



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 12:41 PM GMT

PDB ID : 3RMB  
Title : Crystal Structure of a replicative DNA polymerase bound to DNA containing  
Thymine Glycol  
Authors : Aller, P.; Duclos, S.; Wallace, S.S.; Doublié, S.  
Deposited on : 2011-04-20  
Resolution : 2.65 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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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

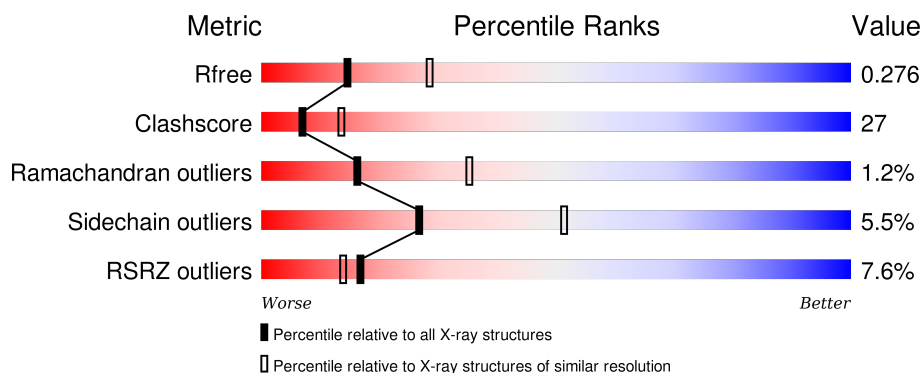
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.65 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	3152 (2.70-2.62)
Clashscore	102246	3524 (2.70-2.62)
Ramachandran outliers	100387	3469 (2.70-2.62)
Sidechain outliers	100360	3469 (2.70-2.62)
RSRZ outliers	91569	3161 (2.70-2.62)

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  $\geq 3$ , 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	A	906	<div> <div>7%</div> <div>53%</div> <div>42%</div> <div>5%</div> </div>
1	B	906	<div> <div>8%</div> <div>59%</div> <div>38%</div> <div>.</div> </div>
1	C	906	<div> <div>%</div> <div>61%</div> <div>36%</div> <div>..</div> </div>
1	D	906	<div> <div>15%</div> <div>49%</div> <div>47%</div> <div>..</div> </div>
2	E	18	<div> <div>6%</div> <div>11%</div> <div>89%</div> </div>

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Mol	Chain	Length	Quality of chain
2	G	18	 22% 78%
2	I	18	 44% 56%
2	K	18	 11% 39% 61%
3	F	14	 21% 79%
3	H	14	 14% 86%
3	J	14	 29% 71%
3	L	14	 7% 21% 93%

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 32166 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 protein called DNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	903	Total	C	N	O	S	4	0	0
			7342	4715	1220	1374	33			
1	B	903	Total	C	N	O	S	0	0	0
			7294	4686	1209	1366	33			
1	C	900	Total	C	N	O	S	0	0	0
			7332	4706	1220	1373	33			
1	D	897	Total	C	N	O	S	0	0	0
			7097	4558	1163	1344	32			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	222	ALA	ASP	ENGINEERED MUTATION	UNP Q38087
A	327	ALA	ASP	ENGINEERED MUTATION	UNP Q38087
A	904	HIS	-	EXPRESSION TAG	UNP Q38087
A	905	HIS	-	EXPRESSION TAG	UNP Q38087
A	906	HIS	-	EXPRESSION TAG	UNP Q38087
B	222	ALA	ASP	ENGINEERED MUTATION	UNP Q38087
B	327	ALA	ASP	ENGINEERED MUTATION	UNP Q38087
B	904	HIS	-	EXPRESSION TAG	UNP Q38087
B	905	HIS	-	EXPRESSION TAG	UNP Q38087
B	906	HIS	-	EXPRESSION TAG	UNP Q38087
C	222	ALA	ASP	ENGINEERED MUTATION	UNP Q38087
C	327	ALA	ASP	ENGINEERED MUTATION	UNP Q38087
C	904	HIS	-	EXPRESSION TAG	UNP Q38087
C	905	HIS	-	EXPRESSION TAG	UNP Q38087
C	906	HIS	-	EXPRESSION TAG	UNP Q38087
D	222	ALA	ASP	ENGINEERED MUTATION	UNP Q38087
D	327	ALA	ASP	ENGINEERED MUTATION	UNP Q38087
D	904	HIS	-	EXPRESSION TAG	UNP Q38087
D	905	HIS	-	EXPRESSION TAG	UNP Q38087
D	906	HIS	-	EXPRESSION TAG	UNP Q38087

