



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 13, 2020 – 06:31 am BST

PDB ID : 5LUC  
Title : Crystal structure of the D183N variant of human Alanine:Glyoxylate Amino-transferase major allele (AGT-Ma) at 1.8 Angstrom; internal aldimine with PLP in the active site  
Authors : Giardina, G.; Cutruzzola, F.; Cellini, B.; Borri Voltattorni, C.; Montioli, R.  
Deposited on : 2016-09-08  
Resolution : 1.80 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.

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
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) : 2.11

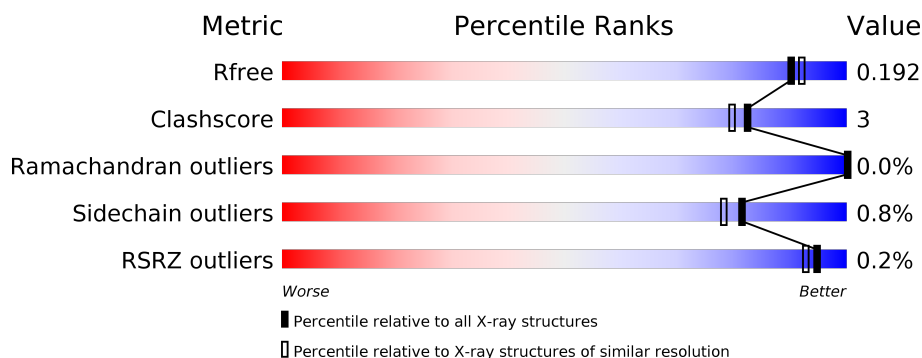
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.80 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	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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 on 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	403	<div> <div>87%</div> <div>8%</div> <div>.</div> </div>
1	B	403	<div> <div>90%</div> <div>6%</div> <div>.</div> </div>
1	E	403	<div> <div>92%</div> <div>.</div> <div>.</div> </div>
1	G	403	<div> <div>87%</div> <div>8%</div> <div>.</div> </div>
1	M	403	<div> <div>89%</div> <div>6%</div> <div>.</div> </div>
1	N	403	<div> <div>90%</div> <div>5%</div> <div>.</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
1	S	403	<div><div></div><div>91%</div><div><div></div><div></div><div></div></div></div>
1	T	403	<div><div></div><div>88%</div><div><div></div><div></div><div></div></div></div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 28283 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 Serine–pyruvate aminotransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	387	Total	C	N	O	S	54	9	0
			3052	1947	537	552	16			
1	B	386	Total	C	N	O	S	6	8	0
			3017	1930	521	548	18			
1	E	386	Total	C	N	O	S	8	4	0
			2966	1899	511	538	18			
1	G	386	Total	C	N	O	S	14	4	0
			2979	1908	514	541	16			
1	M	386	Total	C	N	O	S	9	3	0
			2979	1905	518	539	17			
1	N	387	Total	C	N	O	S	7	1	0
			2965	1897	512	540	16			
1	S	386	Total	C	N	O	S	6	3	0
			2973	1901	515	540	17			
1	T	386	Total	C	N	O	S	6	3	0
			2966	1897	514	539	16			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	MET	-	initiating methionine	UNP P21549
A	-9	GLY	-	expression tag	UNP P21549
A	-8	GLY	-	expression tag	UNP P21549
A	-7	SER	-	expression tag	UNP P21549
A	-6	HIS	-	expression tag	UNP P21549
A	-5	HIS	-	expression tag	UNP P21549
A	-4	HIS	-	expression tag	UNP P21549
A	-3	HIS	-	expression tag	UNP P21549
A	-2	HIS	-	expression tag	UNP P21549
A	-1	HIS	-	expression tag	UNP P21549
A	0	GLY	-	expression tag	UNP P21549
A	183	ASN	ASP	engineered mutation	UNP P21549
B	-10	MET	-	initiating methionine	UNP P21549

