



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 09:44 PM GMT

PDB ID : 1Q9X
Title : Crystal structure of Enterobacteria phage RB69 gp43 DNA polymerase complexed with tetrahydrofuran containing DNA
Authors : Freisinger, E.; Grollman, A.P.; Miller, H.; Kisker, C.
Deposited on : 2003-08-26
Resolution : 2.69 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

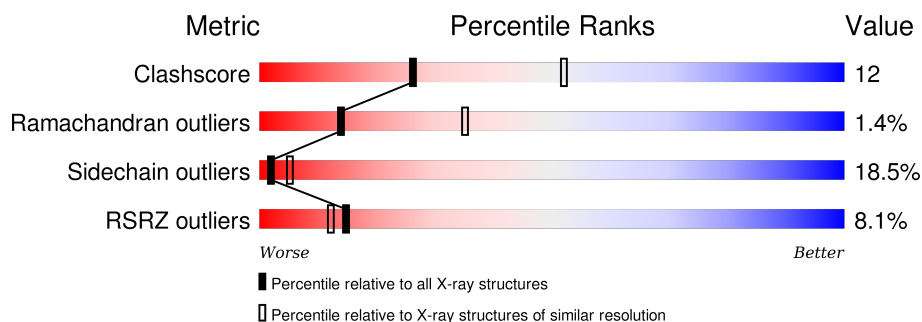
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.69 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))
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

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>33%</div> <div> <div>22%</div> <div>33%</div> <div>44%</div> </div> </div>
1	F	18	<div> <div>22%</div> <div> <div>33%</div> <div>33%</div> <div>33%</div> </div> </div>
1	G	18	<div> <div>17%</div> <div> <div>28%</div> <div>33%</div> <div>39%</div> </div> </div>
1	H	18	<div> <div>17%</div> <div> <div>33%</div> <div>44%</div> <div>22%</div> </div> </div>
2	I	13	<div> <div>23%</div> <div> <div>8%</div> <div>54%</div> <div>38%</div> </div> </div>
2	J	13	<div> <div>15%</div> <div> <div>31%</div> <div>38%</div> <div>31%</div> </div> </div>
2	K	13	<div> <div>8%</div> <div> <div>62%</div> <div>31%</div> </div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	L	13	
3	A	903	
3	B	903	
3	C	903	
3	D	903	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	DGP	F	908	-	-	-	X
5	DGP	G	908	-	-	-	X
5	DGP	H	908	-	-	-	X
5	DGP	K	955	-	-	-	X
5	DGP	L	955	-	-	-	X
6	3DR	F	912	-	-	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 32756 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'-GCGGACTGCTTAC(dideoxycytidine)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	18	Total	C	N	O	P	0	0	0
			370	175	74	104	17			
1	F	18	Total	C	N	O	P	0	0	0
			370	175	74	104	17			
1	G	18	Total	C	N	O	P	0	0	0
			370	175	74	104	17			
1	H	18	Total	C	N	O	P	0	0	0
			370	175	74	104	17			

- Molecule 2 is a DNA chain called 5'-AC(tetrahydrofuran)GGTAAGCAGTCCGCGG-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	I	13	Total	C	N	O	P	0	0	0
			263	126	48	77	12			
2	J	13	Total	C	N	O	P	0	0	0
			263	126	48	77	12			
2	K	13	Total	C	N	O	P	0	0	0
			263	126	48	77	12			
2	L	13	Total	C	N	O	P	0	0	0
			263	126	48	77	12			

- Molecule 3 is a protein called DNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	903	Total	C	N	O	S	0	0	0
			7365	4730	1226	1376	33			
3	B	903	Total	C	N	O	S	0	0	0
			7365	4730	1226	1376	33			
3	C	903	Total	C	N	O	S	0	0	0
			7365	4730	1226	1376	33			
3	D	903	Total	C	N	O	S	0	0	0
			7365	4730	1226	1376	33			

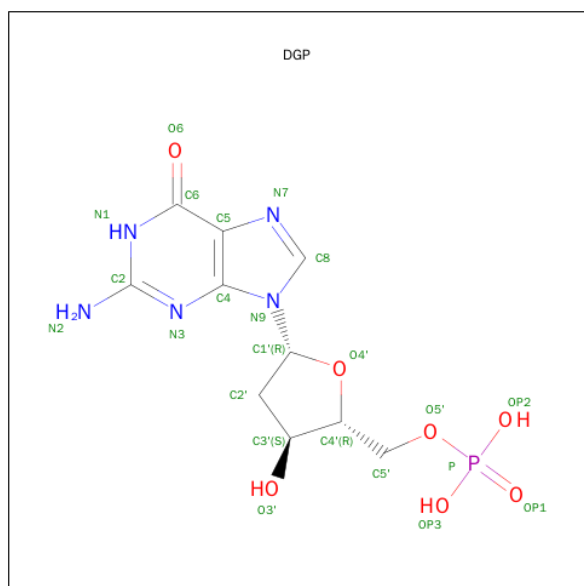
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	222	ALA	ASP	ENGINEERED	UNP Q38087
A	327	ALA	ASP	ENGINEERED	UNP Q38087
B	222	ALA	ASP	ENGINEERED	UNP Q38087
B	327	ALA	ASP	ENGINEERED	UNP Q38087
C	222	ALA	ASP	ENGINEERED	UNP Q38087
C	327	ALA	ASP	ENGINEERED	UNP Q38087
D	222	ALA	ASP	ENGINEERED	UNP Q38087
D	327	ALA	ASP	ENGINEERED	UNP Q38087

