



# wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 11, 2017 – 08:22 PM EST

PDB ID : 6AP4  
Title : Crystal structure of the DNA polymerase III subunit beta from *Acinetobacter baumannii*  
Authors : McGrath, A.E.; Oakley, A.J.  
Deposited on : unknown  
Resolution : 2.95 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
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030345
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	rb-20030345

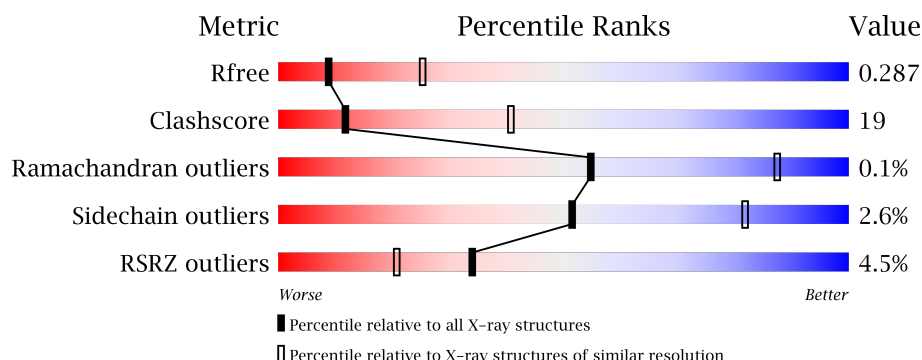
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.95 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))
$R_{free}$	100719	2395 (3.00-2.92)
Clashscore	112137	2773 (3.00-2.92)
Ramachandran outliers	110173	2680 (3.00-2.92)
Sidechain outliers	110143	2683 (3.00-2.92)
RSRZ outliers	101464	2421 (3.00-2.92)

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	388	<div> <div>3%</div> <div>69%</div> <div>29%</div> <div>.</div> </div>
1	B	388	<div> <div>%</div> <div>70%</div> <div>28%</div> <div>..</div> </div>
1	C	388	<div> <div>2%</div> <div>70%</div> <div>26%</div> <div>..</div> </div>
1	D	388	<div> <div>3%</div> <div>69%</div> <div>28%</div> <div>..</div> </div>
1	E	388	<div> <div>73%</div> <div>24%</div> <div>..</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	388	
1	G	388	
1	H	388	
1	I	388	
1	J	388	
1	K	388	
1	L	388	
1	M	388	
1	N	388	
1	O	388	
1	P	388	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 46780 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 III subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	378	Total	C	N	O	S	0	0	0
			2938	1836	515	575	12			
1	B	382	Total	C	N	O	S	0	0	0
			2964	1852	518	582	12			
1	C	379	Total	C	N	O	S	0	0	0
			2942	1842	514	574	12			
1	D	382	Total	C	N	O	S	0	0	0
			2962	1853	520	578	11			
1	E	382	Total	C	N	O	S	0	0	0
			2965	1852	519	582	12			
1	F	379	Total	C	N	O	S	0	0	0
			2942	1839	515	576	12			
1	G	378	Total	C	N	O	S	0	0	0
			2941	1840	516	573	12			
1	H	383	Total	C	N	O	S	0	0	0
			2957	1848	517	580	12			
1	I	370	Total	C	N	O	S	0	0	0
			2874	1804	503	555	12			
1	J	384	Total	C	N	O	S	0	0	0
			2981	1862	525	582	12			
1	K	365	Total	C	N	O	S	0	1	0
			2830	1773	497	547	13			
1	L	356	Total	C	N	O	S	0	0	0
			2735	1710	476	537	12			
1	M	378	Total	C	N	O	S	0	0	0
			2929	1833	510	574	12			
1	N	372	Total	C	N	O	S	0	0	0
			2891	1812	507	560	12			
1	O	357	Total	C	N	O	S	0	0	0
			2768	1741	486	530	11			
1	P	377	Total	C	N	O	S	0	0	0
			2914	1823	508	571	12			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	HIS	-	expression tag	UNP V5V7W3
A	-4	HIS	-	expression tag	UNP V5V7W3
A	-3	HIS	-	expression tag	UNP V5V7W3
A	-2	HIS	-	expression tag	UNP V5V7W3
A	-1	HIS	-	expression tag	UNP V5V7W3
A	0	HIS	-	expression tag	UNP V5V7W3
B	-5	HIS	-	expression tag	UNP V5V7W3
B	-4	HIS	-	expression tag	UNP V5V7W3
B	-3	HIS	-	expression tag	UNP V5V7W3
B	-2	HIS	-	expression tag	UNP V5V7W3
B	-1	HIS	-	expression tag	UNP V5V7W3
B	0	HIS	-	expression tag	UNP V5V7W3
C	-5	HIS	-	expression tag	UNP V5V7W3
C	-4	HIS	-	expression tag	UNP V5V7W3
C	-3	HIS	-	expression tag	UNP V5V7W3
C	-2	HIS	-	expression tag	UNP V5V7W3
C	-1	HIS	-	expression tag	UNP V5V7W3
C	0	HIS	-	expression tag	UNP V5V7W3
D	-5	HIS	-	expression tag	UNP V5V7W3
D	-4	HIS	-	expression tag	UNP V5V7W3
D	-3	HIS	-	expression tag	UNP V5V7W3
D	-2	HIS	-	expression tag	UNP V5V7W3
D	-1	HIS	-	expression tag	UNP V5V7W3
D	0	HIS	-	expression tag	UNP V5V7W3
E	-5	HIS	-	expression tag	UNP V5V7W3
E	-4	HIS	-	expression tag	UNP V5V7W3
E	-3	HIS	-	expression tag	UNP V5V7W3
E	-2	HIS	-	expression tag	UNP V5V7W3
E	-1	HIS	-	expression tag	UNP V5V7W3
E	0	HIS	-	expression tag	UNP V5V7W3
F	-5	HIS	-	expression tag	UNP V5V7W3
F	-4	HIS	-	expression tag	UNP V5V7W3
F	-3	HIS	-	expression tag	UNP V5V7W3
F	-2	HIS	-	expression tag	UNP V5V7W3
F	-1	HIS	-	expression tag	UNP V5V7W3
F	0	HIS	-	expression tag	UNP V5V7W3
G	-5	HIS	-	expression tag	UNP V5V7W3
G	-4	HIS	-	expression tag	UNP V5V7W3
G	-3	HIS	-	expression tag	UNP V5V7W3
G	-2	HIS	-	expression tag	UNP V5V7W3
G	-1	HIS	-	expression tag	UNP V5V7W3
G	0	HIS	-	expression tag	UNP V5V7W3

