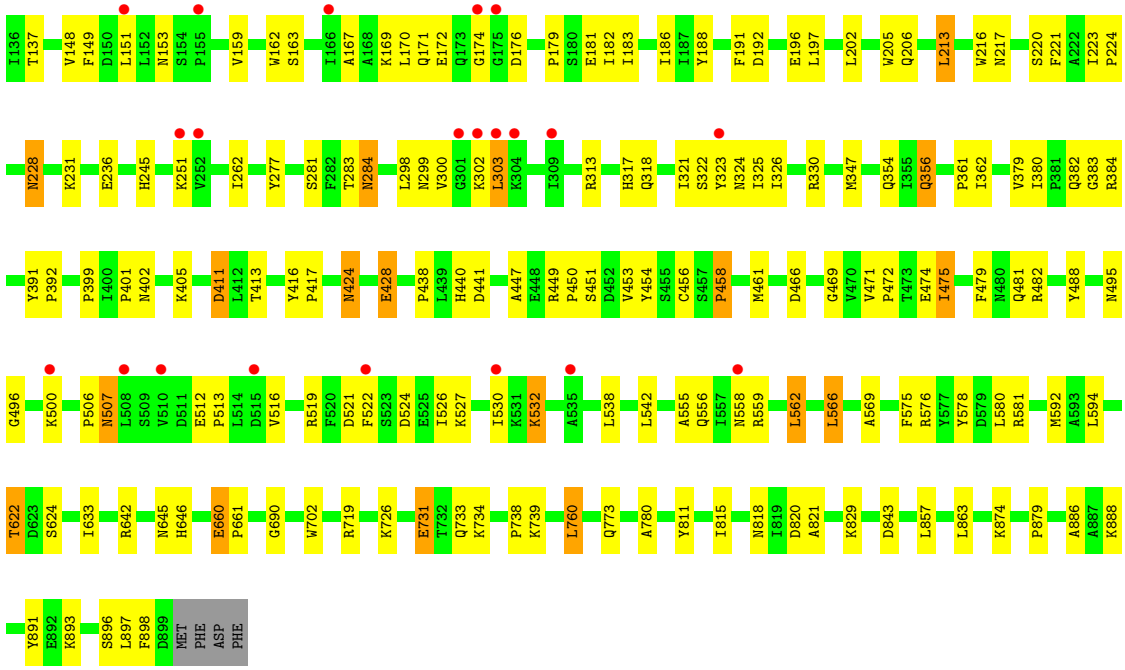
• Molecule 3: DNA polymerase

Chain B:



