



# wwPDB X-ray Structure Validation Summary Report i

Nov 7, 2023 – 06:44 PM JST

PDB ID : 8H2N  
Title : gp96 RNA polymerase from P23-45 phage (crystal 2)  
Authors : Chaban, A.; Sokolova, M.L.; Tagami, S.  
Deposited on : 2022-10-06  
Resolution : 4.41 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  
<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>  
with specific help available everywhere you see the i symbol.

The types of validation reports are described at  
<http://www.wwpdb.org/validation/2017/FAQs#types>.

---

The following versions of software and data (see [references](#) ①) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

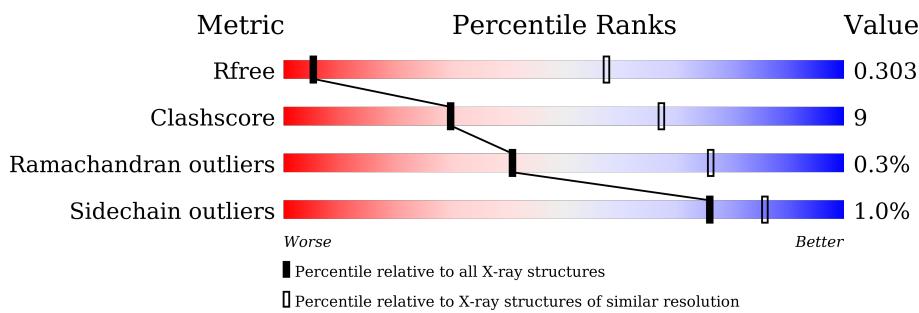
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## X-RAY DIFFRACTION

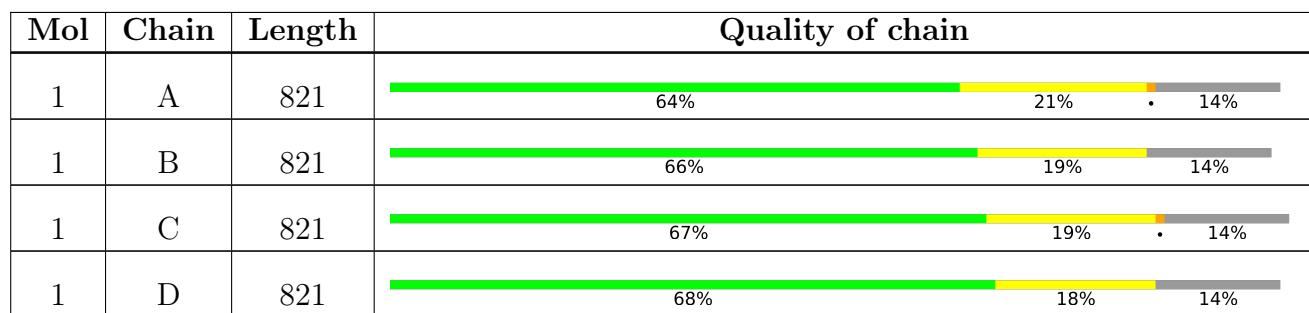
The reported resolution of this entry is 4.41 Å.

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))
$R_{free}$	130704	1046 (5.04-3.80)
Clashscore	141614	1114 (5.04-3.80)
Ramachandran outliers	138981	1061 (5.04-3.80)
Sidechain outliers	138945	1043 (5.04-3.80)

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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. 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  $\leq 5\%$ .



