



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 01:37 PM GMT

PDB ID : 3U61  
Title : Structure of T4 Bacteriophage Clamp Loader Bound To Closed Clamp, DNA and ATP Analog and ADP  
Authors : Kelch, B.A.; Makino, D.L.; O'Donnell, M.; Kuriyan, J.  
Deposited on : 2011-10-11  
Resolution : 3.20 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

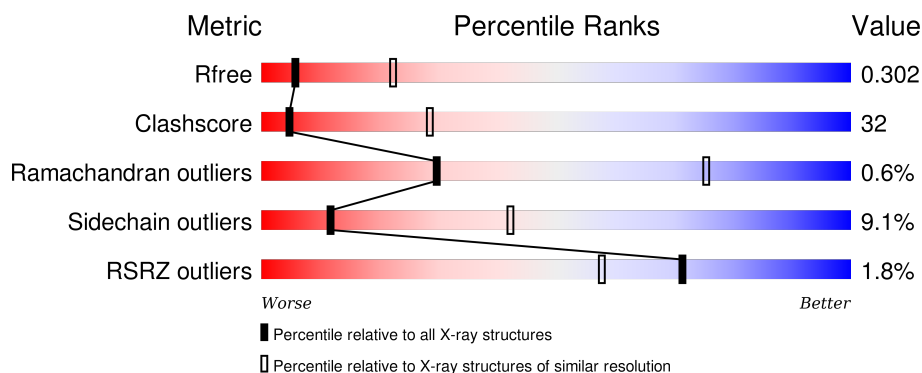
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 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	1124 (3.24-3.16)
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)

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	B	324	<div> <div>2%</div> <div>42%</div> <div>48%</div> <div>6%</div> </div>
1	C	324	<div> <div>%</div> <div>47%</div> <div>45%</div> <div>6%</div> </div>
1	D	324	<div> <div>2%</div> <div>49%</div> <div>42%</div> <div>8%</div> </div>
1	E	324	<div> <div>4%</div> <div>44%</div> <div>42%</div> <div>5%</div> <div>9%</div> </div>
2	A	199	<div> <div>2%</div> <div>34%</div> <div>53%</div> <div>11%</div> </div>

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Mol	Chain	Length	Quality of chain
3	F	228	
3	G	228	
3	H	228	
4	I	20	
5	J	10	

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
6	ADP	B	700	-	-	X	-
7	MG	C	800	-	-	-	X
7	MG	D	800	-	-	-	X

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 16748 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 accessory protein 44.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	305	Total	C	N	O	S	0	0	0
			2407	1525	412	454	16			
1	C	319	Total	C	N	O	S	0	0	0
			2503	1583	430	473	17			
1	D	320	Total	C	N	O	S	0	0	0
			2514	1590	432	475	17			
1	E	294	Total	C	N	O	S	0	0	0
			2292	1451	394	432	15			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-4	GLY	-	EXPRESSION TAG	UNP P04526
B	-3	PRO	-	EXPRESSION TAG	UNP P04526
B	-2	GLY	-	EXPRESSION TAG	UNP P04526
B	-1	GLY	-	EXPRESSION TAG	UNP P04526
B	0	SER	-	EXPRESSION TAG	UNP P04526
C	-4	GLY	-	EXPRESSION TAG	UNP P04526
C	-3	PRO	-	EXPRESSION TAG	UNP P04526
C	-2	GLY	-	EXPRESSION TAG	UNP P04526
C	-1	GLY	-	EXPRESSION TAG	UNP P04526
C	0	SER	-	EXPRESSION TAG	UNP P04526
D	-4	GLY	-	EXPRESSION TAG	UNP P04526
D	-3	PRO	-	EXPRESSION TAG	UNP P04526
D	-2	GLY	-	EXPRESSION TAG	UNP P04526
D	-1	GLY	-	EXPRESSION TAG	UNP P04526
D	0	SER	-	EXPRESSION TAG	UNP P04526
E	-4	GLY	-	EXPRESSION TAG	UNP P04526
E	-3	PRO	-	EXPRESSION TAG	UNP P04526
E	-2	GLY	-	EXPRESSION TAG	UNP P04526
E	-1	GLY	-	EXPRESSION TAG	UNP P04526
E	0	SER	-	EXPRESSION TAG	UNP P04526

