



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 14, 2026 – 08:16 PM UTC

PDB ID : 4PIW / pdb\_00004piw  
Title : Crystal structure of sugar aminotransferase WecE from Escherichia coli K-12  
Authors : Wang, F.; Xu, W.; Helmich, K.E.; Singh, S.; Yennamalli, R.M.; Miller, M.D.;  
Bingman, C.A.; Thorson, J.S.; Phillips Jr., G.N.; Enzyme Discovery for Nat-  
ural Product Biosynthesis (NatPro)  
Deposited on : 2014-05-09  
Resolution : 2.70 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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

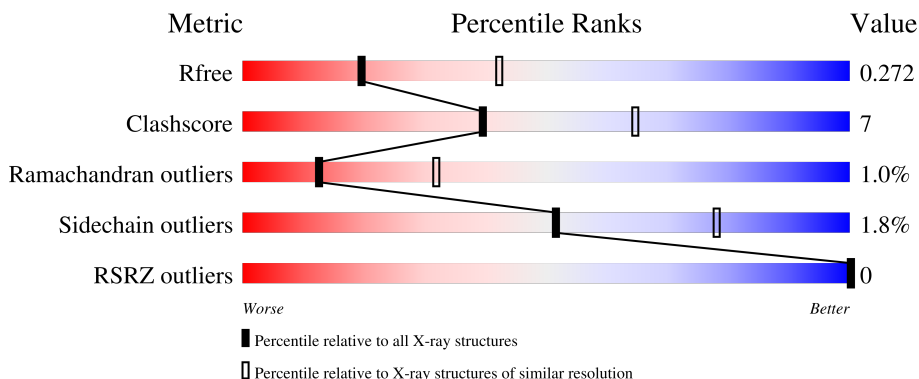
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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))
$R_{free}$	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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  $\leq 5\%$ . 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	396	73% 16% • 9%
1	B	396	74% 16% • 9%
1	C	396	73% 17% • 9%
1	D	396	73% 16% • 9%
1	E	396	76% 14% • 9%

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Mol	Chain	Length	Quality of chain
1	F	396	 72% 18% • 9%
1	G	396	 74% 16% • 9%
1	H	396	 74% 17% • 9%

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 22917 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 TDP-4-keto-6-deoxy-D-glucose transaminase family protein.

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S	Se			
1	A	360	2823	1796	481	527	1	7	11	0	0	0
1	B	362	2839	1807	483	529	1	7	12	0	0	0
1	C	362	2838	1805	483	531	1	7	11	0	0	0
1	D	361	2831	1802	482	528	1	7	11	0	0	0
1	E	362	2839	1807	483	529	1	7	12	0	0	0
1	F	359	2809	1785	479	526	1	7	11	0	0	0
1	G	361	2825	1796	481	528	1	7	12	0	0	0
1	H	361	2825	1796	481	528	1	7	12	0	0	0

There are 160 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MSE	-	expression tag	UNP N2U028
A	-18	GLY	-	expression tag	UNP N2U028
A	-17	SER	-	expression tag	UNP N2U028
A	-16	SER	-	expression tag	UNP N2U028
A	-15	HIS	-	expression tag	UNP N2U028
A	-14	HIS	-	expression tag	UNP N2U028
A	-13	HIS	-	expression tag	UNP N2U028
A	-12	HIS	-	expression tag	UNP N2U028
A	-11	HIS	-	expression tag	UNP N2U028
A	-10	HIS	-	expression tag	UNP N2U028
A	-9	SER	-	expression tag	UNP N2U028
A	-8	SER	-	expression tag	UNP N2U028
A	-7	GLY	-	expression tag	UNP N2U028