## 2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 22384 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 Tape tail measure protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	709	Total	C 5595	N 3533	O 979	Se 1077	6	0	0
1	B	709	Total	C 5595	N 3533	O 979	Se 1077	6	0	0
1	C	709	Total	C 5595	N 3533	O 979	Se 1077	6	0	0
1	D	709	Total	C 5595	N 3533	O 979	Se 1077	6	0	0

There are 92 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	304	MSE	-	initiating methionine	UNP A7XXD0
A	305	ALA	-	expression tag	UNP A7XXD0
A	306	HIS	-	expression tag	UNP A7XXD0
A	307	HIS	-	expression tag	UNP A7XXD0
A	308	HIS	-	expression tag	UNP A7XXD0
A	309	HIS	-	expression tag	UNP A7XXD0
A	310	HIS	-	expression tag	UNP A7XXD0
A	311	HIS	-	expression tag	UNP A7XXD0
A	312	SER	-	expression tag	UNP A7XXD0
A	313	ALA	-	expression tag	UNP A7XXD0
A	314	ALA	-	expression tag	UNP A7XXD0
A	315	LEU	-	expression tag	UNP A7XXD0
A	316	GLU	-	expression tag	UNP A7XXD0
A	317	VAL	-	expression tag	UNP A7XXD0
A	318	LEU	-	expression tag	UNP A7XXD0
A	319	PHE	-	expression tag	UNP A7XXD0
A	320	GLN	-	expression tag	UNP A7XXD0
A	321	GLY	-	expression tag	UNP A7XXD0
A	322	PRO	-	expression tag	UNP A7XXD0
A	323	GLY	-	expression tag	UNP A7XXD0
A	324	ARG	-	expression tag	UNP A7XXD0

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
A	325	ASN	-	expression tag	UNP A7XXD0
A	326	ASN	-	expression tag	UNP A7XXD0
B	304	MSE	-	initiating methionine	UNP A7XXD0
B	305	ALA	-	expression tag	UNP A7XXD0
B	306	HIS	-	expression tag	UNP A7XXD0
B	307	HIS	-	expression tag	UNP A7XXD0
B	308	HIS	-	expression tag	UNP A7XXD0
B	309	HIS	-	expression tag	UNP A7XXD0
B	310	HIS	-	expression tag	UNP A7XXD0
B	311	HIS	-	expression tag	UNP A7XXD0
B	312	SER	-	expression tag	UNP A7XXD0
B	313	ALA	-	expression tag	UNP A7XXD0
B	314	ALA	-	expression tag	UNP A7XXD0
B	315	LEU	-	expression tag	UNP A7XXD0
B	316	GLU	-	expression tag	UNP A7XXD0
B	317	VAL	-	expression tag	UNP A7XXD0
B	318	LEU	-	expression tag	UNP A7XXD0
B	319	PHE	-	expression tag	UNP A7XXD0
B	320	GLN	-	expression tag	UNP A7XXD0
B	321	GLY	-	expression tag	UNP A7XXD0
B	322	PRO	-	expression tag	UNP A7XXD0
B	323	GLY	-	expression tag	UNP A7XXD0
B	324	ARG	-	expression tag	UNP A7XXD0
B	325	ASN	-	expression tag	UNP A7XXD0
B	326	ASN	-	expression tag	UNP A7XXD0
C	304	MSE	-	initiating methionine	UNP A7XXD0
C	305	ALA	-	expression tag	UNP A7XXD0
C	306	HIS	-	expression tag	UNP A7XXD0
C	307	HIS	-	expression tag	UNP A7XXD0
C	308	HIS	-	expression tag	UNP A7XXD0
C	309	HIS	-	expression tag	UNP A7XXD0
C	310	HIS	-	expression tag	UNP A7XXD0
C	311	HIS	-	expression tag	UNP A7XXD0
C	312	SER	-	expression tag	UNP A7XXD0
C	313	ALA	-	expression tag	UNP A7XXD0
C	314	ALA	-	expression tag	UNP A7XXD0
C	315	LEU	-	expression tag	UNP A7XXD0
C	316	GLU	-	expression tag	UNP A7XXD0
C	317	VAL	-	expression tag	UNP A7XXD0
C	318	LEU	-	expression tag	UNP A7XXD0
C	319	PHE	-	expression tag	UNP A7XXD0
C	320	GLN	-	expression tag	UNP A7XXD0