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Chain	Residue	Modelled	Actual	Comment	Reference
H	-5	HIS	-	expression tag	UNP V5V7W3
H	-4	HIS	-	expression tag	UNP V5V7W3
H	-3	HIS	-	expression tag	UNP V5V7W3
H	-2	HIS	-	expression tag	UNP V5V7W3
H	-1	HIS	-	expression tag	UNP V5V7W3
H	0	HIS	-	expression tag	UNP V5V7W3
I	-5	HIS	-	expression tag	UNP V5V7W3
I	-4	HIS	-	expression tag	UNP V5V7W3
I	-3	HIS	-	expression tag	UNP V5V7W3
I	-2	HIS	-	expression tag	UNP V5V7W3
I	-1	HIS	-	expression tag	UNP V5V7W3
I	0	HIS	-	expression tag	UNP V5V7W3
J	-5	HIS	-	expression tag	UNP V5V7W3
J	-4	HIS	-	expression tag	UNP V5V7W3
J	-3	HIS	-	expression tag	UNP V5V7W3
J	-2	HIS	-	expression tag	UNP V5V7W3
J	-1	HIS	-	expression tag	UNP V5V7W3
J	0	HIS	-	expression tag	UNP V5V7W3
K	-5	HIS	-	expression tag	UNP V5V7W3
K	-4	HIS	-	expression tag	UNP V5V7W3
K	-3	HIS	-	expression tag	UNP V5V7W3
K	-2	HIS	-	expression tag	UNP V5V7W3
K	-1	HIS	-	expression tag	UNP V5V7W3
K	0	HIS	-	expression tag	UNP V5V7W3
L	-5	HIS	-	expression tag	UNP V5V7W3
L	-4	HIS	-	expression tag	UNP V5V7W3
L	-3	HIS	-	expression tag	UNP V5V7W3
L	-2	HIS	-	expression tag	UNP V5V7W3
L	-1	HIS	-	expression tag	UNP V5V7W3
L	0	HIS	-	expression tag	UNP V5V7W3
M	-5	HIS	-	expression tag	UNP V5V7W3
M	-4	HIS	-	expression tag	UNP V5V7W3
M	-3	HIS	-	expression tag	UNP V5V7W3
M	-2	HIS	-	expression tag	UNP V5V7W3
M	-1	HIS	-	expression tag	UNP V5V7W3
M	0	HIS	-	expression tag	UNP V5V7W3
N	-5	HIS	-	expression tag	UNP V5V7W3
N	-4	HIS	-	expression tag	UNP V5V7W3
N	-3	HIS	-	expression tag	UNP V5V7W3
N	-2	HIS	-	expression tag	UNP V5V7W3
N	-1	HIS	-	expression tag	UNP V5V7W3
N	0	HIS	-	expression tag	UNP V5V7W3

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Chain	Residue	Modelled	Actual	Comment	Reference
O	-5	HIS	-	expression tag	UNP V5V7W3
O	-4	HIS	-	expression tag	UNP V5V7W3
O	-3	HIS	-	expression tag	UNP V5V7W3
O	-2	HIS	-	expression tag	UNP V5V7W3
O	-1	HIS	-	expression tag	UNP V5V7W3
O	0	HIS	-	expression tag	UNP V5V7W3
P	-5	HIS	-	expression tag	UNP V5V7W3
P	-4	HIS	-	expression tag	UNP V5V7W3
P	-3	HIS	-	expression tag	UNP V5V7W3
P	-2	HIS	-	expression tag	UNP V5V7W3
P	-1	HIS	-	expression tag	UNP V5V7W3
P	0	HIS	-	expression tag	UNP V5V7W3

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	J	1	Total Mg 1 1	0	0
2	C	1	Total Mg 1 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	14	Total O 14 14	0	0
3	B	14	Total O 14 14	0	0
3	C	15	Total O 15 15	0	0
3	D	30	Total O 30 30	0	0
3	E	47	Total O 47 47	0	0
3	F	11	Total O 11 11	0	0
3	G	22	Total O 22 22	0	0
3	H	8	Total O 8 8	0	0
3	I	5	Total O 5 5	0	0

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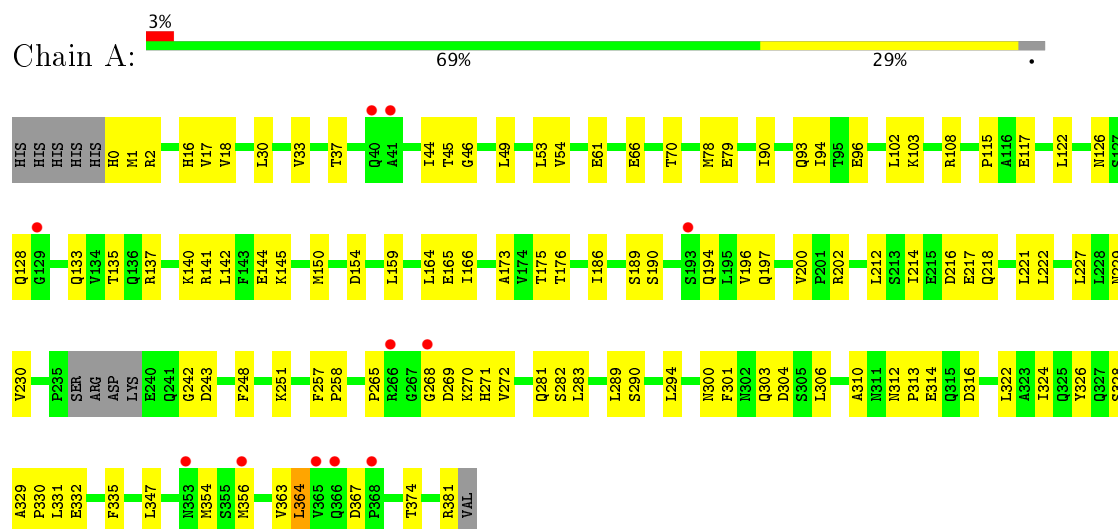
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	J	17	Total 17	O 17	0	0
3	K	9	Total 9	O 9	0	0
3	L	10	Total 10	O 10	0	0
3	M	18	Total 18	O 18	0	0
3	N	9	Total 9	O 9	0	0
3	O	6	Total 6	O 6	0	0
3	P	10	Total 10	O 10	0	0



