



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 01:39 PM GMT

PDB ID : 3U6X  
Title : Phage TP901-1 baseplate tripod  
Authors : Veesler, D.; Spinelli, S.; Mahony, J.; Lichiere, J.; Blangy, S.; Bricogne, G.;  
Legrand, P.; Ortiz-Lombardia, M.; Campanacci, V.I.; van Sinderen, D.; Cam-  
billau, C.  
Deposited on : 2011-10-13  
Resolution : 2.60 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

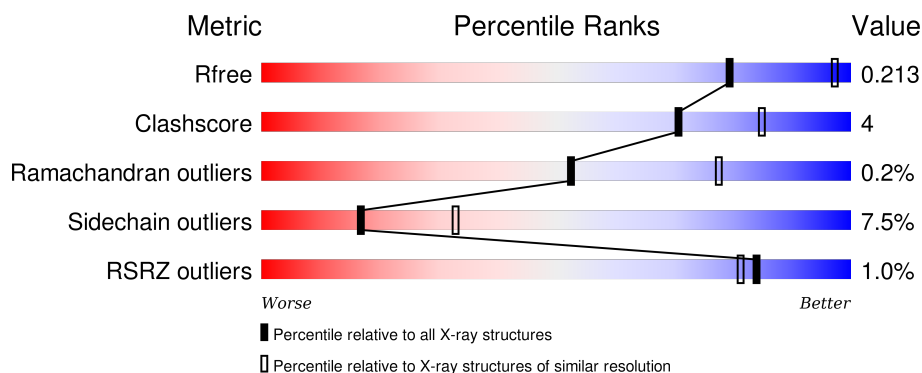
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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.





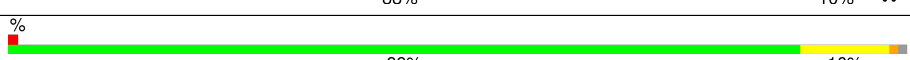
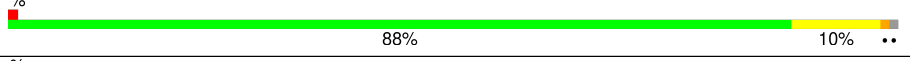
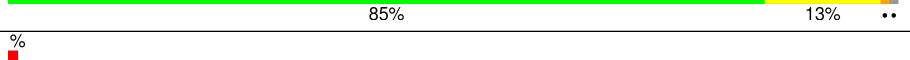
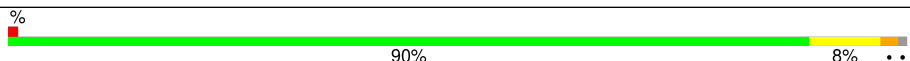
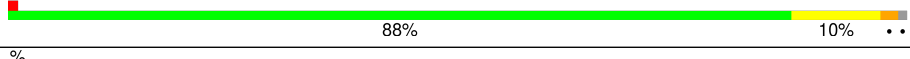
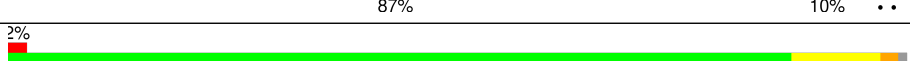

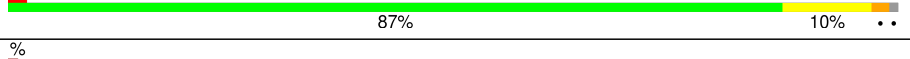

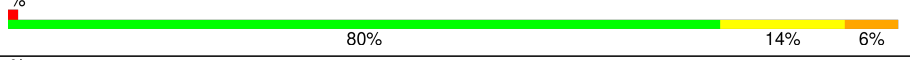
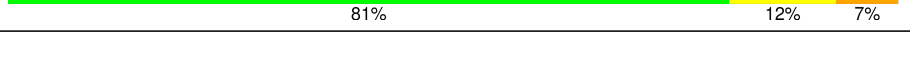






Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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	164	<div> <div></div> <div>88% 10% ..</div> </div>
1	B	164	<div> <div>2%</div> <div>89% 9% ..</div> </div>
1	C	164	<div> <div></div> <div>86% 11% ..</div> </div>
1	D	164	<div> <div></div> <div>87% 11% ..</div> </div>
1	E	164	<div> <div></div> <div>89% 10% ..</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	164	
1	G	164	
1	H	164	
1	I	164	
1	J	164	
1	K	164	
1	L	164	
1	M	164	
1	N	164	
1	O	164	
1	P	164	
1	Q	164	
1	R	164	
2	S	105	
2	T	105	
2	U	105	
2	X	105	
2	Y	105	
2	Z	105	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 30080 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 BPP.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	163	Total	C	N	O	S	0	0	0
			1204	746	214	239	5			
1	B	163	Total	C	N	O	S	0	0	0
			1204	746	214	239	5			
1	C	163	Total	C	N	O	S	0	0	0
			1204	746	214	239	5			
1	D	163	Total	C	N	O	S	0	0	0
			1204	746	214	239	5			
1	E	163	Total	C	N	O	S	0	0	0
			1204	746	214	239	5			
1	F	163	Total	C	N	O	S	0	0	0
			1204	746	214	239	5			
1	G	163	Total	C	N	O	S	0	0	0
			1204	746	214	239	5			
1	H	163	Total	C	N	O	S	0	0	0
			1204	746	214	239	5			
1	I	163	Total	C	N	O	S	0	0	0
			1204	746	214	239	5			
1	J	163	Total	C	N	O	S	0	0	0
			1204	746	214	239	5			
1	K	163	Total	C	N	O	S	0	0	0
			1204	746	214	239	5			
1	L	163	Total	C	N	O	S	0	0	0
			1204	746	214	239	5			
1	M	163	Total	C	N	O	S	0	0	0
			1204	746	214	239	5			
1	N	163	Total	C	N	O	S	0	0	0
			1200	744	214	237	5			
1	O	163	Total	C	N	O	S	0	0	0
			1204	746	214	239	5			
1	P	163	Total	C	N	O	S	0	0	0
			1204	746	214	239	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	163	Total	C	N	O	S	0	0	0
			1204	746	214	239	5			
1	R	163	Total	C	N	O	S	0	0	0
			1204	746	214	239	5			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	164	HIS	-	EXPRESSION TAG	UNP Q9G096
B	164	HIS	-	EXPRESSION TAG	UNP Q9G096
C	164	HIS	-	EXPRESSION TAG	UNP Q9G096
D	164	HIS	-	EXPRESSION TAG	UNP Q9G096
E	164	HIS	-	EXPRESSION TAG	UNP Q9G096
F	164	HIS	-	EXPRESSION TAG	UNP Q9G096
G	164	HIS	-	EXPRESSION TAG	UNP Q9G096
H	164	HIS	-	EXPRESSION TAG	UNP Q9G096
I	164	HIS	-	EXPRESSION TAG	UNP Q9G096
J	164	HIS	-	EXPRESSION TAG	UNP Q9G096
K	164	HIS	-	EXPRESSION TAG	UNP Q9G096
L	164	HIS	-	EXPRESSION TAG	UNP Q9G096
M	164	HIS	-	EXPRESSION TAG	UNP Q9G096
N	164	HIS	-	EXPRESSION TAG	UNP Q9G096
O	164	HIS	-	EXPRESSION TAG	UNP Q9G096
P	164	HIS	-	EXPRESSION TAG	UNP Q9G096
Q	164	HIS	-	EXPRESSION TAG	UNP Q9G096
R	164	HIS	-	EXPRESSION TAG	UNP Q9G096

- Molecule 2 is a protein called ORF48.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	S	105	Total	C	N	O	S	0	0	0
			817	530	124	160	3			
2	T	105	Total	C	N	O	S	0	0	0
			817	530	124	160	3			
2	U	105	Total	C	N	O	S	0	0	0
			817	530	124	160	3			
2	X	105	Total	C	N	O	S	0	0	0
			817	530	124	160	3			
2	Y	105	Total	C	N	O	S	0	0	0
			817	530	124	160	3			
2	Z	105	Total	C	N	O	S	0	0	0
			817	530	124	160	3			

