



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 14, 2020 – 05:34 am BST

PDB ID : 6DNA  
Title : Crystal structure of T110A mutant human Glutamate oxaloacetate transaminase 1 (GOT1)  
Authors : Assar, Z.; Holt, M.C.; Stein, A.J.; Lairson, L.; Lyssiotis, C.A.  
Deposited on : 2018-06-06  
Resolution : 3.00 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

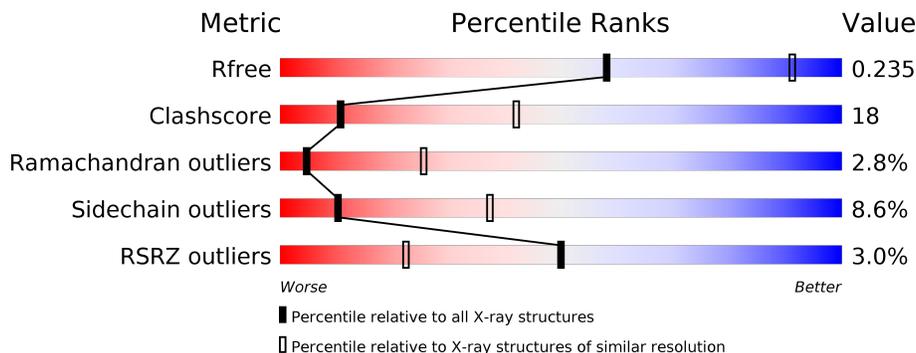
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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	408	<div style="display: flex; align-items: center;"> <div style="width: 3%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 68%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 19%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">3%      71%      19%      • • •</p>
1	B	408	<div style="display: flex; align-items: center;"> <div style="width: 3%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 70%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 18%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 3%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">3%      73%      18%      5%      • •</p>
1	C	408	<div style="display: flex; align-items: center;"> <div style="width: 0%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 73%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 19%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">%      73%      19%      • • •</p>
1	D	408	<div style="display: flex; align-items: center;"> <div style="width: 4%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 68%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 20%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">4%      72%      20%      • •</p>
1	E	408	<div style="display: flex; align-items: center;"> <div style="width: 4%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 65%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 21%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">4%      69%      21%      5%      • •</p>
1	F	408	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 65%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 21%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">2%      67%      21%      5%      • 6%</p>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

<b>Mol</b>	<b>Type</b>	<b>Chain</b>	<b>Res</b>	<b>Chirality</b>	<b>Geometry</b>	<b>Clashes</b>	<b>Electron density</b>
3	PLP	E	501	-	-	X	-

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 18520 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 Aspartate aminotransferase, cytoplasmic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	390	Total 3029	C 1932	N 529	O 559	S 9	0	2	0
1	B	395	Total 3104	C 1985	N 537	O 573	S 9	0	4	0
1	C	391	Total 3049	C 1947	N 531	O 562	S 9	0	2	0
1	D	396	Total 3089	C 1968	N 542	O 570	S 9	0	3	0
1	E	393	Total 3095	C 1979	N 536	O 571	S 9	0	3	0
1	F	383	Total 3013	C 1925	N 523	O 556	S 9	0	4	0

There are 24 discrepancies between the modelled and reference sequences:

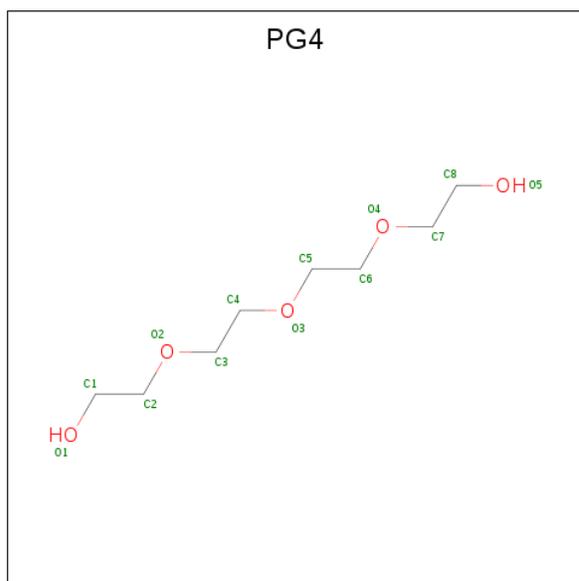
Chain	Residue	Modelled	Actual	Comment	Reference
A	110	ALA	THR	engineered mutation	UNP P17174
A	411	LYS	-	expression tag	UNP P17174
A	412	ILE	-	expression tag	UNP P17174
A	413	GLN	-	expression tag	UNP P17174
B	110	ALA	THR	engineered mutation	UNP P17174
B	411	LYS	-	expression tag	UNP P17174
B	412	ILE	-	expression tag	UNP P17174
B	413	GLN	-	expression tag	UNP P17174
C	110	ALA	THR	engineered mutation	UNP P17174
C	411	LYS	-	expression tag	UNP P17174
C	412	ILE	-	expression tag	UNP P17174
C	413	GLN	-	expression tag	UNP P17174
D	110	ALA	THR	engineered mutation	UNP P17174
D	411	LYS	-	expression tag	UNP P17174
D	412	ILE	-	expression tag	UNP P17174
D	413	GLN	-	expression tag	UNP P17174
E	110	ALA	THR	engineered mutation	UNP P17174