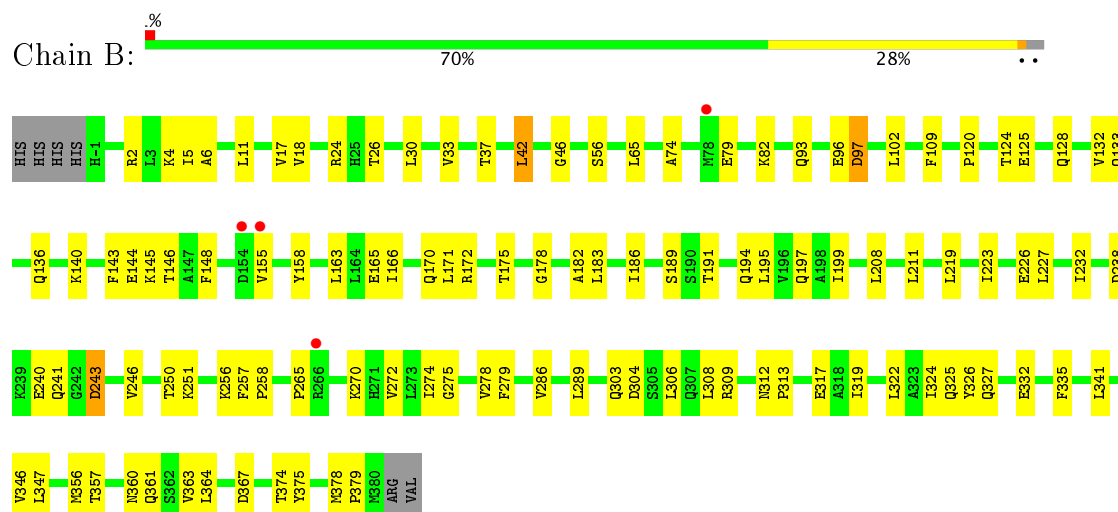
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: DNA polymerase III subunit beta