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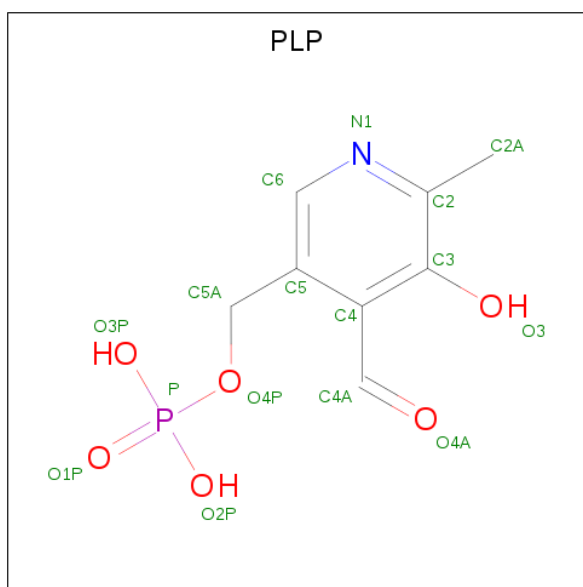
Chain	Residue	Modelled	Actual	Comment	Reference
B	-9	GLY	-	expression tag	UNP P21549
B	-8	GLY	-	expression tag	UNP P21549
B	-7	SER	-	expression tag	UNP P21549
B	-6	HIS	-	expression tag	UNP P21549
B	-5	HIS	-	expression tag	UNP P21549
B	-4	HIS	-	expression tag	UNP P21549
B	-3	HIS	-	expression tag	UNP P21549
B	-2	HIS	-	expression tag	UNP P21549
B	-1	HIS	-	expression tag	UNP P21549
B	0	GLY	-	expression tag	UNP P21549
B	183	ASN	ASP	engineered mutation	UNP P21549
E	-10	MET	-	initiating methionine	UNP P21549
E	-9	GLY	-	expression tag	UNP P21549
E	-8	GLY	-	expression tag	UNP P21549
E	-7	SER	-	expression tag	UNP P21549
E	-6	HIS	-	expression tag	UNP P21549
E	-5	HIS	-	expression tag	UNP P21549
E	-4	HIS	-	expression tag	UNP P21549
E	-3	HIS	-	expression tag	UNP P21549
E	-2	HIS	-	expression tag	UNP P21549
E	-1	HIS	-	expression tag	UNP P21549
E	0	GLY	-	expression tag	UNP P21549
E	183	ASN	ASP	engineered mutation	UNP P21549
G	-10	MET	-	initiating methionine	UNP P21549
G	-9	GLY	-	expression tag	UNP P21549
G	-8	GLY	-	expression tag	UNP P21549
G	-7	SER	-	expression tag	UNP P21549
G	-6	HIS	-	expression tag	UNP P21549
G	-5	HIS	-	expression tag	UNP P21549
G	-4	HIS	-	expression tag	UNP P21549
G	-3	HIS	-	expression tag	UNP P21549
G	-2	HIS	-	expression tag	UNP P21549
G	-1	HIS	-	expression tag	UNP P21549
G	0	GLY	-	expression tag	UNP P21549
G	183	ASN	ASP	engineered mutation	UNP P21549
M	-10	MET	-	initiating methionine	UNP P21549
M	-9	GLY	-	expression tag	UNP P21549
M	-8	GLY	-	expression tag	UNP P21549
M	-7	SER	-	expression tag	UNP P21549
M	-6	HIS	-	expression tag	UNP P21549
M	-5	HIS	-	expression tag	UNP P21549
M	-4	HIS	-	expression tag	UNP P21549