- Molecule 2 is a protein called DNA polymerase accessory protein 62.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	178	Total	C	N	O	S	0	0	0
			1416	909	233	268	6			

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	188	GLY	-	EXPRESSION TAG	UNP P04527
A	189	LEU	-	EXPRESSION TAG	UNP P04527
A	190	GLU	-	EXPRESSION TAG	UNP P04527
A	191	HIS	-	EXPRESSION TAG	UNP P04527
A	192	HIS	-	EXPRESSION TAG	UNP P04527
A	193	HIS	-	EXPRESSION TAG	UNP P04527
A	194	HIS	-	EXPRESSION TAG	UNP P04527
A	195	HIS	-	EXPRESSION TAG	UNP P04527
A	196	HIS	-	EXPRESSION TAG	UNP P04527
A	197	HIS	-	EXPRESSION TAG	UNP P04527
A	198	HIS	-	EXPRESSION TAG	UNP P04527
A	199	HIS	-	EXPRESSION TAG	UNP P04527
A	200	HIS	-	EXPRESSION TAG	UNP P04527

- Molecule 3 is a protein called DNA polymerase processivity component.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	228	Total	C	N	O	Se	0	0	0
			1750	1113	288	343	6			
3	H	228	Total	C	N	O	Se	0	0	0
			1750	1113	288	343	6			
3	F	222	Total	C	N	O	Se	0	0	0
			1699	1083	280	330	6			

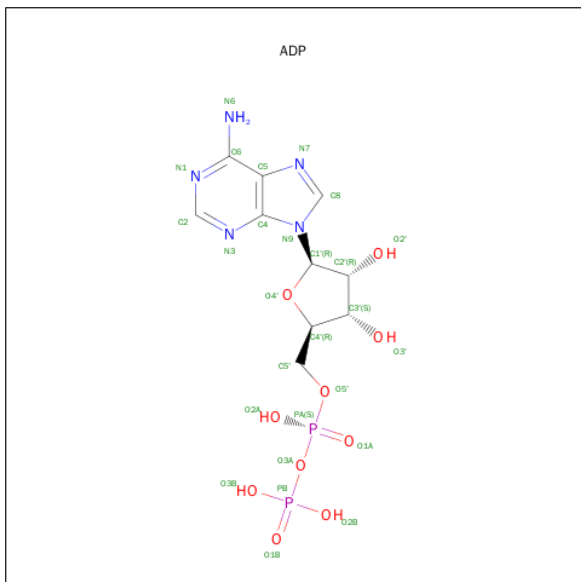
- Molecule 4 is a DNA chain called Template DNA strand.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	I	8	Total	C	N	O	P	0	0	0
			163	79	29	48	7			

- Molecule 5 is a DNA chain called Primer DNA strand.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	J	8	Total	C	N	O	P	0	0	0
			162	77	31	46	8			

- Molecule 6 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).

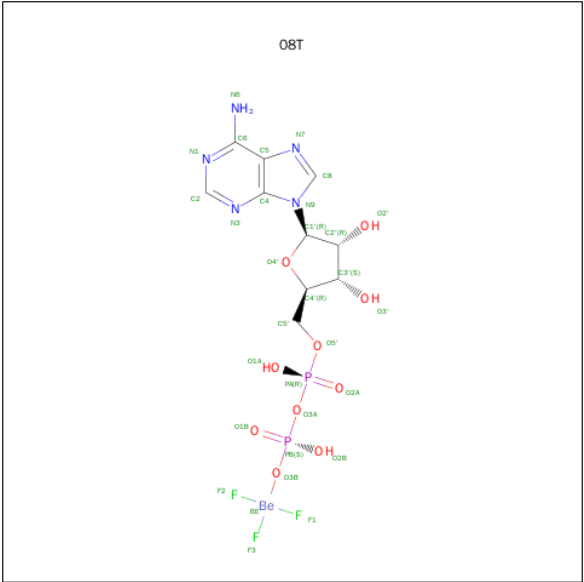


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1	Total	Mg	0	0
			1	1		
7	D	1	Total	Mg	0	0
			1	1		
7	C	1	Total	Mg	0	0
			1	1		