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	18	Total	C	N	O	P	0	0	0
			369	174	72	106	17			
2	G	18	Total	C	N	O	P	0	0	0
			369	174	72	106	17			
2	I	18	Total	C	N	O	P	0	0	0
			369	174	72	106	17			
2	K	18	Total	C	N	O	P	0	0	0
			369	174	72	106	17			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	14	Total	C	N	O	P	0	0	0
			280	134	50	83	13			
3	H	14	Total	C	N	O	P	0	0	0
			280	134	50	83	13			
3	J	14	Total	C	N	O	P	0	0	0
			280	134	50	83	13			
3	L	14	Total	C	N	O	P	0	0	0
			280	134	50	83	13			

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



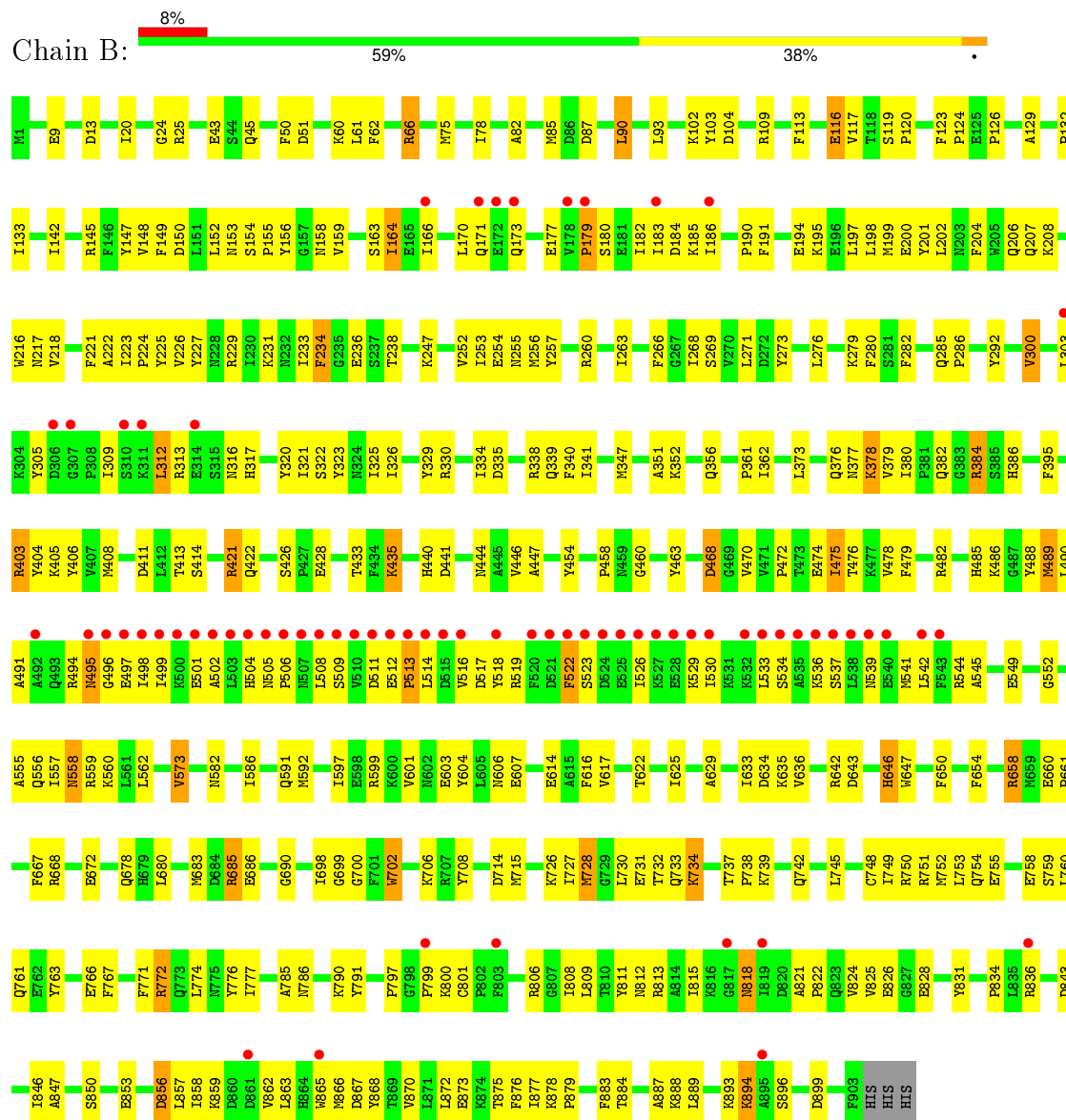
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total O S 5 4 1	0	0