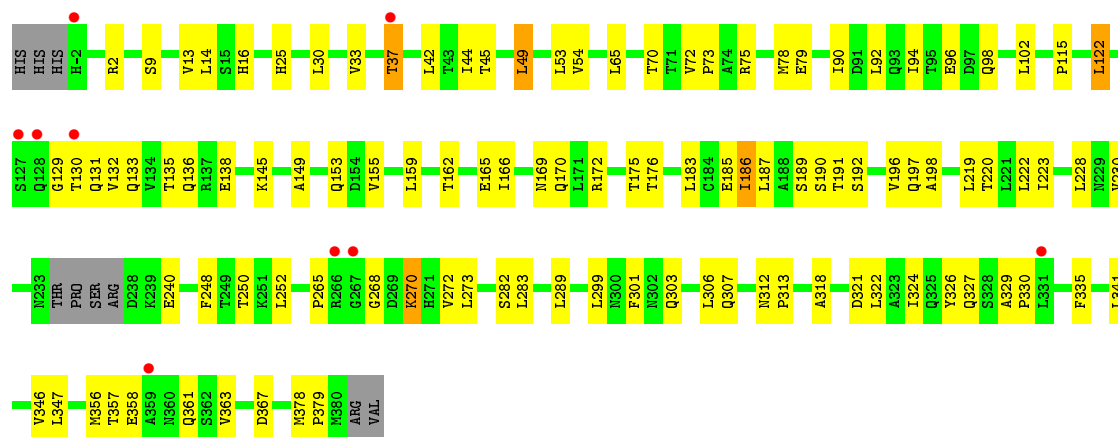


#### • Molecule 1: DNA polymerase III subunit beta

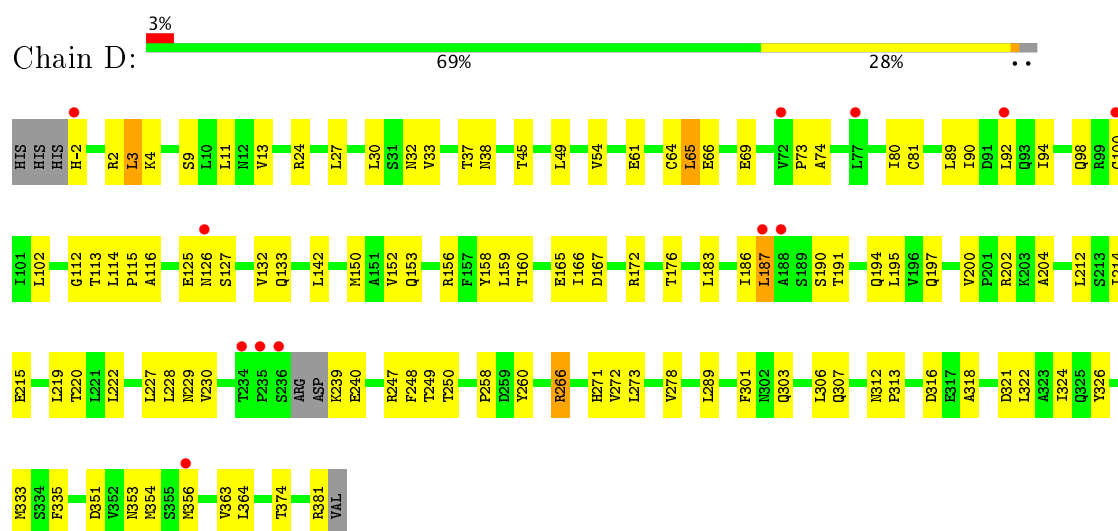


#### • Molecule 1: DNA polymerase III subunit beta

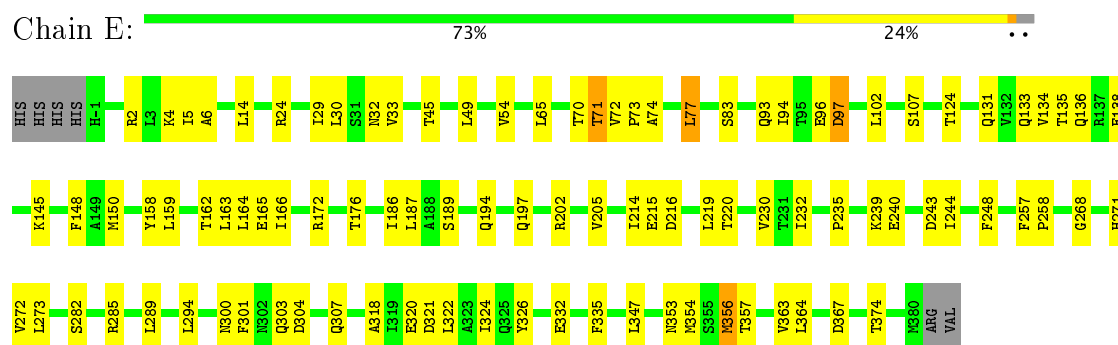




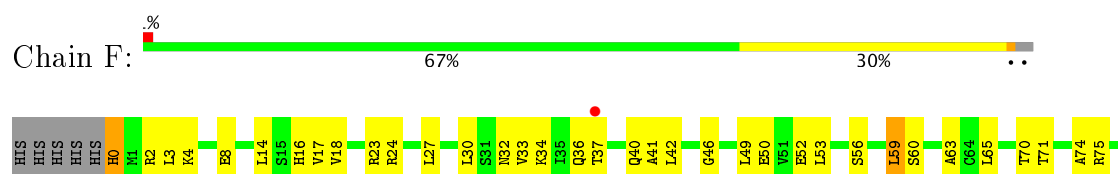
• Molecule 1: DNA polymerase III subunit beta