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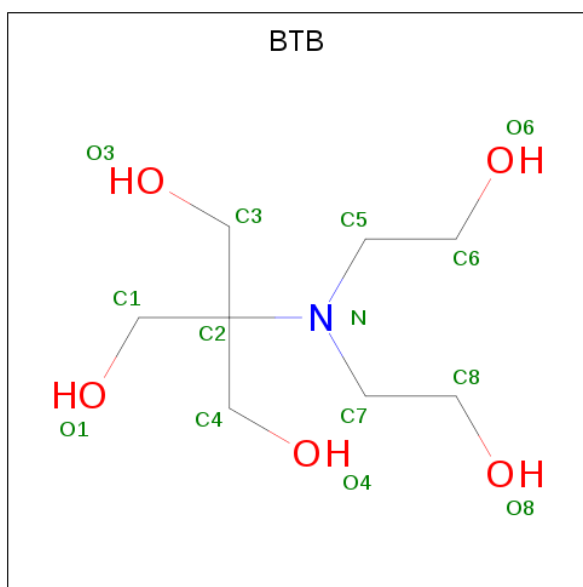
Chain	Residue	Modelled	Actual	Comment	Reference
M	-3	HIS	-	expression tag	UNP P21549
M	-2	HIS	-	expression tag	UNP P21549
M	-1	HIS	-	expression tag	UNP P21549
M	0	GLY	-	expression tag	UNP P21549
M	183	ASN	ASP	engineered mutation	UNP P21549
N	-10	MET	-	initiating methionine	UNP P21549
N	-9	GLY	-	expression tag	UNP P21549
N	-8	GLY	-	expression tag	UNP P21549
N	-7	SER	-	expression tag	UNP P21549
N	-6	HIS	-	expression tag	UNP P21549
N	-5	HIS	-	expression tag	UNP P21549
N	-4	HIS	-	expression tag	UNP P21549
N	-3	HIS	-	expression tag	UNP P21549
N	-2	HIS	-	expression tag	UNP P21549
N	-1	HIS	-	expression tag	UNP P21549
N	0	GLY	-	expression tag	UNP P21549
N	183	ASN	ASP	engineered mutation	UNP P21549
S	-10	MET	-	initiating methionine	UNP P21549
S	-9	GLY	-	expression tag	UNP P21549
S	-8	GLY	-	expression tag	UNP P21549
S	-7	SER	-	expression tag	UNP P21549
S	-6	HIS	-	expression tag	UNP P21549
S	-5	HIS	-	expression tag	UNP P21549
S	-4	HIS	-	expression tag	UNP P21549
S	-3	HIS	-	expression tag	UNP P21549
S	-2	HIS	-	expression tag	UNP P21549
S	-1	HIS	-	expression tag	UNP P21549
S	0	GLY	-	expression tag	UNP P21549
S	183	ASN	ASP	engineered mutation	UNP P21549
T	-10	MET	-	initiating methionine	UNP P21549
T	-9	GLY	-	expression tag	UNP P21549
T	-8	GLY	-	expression tag	UNP P21549
T	-7	SER	-	expression tag	UNP P21549
T	-6	HIS	-	expression tag	UNP P21549
T	-5	HIS	-	expression tag	UNP P21549
T	-4	HIS	-	expression tag	UNP P21549
T	-3	HIS	-	expression tag	UNP P21549
T	-2	HIS	-	expression tag	UNP P21549
T	-1	HIS	-	expression tag	UNP P21549
T	0	GLY	-	expression tag	UNP P21549
T	183	ASN	ASP	engineered mutation	UNP P21549

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: C<sub>8</sub>H<sub>10</sub>NO<sub>6</sub>P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	E	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	G	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	M	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	N	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	S	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	T	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

- Molecule 3 is 2-[BIS-(2-HYDROXY-ETHYL)-AMINO]-2-HYDROXYMETHYL-PROPAN E-1,3-DIOL (three-letter code: BTB) (formula: C<sub>8</sub>H<sub>19</sub>NO<sub>5</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	E	1	Total	C	N	O	0	0
			14	8	1	5		
3	G	1	Total	C	N	O	0	0
			14	8	1	5		
3	M	1	Total	C	N	O	0	0
			14	8	1	5		
3	N	1	Total	C	N	O	0	0
			14	8	1	5		
3	S	1	Total	C	N	O	0	0
			14	8	1	5		
3	T	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	538	Total	O	0	0
			538	538		
4	B	512	Total	O	0	0
			512	512		
4	E	497	Total	O	0	0
			497	497		
4	G	497	Total	O	0	0
			497	497		