- Molecule 3 is BROMIDE ION (three-letter code: BR) (formula: Br).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	P	1	Total Br 1 1	0	0
3	G	1	Total Br 1 1	0	0
3	Q	1	Total Br 1 1	0	0
3	D	1	Total Br 1 1	0	0
3	K	1	Total Br 1 1	0	0
3	E	2	Total Br 2 2	0	0
3	H	2	Total Br 2 2	0	0
3	I	1	Total Br 1 1	0	0
3	Z	1	Total Br 1 1	0	0
3	T	1	Total Br 1 1	0	0
3	N	1	Total Br 1 1	0	0
3	U	1	Total Br 1 1	0	0
3	X	1	Total Br 1 1	0	0
3	O	1	Total Br 1 1	0	0
3	Y	1	Total Br 1 1	0	0
3	S	1	Total Br 1 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	151	Total O 151 151	0	0
4	B	168	Total O 168 168	0	0
4	C	184	Total O 184 184	0	0

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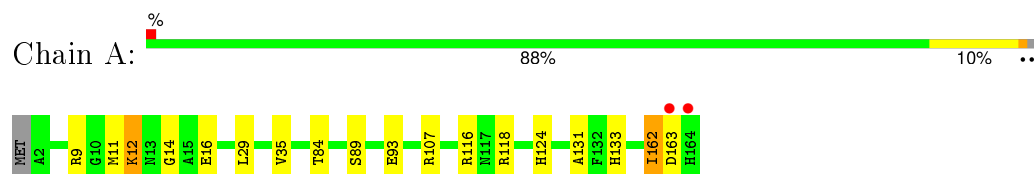
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	181	Total 181	O 181	0	0
4	E	166	Total 166	O 166	0	0
4	F	191	Total 191	O 191	0	0
4	G	128	Total 128	O 128	0	0
4	H	165	Total 165	O 165	0	0
4	I	132	Total 132	O 132	0	0
4	J	189	Total 189	O 189	0	0
4	K	169	Total 169	O 169	0	0
4	L	155	Total 155	O 155	0	0
4	M	158	Total 158	O 158	0	0
4	N	174	Total 174	O 174	0	0
4	O	161	Total 161	O 161	0	0
4	P	90	Total 90	O 90	0	0
4	Q	120	Total 120	O 120	0	0
4	R	107	Total 107	O 107	0	0
4	S	140	Total 140	O 140	0	0
4	T	141	Total 141	O 141	0	0
4	U	116	Total 116	O 116	0	0
4	X	106	Total 106	O 106	0	0
4	Y	97	Total 97	O 97	0	0
4	Z	103	Total 103	O 103	0	0

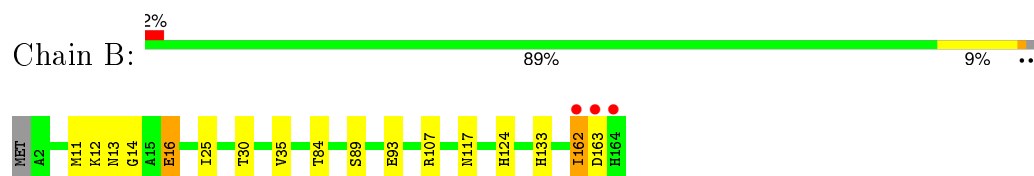
### 3 Residue-property plots [i](#)

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.