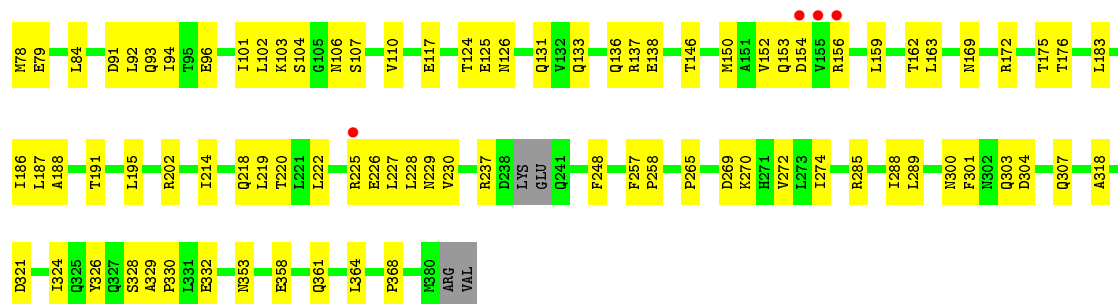


• Molecule 1: DNA polymerase III subunit beta

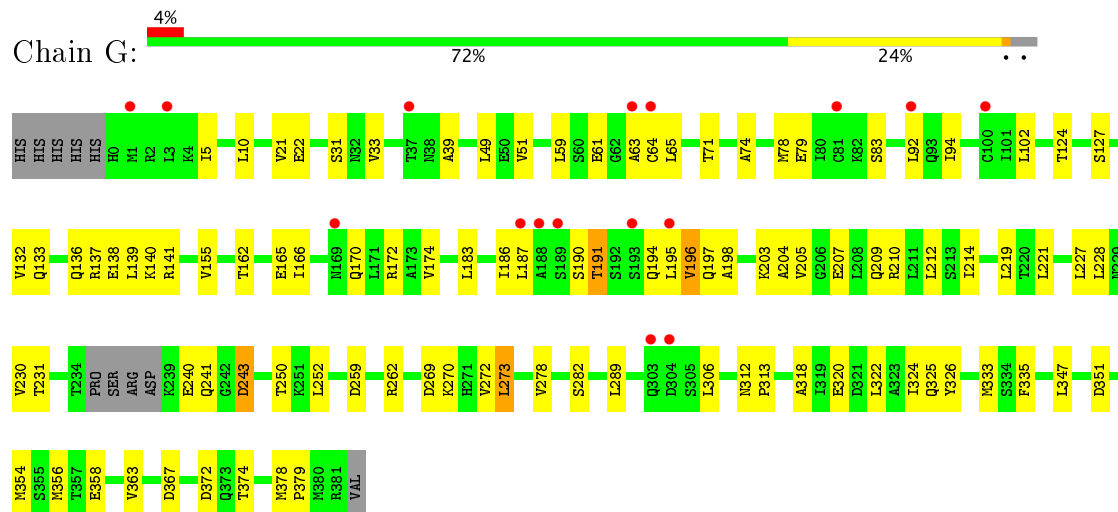


• Molecule 1: DNA polymerase III subunit beta

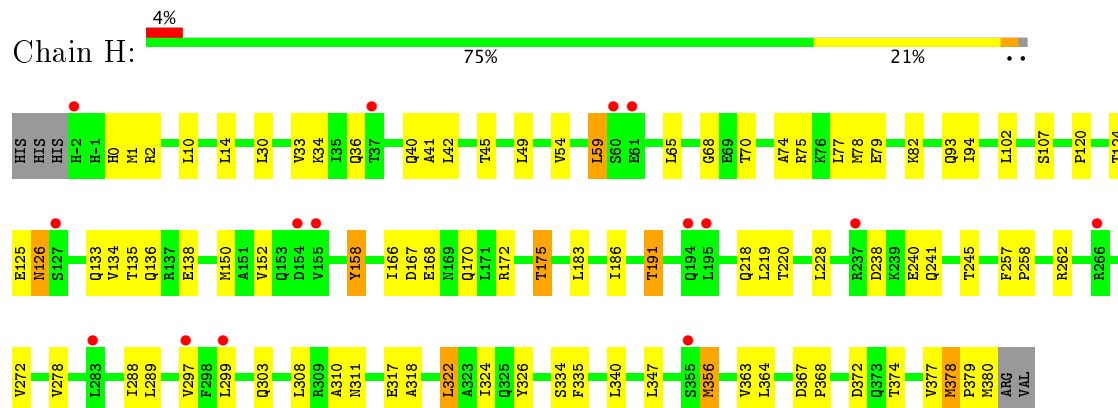




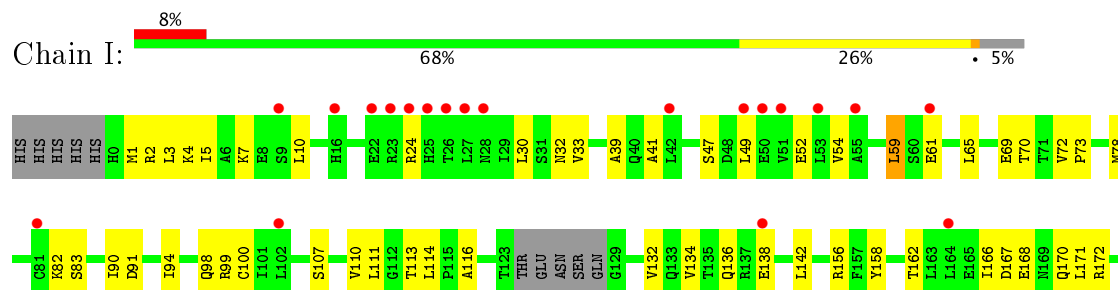
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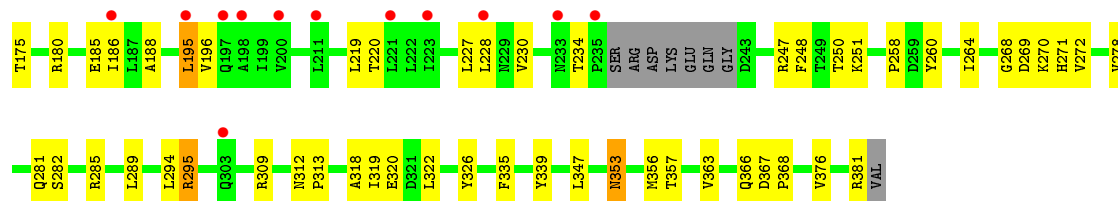


• Molecule 1: DNA polymerase III subunit beta

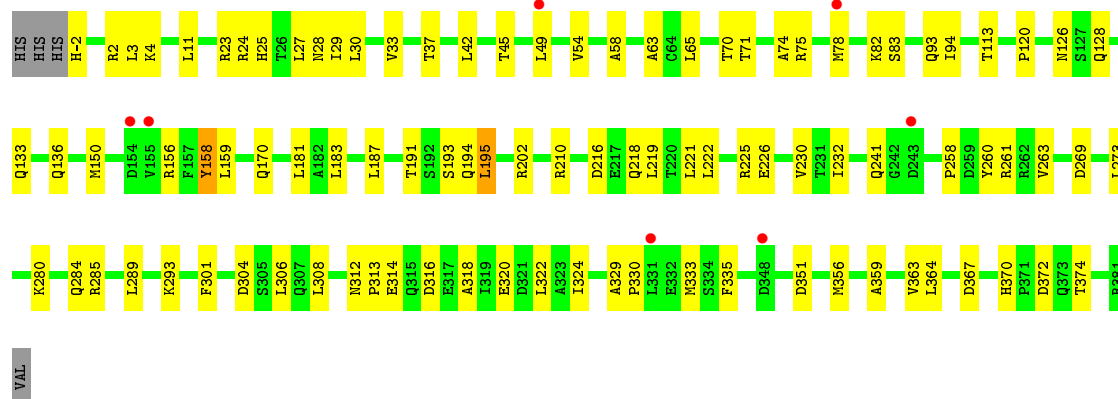
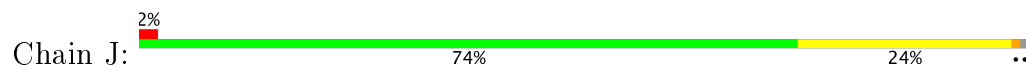