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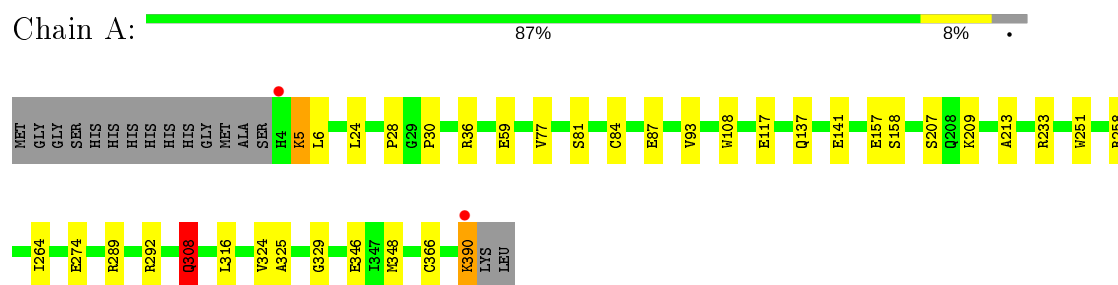
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	M	525	Total 525	O 525	0	0
4	N	529	Total 529	O 529	0	0
4	S	548	Total 548	O 548	0	0
4	T	508	Total 508	O 508	0	0

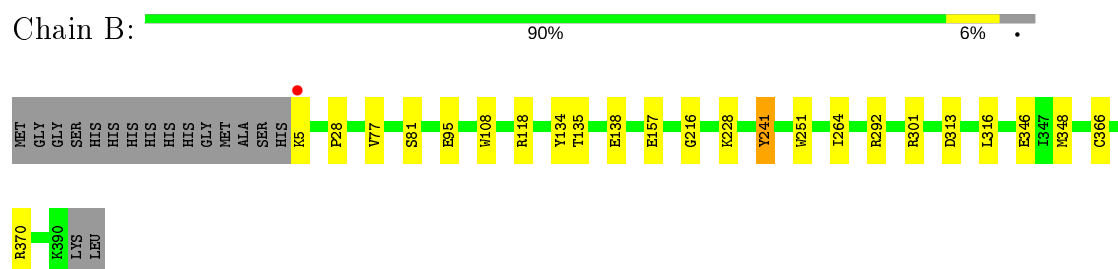
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

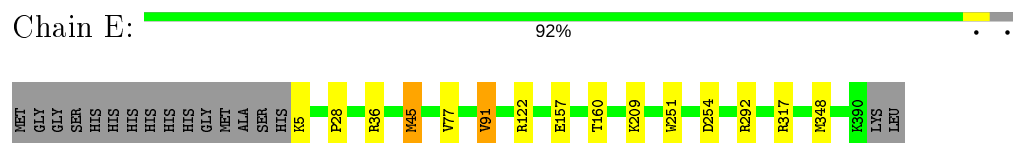
- Molecule 1: Serine-pyruvate aminotransferase



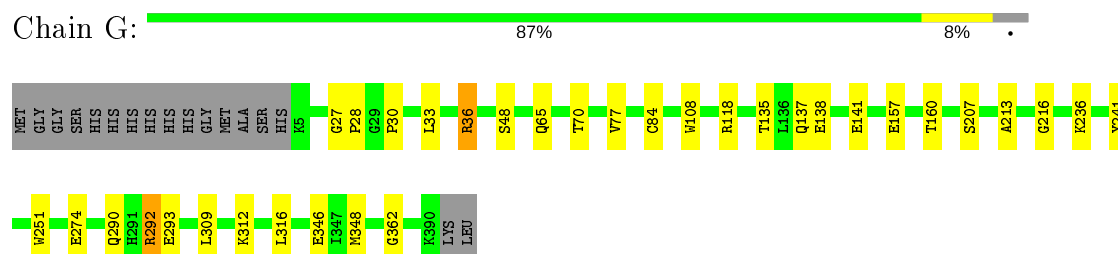
- Molecule 1: Serine-pyruvate aminotransferase