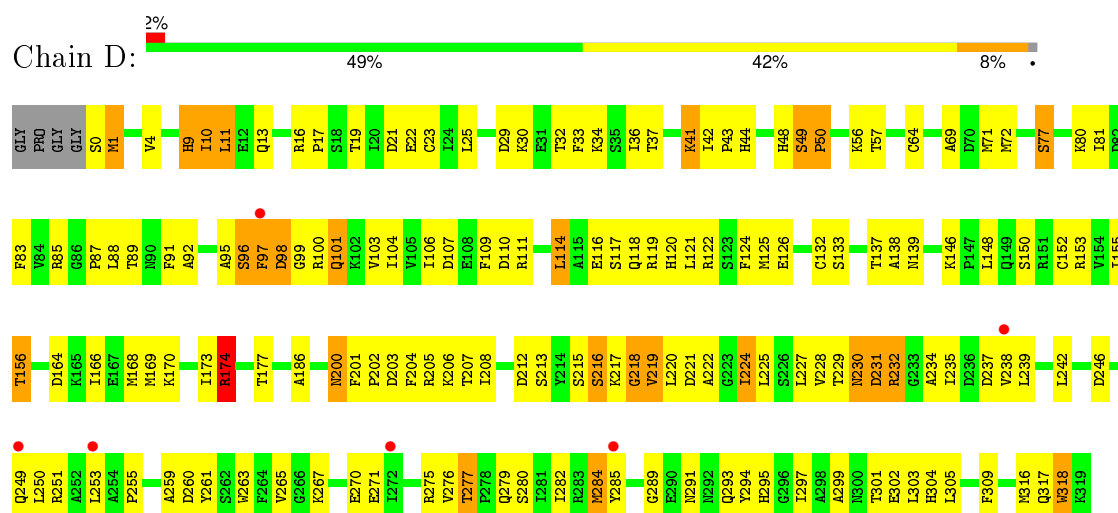
- Molecule 8 is [|(2R,3S,4R,5R)-5-(6-AMINOPURIN-9-YL)-3,4-BIS(OXIDANYL)OXOLAN-2-YL]METHOXY-OXIDANYL-PHOSPHORYL]OXY-OXIDANYL-PHOSPHORYL]OXY-TRIS(FLUORANYL)BERYLLIUM (three-letter code: 08T) (formula:  $C_{10}H_{14}BeF_3N_5O_{10}P_2$ ).



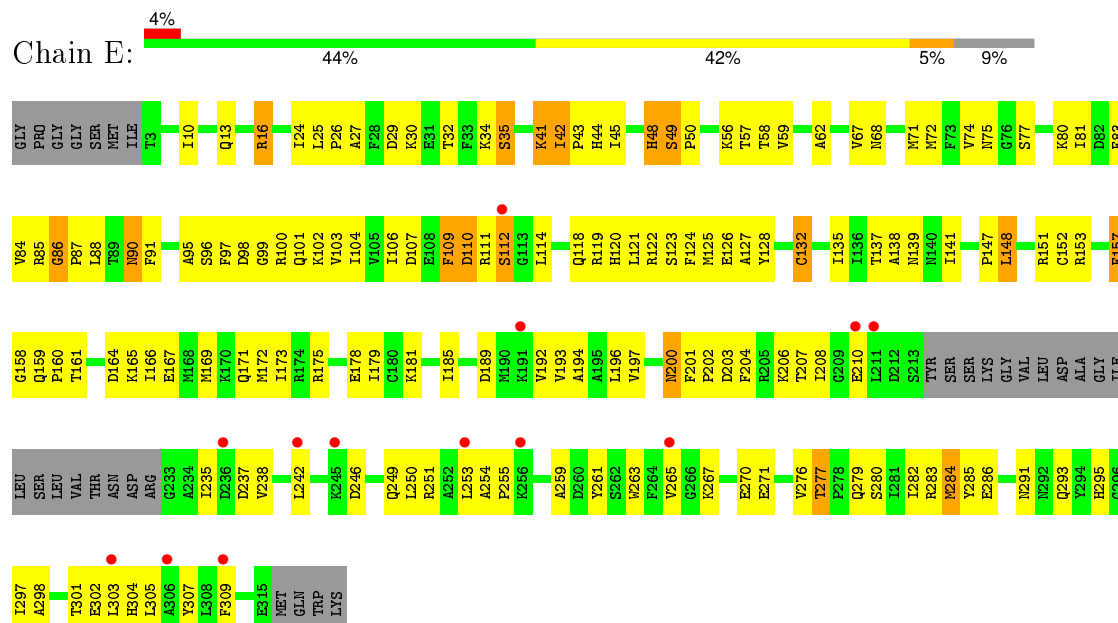
Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
8	C	1	Total	Be	C	F	N	O	P	0	0
			31	1	10	3	5	10	2		
8	D	1	Total	Be	C	F	N	O	P	0	0
			31	1	10	3	5	10	2		