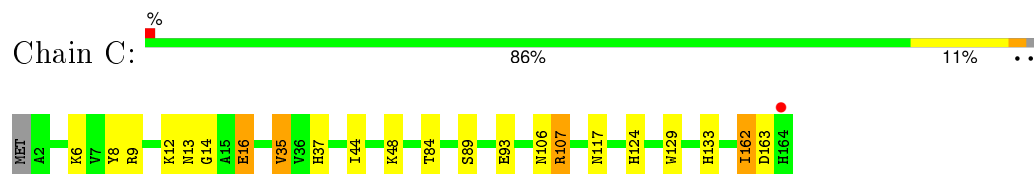
- Molecule 1: BPP



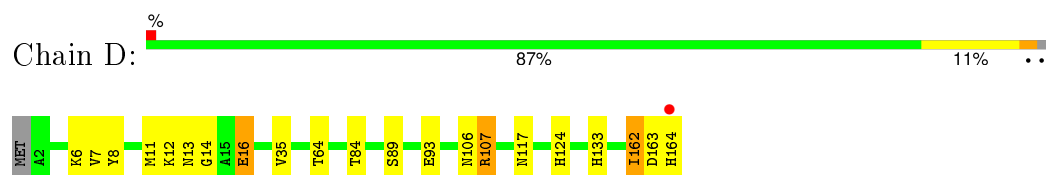
- Molecule 1: BPP



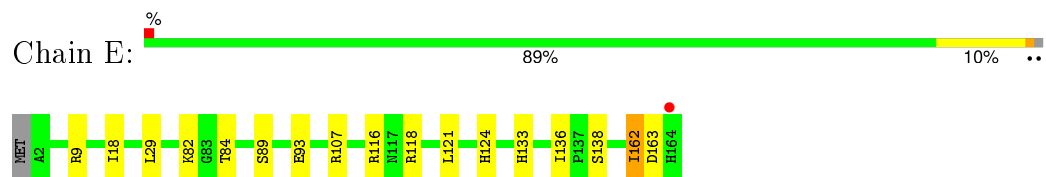
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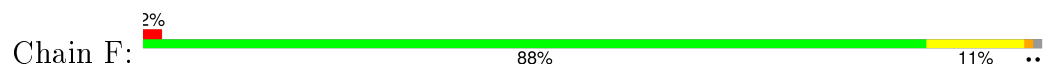
- Molecule 1: BPP



- Molecule 1: BPP



- Molecule 1: BPP

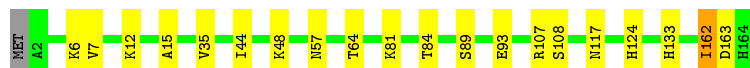






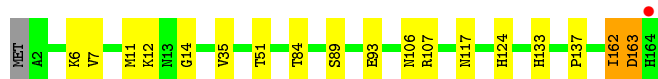
- Molecule 1: BPP

Chain G: 87% 12% ..



- Molecule 1: BPP

Chain H: 88% 10% ..



- Molecule 1: BPP

Chain I: 89% 10% ..



- Molecule 1: BPP

Chain J: 88% 10% ..



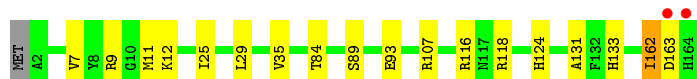
- Molecule 1: BPP

Chain K: 85% 13% ..



- Molecule 1: BPP

Chain L: 88% 10% ..

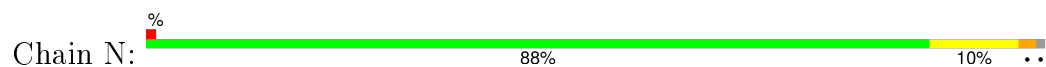


- Molecule 1: BPP

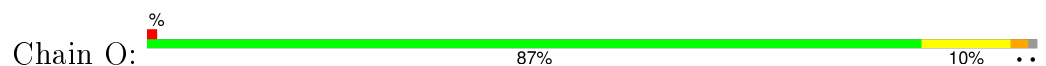
Chain M: 90% 8% ..



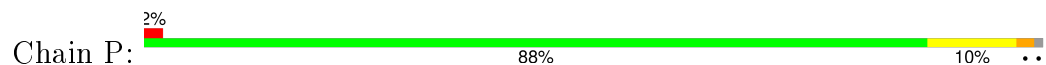
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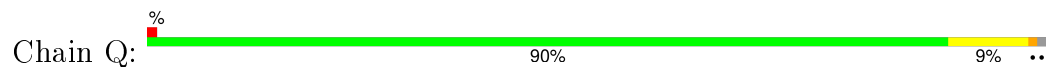
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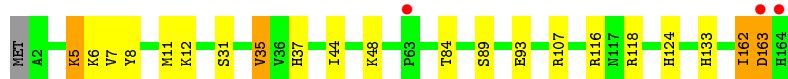
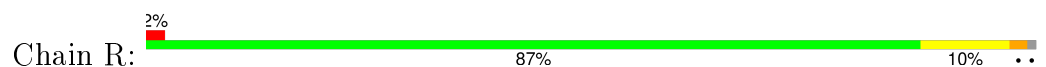
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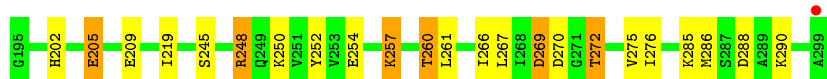
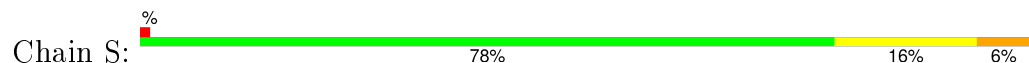
- Molecule 1: BPP