- Molecule 5 is water.

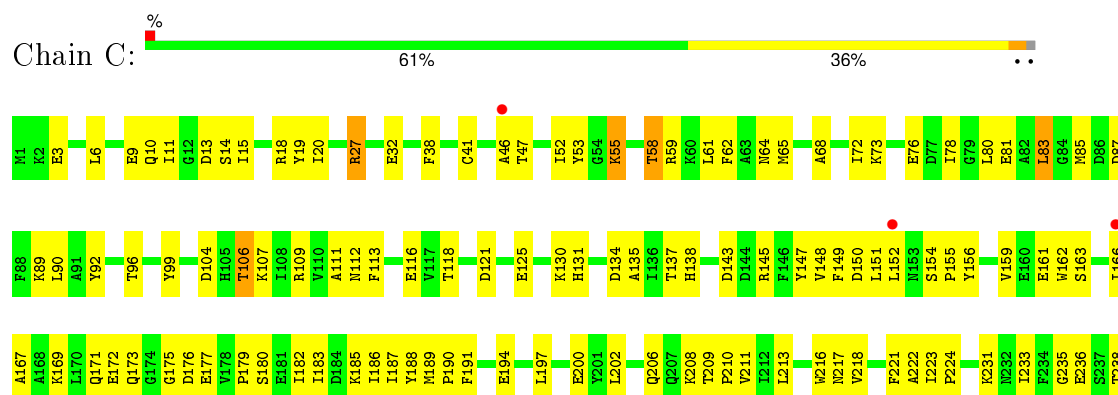
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	111	Total O 111 111	0	0
5	B	129	Total O 129 129	0	0
5	C	178	Total O 178 178	0	0
5	D	33	Total O 33 33	0	0
5	E	5	Total O 5 5	0	0
5	F	4	Total O 4 4	0	0
5	G	11	Total O 11 11	0	0
5	H	4	Total O 4 4	0	0
5	I	13	Total O 13 13	0	0
5	J	7	Total O 7 7	0	0
5	K	3	Total O 3 3	0	0
5	L	2	Total O 2 2	0	0