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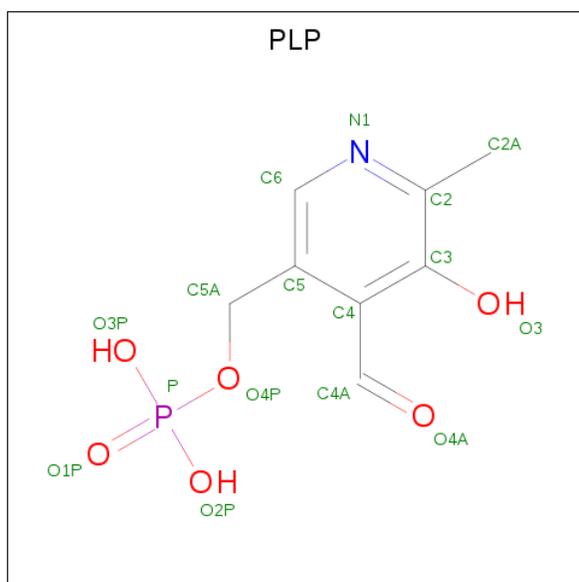
Chain	Residue	Modelled	Actual	Comment	Reference
E	411	LYS	-	expression tag	UNP P17174
E	412	ILE	-	expression tag	UNP P17174
E	413	GLN	-	expression tag	UNP P17174
F	110	ALA	THR	engineered mutation	UNP P17174
F	411	LYS	-	expression tag	UNP P17174
F	412	ILE	-	expression tag	UNP P17174
F	413	GLN	-	expression tag	UNP P17174

- Molecule 2 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: C<sub>8</sub>H<sub>18</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			13	8	5		
2	B	1	Total	C	O	0	0
			10	6	4		
2	D	1	Total	C	O	0	0
			13	8	5		

- Molecule 3 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
			Total	C	N	O	P		
3	A	1	Total 16	8	1	6	1	0	0
3	B	1	Total 16	8	1	6	1	0	0
3	C	1	Total 16	8	1	6	1	0	0
3	D	1	Total 16	8	1	6	1	0	0
3	E	1	Total 16	8	1	6	1	0	0
3	F	1	Total 16	8	1	6	1	0	0

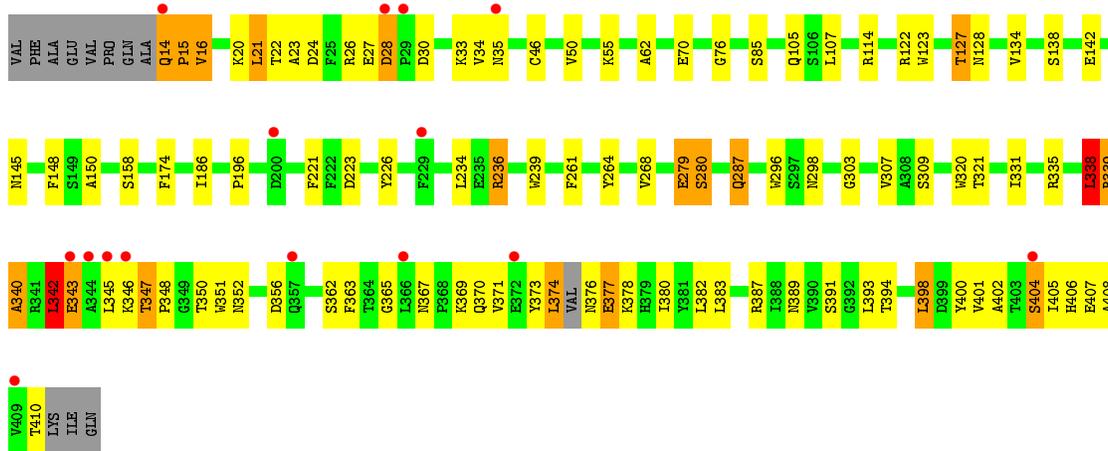
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total 1	O 1	0	0
4	C	3	Total 3	O 3	0	0
4	E	3	Total 3	O 3	0	0
4	F	2	Total 2	O 2	0	0