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

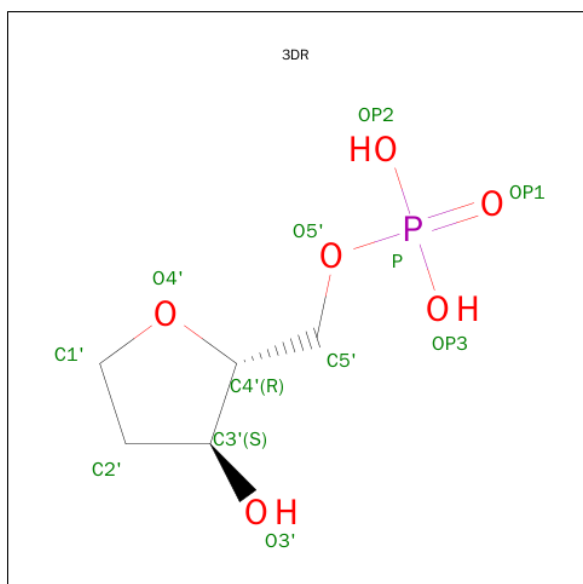
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	2	Total Ca 2 2	0	0
4	A	2	Total Ca 2 2	0	0
4	D	2	Total Ca 2 2	0	0
4	C	2	Total Ca 2 2	0	0

- Molecule 5 is 2'-DEOXYGUANOSINE-5'-MONOPHOSPHATE (three-letter code: DGP) (formula: C₁₀H₁₄N₅O₇P).



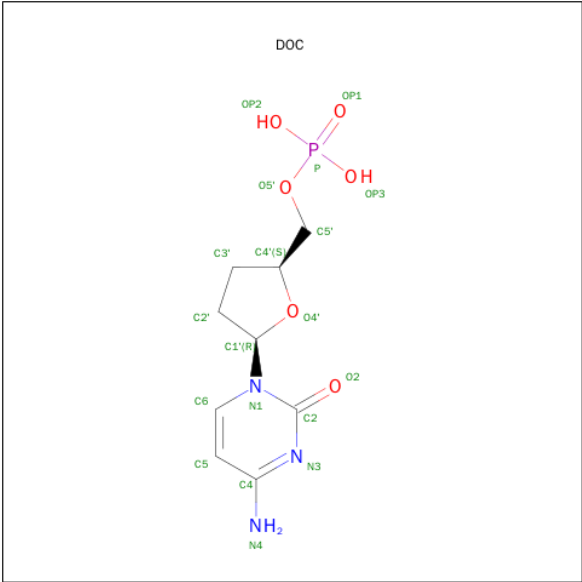
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	F	1	Total C N O 19 10 5 4	0	0
5	G	1	Total O 1 1	0	0
5	G	1	Total C N O P 22 10 5 6 1	0	0
5	H	1	Total C N O 19 10 5 4	0	0
5	K	1	Total C N O P 22 10 5 6 1	0	0
5	L	1	Total C N O P 22 10 5 6 1	0	0

- Molecule 6 is 1',2'-DIDEOXYRIBOFURANOSE-5'-PHOSPHATE (three-letter code: 3DR) (formula: C₅H₁₁O₆P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	E	1	Total C O P 11 5 5 1	0	0
6	F	1	Total C O P 11 5 5 1	0	0
6	G	1	Total C O P 11 5 5 1	0	0
6	H	1	Total C O P 11 5 5 1	0	0

- Molecule 7 is 2',3'-Dideoxycytidine-5'-monophosphate (three-letter code: DOC) (formula: C₉H₁₄N₃O₆P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	I	1	Total	C	N	O	P	0	0
			18	9	3	5	1		
7	J	1	Total	C	N	O	P	0	0
			18	9	3	5	1		
7	K	1	Total	C	N	O	P	0	0
			18	9	3	5	1		
7	L	1	Total	C	N	O	P	0	0
			18	9	3	5	1		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	112	Total	O	0	0
			112	112		
8	B	129	Total	O	0	0
			129	129		
8	C	126	Total	O	0	0
			126	126		
8	D	111	Total	O	0	0
			111	111		
8	E	11	Total	O	0	0
			11	11		
8	F	8	Total	O	0	0
			8	8		
8	G	7	Total	O	0	0
			7	7		
8	H	8	Total	O	0	0
			8	8		

Continued on next page...

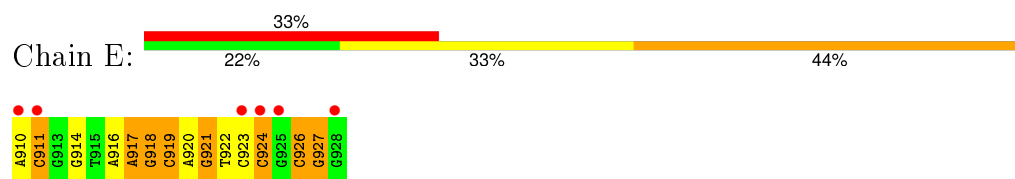
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	I	11	Total 11	O 11	0	0
8	J	6	Total 6	O 6	0	0
8	K	3	Total 3	O 3	0	0
8	L	3	Total 3	O 3	0	0

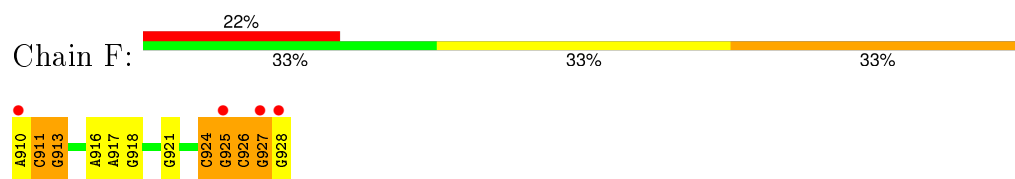
3 Residue-property plots [i](#)

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.