• Molecule 1: DNA polymerase III subunit beta

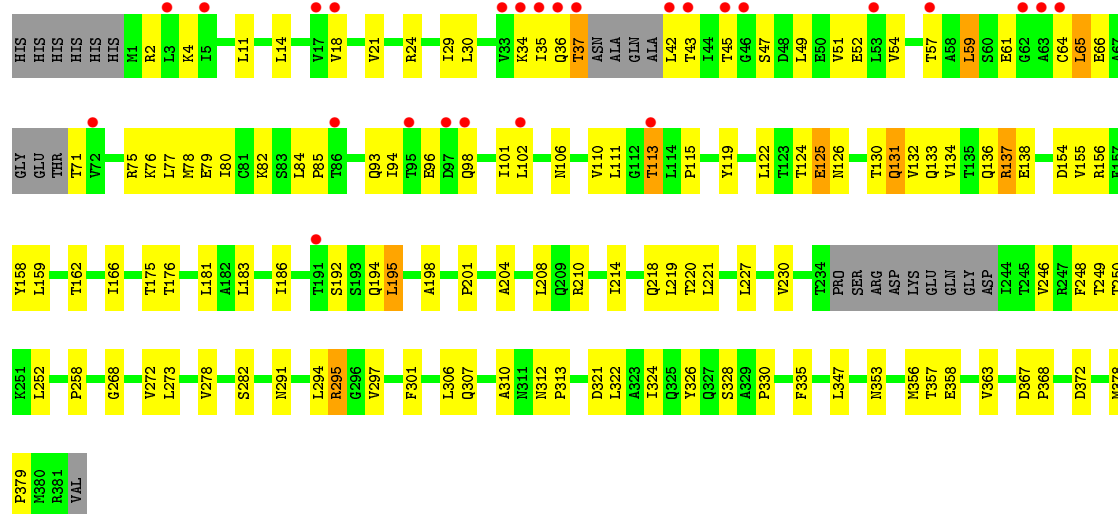




• Molecule 1: DNA polymerase III subunit beta

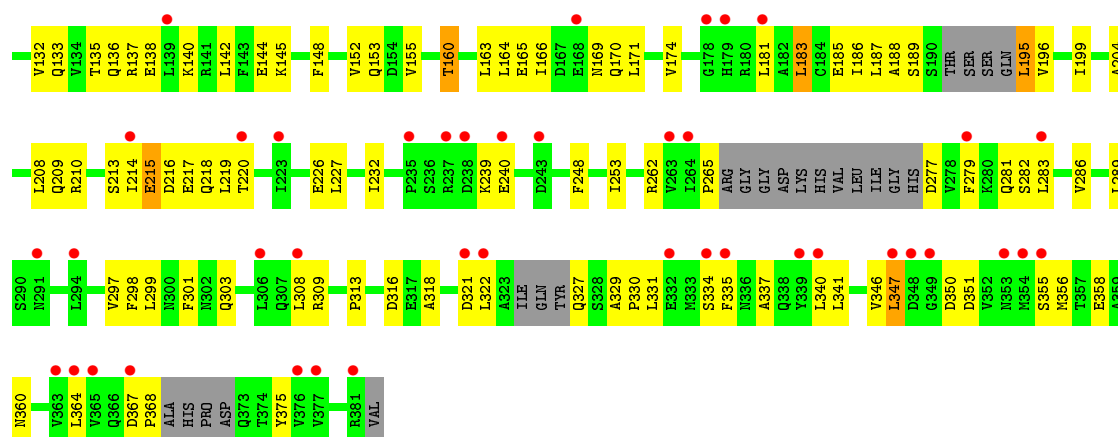


• Molecule 1: DNA polymerase III subunit beta

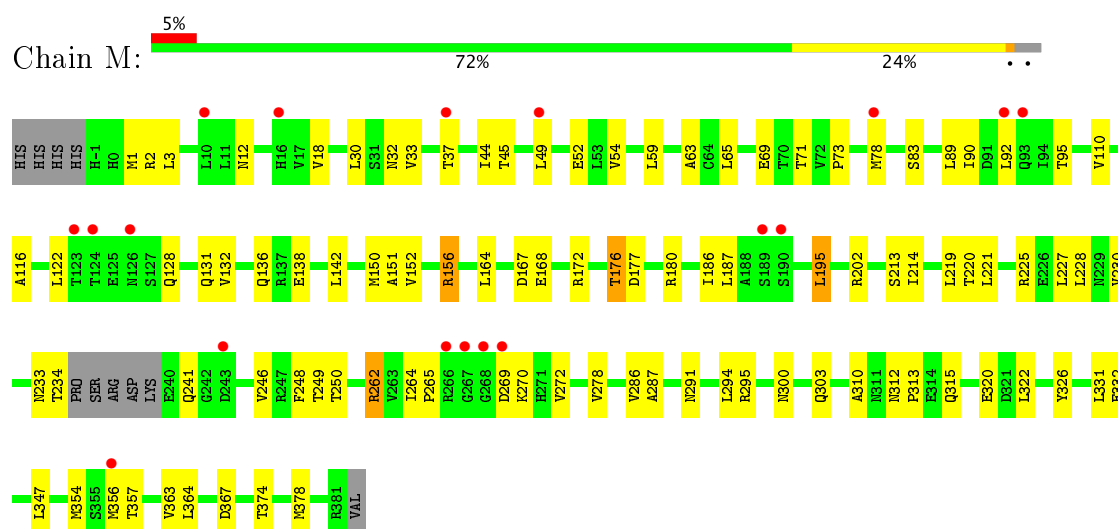


• Molecule 1: DNA polymerase III subunit beta

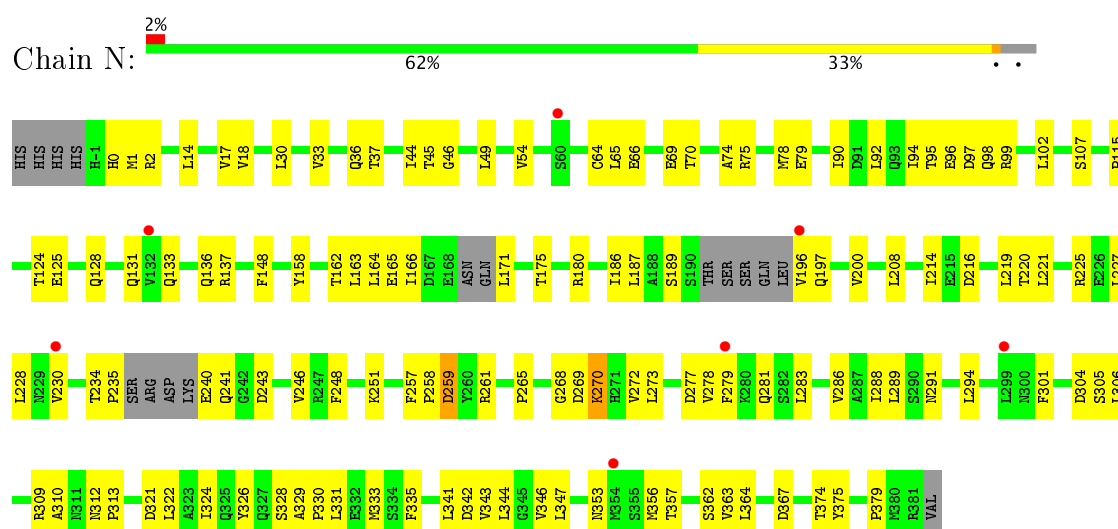




• Molecule 1: DNA polymerase III subunit beta

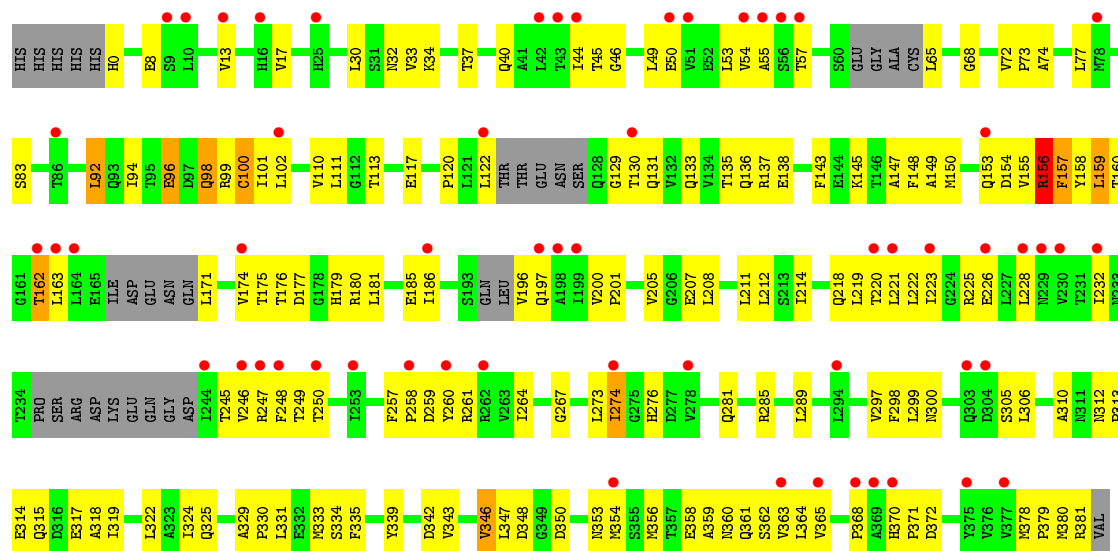


• Molecule 1: DNA polymerase III subunit beta

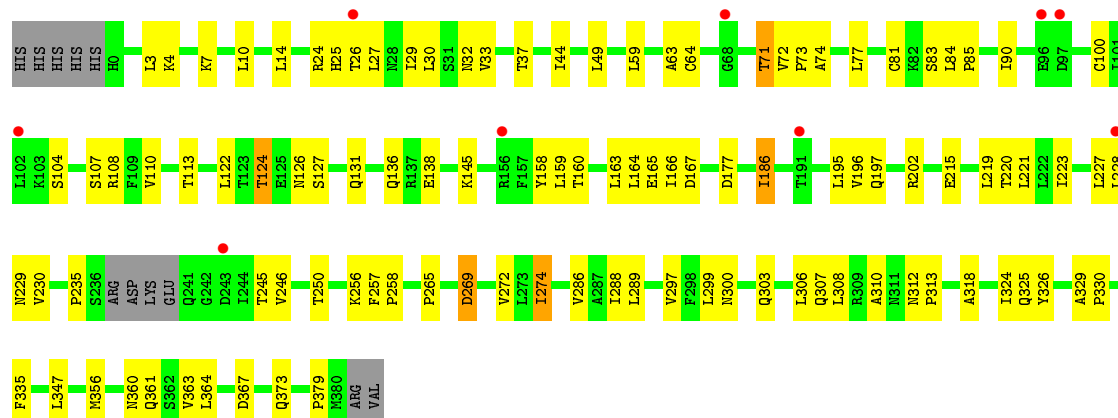


• Molecule 1: DNA polymerase III subunit beta





• Molecule 1: DNA polymerase III subunit beta



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	72.71 Å   328.60 Å   147.50 Å 90.00°   91.53°   90.00°	Depositor
Resolution (Å)	164.30 – 2.95 49.06 – 2.95	Depositor EDS
% Data completeness (in resolution range)	92.5 (164.30-2.95) 85.5 (49.06-2.95)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.96 (at 2.96 Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, $R_{free}$	0.248 , 0.287 0.243 , 0.287	Depositor DCC
$R_{free}$ test set	6717 reflections (5.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	49.6	Xtriage
Anisotropy	0.038	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 10.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.079 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	46780	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.83% 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, 0.333 respectively for untwinned datasets, and 0.375, 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: MG