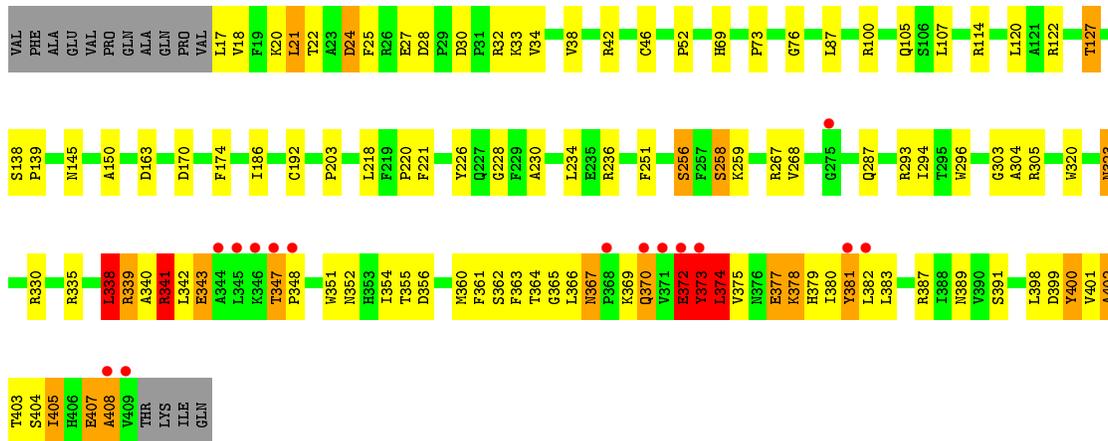




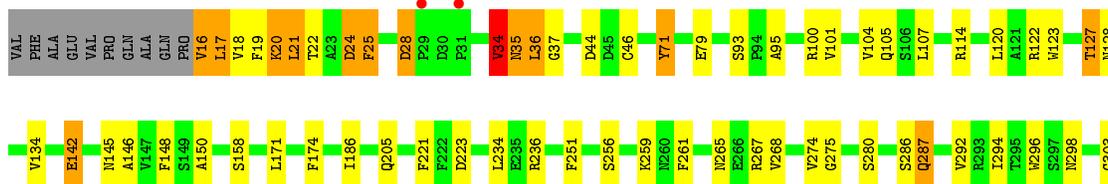
• Molecule 1: Aspartate aminotransferase, cytoplasmic

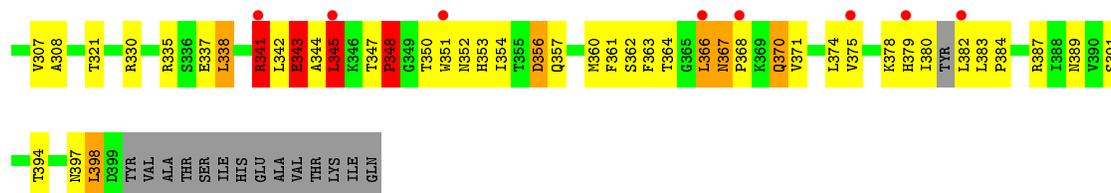


• Molecule 1: Aspartate aminotransferase, cytoplasmic



• Molecule 1: Aspartate aminotransferase, cytoplasmic





## 4 Data and refinement statistics i

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	257.70Å 148.63Å 83.18Å 90.00° 89.98° 90.00°	Depositor
Resolution (Å)	48.70 – 3.00 48.70 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.70-3.00) 99.1 (48.70-3.00)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	65.47 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.8.0230	Depositor
R, $R_{free}$	0.184 , 0.211 0.206 , 0.235	Depositor DCC
$R_{free}$ test set	3047 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	83.8	Xtriage
Anisotropy	0.110	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 64.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	0.000 for -1/2*h-3/2*k,-1/2*h+1/2*k,-l 0.000 for -1/2*h+3/2*k,1/2*h+1/2*k,-l 0.076 for 1/2*h-3/2*k,-1/2*h-1/2*k,-l 0.077 for 1/2*h+3/2*k,1/2*h-1/2*k,-l 0.000 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	18520	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.52% 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: PG4, 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	0.56	0/3108	0.77	0/4230
1	B	0.57	1/3192 (0.0%)	0.75	4/4343 (0.1%)
1	C	0.55	0/3129	0.73	1/4260 (0.0%)
1	D	0.54	0/3171	0.77	1/4315 (0.0%)
1	E	0.58	0/3180	0.76	1/4326 (0.0%)
1	F	0.53	0/3097	0.75	2/4211 (0.0%)
All	All	0.55	1/18877 (0.0%)	0.76	9/25685 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	6
1	B	0	4
1	C	0	2
1	D	0	1
1	E	0	6
1	F	0	3
All	All	0	22