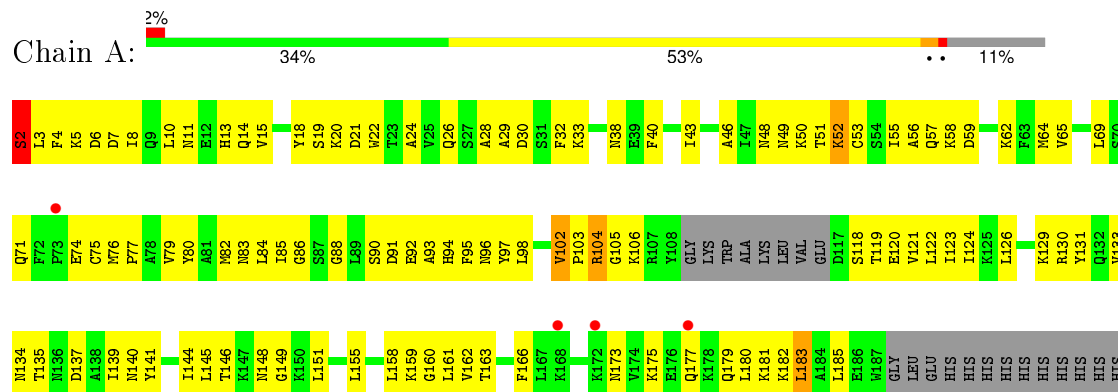




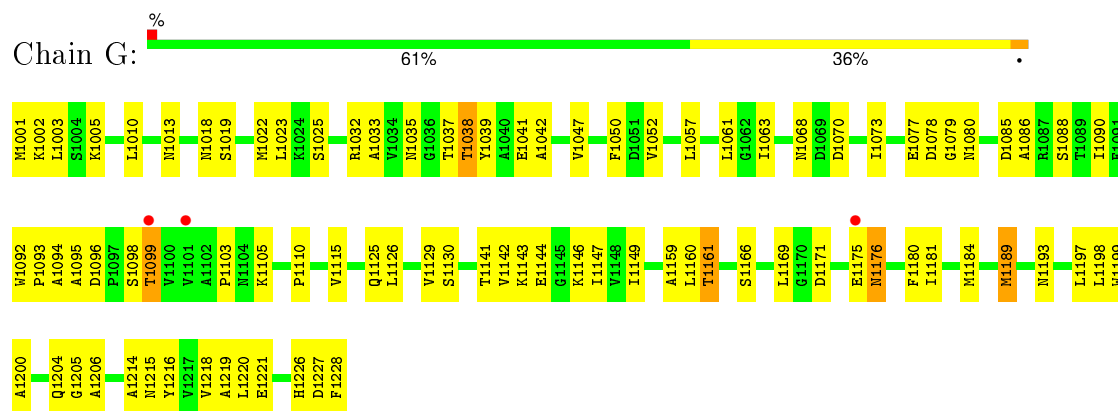
- Molecule 1: DNA polymerase accessory protein 44