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	LEU	-	expression tag	UNP N2U028
A	-5	VAL	-	expression tag	UNP N2U028
A	-4	PRO	-	expression tag	UNP N2U028
A	-3	ARG	-	expression tag	UNP N2U028
A	-2	GLY	-	expression tag	UNP N2U028
A	-1	SER	-	expression tag	UNP N2U028
A	0	HIS	-	expression tag	UNP N2U028
B	-19	MSE	-	expression tag	UNP N2U028
B	-18	GLY	-	expression tag	UNP N2U028
B	-17	SER	-	expression tag	UNP N2U028
B	-16	SER	-	expression tag	UNP N2U028
B	-15	HIS	-	expression tag	UNP N2U028
B	-14	HIS	-	expression tag	UNP N2U028
B	-13	HIS	-	expression tag	UNP N2U028
B	-12	HIS	-	expression tag	UNP N2U028
B	-11	HIS	-	expression tag	UNP N2U028
B	-10	HIS	-	expression tag	UNP N2U028
B	-9	SER	-	expression tag	UNP N2U028
B	-8	SER	-	expression tag	UNP N2U028
B	-7	GLY	-	expression tag	UNP N2U028
B	-6	LEU	-	expression tag	UNP N2U028
B	-5	VAL	-	expression tag	UNP N2U028
B	-4	PRO	-	expression tag	UNP N2U028
B	-3	ARG	-	expression tag	UNP N2U028
B	-2	GLY	-	expression tag	UNP N2U028
B	-1	SER	-	expression tag	UNP N2U028
B	0	HIS	-	expression tag	UNP N2U028
C	-19	MSE	-	expression tag	UNP N2U028
C	-18	GLY	-	expression tag	UNP N2U028
C	-17	SER	-	expression tag	UNP N2U028
C	-16	SER	-	expression tag	UNP N2U028
C	-15	HIS	-	expression tag	UNP N2U028
C	-14	HIS	-	expression tag	UNP N2U028
C	-13	HIS	-	expression tag	UNP N2U028
C	-12	HIS	-	expression tag	UNP N2U028
C	-11	HIS	-	expression tag	UNP N2U028
C	-10	HIS	-	expression tag	UNP N2U028
C	-9	SER	-	expression tag	UNP N2U028
C	-8	SER	-	expression tag	UNP N2U028
C	-7	GLY	-	expression tag	UNP N2U028
C	-6	LEU	-	expression tag	UNP N2U028
C	-5	VAL	-	expression tag	UNP N2U028

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-4	PRO	-	expression tag	UNP N2U028
C	-3	ARG	-	expression tag	UNP N2U028
C	-2	GLY	-	expression tag	UNP N2U028
C	-1	SER	-	expression tag	UNP N2U028
C	0	HIS	-	expression tag	UNP N2U028
D	-19	MSE	-	expression tag	UNP N2U028
D	-18	GLY	-	expression tag	UNP N2U028
D	-17	SER	-	expression tag	UNP N2U028
D	-16	SER	-	expression tag	UNP N2U028
D	-15	HIS	-	expression tag	UNP N2U028
D	-14	HIS	-	expression tag	UNP N2U028
D	-13	HIS	-	expression tag	UNP N2U028
D	-12	HIS	-	expression tag	UNP N2U028
D	-11	HIS	-	expression tag	UNP N2U028
D	-10	HIS	-	expression tag	UNP N2U028
D	-9	SER	-	expression tag	UNP N2U028
D	-8	SER	-	expression tag	UNP N2U028
D	-7	GLY	-	expression tag	UNP N2U028
D	-6	LEU	-	expression tag	UNP N2U028
D	-5	VAL	-	expression tag	UNP N2U028
D	-4	PRO	-	expression tag	UNP N2U028
D	-3	ARG	-	expression tag	UNP N2U028
D	-2	GLY	-	expression tag	UNP N2U028
D	-1	SER	-	expression tag	UNP N2U028
D	0	HIS	-	expression tag	UNP N2U028
E	-19	MSE	-	expression tag	UNP N2U028
E	-18	GLY	-	expression tag	UNP N2U028
E	-17	SER	-	expression tag	UNP N2U028
E	-16	SER	-	expression tag	UNP N2U028
E	-15	HIS	-	expression tag	UNP N2U028
E	-14	HIS	-	expression tag	UNP N2U028
E	-13	HIS	-	expression tag	UNP N2U028
E	-12	HIS	-	expression tag	UNP N2U028
E	-11	HIS	-	expression tag	UNP N2U028
E	-10	HIS	-	expression tag	UNP N2U028
E	-9	SER	-	expression tag	UNP N2U028
E	-8	SER	-	expression tag	UNP N2U028
E	-7	GLY	-	expression tag	UNP N2U028
E	-6	LEU	-	expression tag	UNP N2U028
E	-5	VAL	-	expression tag	UNP N2U028
E	-4	PRO	-	expression tag	UNP N2U028
E	-3	ARG	-	expression tag	UNP N2U028