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	370	GLN	N-CA	5.35	1.57	1.46

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	373	TYR	CB-CG-CD2	6.77	125.06	121.00
1	B	373	TYR	CB-CG-CD1	-6.16	117.30	121.00
1	B	15	PRO	CA-N-CD	-6.07	103.00	111.50
1	C	242	ARG	NE-CZ-NH1	5.81	123.20	120.30
1	F	71	TYR	CB-CG-CD1	5.76	124.46	121.00

There are no chirality outliers.

5 of 22 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	167	ARG	Sidechain
1	A	216	ARG	Sidechain
1	A	236	ARG	Sidechain
1	A	350	THR	Peptide
1	A	86	ARG	Sidechain

## 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	3029	0	2902	85	0
1	B	3104	0	2993	123	0
1	C	3049	0	2934	68	0
1	D	3089	0	2985	109	0
1	E	3095	0	2995	128	0
1	F	3013	0	2915	187	0
2	A	13	0	18	0	0
2	B	10	0	13	0	0
2	D	13	0	18	0	0
3	A	16	0	7	1	0
3	B	16	0	7	2	0
3	C	16	0	7	2	0
3	D	16	0	7	2	0
3	E	16	0	7	6	0
3	F	16	0	7	4	0
4	B	1	0	0	0	0
4	C	3	0	0	0	0
4	E	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	F	2	0	0	0	0
All	All	18520	0	17815	663	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 18.

The worst 5 of 663 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:F:21:LEU:HA	1:F:25:PHE:CD2	1.41	1.56
1:B:382:LEU:CD2	1:B:388:ILE:HG23	1.49	1.41
1:F:21:LEU:HA	1:F:25:PHE:CE2	1.59	1.37
1:F:17:LEU:O	1:F:20:LYS:CD	1.76	1.33
1:F:17:LEU:O	1:F:20:LYS:CE	1.74	1.32

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	385/408 (94%)	344 (89%)	22 (6%)	19 (5%)	2	13
1	B	395/408 (97%)	358 (91%)	28 (7%)	9 (2%)	6	30
1	C	389/408 (95%)	355 (91%)	25 (6%)	9 (2%)	6	30
1	D	395/408 (97%)	355 (90%)	31 (8%)	9 (2%)	6	30
1	E	394/408 (97%)	347 (88%)	35 (9%)	12 (3%)	4	24
1	F	383/408 (94%)	353 (92%)	23 (6%)	7 (2%)	8	37
All	All	2341/2448 (96%)	2112 (90%)	164 (7%)	65 (3%)	5	25

5 of 65 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	17	LEU
1	A	26	ARG
1	A	29	PRO
1	A	33	LYS
1	A	347	THR

### 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	313/346 (90%)	288 (92%)	25 (8%)	12	40
1	B	324/346 (94%)	291 (90%)	33 (10%)	7	28
1	C	316/346 (91%)	293 (93%)	23 (7%)	14	44
1	D	321/346 (93%)	290 (90%)	31 (10%)	8	31
1	E	323/346 (93%)	294 (91%)	29 (9%)	9	35
1	F	315/346 (91%)	281 (89%)	34 (11%)	6	26
All	All	1912/2076 (92%)	1737 (91%)	175 (9%)	10	34

5 of 175 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	398	LEU
1	D	298	ASN
1	F	286	SER
1	D	14	GLN
1	D	145[A]	ASN

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

Mol	Chain	Res	Type
1	D	283	GLN
1	D	379	HIS
1	F	302	GLN
1	D	298	ASN

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Mol	Chain	Res	Type
1	D	323	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](#)

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](#)