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
C	321	GLY	-	expression tag	UNP A7XXD0
C	322	PRO	-	expression tag	UNP A7XXD0
C	323	GLY	-	expression tag	UNP A7XXD0
C	324	ARG	-	expression tag	UNP A7XXD0
C	325	ASN	-	expression tag	UNP A7XXD0
C	326	ASN	-	expression tag	UNP A7XXD0
D	304	MSE	-	initiating methionine	UNP A7XXD0
D	305	ALA	-	expression tag	UNP A7XXD0
D	306	HIS	-	expression tag	UNP A7XXD0
D	307	HIS	-	expression tag	UNP A7XXD0
D	308	HIS	-	expression tag	UNP A7XXD0
D	309	HIS	-	expression tag	UNP A7XXD0
D	310	HIS	-	expression tag	UNP A7XXD0
D	311	HIS	-	expression tag	UNP A7XXD0
D	312	SER	-	expression tag	UNP A7XXD0
D	313	ALA	-	expression tag	UNP A7XXD0
D	314	ALA	-	expression tag	UNP A7XXD0
D	315	LEU	-	expression tag	UNP A7XXD0
D	316	GLU	-	expression tag	UNP A7XXD0
D	317	VAL	-	expression tag	UNP A7XXD0
D	318	LEU	-	expression tag	UNP A7XXD0
D	319	PHE	-	expression tag	UNP A7XXD0
D	320	GLN	-	expression tag	UNP A7XXD0
D	321	GLY	-	expression tag	UNP A7XXD0
D	322	PRO	-	expression tag	UNP A7XXD0
D	323	GLY	-	expression tag	UNP A7XXD0
D	324	ARG	-	expression tag	UNP A7XXD0
D	325	ASN	-	expression tag	UNP A7XXD0
D	326	ASN	-	expression tag	UNP A7XXD0

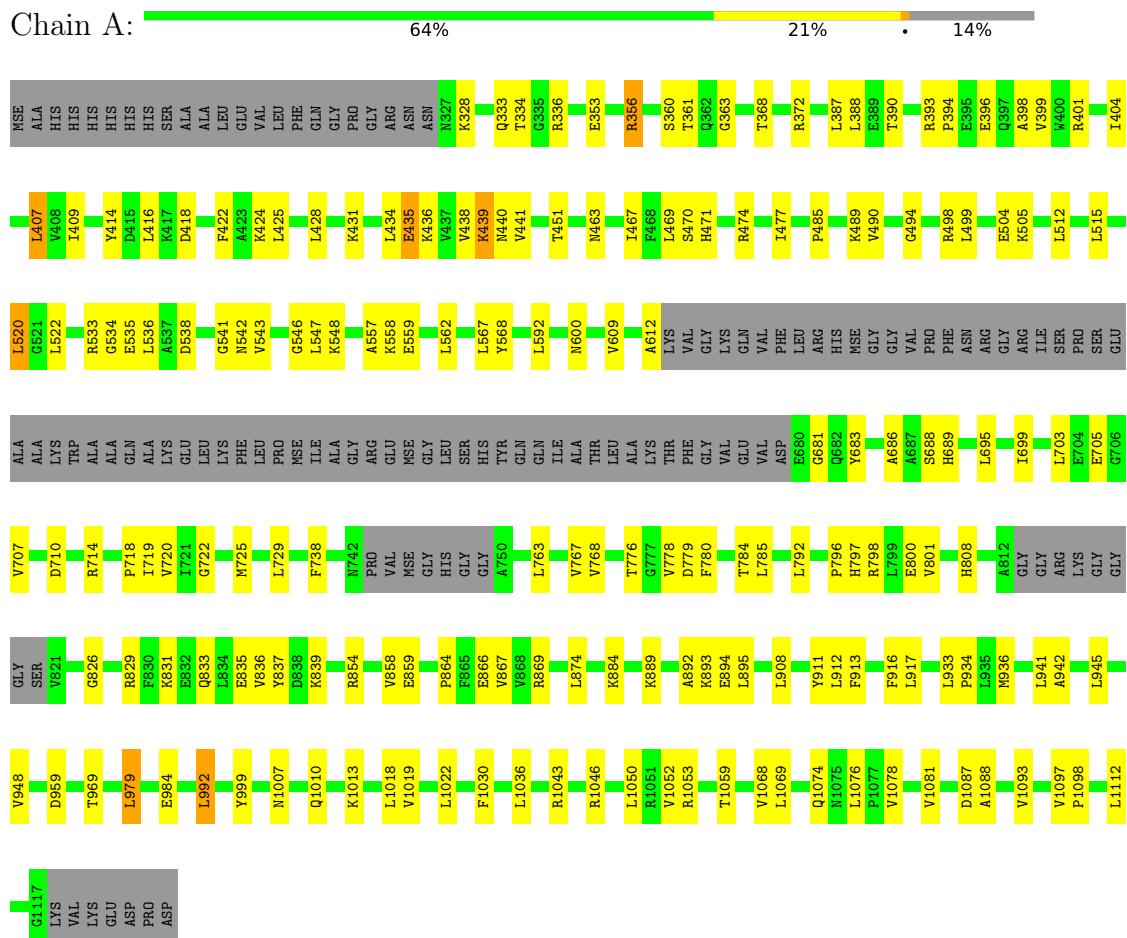
- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