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-2	GLY	-	expression tag	UNP N2U028
E	-1	SER	-	expression tag	UNP N2U028
E	0	HIS	-	expression tag	UNP N2U028
F	-19	MSE	-	expression tag	UNP N2U028
F	-18	GLY	-	expression tag	UNP N2U028
F	-17	SER	-	expression tag	UNP N2U028
F	-16	SER	-	expression tag	UNP N2U028
F	-15	HIS	-	expression tag	UNP N2U028
F	-14	HIS	-	expression tag	UNP N2U028
F	-13	HIS	-	expression tag	UNP N2U028
F	-12	HIS	-	expression tag	UNP N2U028
F	-11	HIS	-	expression tag	UNP N2U028
F	-10	HIS	-	expression tag	UNP N2U028
F	-9	SER	-	expression tag	UNP N2U028
F	-8	SER	-	expression tag	UNP N2U028
F	-7	GLY	-	expression tag	UNP N2U028
F	-6	LEU	-	expression tag	UNP N2U028
F	-5	VAL	-	expression tag	UNP N2U028
F	-4	PRO	-	expression tag	UNP N2U028
F	-3	ARG	-	expression tag	UNP N2U028
F	-2	GLY	-	expression tag	UNP N2U028
F	-1	SER	-	expression tag	UNP N2U028
F	0	HIS	-	expression tag	UNP N2U028
G	-19	MSE	-	expression tag	UNP N2U028
G	-18	GLY	-	expression tag	UNP N2U028
G	-17	SER	-	expression tag	UNP N2U028
G	-16	SER	-	expression tag	UNP N2U028
G	-15	HIS	-	expression tag	UNP N2U028
G	-14	HIS	-	expression tag	UNP N2U028
G	-13	HIS	-	expression tag	UNP N2U028
G	-12	HIS	-	expression tag	UNP N2U028
G	-11	HIS	-	expression tag	UNP N2U028
G	-10	HIS	-	expression tag	UNP N2U028
G	-9	SER	-	expression tag	UNP N2U028
G	-8	SER	-	expression tag	UNP N2U028
G	-7	GLY	-	expression tag	UNP N2U028
G	-6	LEU	-	expression tag	UNP N2U028
G	-5	VAL	-	expression tag	UNP N2U028
G	-4	PRO	-	expression tag	UNP N2U028
G	-3	ARG	-	expression tag	UNP N2U028
G	-2	GLY	-	expression tag	UNP N2U028
G	-1	SER	-	expression tag	UNP N2U028

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Chain	Residue	Modelled	Actual	Comment	Reference
G	0	HIS	-	expression tag	UNP N2U028
H	-19	MSE	-	expression tag	UNP N2U028
H	-18	GLY	-	expression tag	UNP N2U028
H	-17	SER	-	expression tag	UNP N2U028
H	-16	SER	-	expression tag	UNP N2U028
H	-15	HIS	-	expression tag	UNP N2U028
H	-14	HIS	-	expression tag	UNP N2U028
H	-13	HIS	-	expression tag	UNP N2U028
H	-12	HIS	-	expression tag	UNP N2U028
H	-11	HIS	-	expression tag	UNP N2U028
H	-10	HIS	-	expression tag	UNP N2U028
H	-9	SER	-	expression tag	UNP N2U028
H	-8	SER	-	expression tag	UNP N2U028
H	-7	GLY	-	expression tag	UNP N2U028
H	-6	LEU	-	expression tag	UNP N2U028
H	-5	VAL	-	expression tag	UNP N2U028
H	-4	PRO	-	expression tag	UNP N2U028
H	-3	ARG	-	expression tag	UNP N2U028
H	-2	GLY	-	expression tag	UNP N2U028
H	-1	SER	-	expression tag	UNP N2U028
H	0	HIS	-	expression tag	UNP N2U028

- Molecule 2 is water.