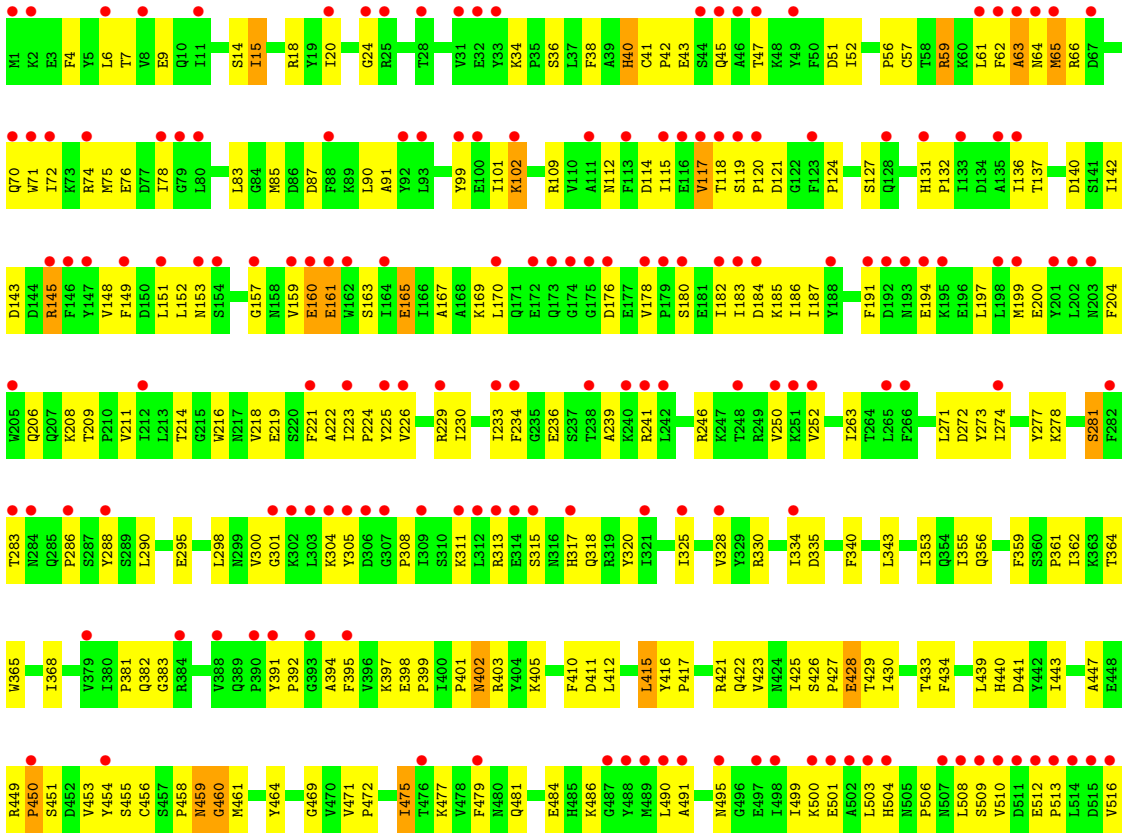
• Molecule 3: DNA polymerase

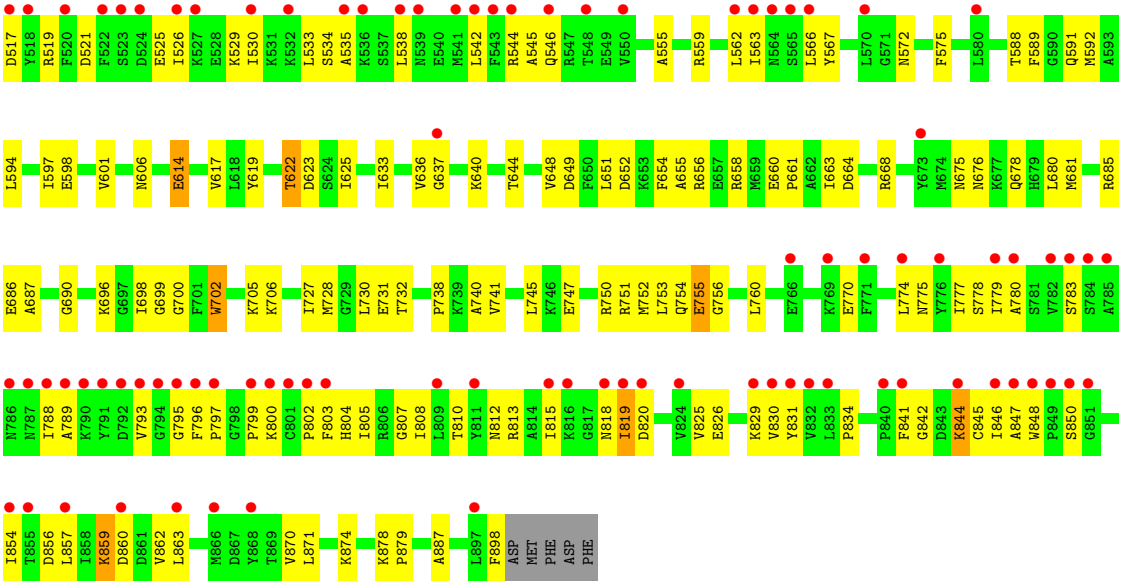
Chain C:



- Molecule 3: DNA polymerase

Chain D:




D517 Y518 R519 F520 D521 F522 S523 D524 E525 I526 K527 E528 K529 I530 K531 K532 L533 S534 A535 K536 S537 L538 N539 E540 M541 L542 F543 R544 A545 Q546 R547 T548 E549 V550 A555 R559 L562 I563 N564 S565 L566 Y567 L570 G571 N572 F575 L580 T588 F589 G590 Q591 M592 A593
L594 I597 E598 V601 N606 E614 V617 L618 Y619 T622 D623 S624 I625 I633 V636 G637 K640 T644 V648 D649 F650 L651 D652 K653 F654 A655 R656 E657 R658 M659 E660 P661 A662 I663 D664 R668 Y673 M674 N675 N676 K677 Q678 H679 L680 M681 R685
E686 A687 G690 K696 G697 I698 G699 G700 F701 W702 K705 K706 I727 M728 G729 L730 E731 T732 P738 K739 A740 V741 L745 K746 E747 R750 R751 M752 L753 Q754 E755 G756 L760 E766 K769 E770 F771 L774 N775 Y776 I777 S778 I779 A780 S781 V782 S783 S784 A785
N786 N787 I788 A789 K790 Y791 D792 V793 G794 G795 F796 P797 G798 P799 K800 C801 P802 F803 H804 I805 R806 G807 I808 L809 T810 Y811 N812 R813 A814 I815 K816 G817 N818 I819 D820 V824 V825 E826 K829 V830 Y831 V832 L833 P834 P840 F841 G842 D843 K844 C845 I846 A847 W848 P849 S850 G851
I854 T855 D856 L857 I858 K859 D860 D861 V862 L863 M866 D867 Y868 T869 V870 L871 K874 K878 P879 A887 L897 F898 ASP MET PHE ASP PHE