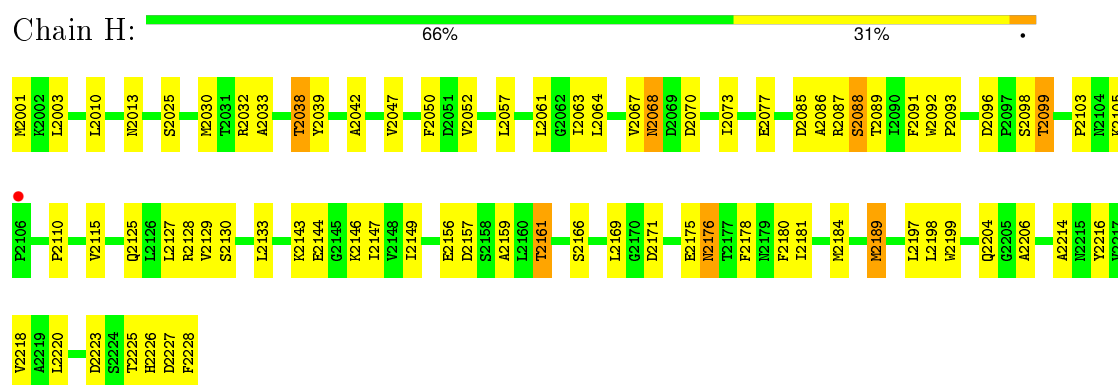
- Molecule 2: DNA polymerase accessory protein 62



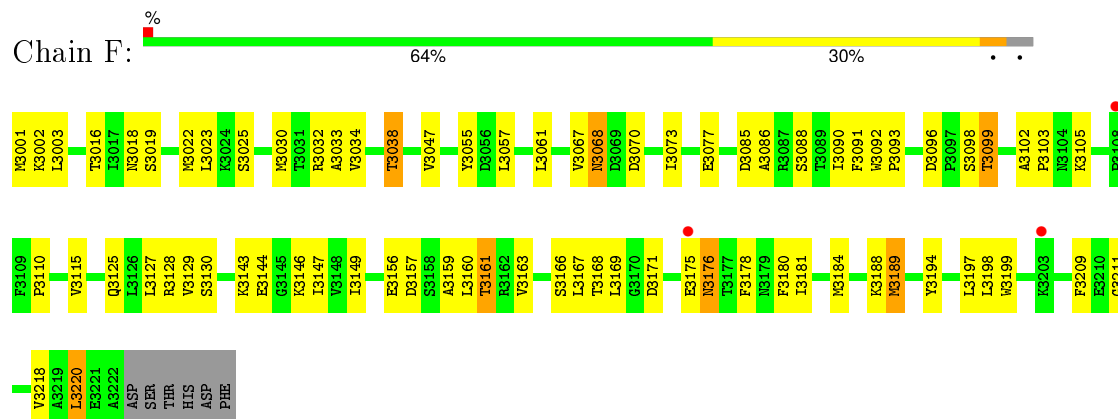
- Molecule 3: DNA polymerase processivity component



- Molecule 3: DNA polymerase processivity component



- Molecule 3: DNA polymerase processivity component



- Molecule 4: Template DNA strand



- Molecule 5: Primer DNA strand



DC	DG	T3	A4	G5	A6	C7	A8	C9	C10
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## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	82.30 Å   137.27 Å   222.78 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	47.65 – 3.20 47.65 – 2.92	Depositor EDS
% Data completeness (in resolution range)	96.2 (47.65-3.20) 89.9 (47.65-2.92)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.12	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.81 (at 2.91 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, $R_{free}$	0.239   ,   0.305 0.238   ,   0.302	Depositor DCC
$R_{free}$ test set	2918 reflections (7.69%)	DCC
Wilson B-factor (Å <sup>2</sup> )	73.1	Xtriage
Anisotropy	0.483	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 59.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 50194 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	16748	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	106.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.99% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ADP, 08T