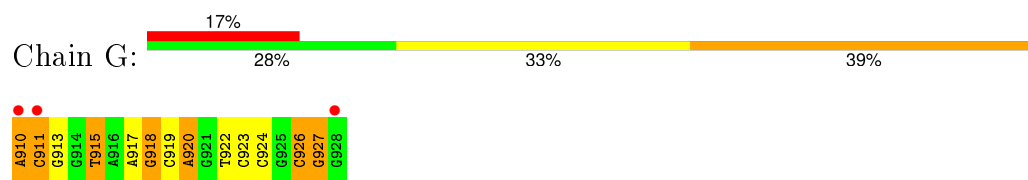
- Molecule 1: 5'-GCGGACTGCTTAC(dideoxycytidine)-3'



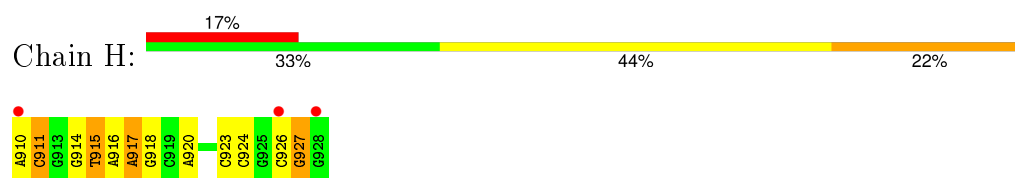
- Molecule 1: 5'-GCGGACTGCTTAC(dideoxycytidine)-3'



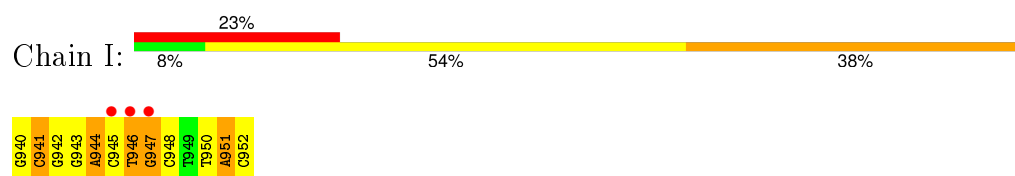
- Molecule 1: 5'-GCGGACTGCTTAC(dideoxycytidine)-3'



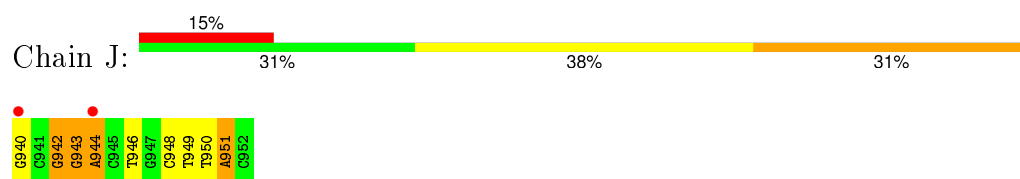
- Molecule 1: 5'-GCGGACTGCTTAC(dideoxycytidine)-3'



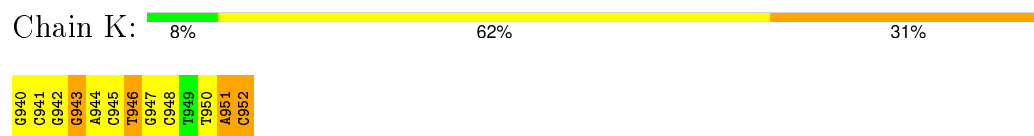
- Molecule 2: 5'-AC(tetrahydrofuran)GGTAAGCAGTCCGCGG-3'



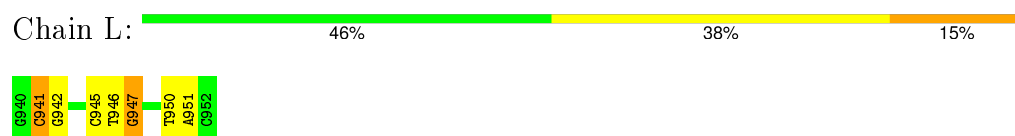
- Molecule 2: 5'-AC(tetrahydrofuran)GGTAAGCAGTCCGCGG-3'