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	0.50	0/2972	0.73	0/4029
1	B	0.52	0/3000	0.75	0/4070
1	C	0.48	0/2977	0.73	0/4035
1	D	0.53	0/2998	0.74	0/4066
1	E	0.60	0/3001	0.79	0/4070
1	F	0.51	0/2976	0.72	0/4035
1	G	0.49	0/2974	0.75	0/4030
1	H	0.46	0/2994	0.70	0/4064
1	I	0.49	0/2907	0.72	0/3940
1	J	0.48	0/3018	0.71	0/4094
1	K	0.51	0/2860	0.75	0/3876
1	L	0.47	0/2759	0.73	0/3736
1	M	0.48	0/2963	0.72	0/4018
1	N	0.47	0/2924	0.71	0/3961
1	O	0.40	0/2797	0.71	1/3786 (0.0%)
1	P	0.45	0/2948	0.70	0/3999
All	All	0.49	0/47068	0.73	1/63809 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	156	ARG	N-CA-C	-5.06	97.34	111.00

There are no chirality outliers.

There are no planarity outliers.



## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2938	0	2992	114	0
1	B	2964	0	3009	117	0
1	C	2942	0	2990	101	0
1	D	2962	0	3006	111	0
1	E	2965	0	3011	89	0
1	F	2942	0	2998	119	0
1	G	2941	0	3001	96	0
1	H	2957	0	2986	108	0
1	I	2874	0	2939	110	0
1	J	2981	0	3025	98	0
1	K	2830	0	2874	131	0
1	L	2735	0	2772	158	0
1	M	2929	0	2975	102	0
1	N	2891	0	2948	149	0
1	O	2768	0	2839	185	0
1	P	2914	0	2963	95	0
2	C	1	0	0	0	0
2	J	1	0	0	0	0
3	A	14	0	0	0	0
3	B	14	0	0	1	0
3	C	15	0	0	0	0
3	D	30	0	0	0	0
3	E	47	0	0	2	0
3	F	11	0	0	1	0
3	G	22	0	0	1	0
3	H	8	0	0	0	0
3	I	5	0	0	0	0
3	J	17	0	0	0	0
3	K	9	0	0	1	0
3	L	10	0	0	0	0
3	M	18	0	0	0	0
3	N	9	0	0	1	0
3	O	6	0	0	0	0
3	P	10	0	0	0	0
All	All	46780	0	47328	1816	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 19.