- Molecule 1: Serine-pyruvate aminotransferase

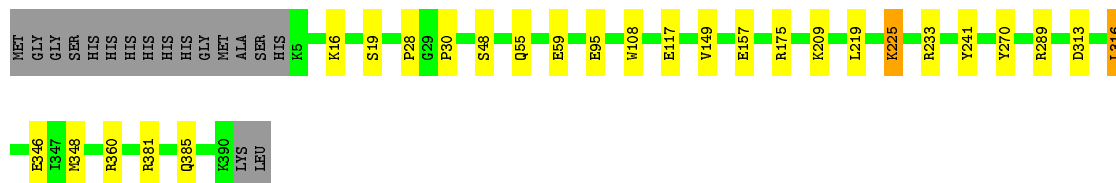


- Molecule 1: Serine-pyruvate aminotransferase




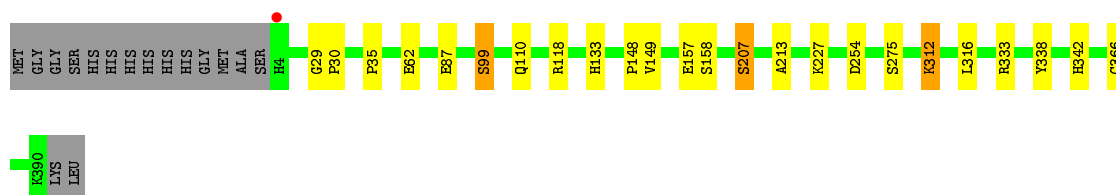
- Molecule 1: Serine-pyruvate aminotransferase

Chain M:  89% 6% •




- Molecule 1: Serine-pyruvate aminotransferase

Chain N:  90% 5% • •




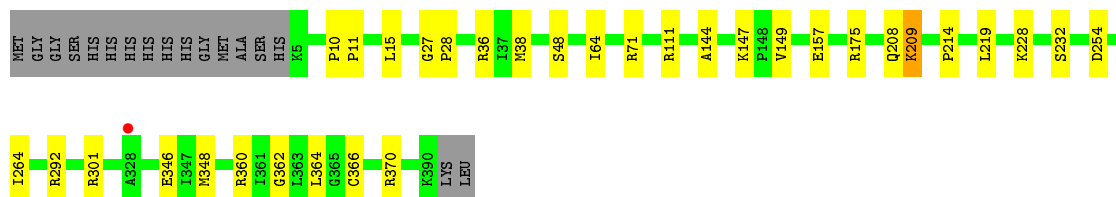
- Molecule 1: Serine-pyruvate aminotransferase

Chain S:  91% • • •



- Molecule 1: Serine-pyruvate aminotransferase

Chain T:  88% 8% •



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	127.60Å 141.11Å 256.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	56.69 – 1.80 57.23 – 1.80	Depositor EDS
% Data completeness (in resolution range)	93.6 (56.69-1.80) 93.7 (57.23-1.80)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.04 (at 1.80Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.163 , 0.192 0.164 , 0.192	Depositor DCC
$R_{free}$ test set	19842 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	15.8	Xtriage
Anisotropy	0.054	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 45.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	28283	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 23.27 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.8170e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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: BTB, PLP