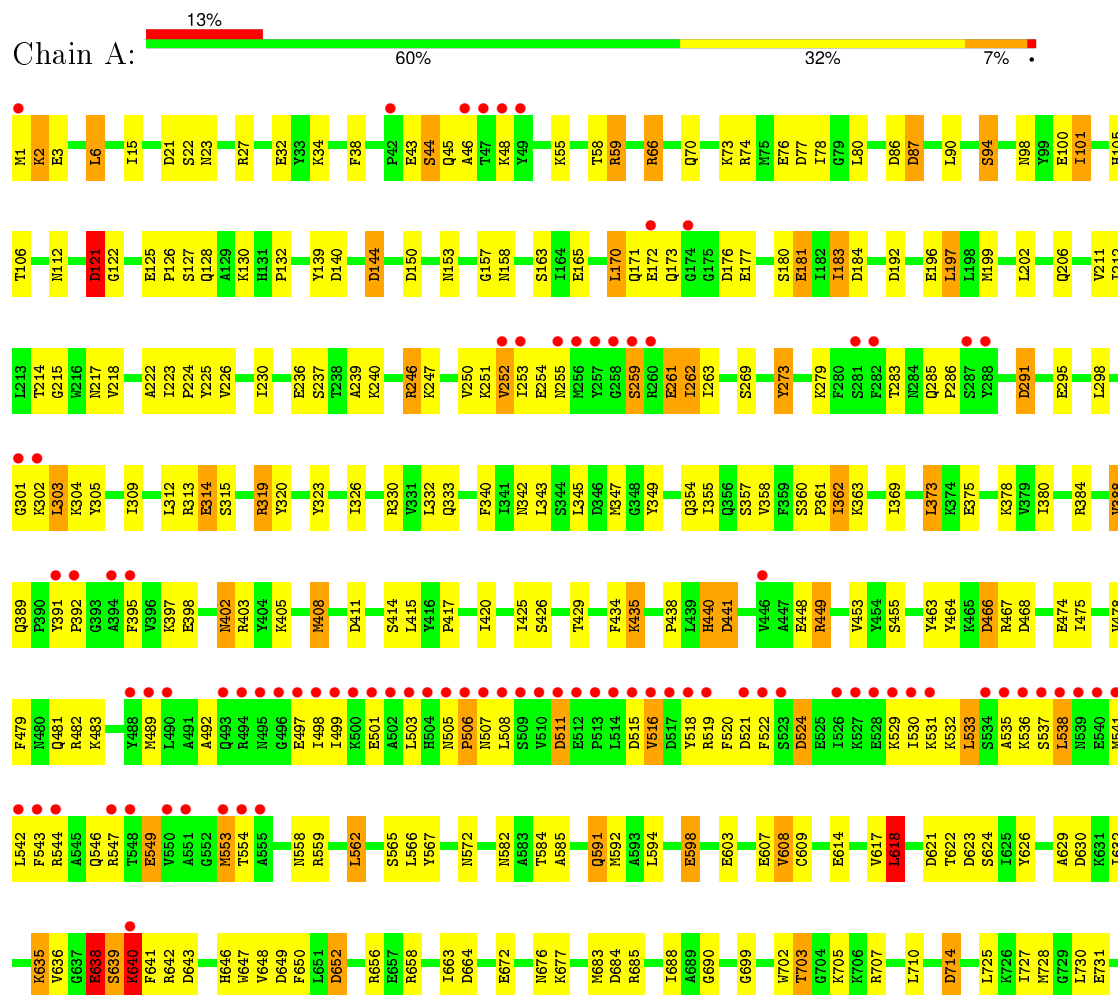
- Molecule 2: 5'-AC(tetrahydrofuran)GGTAAGCAGTCCGCGG-3'

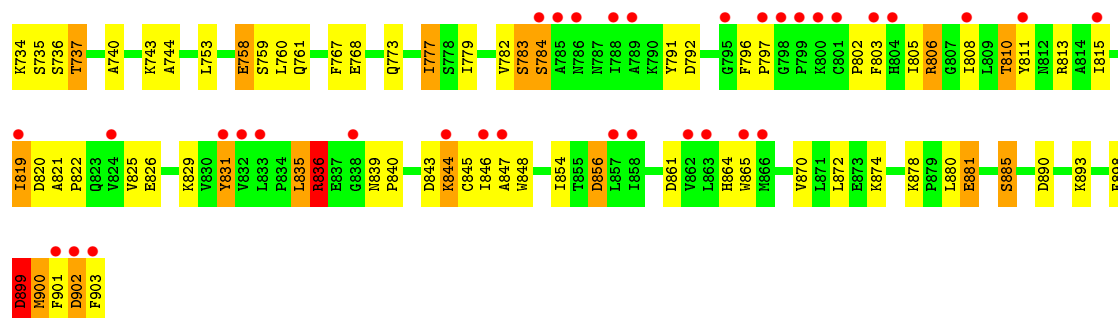


- Molecule 2: 5'-AC(tetrahydrofuran)GGTAAGCAGTCCGCGG-3'