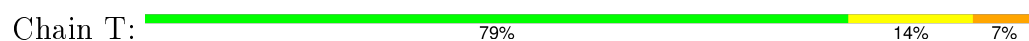
- Molecule 1: BPP

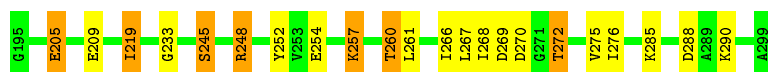


- Molecule 2: ORF48

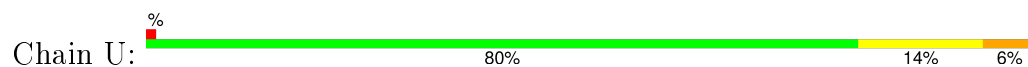


- Molecule 2: ORF48

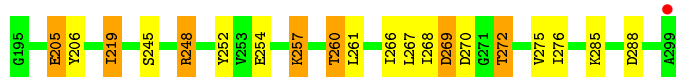
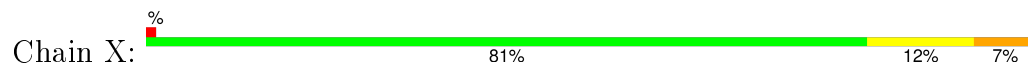




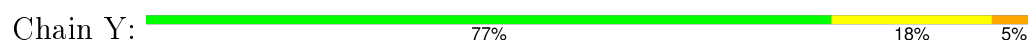
- Molecule 2: ORF48



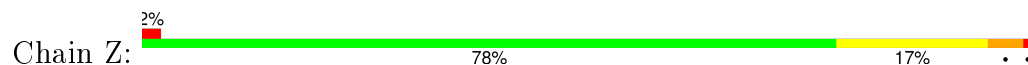
- Molecule 2: ORF48



- Molecule 2: ORF48



- Molecule 2: ORF48



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	149.96Å 237.42Å 152.21Å 90.00° 115.67° 90.00°	Depositor
Resolution (Å)	49.74 – 2.60 49.74 – 2.60	Depositor EDS
% Data completeness (in resolution range)	(Not available) (49.74-2.60) 98.3 (49.74-2.60)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.47 (at 2.61Å)	Xtriage
Refinement program	BUSTER 2.9.2	Depositor
R, $R_{free}$	0.178 , 0.206 0.187 , 0.213	Depositor DCC
$R_{free}$ test set	28781 reflections (11.09%)	DCC
Wilson B-factor (Å <sup>2</sup> )	37.1	Xtriage
Anisotropy	1.026	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 64.0	EDS
Estimated twinning fraction	0.017 for l,-k,h	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	2 of 288313 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	30080	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.60% 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: BR

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	0.48	0/1227	0.72	0/1662
1	B	0.49	0/1227	0.70	0/1662
1	C	0.48	0/1227	0.72	0/1662
1	D	0.47	0/1227	0.70	0/1662
1	E	0.50	0/1227	0.71	0/1662
1	F	0.50	0/1227	0.71	0/1662
1	G	0.46	0/1227	0.71	0/1662
1	H	0.45	0/1227	0.70	0/1662
1	I	0.46	0/1227	0.72	0/1662
1	J	0.50	0/1227	0.72	0/1662
1	K	0.49	0/1227	0.73	0/1662
1	L	0.49	0/1227	0.70	0/1662
1	M	0.47	0/1227	0.70	0/1662
1	N	0.48	0/1223	0.70	0/1657
1	O	0.52	0/1227	0.70	0/1662
1	P	0.41	0/1227	0.68	0/1662
1	Q	0.45	0/1227	0.67	0/1662
1	R	0.46	0/1227	0.70	0/1662
2	S	0.55	0/834	0.79	0/1129
2	T	0.52	0/834	0.79	0/1129
2	U	0.54	0/834	0.80	0/1129
2	X	0.48	0/834	0.76	0/1129
2	Y	0.50	0/834	0.78	0/1129
2	Z	0.51	0/834	0.79	0/1129
All	All	0.48	0/27086	0.72	0/36685