• Molecule 1: DNA polymerase

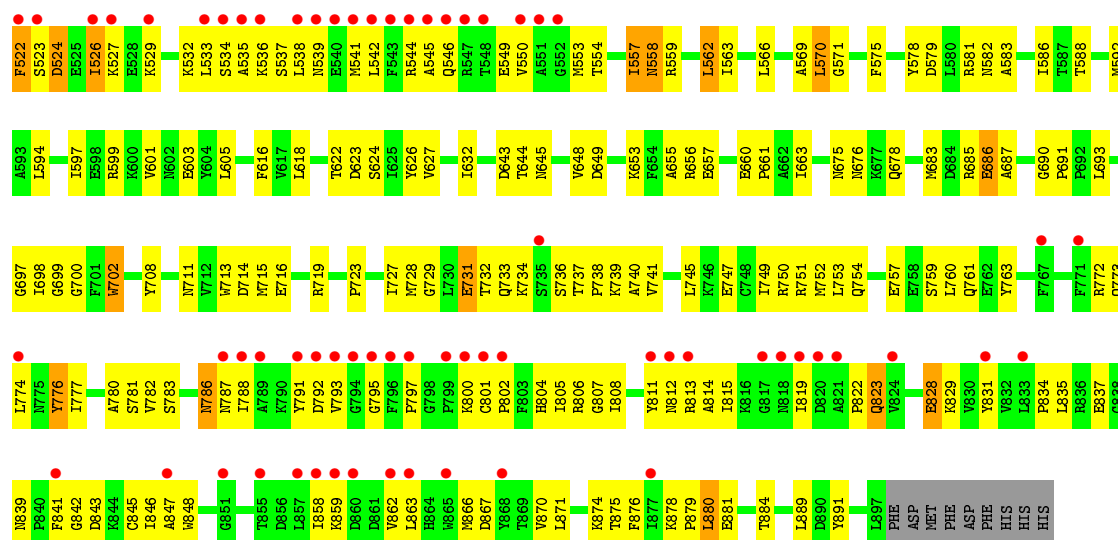


• Molecule 1: DNA polymerase

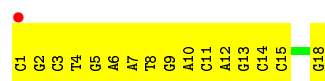




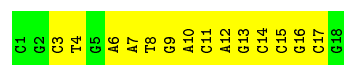




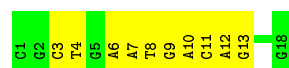
• Molecule 2: DNA (5'-D(\*CP\*GP\*CP\*(CTG)P\*GP\*AP\*AP\*TP\*GP\*AP\*CP\*AP\*GP\*CP\*C  
P\*GP\*CP\*G)-3')



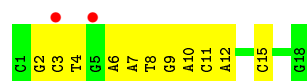
• Molecule 2: DNA (5'-D(\*CP\*GP\*CP\*(CTG)P\*GP\*AP\*AP\*TP\*GP\*AP\*CP\*AP\*GP\*CP\*C  
P\*GP\*CP\*G)-3')




• Molecule 2: DNA (5'-D(\*CP\*GP\*CP\*(CTG)P\*GP\*AP\*AP\*TP\*GP\*AP\*CP\*AP\*GP\*CP\*C  
P\*GP\*CP\*G)-3')



• Molecule 2: DNA (5'-D(\*CP\*GP\*CP\*(CTG)P\*GP\*AP\*AP\*TP\*GP\*AP\*CP\*AP\*GP\*CP\*C  
P\*GP\*CP\*G)-3')



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

Chain F:  21% 79%

G101	G102	G103	G104	C105	T106	G107	T108	C109	A110	T111	T112	C113	A114
Green	Green	Yellow	Yellow	Yellow	Yellow	Green	Yellow	Yellow	Yellow	Yellow	Yellow	Yellow	Yellow

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

Chain H:  14% 86%

G101	G102	G103	G104	C105	T106	G107	T108	C109	A110	T111	T112	C113	A114
Yellow	Yellow	Green	Yellow	Yellow	Yellow	Green	Yellow	Yellow	Yellow	Yellow	Yellow	Yellow	Yellow

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

Chain J:  29% 71%

G101	C102	G103	G104	C105	T106	A110	T111	T112	C113	A114
Green	Yellow	Yellow	Yellow	Yellow	Yellow	Yellow	Yellow	Yellow	Yellow	Yellow