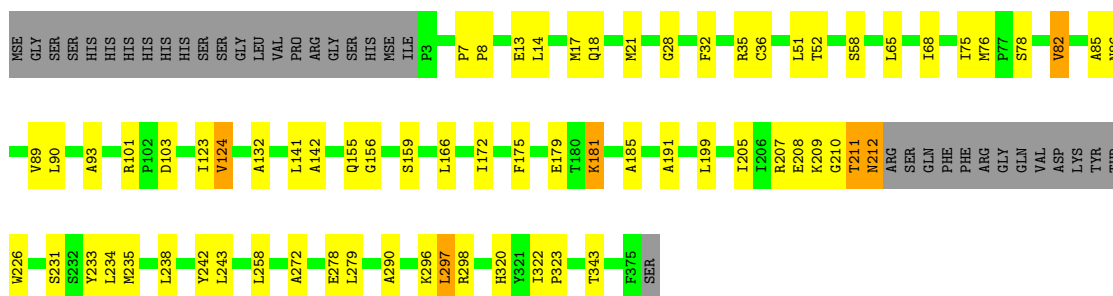
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	27	Total O 27 27	0	0
2	B	27	Total O 27 27	0	0
2	C	37	Total O 37 37	0	0
2	D	32	Total O 32 32	0	0
2	E	26	Total O 26 26	0	0
2	F	22	Total O 22 22	0	0
2	G	50	Total O 50 50	0	0
2	H	67	Total O 67 67	0	0

### 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 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.

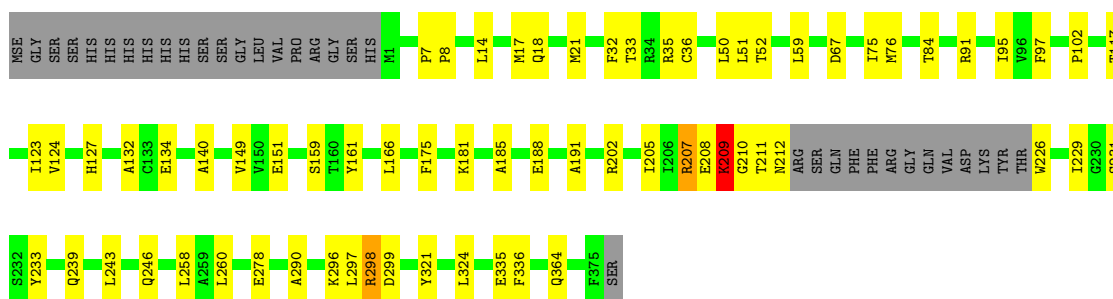
- Molecule 1: TDP-4-keto-6-deoxy-D-glucose transaminase family protein

Chain A: 



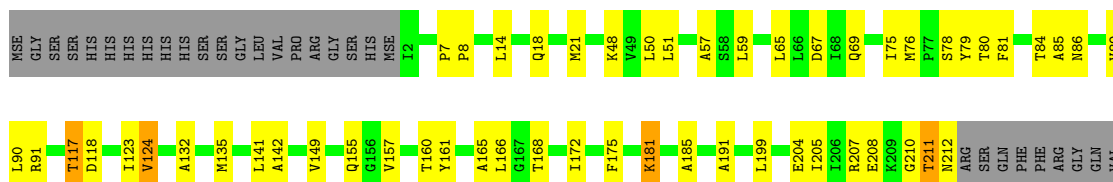
- Molecule 1: TDP-4-keto-6-deoxy-D-glucose transaminase family protein

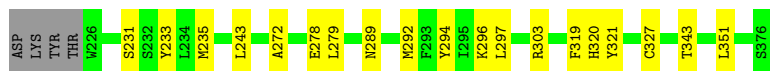
Chain B: 