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	B	0.52	0/2450	0.71	0/3303
1	C	0.58	0/2546	0.75	1/3434 (0.0%)
1	D	0.54	0/2558	0.77	3/3449 (0.1%)
1	E	0.52	0/2331	0.73	1/3144 (0.0%)
2	A	0.48	0/1440	0.74	0/1938
3	F	0.52	0/1721	0.65	0/2324
3	G	0.59	0/1774	0.67	0/2395
3	H	0.50	0/1774	0.63	0/2395
4	I	1.03	0/182	1.86	7/280 (2.5%)
5	J	1.03	0/181	2.09	13/276 (4.7%)
All	All	0.55	0/16957	0.77	25/22938 (0.1%)

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	C	0	1
1	D	0	1
1	E	0	2
2	A	0	2
3	F	0	1
All	All	0	7

There are no bond length outliers.

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	J	3	DT	O4'-C1'-N1	9.74	114.82	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	J	3	DT	C5-C4-O4	-8.25	119.12	124.90
5	J	7	DC	O4'-C1'-N1	8.20	113.74	108.00
5	J	8	DA	O4'-C1'-N9	7.47	113.23	108.00
5	J	5	DG	O4'-C1'-C2'	-7.41	99.97	105.90

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	2	SER	Peptide
1	C	128	TYR	Mainchain
1	D	217	LYS	Mainchain
1	E	157	PHE	Peptide
1	E	49	SER	Peptide

## 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	B	2407	0	2424	182	0
1	C	2503	0	2524	231	0
1	D	2514	0	2543	245	0
1	E	2292	0	2302	198	0
2	A	1416	0	1431	146	0
3	F	1699	0	1716	72	1
3	G	1750	0	1752	112	1
3	H	1750	0	1752	66	0
4	I	163	0	93	18	0
5	J	162	0	90	6	0
6	B	27	0	12	10	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
7	D	1	0	0	0	0
8	C	31	0	13	5	0
8	D	31	0	13	1	0
All	All	16748	0	16665	1056	1

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 32.

The worst 5 of 1056 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:C:97:PHE:CD1	3:G:1204:GLN:HB3	1.57	1.40
1:C:9:HIS:CD2	1:D:41:LYS:HB3	1.73	1.22
1:D:174:ARG:HH11	1:D:174:ARG:CB	1.53	1.20
1:D:174:ARG:HB3	1:D:174:ARG:NH1	1.55	1.20
1:C:174:ARG:HB3	1:C:174:ARG:NH1	1.55	1.18

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:1193:ASN:OD1	3:F:3176:ASN:ND2[4_445]	2.12	0.08

## 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	B	301/324 (93%)	282 (94%)	18 (6%)	1 (0%)	46	85
1	C	317/324 (98%)	302 (95%)	11 (4%)	4 (1%)	15	59
1	D	318/324 (98%)	300 (94%)	13 (4%)	5 (2%)	12	54
1	E	290/324 (90%)	277 (96%)	12 (4%)	1 (0%)	46	85
2	A	174/199 (87%)	140 (80%)	33 (19%)	1 (1%)	30	75
3	F	220/228 (96%)	217 (99%)	3 (1%)	0	100	100
3	G	226/228 (99%)	223 (99%)	3 (1%)	0	100	100
3	H	226/228 (99%)	222 (98%)	4 (2%)	0	100	100
All	All	2072/2179 (95%)	1963 (95%)	97 (5%)	12 (1%)	30	75

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	219	VAL
1	C	97	PHE
1	D	234	ALA
1	B	259	ALA
1	C	259	ALA

### 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	B	266/279 (95%)	239 (90%)	27 (10%)	9	36
1	C	276/279 (99%)	244 (88%)	32 (12%)	7	30
1	D	278/279 (100%)	248 (89%)	30 (11%)	8	33
1	E	250/279 (90%)	225 (90%)	25 (10%)	9	37
2	A	154/174 (88%)	143 (93%)	11 (7%)	18	57
3	F	183/183 (100%)	170 (93%)	13 (7%)	18	57
3	G	189/183 (103%)	177 (94%)	12 (6%)	22	63
3	H	189/183 (103%)	177 (94%)	12 (6%)	22	63
All	All	1785/1839 (97%)	1623 (91%)	162 (9%)	12	42