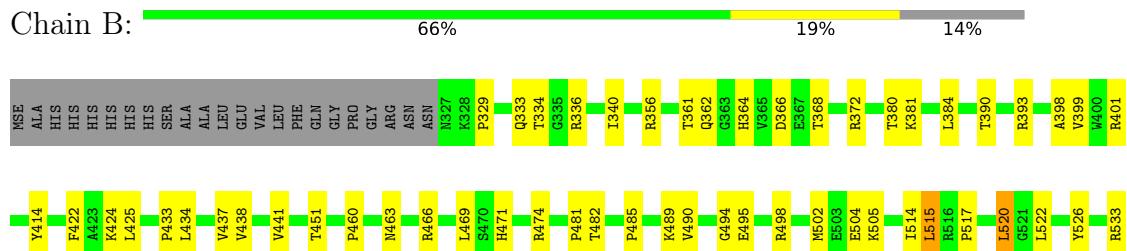
### 3 Residue-property plots [\(i\)](#)

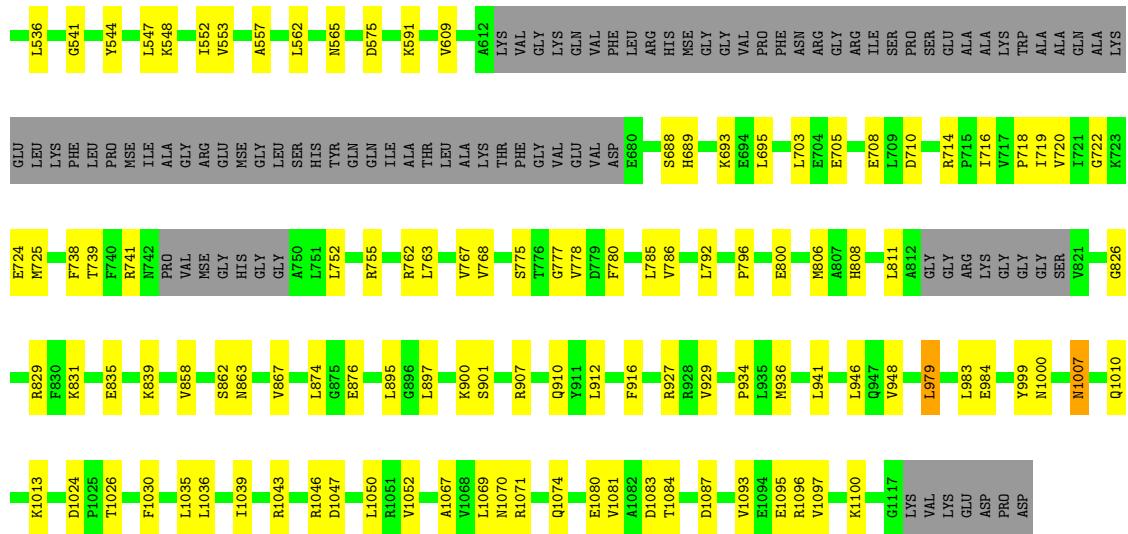
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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: Tape tail measure protein