- Molecule 1: TDP-4-keto-6-deoxy-D-glucose transaminase family protein

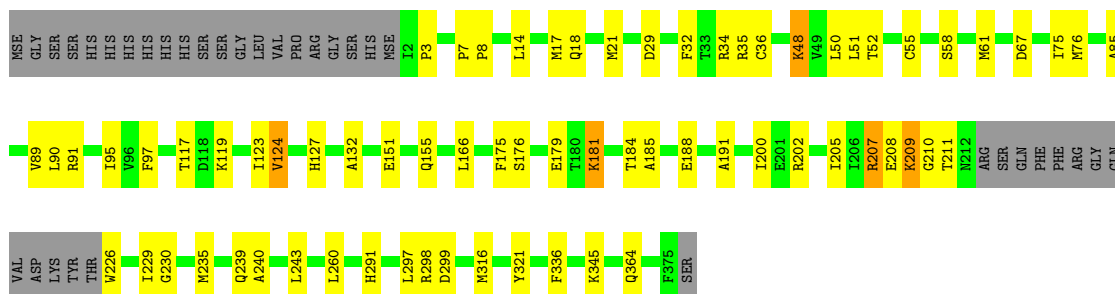
Chain C: 





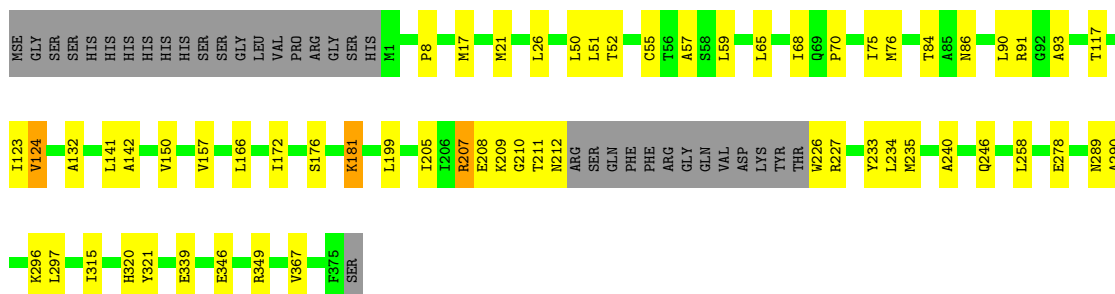
- Molecule 1: TDP-4-keto-6-deoxy-D-glucose transaminase family protein

Chain D: 73% 16% 9%



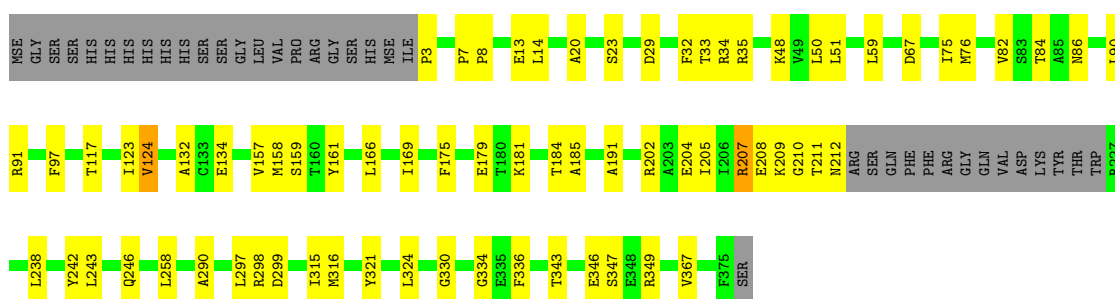
- Molecule 1: TDP-4-keto-6-deoxy-D-glucose transaminase family protein

Chain E: 76% 14% 9%



- Molecule 1: TDP-4-keto-6-deoxy-D-glucose transaminase family protein

Chain F: 72% 18% 9%



- Molecule 1: TDP-4-keto-6-deoxy-D-glucose transaminase family protein

Chain G: 74% 16% 9%





## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	125.34Å 87.48Å 161.55Å 90.00° 91.10° 90.00°	Depositor
Resolution (Å)	48.80 – 2.70 48.80 – 2.70	Depositor EDS
% Data completeness (in resolution range)	89.8 (48.80-2.70) 75.8 (48.80-2.70)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.30 (at 2.61Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1678)	Depositor
R, $R_{free}$	0.236 , 0.275 0.237 , 0.272	Depositor DCC
$R_{free}$ test set	1677 reflections (1.55%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	32.0	Xtriage
Anisotropy	0.866	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 18.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.128 for h,-k,-l	Xtriage
Reported twinning fraction	0.150 for h,-k,-l	Depositor
Outliers	0 of 86071 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	22917	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.87% 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 [i](#)