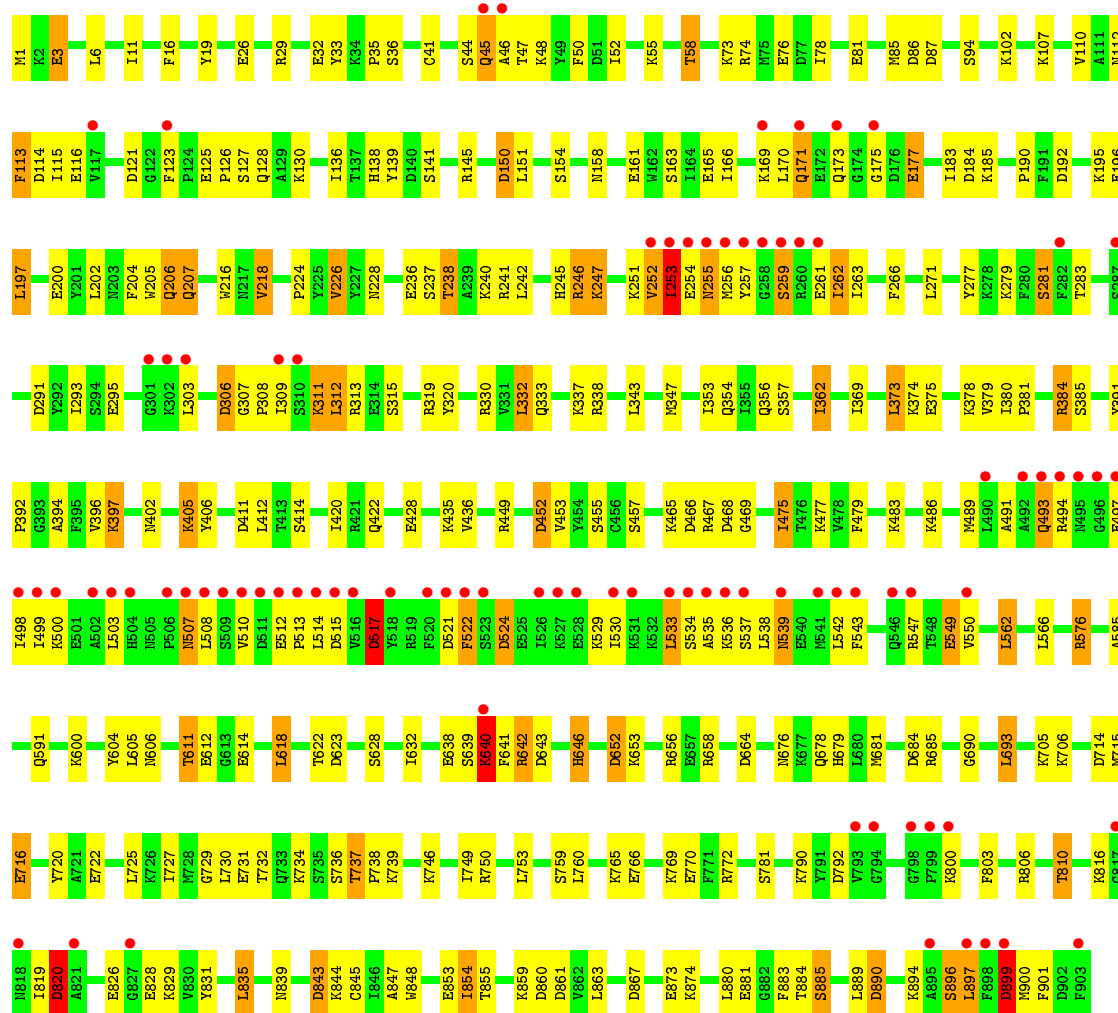


- Molecule 3: DNA polymerase

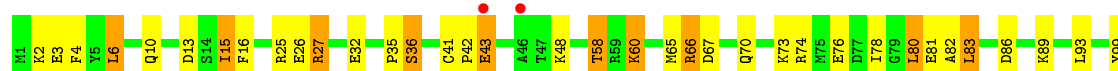


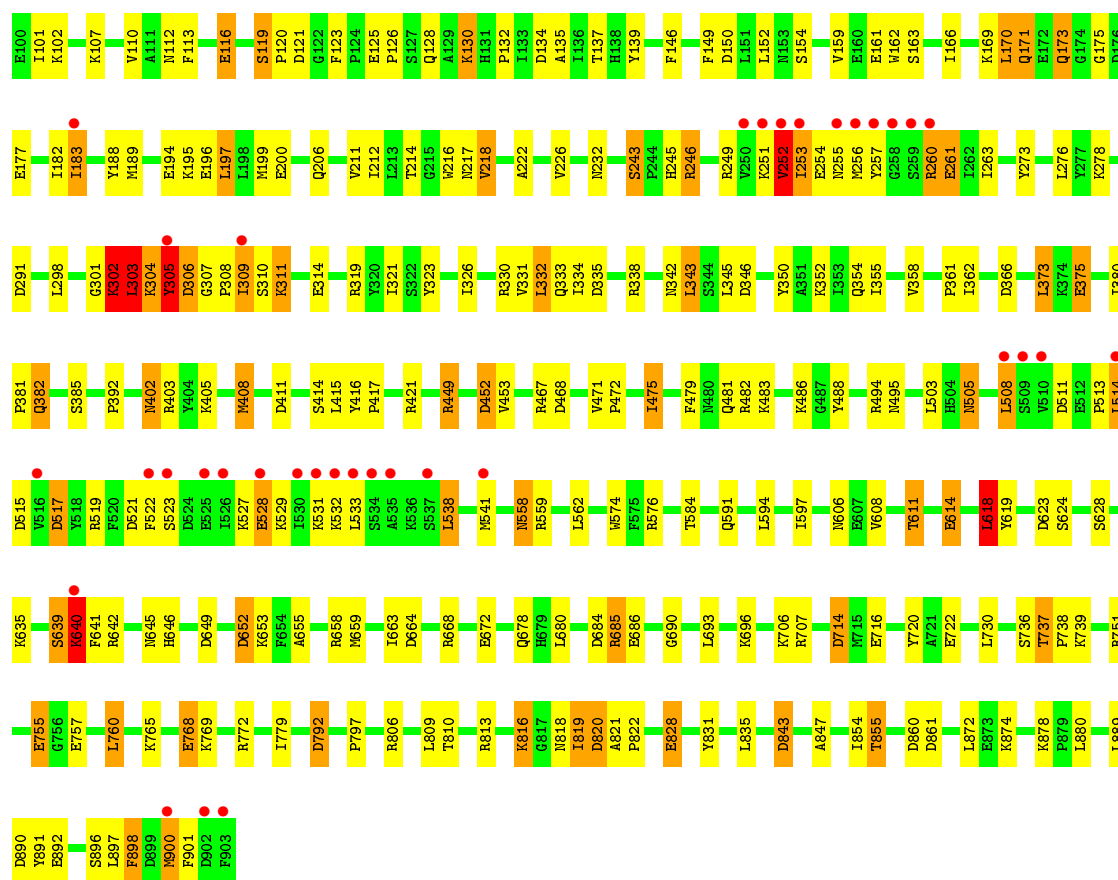


• Molecule 3: DNA polymerase

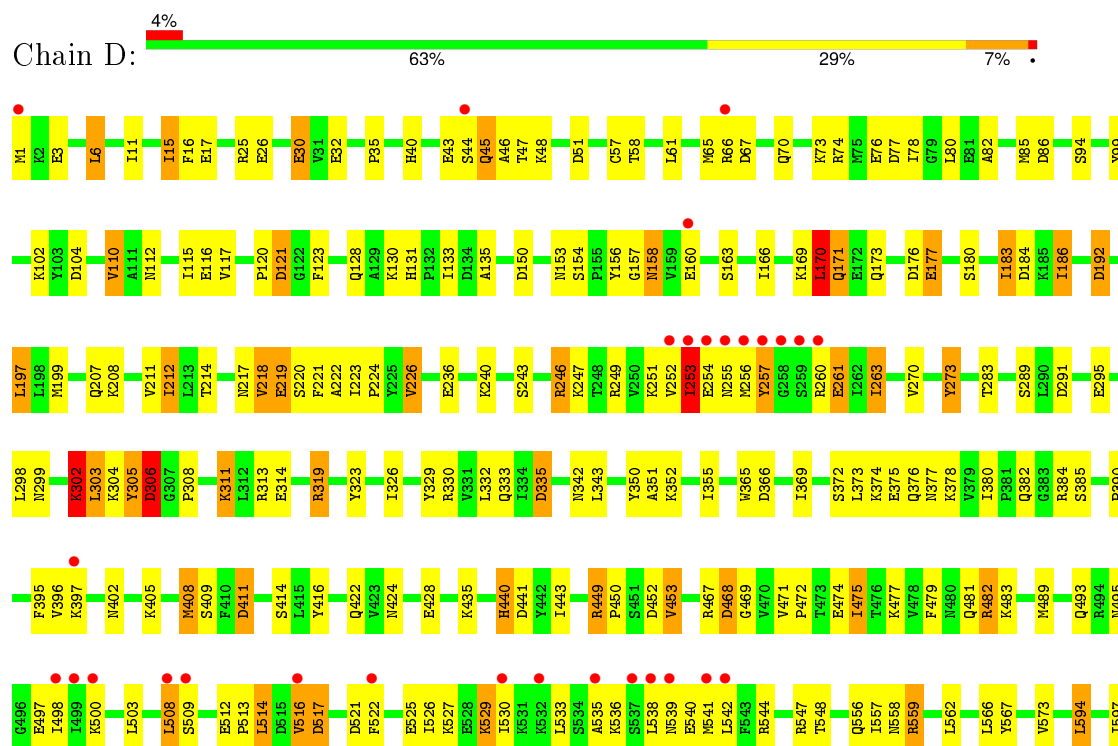


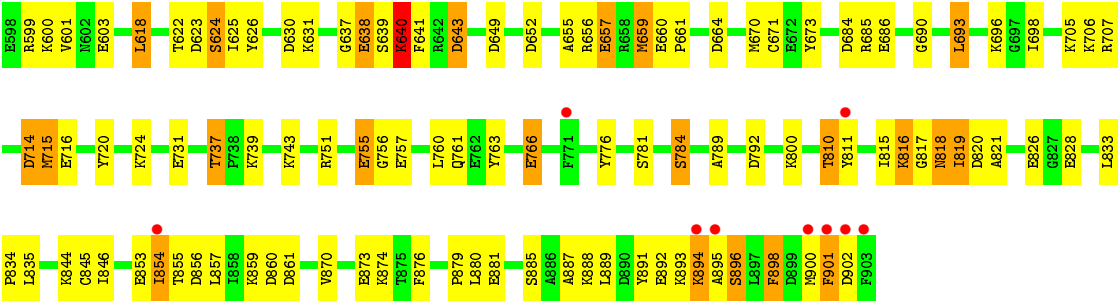
• Molecule 3: DNA polymerase





• 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	131.95Å 122.24Å 165.36Å 90.00° 96.85° 90.00°	Depositor
Resolution (Å)	47.00 – 2.69 45.07 – 2.70	Depositor EDS
% Data completeness (in resolution range)	94.7 (47.00-2.69) 95.1 (45.07-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.48 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.215 , 0.288 (Not available) , (Not available)	Depositor DCC
R_{free} test set	NotAvailable	DCC
Wilson B-factor (Å ²)	58.9	Xtriage
Anisotropy	0.324	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 57.9	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 135577 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	32756	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.88% 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: DOC, CA, DGP, 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	1.19	0/415	2.02	23/637 (3.6%)
1	F	1.07	0/415	1.77	8/637 (1.3%)
1	G	1.28	2/415 (0.5%)	2.14	18/637 (2.8%)
1	H	1.43	4/415 (1.0%)	1.90	13/637 (2.0%)
2	I	1.06	0/294	1.78	9/452 (2.0%)
2	J	1.15	0/294	1.90	7/452 (1.5%)
2	K	1.20	0/294	1.89	9/452 (2.0%)
2	L	1.25	1/294 (0.3%)	1.84	6/452 (1.3%)
3	A	0.56	0/7545	0.83	32/10196 (0.3%)
3	B	0.62	0/7545	0.83	28/10196 (0.3%)
3	C	0.65	0/7545	0.87	26/10196 (0.3%)
3	D	0.60	0/7545	0.83	27/10196 (0.3%)
All	All	0.68	7/33016 (0.0%)	0.99	206/45140 (0.5%)

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
3	B	0	1
3	C	0	1
All	All	0	2