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	1.01	11/3125 (0.4%)	0.97	12/4241 (0.3%)
1	B	0.98	7/3086 (0.2%)	0.85	3/4190 (0.1%)
1	E	0.98	4/3035 (0.1%)	1.03	13/4127 (0.3%)
1	G	0.97	6/3048 (0.2%)	0.86	3/4141 (0.1%)
1	M	0.97	4/3048 (0.1%)	0.90	7/4140 (0.2%)
1	N	1.04	9/3034 (0.3%)	0.87	2/4125 (0.0%)
1	S	1.00	6/3042 (0.2%)	0.90	6/4134 (0.1%)
1	T	1.00	7/3035 (0.2%)	0.89	6/4127 (0.1%)
All	All	0.99	54/24453 (0.2%)	0.91	52/33225 (0.2%)

The worst 5 of 54 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	366	CYS	CB-SG	-10.27	1.64	1.82
1	B	366	CYS	CB-SG	-8.41	1.68	1.82
1	E	122	ARG	CZ-NH2	-7.80	1.23	1.33
1	T	366	CYS	CB-SG	-7.76	1.69	1.82
1	S	36	ARG	CB-CG	-7.53	1.32	1.52

The worst 5 of 52 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	122	ARG	NE-CZ-NH2	27.20	133.90	120.30
1	E	122	ARG	NE-CZ-NH1	-15.90	112.35	120.30
1	A	289[A]	ARG	NE-CZ-NH2	13.77	127.18	120.30
1	A	289[B]	ARG	NE-CZ-NH2	13.77	127.18	120.30
1	S	7	LEU	CA-CB-CG	9.58	137.34	115.30

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	3052	0	3071	24	0
1	B	3017	0	3038	12	0
1	E	2966	0	2944	6	0
1	G	2979	0	2987	24	0
1	M	2979	0	2992	17	0
1	N	2965	0	2967	10	0
1	S	2973	0	2972	9	0
1	T	2966	0	2962	21	0
2	A	15	0	7	2	0
2	B	15	0	6	1	0
2	E	15	0	7	1	0
2	G	15	0	7	1	0
2	M	15	0	7	2	0
2	N	15	0	7	0	0
2	S	15	0	6	0	0
2	T	15	0	7	0	0
3	A	14	0	19	0	0
3	B	14	0	19	1	0
3	E	14	0	19	0	0
3	G	14	0	19	0	0
3	M	14	0	19	0	0
3	N	14	0	19	1	0
3	S	14	0	19	1	0
3	T	14	0	19	1	0
4	A	538	0	0	7	0
4	B	512	0	0	5	5
4	E	497	0	0	3	2
4	G	497	0	0	7	0
4	M	525	0	0	9	2
4	N	529	0	0	2	0
4	S	548	0	0	5	1
4	T	508	0	0	7	2
All	All	28283	0	24139	122	6

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 3.

The worst 5 of 122 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:M:28:PRO:HD2	1:M:348[B]:MET:HG2	1.47	0.93
1:N:333:ARG:NH1	4:N:502:HOH:O	2.17	0.77
1:M:117:GLU:OE2	4:M:501:HOH:O	2.04	0.76
1:A:141:GLU:OE1	4:A:501:HOH:O	2.02	0.75
1:S:292:ARG:NH1	4:S:502:HOH:O	2.07	0.72

The worst 5 of 6 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)
4:E:738:HOH:O	4:S:943:HOH:O[4_545]	1.96	0.24
4:B:675:HOH:O	4:E:694:HOH:O[1_565]	2.01	0.19
4:B:772:HOH:O	4:M:786:HOH:O[3_555]	2.02	0.18
4:B:533:HOH:O	4:M:519:HOH:O[3_555]	2.05	0.15
4:B:505:HOH:O	4:T:619:HOH:O[4_555]	2.16	0.04

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	394/403 (98%)	386 (98%)	7 (2%)	1 (0%)	41	27
1	B	392/403 (97%)	387 (99%)	5 (1%)	0	100	100
1	E	388/403 (96%)	383 (99%)	5 (1%)	0	100	100
1	G	388/403 (96%)	382 (98%)	6 (2%)	0	100	100
1	M	387/403 (96%)	379 (98%)	8 (2%)	0	100	100
1	N	386/403 (96%)	380 (98%)	6 (2%)	0	100	100
1	S	387/403 (96%)	380 (98%)	7 (2%)	0	100	100
1	T	387/403 (96%)	380 (98%)	7 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	3109/3224 (96%)	3057 (98%)	51 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	233	ARG