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

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	1204	0	1184	13	0
1	B	1204	0	1184	9	0
1	C	1204	0	1184	21	0
1	D	1204	0	1184	16	0
1	E	1204	0	1184	16	0
1	F	1204	0	1184	9	1
1	G	1204	0	1184	9	0
1	H	1204	0	1184	15	0
1	I	1204	0	1184	12	0
1	J	1204	0	1184	9	1
1	K	1204	0	1184	17	0
1	L	1204	0	1184	14	0
1	M	1204	0	1184	12	0
1	N	1200	0	1180	17	0
1	O	1204	0	1184	13	0
1	P	1204	0	1184	9	0
1	Q	1204	0	1184	12	0
1	R	1204	0	1184	15	0
2	S	817	0	811	10	0
2	T	817	0	811	12	0
2	U	817	0	811	14	0
2	X	817	0	811	11	0
2	Y	817	0	811	13	0
2	Z	817	0	811	13	0
3	D	1	0	0	0	0
3	E	2	0	0	0	0
3	G	1	0	0	0	0
3	H	2	0	0	0	0
3	I	1	0	0	0	0
3	K	1	0	0	0	0
3	N	1	0	0	0	0
3	O	1	0	0	0	0
3	P	1	0	0	0	0
3	Q	1	0	0	0	0
3	S	1	0	0	0	0
3	T	1	0	0	0	0
3	U	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	X	1	0	0	0	0
3	Y	1	0	0	0	0
3	Z	1	0	0	0	0
4	A	151	0	0	1	0
4	B	168	0	0	0	0
4	C	184	0	0	1	0
4	D	181	0	0	1	0
4	E	166	0	0	1	0
4	F	191	0	0	0	0
4	G	128	0	0	1	0
4	H	165	0	0	1	0
4	I	132	0	0	0	0
4	J	189	0	0	3	0
4	K	169	0	0	1	0
4	L	155	0	0	1	0
4	M	158	0	0	3	0
4	N	174	0	0	2	0
4	O	161	0	0	1	0
4	P	90	0	0	0	0
4	Q	120	0	0	1	0
4	R	107	0	0	1	0
4	S	140	0	0	0	0
4	T	141	0	0	1	0
4	U	116	0	0	2	0
4	X	106	0	0	0	0
4	Y	97	0	0	1	0
4	Z	103	0	0	0	0
All	All	30080	0	26174	232	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 4.

The worst 5 of 232 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)
2:Z:257:LYS:O	2:Z:260:THR:HG22	1.62	0.99
2:T:257:LYS:O	2:T:260:THR:HG22	1.71	0.91
1:D:7:VAL:HG13	1:D:11:MET:HE1	1.56	0.87
2:X:257:LYS:O	2:X:260:THR:HG22	1.77	0.85
1:D:133:HIS:HD2	1:F:124:HIS:ND1	1.75	0.84

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)
1:F:8:TYR:OH	1:J:111:ASN:OD1[2_445]	2.19	0.01