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	926	DC	C4-C5	9.24	1.50	1.43
1	G	926	DC	C4-C5	6.59	1.48	1.43
1	H	926	DC	N1-C2	6.51	1.46	1.40
1	H	926	DC	N1-C6	6.47	1.41	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	926	DC	N1-C2	5.28	1.45	1.40

The worst 5 of 206 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	911	DC	C1'-O4'-C4'	-13.14	96.96	110.10
1	G	911	DC	O4'-C1'-N1	12.56	116.80	108.00
1	E	918	DG	O4'-C1'-N9	12.30	116.61	108.00
2	K	943	DG	O4'-C1'-N9	11.64	116.15	108.00
1	E	919	DC	O4'-C1'-N1	10.99	115.69	108.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	B	640	LYS	Peptide
3	C	252	VAL	Peptide

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	370	0	202	16	0
1	F	370	0	202	13	0
1	G	370	0	202	11	0
1	H	370	0	202	10	0
2	I	263	0	147	16	0
2	J	263	0	147	9	0
2	K	263	0	147	6	0
2	L	263	0	147	3	0
3	A	7365	0	7257	191	0
3	B	7365	0	7258	158	0
3	C	7365	0	7258	172	0
3	D	7365	0	7258	188	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	2	0	0	0	0
5	F	19	0	12	0	0
5	G	23	0	12	2	0
5	H	19	0	12	3	0
5	K	22	0	12	1	0
5	L	22	0	12	1	0
6	E	11	0	8	1	0
6	F	11	0	8	3	0
6	G	11	0	8	3	0
6	H	11	0	8	0	0
7	I	18	0	12	2	0
7	J	18	0	12	1	0
7	K	18	0	12	1	0
7	L	18	0	12	0	0
8	A	112	0	0	16	0
8	B	129	0	0	18	0
8	C	126	0	0	21	0
8	D	111	0	0	18	0
8	E	11	0	0	3	0
8	F	8	0	0	0	0
8	G	7	0	0	2	0
8	H	8	0	0	2	0
8	I	11	0	0	3	0
8	J	6	0	0	0	0
8	K	3	0	0	0	0
8	L	3	0	0	0	0
All	All	32756	0	30567	769	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 12.

The worst 5 of 769 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:253:ILE:HG22	3:A:261:GLU:HB3	1.28	1.13
3:C:514:LEU:H	3:C:541:MET:HE2	1.11	1.12
3:C:171:GLN:NE2	3:C:177:GLU:HB2	1.66	1.10
3:C:89:LYS:HE2	3:C:354:GLN:HE22	1.13	1.06
3:A:253:ILE:HG22	3:A:261:GLU:CB	1.91	1.01

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	901/903 (100%)	805 (89%)	81 (9%)	15 (2%)	11	29
3	B	901/903 (100%)	830 (92%)	62 (7%)	9 (1%)	19	45
3	C	901/903 (100%)	827 (92%)	60 (7%)	14 (2%)	12	30
3	D	901/903 (100%)	823 (91%)	64 (7%)	14 (2%)	12	30
All	All	3604/3612 (100%)	3285 (91%)	267 (7%)	52 (1%)	14	35

5 of 52 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	22	SER
3	A	45	GLN
3	A	639	SER
3	A	640	LYS
3	A	902	ASP

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	A	798/800 (100%)	636 (80%)	162 (20%)	1	4
3	B	798/800 (100%)	640 (80%)	158 (20%)	1	4
3	C	798/800 (100%)	669 (84%)	129 (16%)	3	7
3	D	798/800 (100%)	656 (82%)	142 (18%)	2	5
All	All	3192/3200 (100%)	2601 (82%)	591 (18%)	2	5

5 of 591 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	B	536	LYS
3	C	43	GLU
3	D	529	LYS
3	B	576	ARG
3	B	810	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 78 such sidechains are listed below:

Mol	Chain	Res	Type
3	B	646	HIS
3	C	158	ASN
3	D	546	GLN
3	B	761	GLN
3	C	98	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 22 ligands modelled in this entry, 8 are monoatomic and 1 is modelled with single atom - leaving 13 for Mogul analysis.

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
6	3DR	E	912	1	7,11,12	0.66	0	8,14,17	0.70	0
5	DGP	F	908	-	17,21,25	1.29	1 (5%)	20,31,38	2.43	4 (20%)
6	3DR	F	912	1	7,11,12	0.49	0	8,14,17	0.74	0
5	DGP	G	908	5,4	16,24,25	1.39	3 (18%)	20,35,38	2.56	6 (30%)
6	3DR	G	912	1	7,11,12	0.86	0	8,14,17	1.08	1 (12%)
5	DGP	H	908	-	17,21,25	1.48	3 (17%)	20,31,38	2.64	8 (40%)
6	3DR	H	912	1	7,11,12	0.66	0	8,14,17	0.75	0
7	DOC	I	953	2	11,19,20	0.89	0	14,26,29	1.38	2 (14%)
7	DOC	J	953	2	11,19,20	0.90	0	14,26,29	1.29	2 (14%)
7	DOC	K	953	2	11,19,20	0.72	0	14,26,29	1.68	3 (21%)
5	DGP	K	955	-	16,24,25	1.35	1 (6%)	20,35,38	2.86	7 (35%)
7	DOC	L	953	2	11,19,20	0.99	0	14,26,29	1.47	2 (14%)
5	DGP	L	955	-	16,24,25	1.30	2 (12%)	20,35,38	2.55	6 (30%)