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

Chain L:  7% 21% 93%

G101	C102	G103	G104	C105	T106	G107	T108	C109	A110	T111	T112	C113	A114
Green	Yellow	Yellow	Yellow	Yellow	Yellow	Yellow	Yellow	Yellow	Yellow	Yellow	Yellow	Yellow	Yellow

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	133.53Å 123.44Å 164.29Å 90.00° 96.84° 90.00°	Depositor
Resolution (Å)	50.00 – 2.65 45.00 – 2.65	Depositor EDS
% Data completeness (in resolution range)	91.5 (50.00-2.65) 96.4 (45.00-2.65)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.87 (at 2.65Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.224 , 0.276 0.227 , 0.276	Depositor DCC
$R_{free}$ test set	13763 reflections (10.49%)	DCC
Wilson B-factor (Å <sup>2</sup> )	48.7	Xtriage
Anisotropy	0.140	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 62.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 290748 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	32166	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.66% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CTG, SO4

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	A	0.41	0/7523	0.62	0/10175
1	B	0.40	0/7475	0.59	0/10121
1	C	0.42	0/7511	0.62	0/10154
1	D	0.33	0/7275	0.56	0/9887
2	E	0.35	0/389	0.72	0/596
2	G	0.47	0/389	0.74	0/596
2	I	0.57	0/389	0.83	0/596
2	K	0.27	0/389	0.65	0/596
3	F	0.27	0/312	0.72	0/478
3	H	0.36	0/312	0.73	0/478
3	J	0.50	0/312	0.80	0/478
3	L	0.26	0/312	0.65	0/478
All	All	0.39	0/32588	0.61	0/44633

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	A	7342	0	7193	401	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	7294	0	7096	374	0
1	C	7332	0	7212	295	0
1	D	7097	0	6752	404	0
2	E	369	0	204	29	0
2	G	369	0	204	31	0
2	I	369	0	204	20	0
2	K	369	0	204	19	0
3	F	280	0	154	25	0
3	H	280	0	154	22	0
3	J	280	0	154	19	0
3	L	280	0	154	14	0
4	C	5	0	0	0	0
5	A	111	0	0	14	0
5	B	129	0	0	11	0
5	C	178	0	0	15	0
5	D	33	0	0	3	0
5	E	5	0	0	0	0
5	F	4	0	0	3	0
5	G	11	0	0	0	0
5	H	4	0	0	1	0
5	I	13	0	0	0	0
5	J	7	0	0	0	0
5	K	3	0	0	1	0
5	L	2	0	0	0	0
All	All	32166	0	29685	1633	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 27.

The worst 5 of 1633 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:85:MET:HE2	1:B:87:ASP:H	1.09	1.15
3:L:104:DG:H2"	3:L:105:DC:H5"	1.19	1.14
1:B:309:ILE:HA	1:B:312:LEU:HB2	1.31	1.11
3:J:104:DG:H2"	3:J:105:DC:H5"	1.22	1.11
2:K:10:DA:H2"	2:K:11:DC:H5"	1.20	1.08

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	
1	A	901/906 (99%)	781 (87%)	105 (12%)	15 (2%)	11	25
1	B	901/906 (99%)	816 (91%)	79 (9%)	6 (1%)	26	51
1	C	898/906 (99%)	818 (91%)	68 (8%)	12 (1%)	15	33
1	D	895/906 (99%)	769 (86%)	115 (13%)	11 (1%)	16	35
All	All	3595/3624 (99%)	3184 (89%)	367 (10%)	44 (1%)	16	35

5 of 44 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	524	ASP
1	A	300	VAL
1	A	773	GLN
1	A	825	VAL
1	A	856	ASP

### 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	
1	A	792/803 (99%)	742 (94%)	50 (6%)	22	44
1	B	780/803 (97%)	738 (95%)	42 (5%)	27	52
1	C	794/803 (99%)	755 (95%)	39 (5%)	31	58
1	D	743/803 (92%)	702 (94%)	41 (6%)	27	51
All	All	3109/3212 (97%)	2937 (94%)	172 (6%)	27	51