## 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	161/164 (98%)	157 (98%)	4 (2%)	0	100	100
1	B	161/164 (98%)	159 (99%)	2 (1%)	0	100	100
1	C	161/164 (98%)	158 (98%)	3 (2%)	0	100	100
1	D	161/164 (98%)	158 (98%)	3 (2%)	0	100	100
1	E	161/164 (98%)	158 (98%)	3 (2%)	0	100	100
1	F	161/164 (98%)	158 (98%)	3 (2%)	0	100	100
1	G	161/164 (98%)	158 (98%)	3 (2%)	0	100	100
1	H	161/164 (98%)	157 (98%)	4 (2%)	0	100	100
1	I	161/164 (98%)	157 (98%)	4 (2%)	0	100	100
1	J	161/164 (98%)	157 (98%)	4 (2%)	0	100	100
1	K	161/164 (98%)	155 (96%)	6 (4%)	0	100	100
1	L	161/164 (98%)	158 (98%)	3 (2%)	0	100	100
1	M	161/164 (98%)	158 (98%)	3 (2%)	0	100	100
1	N	161/164 (98%)	157 (98%)	4 (2%)	0	100	100
1	O	161/164 (98%)	157 (98%)	4 (2%)	0	100	100
1	P	161/164 (98%)	158 (98%)	3 (2%)	0	100	100
1	Q	161/164 (98%)	157 (98%)	4 (2%)	0	100	100
1	R	161/164 (98%)	156 (97%)	5 (3%)	0	100	100
2	S	103/105 (98%)	96 (93%)	6 (6%)	1 (1%)	19	39

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	T	103/105 (98%)	96 (93%)	6 (6%)	1 (1%)	19	39
2	U	103/105 (98%)	96 (93%)	6 (6%)	1 (1%)	19	39
2	X	103/105 (98%)	95 (92%)	7 (7%)	1 (1%)	19	39
2	Y	103/105 (98%)	97 (94%)	4 (4%)	2 (2%)	10	19
2	Z	103/105 (98%)	97 (94%)	4 (4%)	2 (2%)	10	19
All	All	3516/3582 (98%)	3410 (97%)	98 (3%)	8 (0%)	52	77

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	S	269	ASP
2	T	269	ASP
2	U	270	ASP
2	X	269	ASP
2	Y	269	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	133/134 (99%)	125 (94%)	8 (6%)	24	47
1	B	133/134 (99%)	124 (93%)	9 (7%)	20	39
1	C	133/134 (99%)	124 (93%)	9 (7%)	20	39
1	D	133/134 (99%)	123 (92%)	10 (8%)	17	33
1	E	133/134 (99%)	128 (96%)	5 (4%)	40	68
1	F	133/134 (99%)	123 (92%)	10 (8%)	17	33
1	G	133/134 (99%)	122 (92%)	11 (8%)	14	27
1	H	133/134 (99%)	125 (94%)	8 (6%)	24	47
1	I	133/134 (99%)	127 (96%)	6 (4%)	34	62
1	J	133/134 (99%)	122 (92%)	11 (8%)	14	27
1	K	133/134 (99%)	126 (95%)	7 (5%)	28	53

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	L	133/134 (99%)	126 (95%)	7 (5%)	28	53
1	M	133/134 (99%)	125 (94%)	8 (6%)	24	47
1	N	132/134 (98%)	124 (94%)	8 (6%)	23	46
1	O	133/134 (99%)	122 (92%)	11 (8%)	14	27
1	P	133/134 (99%)	121 (91%)	12 (9%)	12	23
1	Q	133/134 (99%)	126 (95%)	7 (5%)	28	53
1	R	133/134 (99%)	124 (93%)	9 (7%)	20	39
2	S	91/91 (100%)	79 (87%)	12 (13%)	5	9
2	T	91/91 (100%)	80 (88%)	11 (12%)	6	11
2	U	91/91 (100%)	82 (90%)	9 (10%)	10	18
2	X	91/91 (100%)	81 (89%)	10 (11%)	8	14
2	Y	91/91 (100%)	80 (88%)	11 (12%)	6	11
2	Z	91/91 (100%)	79 (87%)	12 (13%)	5	9
All	All	2939/2958 (99%)	2718 (92%)	221 (8%)	17	33

5 of 221 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	162	ILE
1	O	101	ASN
2	Y	260	THR
1	M	35	VAL
1	N	93	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 31 such sidechains are listed below:

Mol	Chain	Res	Type
1	H	133	HIS
1	J	133	HIS
1	Q	133	HIS
1	I	106	ASN
1	K	106	ASN

### 5.3.3 RNA ⓘ

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 18 ligands modelled in this entry, 18 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 [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	A	163/164 (99%)	-0.49	2 (1%) 81 77	26, 43, 67, 132	0
1	B	163/164 (99%)	-0.50	3 (1%) 71 66	27, 43, 64, 142	0
1	C	163/164 (99%)	-0.46	1 (0%) 90 88	23, 41, 61, 122	0
1	D	163/164 (99%)	-0.53	1 (0%) 90 88	24, 42, 62, 129	0
1	E	163/164 (99%)	-0.56	1 (0%) 90 88	25, 39, 67, 123	0
1	F	163/164 (99%)	-0.46	3 (1%) 71 66	25, 40, 63, 144	0
1	G	163/164 (99%)	-0.49	0 100 100	33, 50, 79, 125	0
1	H	163/164 (99%)	-0.42	1 (0%) 90 88	30, 45, 65, 130	0
1	I	163/164 (99%)	-0.42	2 (1%) 81 77	32, 50, 74, 134	0
1	J	163/164 (99%)	-0.44	2 (1%) 81 77	24, 40, 66, 151	0
1	K	163/164 (99%)	-0.48	1 (0%) 90 88	23, 38, 61, 128	0
1	L	163/164 (99%)	-0.50	2 (1%) 81 77	28, 41, 69, 128	0
1	M	163/164 (99%)	-0.41	2 (1%) 81 77	27, 44, 68, 147	0
1	N	163/164 (99%)	-0.53	1 (0%) 90 88	27, 44, 65, 139	0
1	O	163/164 (99%)	-0.53	2 (1%) 81 77	26, 41, 65, 127	0
1	P	163/164 (99%)	-0.17	3 (1%) 71 66	37, 65, 91, 145	0
1	Q	163/164 (99%)	-0.42	1 (0%) 90 88	36, 53, 73, 131	0
1	R	163/164 (99%)	-0.35	3 (1%) 71 66	37, 57, 78, 138	0
2	S	105/105 (100%)	-0.50	1 (0%) 84 81	26, 39, 64, 104	0
2	T	105/105 (100%)	-0.60	0 100 100	28, 42, 69, 110	0
2	U	105/105 (100%)	-0.56	1 (0%) 84 81	31, 43, 68, 107	0
2	X	105/105 (100%)	-0.33	1 (0%) 84 81	37, 56, 79, 117	0
2	Y	105/105 (100%)	-0.55	0 100 100	33, 47, 70, 105	0
2	Z	105/105 (100%)	-0.58	2 (1%) 70 64	37, 49, 71, 115	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
All	All	3564/3582 (99%)	-0.47	36 (1%) 84 81	23, 46, 74, 151	0

The worst 5 of 36 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	164	HIS	11.6
1	M	164	HIS	9.1
1	F	164	HIS	8.8
1	B	164	HIS	8.3
1	P	164	HIS	7.0

## 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(Å <sup>2</sup> )	Q<0.9
3	BR	G	201	1/1	0.99	0.10	-1.47	61,61,61,61	0
3	BR	P	201	1/1	0.98	0.09	-2.89	84,84,84,84	0
3	BR	E	202	1/1	0.94	0.11	-2.94	103,103,103,103	0
3	BR	O	201	1/1	0.98	0.08	-3.52	90,90,90,90	0
3	BR	H	202	1/1	0.99	0.08	-5.02	100,100,100,100	0
3	BR	D	201	1/1	0.99	0.07	-6.60	84,84,84,84	0
3	BR	Q	201	1/1	0.96	0.17	-	94,94,94,94	0
3	BR	N	201	1/1	0.98	0.10	-	95,95,95,95	0
3	BR	U	301	1/1	0.99	0.14	-	42,42,42,42	0
3	BR	S	301	1/1	1.00	0.15	-	38,38,38,38	0
3	BR	Z	301	1/1	0.99	0.13	-	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	BR	I	201	1/1	0.98	0.14	-	83,83,83,83	0
3	BR	H	201	1/1	0.98	0.19	-	89,89,89,89	0
3	BR	K	201	1/1	0.98	0.14	-	80,80,80,80	0
3	BR	Y	301	1/1	0.99	0.12	-	45,45,45,45	0
3	BR	E	201	1/1	0.98	0.14	-	80,80,80,80	0
3	BR	T	301	1/1	0.99	0.14	-	45,45,45,45	0
3	BR	X	301	1/1	0.99	0.11	-	52,52,52,52	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.