### 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	326/334 (98%)	321 (98%)	5 (2%)	65	56
1	B	323/334 (97%)	322 (100%)	1 (0%)	92	91
1	E	309/334 (92%)	308 (100%)	1 (0%)	92	91
1	G	315/334 (94%)	314 (100%)	1 (0%)	92	91
1	M	316/334 (95%)	315 (100%)	1 (0%)	92	91
1	N	314/334 (94%)	311 (99%)	3 (1%)	76	71
1	S	314/334 (94%)	310 (99%)	4 (1%)	69	62
1	T	313/334 (94%)	310 (99%)	3 (1%)	76	71
All	All	2530/2672 (95%)	2511 (99%)	19 (1%)	81	78

5 of 19 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	M	157	GLU
1	N	157	GLU
1	S	309	LEU
1	G	36	ARG
1	T	36	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:



Mol	Chain	Res	Type
1	B	308	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](#)

16 ligands 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	$\# Z  > 2$
3	BTB	S	402	-	13,13,13	1.20	2 (15%)	7,16,16	0.83	0
3	BTB	B	402	-	13,13,13	0.74	0	7,16,16	0.96	0
3	BTB	M	402	-	13,13,13	0.83	0	7,16,16	0.97	0
2	PLP	G	401	1	15,15,16	2.37	9 (60%)	20,22,23	2.36	6 (30%)
3	BTB	N	402	-	13,13,13	0.80	0	7,16,16	1.14	1 (14%)
2	PLP	B	401	1	15,15,16	2.50	7 (46%)	20,22,23	2.08	6 (30%)
2	PLP	A	401	1	15,15,16	2.44	5 (33%)	20,22,23	2.34	5 (25%)
3	BTB	T	402	-	13,13,13	0.90	1 (7%)	7,16,16	0.53	0
3	BTB	G	402	-	13,13,13	1.01	0	7,16,16	1.18	0
2	PLP	M	401	1	15,15,16	2.83	5 (33%)	20,22,23	2.28	7 (35%)
3	BTB	A	402	-	13,13,13	0.98	1 (7%)	7,16,16	0.60	0
3	BTB	E	402	-	13,13,13	1.23	1 (7%)	7,16,16	0.40	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	PLP	T	401	1	15,15,16	2.28	5 (33%)	20,22,23	2.60	8 (40%)
2	PLP	E	401	1	15,15,16	2.59	8 (53%)	20,22,23	2.36	4 (20%)
2	PLP	S	401	1	15,15,16	2.06	2 (13%)	20,22,23	4.09	8 (40%)
2	PLP	N	401	1	15,15,16	2.40	8 (53%)	20,22,23	2.31	4 (20%)

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
3	BTB	S	402	-	-	3/21/21/21	-
3	BTB	B	402	-	-	4/21/21/21	-
3	BTB	M	402	-	-	0/21/21/21	-
2	PLP	G	401	1	-	0/6/6/8	0/1/1/1
3	BTB	N	402	-	-	3/21/21/21	-
2	PLP	B	401	1	-	2/6/6/8	0/1/1/1
2	PLP	A	401	1	-	4/6/6/8	0/1/1/1
3	BTB	T	402	-	-	0/21/21/21	-
3	BTB	G	402	-	-	3/21/21/21	-
2	PLP	M	401	1	-	3/6/6/8	0/1/1/1
3	BTB	A	402	-	-	3/21/21/21	-
3	BTB	E	402	-	-	4/21/21/21	-
2	PLP	T	401	1	-	3/6/6/8	0/1/1/1
2	PLP	E	401	1	-	4/6/6/8	0/1/1/1
2	PLP	S	401	1	-	1/6/6/8	0/1/1/1
2	PLP	N	401	1	-	3/6/6/8	0/1/1/1