9 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	PLP	F	501	-	16,16,16	2.73	3 (18%)	20,23,23	1.81	7 (35%)
3	PLP	C	501	-	16,16,16	2.80	3 (18%)	20,23,23	1.60	6 (30%)
2	PG4	A	501	-	12,12,12	0.64	0	11,11,11	0.35	0
3	PLP	B	502	-	16,16,16	2.90	3 (18%)	20,23,23	1.45	2 (10%)
3	PLP	A	502	-	16,16,16	2.90	3 (18%)	20,23,23	1.81	5 (25%)
3	PLP	E	501	-	16,16,16	2.75	3 (18%)	20,23,23	2.01	5 (25%)
3	PLP	D	502	-	16,16,16	2.42	3 (18%)	20,23,23	1.93	6 (30%)
2	PG4	B	501	-	9,9,12	0.64	0	8,8,11	0.48	0
2	PG4	D	501	-	12,12,12	0.54	0	11,11,11	0.26	0

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	PLP	F	501	-	-	5/8/8/8	0/1/1/1
3	PLP	C	501	-	-	3/8/8/8	0/1/1/1
2	PG4	A	501	-	-	4/10/10/10	-
3	PLP	B	502	-	-	3/8/8/8	0/1/1/1
3	PLP	A	502	-	-	0/8/8/8	0/1/1/1
3	PLP	E	501	-	-	2/8/8/8	0/1/1/1
3	PLP	D	502	-	-	1/8/8/8	0/1/1/1
2	PG4	B	501	-	-	5/7/7/10	-
2	PG4	D	501	-	-	5/10/10/10	-

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	502	PLP	C3-C2	8.11	1.49	1.40
3	A	502	PLP	C3-C2	7.93	1.48	1.40
3	F	501	PLP	C3-C2	7.60	1.48	1.40
3	E	501	PLP	C3-C2	7.49	1.48	1.40
3	C	501	PLP	C3-C2	6.73	1.47	1.40

The worst 5 of 31 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	502	PLP	O4P-C5A-C5	5.04	118.96	109.35
3	E	501	PLP	C4-C3-C2	-4.87	117.18	120.19
3	D	502	PLP	O4P-C5A-C5	4.74	118.38	109.35
3	F	501	PLP	O4P-C5A-C5	4.53	117.98	109.35
3	E	501	PLP	O4P-C5A-C5	4.11	117.19	109.35

There are no chirality outliers.

5 of 28 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	F	501	PLP	C4-C5-C5A-O4P
3	F	501	PLP	C6-C5-C5A-O4P
3	F	501	PLP	C5A-O4P-P-O2P
3	F	501	PLP	C5A-O4P-P-O3P
3	C	501	PLP	C5A-O4P-P-O2P

There are no ring outliers.

6 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	501	PLP	4	0
3	C	501	PLP	2	0
3	B	502	PLP	2	0
3	A	502	PLP	1	0
3	E	501	PLP	6	0
3	D	502	PLP	2	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	390/408 (95%)	-0.11	12 (3%)	49 21	38, 68, 113, 168	2 (0%)
1	B	395/408 (96%)	-0.04	14 (3%)	44 18	38, 75, 128, 228	1 (0%)
1	C	391/408 (95%)	-0.17	4 (1%)	82 59	37, 72, 109, 156	1 (0%)
1	D	396/408 (97%)	-0.11	15 (3%)	40 16	42, 70, 124, 208	1 (0%)
1	E	393/408 (96%)	-0.04	15 (3%)	40 16	40, 75, 123, 213	0
1	F	383/408 (93%)	-0.06	10 (2%)	56 27	35, 77, 126, 159	1 (0%)
All	All	2348/2448 (95%)	-0.09	70 (2%)	50 22	35, 73, 120, 228	6 (0%)

The worst 5 of 70 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	409	VAL	16.6
1	A	382	LEU	13.4
1	A	347	THR	12.8
1	E	347	THR	11.8
1	D	344	ALA	7.9

### 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. 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
2	PG4	A	501	13/13	0.80	0.24	87,99,115,123	0
3	PLP	B	502	16/16	0.80	0.47	101,111,159,163	10
3	PLP	A	502	16/16	0.81	0.56	96,121,141,145	10
3	PLP	E	501	16/16	0.81	0.37	102,116,133,137	16
3	PLP	C	501	16/16	0.81	0.46	122,136,158,166	10
2	PG4	B	501	10/13	0.88	0.22	75,81,88,91	0
2	PG4	D	501	13/13	0.88	0.18	85,99,107,108	0
3	PLP	D	502	16/16	0.90	0.28	78,101,143,148	10
3	PLP	F	501	16/16	0.92	0.35	75,90,106,110	10

## 6.5 Other polymers [i](#)

There are no such residues in this entry.