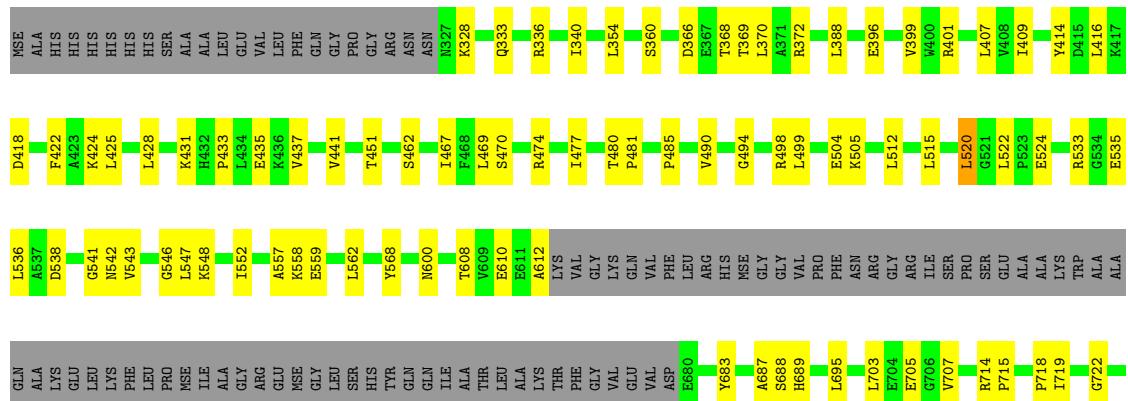
- Molecule 1: Tape tail measure protein





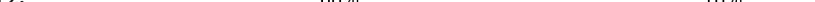
- Molecule 1: Tape tail measure protein

Chain C:  67% 19% • 14%

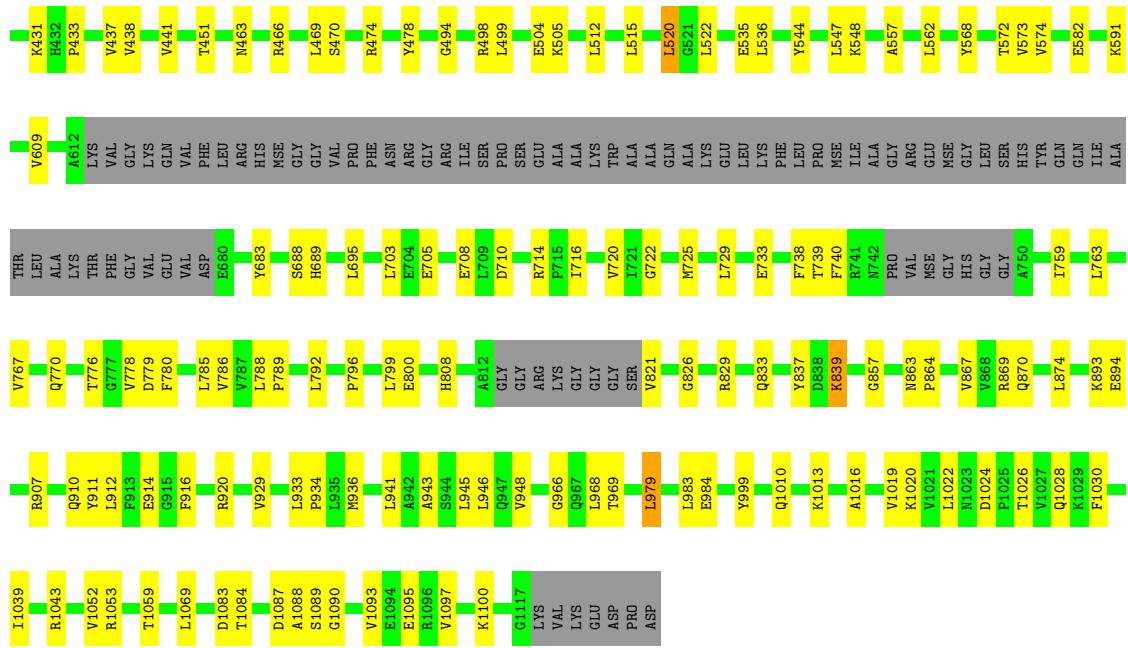




- Molecule 1: Tape tail measure protein

Chain D:  68% 18% 14%





## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	118.16 Å    128.91 Å    136.76 Å 90.00°    96.84°    90.00°	Depositor
Resolution (Å)	44.37 – 4.41 47.95 – 4.41	Depositor EDS
% Data completeness (in resolution range)	99.2 (44.37-4.41) 82.0 (47.95-4.41)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) >$ <sup>1</sup>	0.58 (at 4.45 Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
$R$ , $R_{free}$	0.245 , 0.303 0.245 , 0.303	Depositor DCC
$R_{free}$ test set	1998 reflections (7.74%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	146.8	Xtriage
Anisotropy	0.140	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 115.1	EDS
L-test for twinning <sup>2</sup>	$<  L  > = 0.44$ , $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.87	EDS
Total number of atoms	22384	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	203.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.55% 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  $< |L| >$ ,  $< L^2 >$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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:  
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	0.27	0/5672	0.47	0/7644
1	B	0.27	0/5672	0.47	0/7644
1	C	0.27	0/5672	0.47	0/7644
1	D	0.26	0/5672	0.46	0/7644
All	All	0.26	0/22688	0.47	0/30576

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	5595	0	5684	120	0
1	B	5595	0	5684	121	0
1	C	5595	0	5684	103	0
1	D	5595	0	5684	94	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