The worst 5 of 1816 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:O:276:HIS:CD2	1:O:347:LEU:HD11	1.53	1.40
1:G:92:LEU:HG	1:G:102:LEU:CD2	1.62	1.28
1:O:276:HIS:CD2	1:O:347:LEU:CD1	2.23	1.19
1:H:1:MET:CE	1:H:70:THR:HG22	1.73	1.19
1:C:162:THR:HG22	1:C:175:THR:CG2	1.72	1.18

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	
1	A	374/388 (96%)	367 (98%)	6 (2%)	1 (0%)	44	79
1	B	380/388 (98%)	375 (99%)	5 (1%)	0	100	100
1	C	375/388 (97%)	365 (97%)	9 (2%)	1 (0%)	44	79
1	D	378/388 (97%)	370 (98%)	8 (2%)	0	100	100
1	E	380/388 (98%)	371 (98%)	9 (2%)	0	100	100
1	F	375/388 (97%)	369 (98%)	6 (2%)	0	100	100
1	G	374/388 (96%)	366 (98%)	8 (2%)	0	100	100
1	H	381/388 (98%)	375 (98%)	6 (2%)	0	100	100
1	I	364/388 (94%)	352 (97%)	11 (3%)	1 (0%)	44	79
1	J	382/388 (98%)	372 (97%)	10 (3%)	0	100	100
1	K	358/388 (92%)	344 (96%)	12 (3%)	2 (1%)	28	67
1	L	344/388 (89%)	336 (98%)	7 (2%)	1 (0%)	44	79
1	M	374/388 (96%)	368 (98%)	5 (1%)	1 (0%)	44	79

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	N	364/388 (94%)	360 (99%)	3 (1%)	1 (0%)	44	79
1	O	345/388 (89%)	334 (97%)	11 (3%)	0	100	100
1	P	373/388 (96%)	359 (96%)	14 (4%)	0	100	100
All	All	5921/6208 (95%)	5783 (98%)	130 (2%)	8 (0%)	55	87

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	K	125	GLU
1	A	265	PRO
1	L	160	THR
1	N	265	PRO
1	K	115	PRO

### 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	330/341 (97%)	326 (99%)	4 (1%)	75	92
1	B	333/341 (98%)	326 (98%)	7 (2%)	59	85
1	C	329/341 (96%)	318 (97%)	11 (3%)	43	77
1	D	331/341 (97%)	325 (98%)	6 (2%)	64	87
1	E	333/341 (98%)	326 (98%)	7 (2%)	59	85
1	F	331/341 (97%)	327 (99%)	4 (1%)	75	92
1	G	329/341 (96%)	323 (98%)	6 (2%)	64	87
1	H	330/341 (97%)	317 (96%)	13 (4%)	37	73
1	I	321/341 (94%)	312 (97%)	9 (3%)	49	80
1	J	334/341 (98%)	328 (98%)	6 (2%)	64	87
1	K	314/341 (92%)	301 (96%)	13 (4%)	35	71
1	L	304/341 (89%)	296 (97%)	8 (3%)	51	82
1	M	328/341 (96%)	321 (98%)	7 (2%)	59	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	N	323/341 (95%)	317 (98%)	6 (2%)	62	87
1	O	309/341 (91%)	292 (94%)	17 (6%)	25	61
1	P	327/341 (96%)	318 (97%)	9 (3%)	49	80
All	All	5206/5456 (95%)	5073 (97%)	133 (3%)	51	82

5 of 133 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	111	LEU
1	K	59	LEU
1	O	348	ASP
1	I	167	ASP
1	J	-2	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 88 such sidechains are listed below:

Mol	Chain	Res	Type
1	H	373	GLN
1	J	133	GLN
1	O	133	GLN
1	I	98	GLN
1	I	218	GLN

### 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 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

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

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, 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	378/388 (97%)	0.15	11 (2%) 52 33	27, 56, 94, 134	0
1	B	382/388 (98%)	-0.01	4 (1%) 82 66	18, 44, 86, 118	0
1	C	379/388 (97%)	0.21	9 (2%) 59 40	30, 54, 92, 114	1 (0%)
1	D	382/388 (98%)	0.07	12 (3%) 49 31	15, 39, 72, 101	1 (0%)
1	E	382/388 (98%)	-0.09	0 100 100	12, 32, 63, 132	0
1	F	379/388 (97%)	0.04	5 (1%) 77 59	26, 46, 76, 121	1 (0%)
1	G	378/388 (97%)	0.22	16 (4%) 37 23	21, 50, 89, 128	2 (0%)
1	H	383/388 (98%)	0.20	15 (3%) 40 25	30, 59, 95, 128	0
1	I	370/388 (95%)	0.49	32 (8%) 11 6	28, 65, 98, 148	3 (0%)
1	J	384/388 (98%)	0.04	7 (1%) 69 50	22, 52, 85, 108	1 (0%)
1	K	365/388 (94%)	0.41	26 (7%) 17 9	22, 51, 110, 134	3 (0%)
1	L	356/388 (91%)	0.63	44 (12%) 4 2	29, 78, 116, 149	1 (0%)
1	M	378/388 (97%)	0.24	18 (4%) 31 19	20, 53, 96, 118	0
1	N	372/388 (95%)	0.27	7 (1%) 67 47	30, 64, 98, 120	2 (0%)
1	O	357/388 (92%)	0.91	58 (16%) 2 1	39, 81, 108, 136	0
1	P	377/388 (97%)	0.25	9 (2%) 59 40	30, 63, 105, 132	0
All	All	6002/6208 (96%)	0.25	273 (4%) 34 21	12, 55, 101, 149	15 (0%)

The worst 5 of 273 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	235	PRO	8.2
1	K	63	ALA	7.3
1	L	354	MET	7.1
1	O	55	ALA	6.5
1	I	235	PRO	6.4

## 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 [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( $\text{\AA}^2$ )	Q<0.9
2	MG	C	401	1/1	0.92	0.14	-1.87	30,30,30,30	0
2	MG	J	401	1/1	0.96	0.09	-2.39	30,30,30,30	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.