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

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

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	0/2847	0.68	0/3840
1	B	0.26	0/2863	0.69	0/3862
1	C	0.27	0/2862	0.69	0/3860
1	D	0.27	0/2855	0.68	0/3852
1	E	0.26	0/2863	0.68	0/3862
1	F	0.26	0/2831	0.68	0/3817
1	G	0.26	0/2847	0.67	0/3839
1	H	0.26	0/2847	0.67	0/3839
All	All	0.26	0/22815	0.68	0/30771

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	2823	0	2783	43	0
1	B	2839	0	2804	41	0
1	C	2838	0	2798	44	0
1	D	2831	0	2792	50	0
1	E	2839	0	2804	33	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	2809	0	2772	39	0
1	G	2825	0	2795	40	0
1	H	2825	0	2795	37	0
2	A	27	0	0	0	0
2	B	27	0	0	1	0
2	C	37	0	0	1	0
2	D	32	0	0	1	0
2	E	26	0	0	0	0
2	F	22	0	0	2	0
2	G	50	0	0	3	0
2	H	67	0	0	4	0
All	All	22917	0	22343	302	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 7.

The worst 5 of 302 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:67:ASP:HB2	1:B:202:ARG:HH12	1.45	0.82
1:H:67:ASP:HB2	1:H:202:ARG:HH12	1.45	0.81
1:A:207:ARG:HG3	1:A:233:TYR:HB2	1.65	0.76
1:D:67:ASP:HB2	1:D:202:ARG:HH12	1.50	0.75
1:G:278:GLU:HB2	1:G:296:LYS:HB2	1.67	0.74

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	355/396 (90%)	338 (95%)	14 (4%)	3 (1%)	<b>16</b> <b>37</b>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	357/396 (90%)	332 (93%)	21 (6%)	4 (1%)	11	29
1	C	357/396 (90%)	339 (95%)	16 (4%)	2 (1%)	21	44
1	D	356/396 (90%)	341 (96%)	11 (3%)	4 (1%)	11	29
1	E	357/396 (90%)	340 (95%)	13 (4%)	4 (1%)	11	29
1	F	354/396 (89%)	332 (94%)	17 (5%)	5 (1%)	9	23
1	G	356/396 (90%)	337 (95%)	16 (4%)	3 (1%)	16	37
1	H	356/396 (90%)	341 (96%)	11 (3%)	4 (1%)	11	29
All	All	2848/3168 (90%)	2700 (95%)	119 (4%)	29 (1%)	12	32

5 of 29 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	209	LYS
1	D	298	ARG
1	E	297	LEU
1	F	298	ARG
1	H	298	ARG

### 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	294/313 (94%)	288 (98%)	6 (2%)	48	76
1	B	296/313 (95%)	290 (98%)	6 (2%)	48	76
1	C	296/313 (95%)	291 (98%)	5 (2%)	53	79
1	D	295/313 (94%)	292 (99%)	3 (1%)	68	86
1	E	296/313 (95%)	286 (97%)	10 (3%)	32	62
1	F	293/313 (94%)	290 (99%)	3 (1%)	68	86
1	G	295/313 (94%)	291 (99%)	4 (1%)	59	82
1	H	295/313 (94%)	290 (98%)	5 (2%)	53	79
All	All	2360/2504 (94%)	2318 (98%)	42 (2%)	51	78

5 of 42 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	321	TYR
1	G	124	VAL
1	E	339	GLU
1	F	207	ARG
1	H	48	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	69	GLN
1	H	212	ASN
1	H	239	GLN
1	H	145	HIS
1	D	212	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