All	All	22384	0	22736	426	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 9.

The worst 5 of 426 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:D:1010:GLN:HE22	1:D:1013:LYS:HE3	1.47	0.79
1:C:1002:ALA:HB1	1:C:1010:GLN:HG3	1.66	0.78
1:C:520:LEU:HD13	1:C:522:LEU:HD13	1.66	0.77
1:A:435:GLU:OE2	1:B:1007:ASN:ND2	2.17	0.77
1:A:547:LEU:HB3	1:A:567:LEU:HG	1.67	0.76

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	701/821 (85%)	645 (92%)	53 (8%)	3 (0%)	34 72
1	B	701/821 (85%)	650 (93%)	51 (7%)	0	100 100
1	C	701/821 (85%)	651 (93%)	46 (7%)	4 (1%)	25 65
1	D	701/821 (85%)	663 (95%)	36 (5%)	2 (0%)	41 76
All	All	2804/3284 (85%)	2609 (93%)	186 (7%)	9 (0%)	41 76

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	435	GLU
1	C	1002	ALA
1	C	1088	ALA
1	C	1097	VAL
1	D	1088	ALA

### 5.3.2 Protein sidechains [\(i\)](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	597/670 (89%)	589 (99%)	8 (1%)	69 82
1	B	597/670 (89%)	593 (99%)	4 (1%)	84 90
1	C	597/670 (89%)	589 (99%)	8 (1%)	69 82
1	D	597/670 (89%)	592 (99%)	5 (1%)	81 89
All	All	2388/2680 (89%)	2363 (99%)	25 (1%)	76 86

5 of 25 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	418	ASP
1	C	520	LEU
1	D	979	LEU
1	C	515	LEU
1	C	907	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	967	GLN
1	B	910	GLN
1	C	1010	GLN
1	D	1010	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 monosaccharides in this entry.

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

Of 4 ligands modelled in this entry, 4 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 [\(i\)](#)

### 6.1 Protein, DNA and RNA chains [\(i\)](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.3 Carbohydrates [\(i\)](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.4 Ligands [\(i\)](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.