The worst 5 of 54 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	M	401	PLP	C5-C4	-7.85	1.31	1.40
2	E	401	PLP	C4A-C4	5.25	1.62	1.51
2	T	401	PLP	C4A-C4	5.09	1.62	1.51
2	S	401	PLP	C4A-C4	5.02	1.62	1.51
2	A	401	PLP	C4A-C4	4.77	1.61	1.51

The worst 5 of 49 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	S	401	PLP	C5A-C5-C6	-10.04	102.86	119.37
2	E	401	PLP	O4P-C5A-C5	9.09	126.68	109.35
2	A	401	PLP	O4P-C5A-C5	8.35	125.26	109.35
2	T	401	PLP	O4P-C5A-C5	8.02	124.64	109.35
2	S	401	PLP	O4P-C5A-C5	7.81	124.23	109.35

There are no chirality outliers.

5 of 40 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	N	402	BTB	C1-C2-C3-O3
3	N	402	BTB	C4-C2-C3-O3
3	N	402	BTB	N-C2-C3-O3
3	B	402	BTB	O1-C1-C2-C3
3	B	402	BTB	O1-C1-C2-C4

There are no ring outliers.

9 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	S	402	BTB	1	0
3	B	402	BTB	1	0
2	G	401	PLP	1	0
3	N	402	BTB	1	0
2	B	401	PLP	1	0
2	A	401	PLP	2	0
3	T	402	BTB	1	0
2	M	401	PLP	2	0
2	E	401	PLP	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 [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	387/403 (96%)	-0.56	2 (0%) 91 89	6, 11, 22, 82	0
1	B	386/403 (95%)	-0.56	1 (0%) 94 92	7, 12, 25, 54	0
1	E	386/403 (95%)	-0.59	0 100 100	7, 12, 23, 44	0
1	G	386/403 (95%)	-0.58	0 100 100	7, 12, 23, 52	0
1	M	386/403 (95%)	-0.60	0 100 100	7, 11, 22, 51	0
1	N	387/403 (96%)	-0.56	1 (0%) 94 92	7, 11, 23, 47	0
1	S	386/403 (95%)	-0.62	0 100 100	7, 11, 21, 58	0
1	T	386/403 (95%)	-0.54	1 (0%) 94 92	6, 11, 22, 54	0
All	All	3090/3224 (95%)	-0.58	5 (0%) 95 93	6, 11, 23, 82	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	4	HIS	3.9
1	N	4	HIS	3.5
1	A	390	LYS	2.9
1	T	328	ALA	2.4
1	B	5	LYS	2.0

### 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

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
3	BTB	G	402	14/14	0.94	0.11	16,20,27,28	0
3	BTB	B	402	14/14	0.95	0.09	14,18,23,24	0
3	BTB	T	402	14/14	0.95	0.09	14,16,23,23	0
3	BTB	E	402	14/14	0.95	0.09	15,19,23,23	0
3	BTB	A	402	14/14	0.95	0.08	16,19,24,28	0
3	BTB	N	402	14/14	0.95	0.11	15,21,23,23	0
3	BTB	S	402	14/14	0.96	0.09	14,18,21,21	0
3	BTB	M	402	14/14	0.96	0.09	14,20,24,25	0
2	PLP	G	401	15/16	0.98	0.09	9,12,16,16	0
2	PLP	E	401	15/16	0.98	0.07	9,11,16,16	0
2	PLP	M	401	15/16	0.98	0.07	9,12,17,17	0
2	PLP	B	401	15/16	0.98	0.08	9,11,14,14	0
2	PLP	S	401	15/16	0.98	0.07	8,11,14,17	0
2	PLP	A	401	15/16	0.98	0.08	9,12,14,14	0
2	PLP	N	401	15/16	0.98	0.08	9,12,15,18	0
2	PLP	T	401	15/16	0.99	0.07	10,12,14,15	0

## 6.5 Other polymers

There are no such residues in this entry.