8 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	LLP	B	181	1	23,24,25	2.54	6 (26%)	25,32,34	1.32	4 (16%)
1	LLP	A	181	1	23,24,25	2.53	6 (26%)	25,32,34	1.26	3 (12%)
1	LLP	D	181	1	23,24,25	2.55	6 (26%)	25,32,34	1.27	3 (12%)
1	LLP	E	181	1	23,24,25	2.53	6 (26%)	25,32,34	1.20	3 (12%)
1	LLP	F	181	1	23,24,25	2.53	6 (26%)	25,32,34	1.25	3 (12%)
1	LLP	C	181	1	23,24,25	2.56	6 (26%)	25,32,34	1.11	3 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	LLP	H	181	1	23,24,25	2.53	6 (26%)	25,32,34	1.23	3 (12%)
1	LLP	G	181	1	23,24,25	2.53	6 (26%)	25,32,34	1.24	3 (12%)

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
1	LLP	B	181	1	-	4/16/17/19	0/1/1/1
1	LLP	A	181	1	-	10/16/17/19	0/1/1/1
1	LLP	D	181	1	-	6/16/17/19	0/1/1/1
1	LLP	E	181	1	-	8/16/17/19	0/1/1/1
1	LLP	F	181	1	-	5/16/17/19	0/1/1/1
1	LLP	C	181	1	-	5/16/17/19	0/1/1/1
1	LLP	H	181	1	-	5/16/17/19	0/1/1/1
1	LLP	G	181	1	-	7/16/17/19	0/1/1/1

The worst 5 of 48 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	181	LLP	C4-C4'	7.47	1.62	1.46
1	E	181	LLP	C4-C4'	7.40	1.62	1.46
1	D	181	LLP	C4-C4'	7.35	1.62	1.46
1	G	181	LLP	C4-C4'	7.30	1.62	1.46
1	F	181	LLP	C4-C4'	7.29	1.62	1.46

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	181	LLP	C4-C4'-NZ	-3.38	108.43	124.04
1	B	181	LLP	C4-C4'-NZ	-3.26	109.01	124.04
1	D	181	LLP	C4-C4'-NZ	-3.16	109.45	124.04
1	H	181	LLP	C4-C4'-NZ	-3.07	109.85	124.04
1	F	181	LLP	CE-NZ-C4'	-3.00	109.11	118.72

There are no chirality outliers.

5 of 50 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	181	LLP	C5'-OP4-P-OP2
1	A	181	LLP	C5'-OP4-P-OP3
1	A	181	LLP	C-CA-CB-CG
1	A	181	LLP	CG-CD-CE-NZ
1	B	181	LLP	CG-CD-CE-NZ

There are no ring outliers.

5 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	181	LLP	1	0
1	D	181	LLP	5	0
1	E	181	LLP	1	0
1	C	181	LLP	1	0
1	G	181	LLP	1	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

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

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	348/396 (87%)	-1.55	0 100 100	21, 30, 44, 66	0
1	B	349/396 (88%)	-1.55	0 100 100	23, 35, 47, 58	0
1	C	350/396 (88%)	-1.54	0 100 100	19, 32, 45, 64	0
1	D	349/396 (88%)	-1.54	0 100 100	20, 34, 50, 64	0
1	E	349/396 (88%)	-1.49	0 100 100	24, 39, 58, 77	0
1	F	347/396 (87%)	-1.35	0 100 100	33, 57, 76, 90	0
1	G	348/396 (87%)	-1.39	0 100 100	26, 48, 65, 82	0
1	H	348/396 (87%)	-1.44	0 100 100	27, 48, 64, 76	0
All	All	2788/3168 (88%)	-1.48	0 100 100	19, 38, 65, 90	0

There are no RSRZ outliers to report.

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	B-factors(Å <sup>2</sup> )	Q<0.9
1	LLP	B	181	24/25	0.99	0.03	22,30,41,41	0
1	LLP	C	181	24/25	0.99	0.04	21,29,38,43	0
1	LLP	E	181	24/25	0.99	0.04	25,32,42,46	0
1	LLP	F	181	24/25	0.99	0.03	40,51,65,68	0
1	LLP	G	181	24/25	0.99	0.05	32,42,48,52	0
1	LLP	H	181	24/25	0.99	0.03	32,40,50,53	0
1	LLP	A	181	24/25	1.00	0.03	21,30,37,40	0
1	LLP	D	181	24/25	1.00	0.03	24,30,38,41	0

### 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 6.4 Ligands [i](#)

There are no ligands in this entry.

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

There are no such residues in this entry.