5 of 172 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	573	VAL
1	C	83	LEU
1	D	557	ILE
1	B	658	ARG
1	B	772	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 94 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	754	GLN
1	C	255	ASN
1	D	678	GLN
1	B	775	ASN
1	C	112	ASN

### 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	$\# Z  > 2$
2	CTG	E	4	3,2	16,23,24	0.69	0	17,35,38	1.03	2 (11%)
2	CTG	G	4	3,2	16,23,24	0.72	0	17,35,38	1.00	2 (11%)
2	CTG	I	4	3,2	16,23,24	0.70	0	17,35,38	1.00	2 (11%)
2	CTG	K	4	3,2	16,23,24	0.77	1 (6%)	17,35,38	0.75	1 (5%)

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
2	CTG	E	4	3,2	-	0/7/45/46	0/2/2/2
2	CTG	G	4	3,2	-	0/7/45/46	0/2/2/2
2	CTG	I	4	3,2	-	0/7/45/46	0/2/2/2
2	CTG	K	4	3,2	-	0/7/45/46	0/2/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	4	CTG	C1'-N1	2.05	1.48	1.45

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	4	CTG	C2'-C1'-N1	-3.09	111.41	115.64
2	G	4	CTG	C2'-C1'-N1	-2.83	111.76	115.64
2	I	4	CTG	C2'-C1'-N1	-2.74	111.88	115.64
2	I	4	CTG	N3-C2-N1	-2.59	114.23	116.82
2	E	4	CTG	N3-C2-N1	-2.43	114.39	116.82

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	4	CTG	3	0
2	G	4	CTG	3	0
2	I	4	CTG	1	0
2	K	4	CTG	2	0

## 5.5 Carbohydrates

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

1 ligand is 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	$\# Z  > 2$
4	SO4	C	907	-	4,4,4	0.27	0	6,6,6	0.09	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
4	SO4	C	907	-	-	0/0/0/0	0/0/0/0

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.

No monomer is involved in short contacts.

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	903/906 (99%)	0.31	65 (7%) 18 16	24, 53, 144, 162	1 (0%)
1	B	903/906 (99%)	0.37	68 (7%) 17 14	20, 59, 157, 172	0
1	C	900/906 (99%)	-0.01	7 (0%) 87 87	17, 47, 89, 109	0
1	D	897/906 (99%)	0.86	138 (15%) 3 2	48, 98, 134, 169	0
2	E	17/18 (94%)	0.44	1 (5%) 26 23	70, 88, 124, 132	0
2	G	17/18 (94%)	-0.20	0 100 100	45, 57, 79, 92	0
2	I	17/18 (94%)	-0.38	0 100 100	32, 38, 85, 94	0
2	K	17/18 (94%)	0.78	2 (11%) 6 4	59, 126, 147, 151	0
3	F	14/14 (100%)	0.54	0 100 100	85, 117, 130, 134	0
3	H	14/14 (100%)	0.15	0 100 100	53, 70, 83, 85	0
3	J	14/14 (100%)	-0.38	0 100 100	30, 45, 93, 99	0
3	L	14/14 (100%)	1.04	3 (21%) 1 1	120, 131, 135, 136	0
All	All	3727/3752 (99%)	0.38	284 (7%) 17 14	17, 62, 132, 172	1 (0%)

The worst 5 of 284 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	510	VAL	15.6
1	B	513	PRO	13.4
1	B	507	ASN	13.4
1	B	511	ASP	10.9
1	B	506	PRO	10.3

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	CTG	G	4	22/23	0.93	0.17	-	65,69,71,71	0
2	CTG	I	4	22/23	0.96	0.17	-	44,50,54,54	0
2	CTG	K	4	22/23	0.64	0.37	-	144,145,151,152	0
2	CTG	E	4	22/23	0.86	0.22	-	102,103,106,107	0

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
4	SO4	C	907	5/5	0.96	0.12	-1.02	89,90,90,90	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.