5 of 162 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	121	LEU
1	E	32	THR
3	F	3025	SER
1	D	146	LYS
1	D	232	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 26 such sidechains are listed below:



Mol	Chain	Res	Type
1	D	101	GLN
1	D	295	HIS
3	H	2190	GLN
1	D	230	ASN
1	D	293	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](#)

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

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 3 are monoatomic - leaving 3 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	ADP	B	700	-	22,29,29	0.99	1 (4%)	27,45,45	2.29	6 (22%)
8	08T	C	700	7	26,33,33	2.88	13 (50%)	28,52,52	5.51	7 (25%)
8	08T	D	700	7	26,33,33	2.90	13 (50%)	28,52,52	6.05	10 (35%)

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	ADP	B	700	-	-	0/12/32/32	0/3/3/3
8	08T	C	700	7	-	0/12/38/38	0/3/3/3
8	08T	D	700	7	-	0/12/38/38	0/3/3/3

The worst 5 of 27 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	C	700	08T	F1-BE	-7.19	1.35	1.54
8	D	700	08T	F1-BE	-6.63	1.37	1.54
8	C	700	08T	F3-BE	-5.56	1.39	1.54
8	D	700	08T	C2'-C3'	-5.49	1.38	1.53
8	D	700	08T	F2-BE	-5.45	1.40	1.54

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	D	700	08T	C1'-N9-C4	-29.49	82.46	126.94
8	C	700	08T	C1'-N9-C4	-26.31	87.26	126.94
8	C	700	08T	N3-C2-N1	-9.65	121.51	128.89
8	D	700	08T	N3-C2-N1	-8.98	122.02	128.89
6	B	700	ADP	N3-C2-N1	-7.09	123.47	128.89

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	700	ADP	10	0
8	C	700	08T	5	0
8	D	700	08T	1	0

## 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 ⓘ

### 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	B	305/324 (94%)	-0.04	6 (1%) 68 54	81, 104, 150, 221	0
1	C	319/324 (98%)	-0.13	2 (0%) 90 84	57, 95, 144, 211	0
1	D	320/324 (98%)	-0.02	6 (1%) 70 55	54, 89, 179, 232	0
1	E	294/324 (90%)	0.09	13 (4%) 38 24	69, 117, 189, 246	0
2	A	178/199 (89%)	0.09	4 (2%) 65 50	81, 120, 181, 223	0
3	F	216/228 (94%)	-0.10	3 (1%) 78 65	70, 96, 159, 252	0
3	G	222/228 (97%)	-0.25	3 (1%) 78 65	58, 84, 130, 188	0
3	H	222/228 (97%)	-0.21	1 (0%) 91 87	71, 95, 143, 200	0
4	I	8/20 (40%)	-0.20	0 100 100	83, 92, 123, 127	0
5	J	8/10 (80%)	-0.05	0 100 100	107, 118, 140, 160	0
All	All	2092/2209 (94%)	-0.07	38 (1%) 71 58	54, 100, 167, 252	0

The worst 5 of 38 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	73	PRO	6.5
2	A	177	GLN	4.9
1	B	214	TYR	4.3
1	D	253	LEU	4.1
1	D	285	TYR	4.1

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

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(Å <sup>2</sup> )	Q<0.9
7	MG	C	800	1/1	0.95	0.46	12.86	83,83,83,83	0
7	MG	D	800	1/1	0.90	0.52	8.46	83,83,83,83	0
8	08T	D	700	31/31	0.94	0.24	0.60	83,83,83,83	0
8	08T	C	700	31/31	0.95	0.22	0.20	83,83,83,83	0
6	ADP	B	700	27/27	0.92	0.18	-1.06	83,83,83,83	0
7	MG	B	800	1/1	0.80	0.29	-	83,83,83,83	0

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

There are no such residues in this entry.