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
6	3DR	E	912	1	-	0/3/15/16	0/1/1/1
5	DGP	F	908	-	-	0/2/18/22	0/3/3/3
6	3DR	F	912	1	-	0/3/15/16	0/1/1/1
5	DGP	G	908	5,4	-	0/3/21/22	0/3/3/3
6	3DR	G	912	1	-	0/3/15/16	0/1/1/1
5	DGP	H	908	-	-	0/2/18/22	0/3/3/3
6	3DR	H	912	1	-	0/3/15/16	0/1/1/1
7	DOC	I	953	2	-	0/3/18/19	0/2/2/2
7	DOC	J	953	2	-	0/3/18/19	0/2/2/2
7	DOC	K	953	2	-	0/3/18/19	0/2/2/2
5	DGP	K	955	-	-	0/3/21/22	0/3/3/3
7	DOC	L	953	2	-	0/3/18/19	0/2/2/2
5	DGP	L	955	-	-	0/3/21/22	0/3/3/3

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	G	908	DGP	C8-N7	-2.36	1.30	1.34
5	H	908	DGP	C8-N7	-2.26	1.30	1.34
5	L	955	DGP	C8-N7	-2.24	1.30	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	H	908	DGP	C4-N3	2.16	1.39	1.35
5	G	908	DGP	C4-N3	2.42	1.39	1.35

The worst 5 of 41 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	955	DGP	C5-C6-N1	-7.72	113.03	123.59
5	H	908	DGP	C5-C6-N1	-7.40	113.47	123.59
5	F	908	DGP	C5-C6-N1	-7.21	113.74	123.59
5	K	955	DGP	C5-C6-N1	-7.04	113.97	123.59
5	G	908	DGP	C5-C6-N1	-6.90	114.16	123.59

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	E	912	3DR	1	0
6	F	912	3DR	3	0
5	G	908	DGP	1	0
6	G	912	3DR	3	0
5	H	908	DGP	3	0
7	I	953	DOC	2	0
7	J	953	DOC	1	0
7	K	953	DOC	1	0
5	K	955	DGP	1	0
5	L	955	DGP	1	0

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 [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(Å²)	Q<0.9	
1	E	18/18 (100%)	1.95	6 (33%)	0	0	76, 92, 130, 152	0
1	F	18/18 (100%)	1.44	4 (22%)	1	1	39, 75, 149, 176	0
1	G	18/18 (100%)	0.75	3 (16%)	2	2	36, 54, 90, 102	0
1	H	18/18 (100%)	0.85	3 (16%)	2	2	44, 67, 128, 131	0
2	I	13/13 (100%)	1.41	3 (23%)	1	1	77, 95, 100, 102	0
2	J	13/13 (100%)	0.62	2 (15%)	3	2	41, 68, 121, 135	0
2	K	13/13 (100%)	-0.07	0	100	100	36, 55, 77, 83	0
2	L	13/13 (100%)	0.21	0	100	100	43, 65, 95, 102	0
3	A	903/903 (100%)	0.96	119 (13%)	4	4	30, 64, 147, 260	0
3	B	903/903 (100%)	0.56	86 (9%)	10	8	30, 53, 121, 222	0
3	C	903/903 (100%)	0.18	37 (4%)	41	41	28, 47, 88, 138	0
3	D	903/903 (100%)	0.38	38 (4%)	40	39	30, 57, 93, 170	0
All	All	3736/3736 (100%)	0.53	301 (8%)	15	12	28, 56, 113, 260	0

The worst 5 of 301 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	508	LEU	16.0
3	A	514	LEU	15.3
3	A	509	SER	15.0
3	A	503	LEU	13.6
3	A	510	VAL	12.9

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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
5	DGP	K	955	22/23	0.58	0.64	9.48	51,60,71,72	15
5	DGP	F	908	19/23	0.77	0.45	9.41	72,75,81,81	0
5	DGP	H	908	19/23	0.81	0.42	7.55	69,71,75,75	0
5	DGP	G	908	22/23	0.78	0.38	7.52	70,72,83,85	0
5	DGP	L	955	22/23	0.62	0.47	4.24	58,66,76,76	15
6	3DR	F	912	11/12	0.91	0.26	2.26	57,59,74,77	0
6	3DR	E	912	11/12	0.76	0.34	1.81	92,98,109,109	0
6	3DR	H	912	11/12	0.91	0.26	1.81	61,66,81,82	0
6	3DR	G	912	11/12	0.92	0.23	0.46	51,55,68,71	0
7	DOC	K	953	18/19	0.97	0.13	-0.44	32,36,40,40	0
7	DOC	I	953	18/19	0.93	0.17	-1.06	74,81,85,89	0
7	DOC	J	953	18/19	0.97	0.10	-1.36	39,42,46,46	0
4	CA	C	1006	1/1	0.87	0.08	-1.69	57,57,57,57	0
7	DOC	L	953	18/19	0.97	0.10	-1.99	39,43,51,52	0
4	CA	A	1002	1/1	0.99	0.05	-4.06	67,67,67,67	0
4	CA	A	1001	1/1	0.80	0.12	-	91,91,91,91	0
4	CA	D	1007	1/1	0.93	0.07	-	55,55,55,55	0
4	CA	C	1005	1/1	0.85	0.19	-	75,75,75,75	0
4	CA	B	1003	1/1	0.88	0.11	-	54,54,54,54	0
5	DGP	G	907	1/23	0.93	0.59	-	84,84,84,84	0
4	CA	B	1004	1/1	0.56	0.14	-	96,96,96,96	0
4	CA	D	1008	1/1	0.64	0.22	-	79,79,79,79	0

6.5 Other polymers ⓘ

There are no such residues in this entry.