4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	1.92 (at 2.37Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.223 , 0.268 0.218 , 0.262	Depositor DCC
R_{free} test set	37523 reflections (9.47%)	wwPDB-VP
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
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	0.94	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.*

[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 (i)

5.1 Standard geometry (i)

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(^{o})	Ideal(^{o})
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 (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	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%)	25 34
3	B	894/896 (100%)	815 (91%)	69 (8%)	10 (1%)	14 18
3	C	890/896 (99%)	841 (94%)	45 (5%)	4 (0%)	34 46
3	D	889/896 (99%)	746 (84%)	116 (13%)	27 (3%)	4 3
All	All	3567/3584 (100%)	3240 (91%)	281 (8%)	46 (1%)	12 15

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 (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	785/793 (99%)	756 (96%)	29 (4%)	34	50
3	B	774/793 (98%)	750 (97%)	24 (3%)	40	57
3	C	781/793 (98%)	741 (95%)	40 (5%)	24	36
3	D	770/793 (97%)	746 (97%)	24 (3%)	40	57
All	All	3110/3172 (98%)	2993 (96%)	117 (4%)	33	49

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

Mol	Chain	Res	Type
3	C	128	GLN
3	D	649	ASP
3	C	440	HIS
3	D	614	GLU
3	D	161	GLU

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

Mol	Chain	Res	Type
3	C	481	GLN
3	D	206	GLN
3	C	507	ASN
3	C	818	ASN
3	D	285	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)

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	I	3	1	8,11,12	0.48	0	9,14,17	1.68	1 (11%)
1	3DR	K	3	1	8,11,12	0.50	0	9,14,17	1.61	1 (11%)
1	3DR	E	3	1	8,11,12	0.50	0	9,14,17	1.64	1 (11%)
1	3DR	G	3	1	8,11,12	0.53	0	9,14,17	1.81	1 (11%)

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

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	3	3DR	O3'-C3'-C2'	4.07	121.23	111.54
1	I	3	3DR	O3'-C3'-C2'	3.80	120.58	111.54
1	K	3	3DR	O3'-C3'-C2'	3.55	120.00	111.54
1	E	3	3DR	O3'-C3'-C2'	3.54	119.98	111.54

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	K	3	3DR	O4'-C4'-C5'-O5'

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	I	3	3DR	1	0
1	K	3	3DR	2	0
1	G	3	3DR	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	17/18 (94%)	0.21	1 (5%)	22	24	54, 75, 126, 146	0
1	G	17/18 (94%)	0.13	1 (5%)	22	24	45, 57, 133, 148	0
1	I	17/18 (94%)	0.08	1 (5%)	22	24	35, 42, 101, 115	0
1	K	17/18 (94%)	1.15	3 (17%)	1	1	45, 123, 161, 169	0
2	F	15/15 (100%)	0.58	1 (6%)	17	19	68, 99, 128, 141	0
2	H	15/15 (100%)	0.36	2 (13%)	3	3	56, 71, 126, 152	0
2	J	15/15 (100%)	0.08	0	100	100	38, 57, 91, 96	0
2	L	15/15 (100%)	1.46	4 (26%)	0	0	126, 131, 153, 157	0
3	A	896/896 (100%)	0.47	55 (6%)	21	23	30, 47, 125, 149	0
3	B	896/896 (100%)	1.00	155 (17%)	1	1	28, 62, 154, 165	0
3	C	892/896 (99%)	0.37	23 (2%)	56	57	23, 48, 83, 106	0
3	D	891/896 (99%)	1.50	251 (28%)	0	0	53, 117, 153, 160	0
All	All	3703/3716 (99%)	0.82	497 (13%)	3	3	23, 62, 148, 169	0

The worst 5 of 497 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	B	516	VAL	13.1
3	A	530	ILE	13.0
3	D	514	LEU	12.4
3	B	508	LEU	11.4
3	D	117	VAL	11.1

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	3DR	K	3	11/12	0.72	0.37	165,167,169,169	0
1	3DR	E	3	11/12	0.75	0.35	138,143,147,147	0
1	3DR	G	3	11/12	0.76	0.27	132,137,146,147	0
1	3DR	I	3	11/12	0.81	0.19	102,105,111,112	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.