



# wwPDB X-ray Structure Validation Summary Report

Feb 27, 2014 – 05:27 AM GMT

PDB ID : 1M32  
Title : Crystal Structure of 2-aminoethylphosphonateTransaminase  
Authors : Chen, C.C.H.; Zhang, H.; Kim, A.D.; Howard, A.; Sheldrick, G.M.; Mariano-Dunnaway, D.; Herzberg, O.  
Deposited on : 2002-06-26  
Resolution : 2.20 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

---

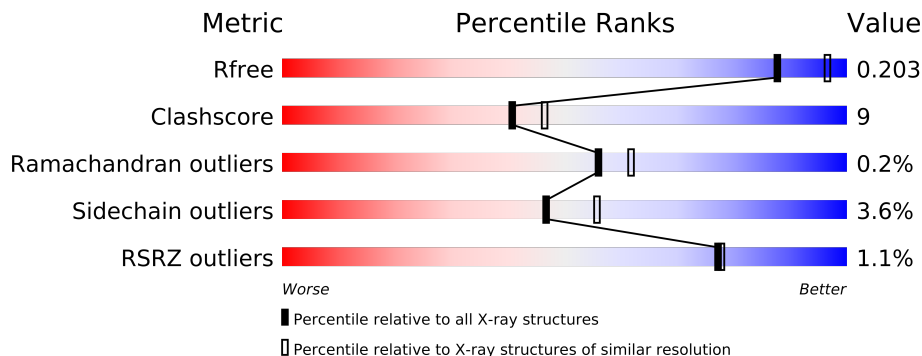
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.20 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))
$R_{free}$	66092	2938 (2.20-2.20)
Clashscore	79885	3751 (2.20-2.20)
Ramachandran outliers	78287	3681 (2.20-2.20)
Sidechain outliers	78261	3682 (2.20-2.20)
RSRZ outliers	66119	2939 (2.20-2.20)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	366	
1	B	366	
1	C	366	
1	D	366	
1	E	366	
1	F	366	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	PO4	B	4602	-	X
2	PO4	C	4604	-	X

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Geometry	Electron density
2	PO4	E	4605	-	X
3	PLP	D	4404	-	X
3	PLP	F	4406	-	X
4	POA	A	4601	-	X
4	POA	C	4603	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 19906 atoms, of which 0 are hydrogen and 0 are deuterium.

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 2-aminoethylphosphonate-pyruvateaminotransferase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	361	Total	C	N	O	S	Se	24	1	0
			2783	1762	479	525	6	11			
1	B	362	Total	C	N	O	S	Se	31	4	0
			2800	1777	480	526	6	11			
1	C	361	Total	C	N	O	S	Se	39	4	0
			2799	1776	479	526	7	11			
1	D	362	Total	C	N	O	S	Se	11	3	0
			2798	1775	480	526	6	11			
1	E	361	Total	C	N	O	S	Se	15	1	0
			2782	1763	478	524	6	11			
1	F	362	Total	C	N	O	S	Se	20	0	0
			2786	1763	480	526	6	11			

There are 66 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	23	MSE	MET	MODIFIED RESIDUE	UNP P96060
A	95	MSE	MET	MODIFIED RESIDUE	UNP P96060
A	98	MSE	MET	MODIFIED RESIDUE	UNP P96060
A	102	MSE	MET	MODIFIED RESIDUE	UNP P96060
A	137	MSE	MET	MODIFIED RESIDUE	UNP P96060
A	146	MSE	MET	MODIFIED RESIDUE	UNP P96060
A	169	MSE	MET	MODIFIED RESIDUE	UNP P96060
A	177	MSE	MET	MODIFIED RESIDUE	UNP P96060
A	232	MSE	MET	MODIFIED RESIDUE	UNP P96060
A	282	MSE	MET	MODIFIED RESIDUE	UNP P96060
A	362	MSE	MET	MODIFIED RESIDUE	UNP P96060
B	23	MSE	MET	MODIFIED RESIDUE	UNP P96060
B	95	MSE	MET	MODIFIED RESIDUE	UNP P96060
B	98	MSE	MET	MODIFIED RESIDUE	UNP P96060
B	102	MSE	MET	MODIFIED RESIDUE	UNP P96060
B	137	MSE	MET	MODIFIED RESIDUE	UNP P96060
B	146	MSE	MET	MODIFIED RESIDUE	UNP P96060

*Continued on next page...*

*Continued from previous page...*

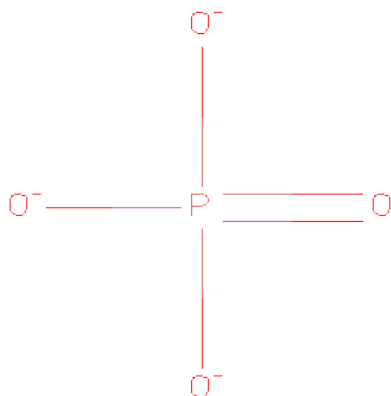
Chain	Residue	Modelled	Actual	Comment	Reference
B	169	MSE	MET	MODIFIED RESIDUE	UNP P96060
B	177	MSE	MET	MODIFIED RESIDUE	UNP P96060
B	232	MSE	MET	MODIFIED RESIDUE	UNP P96060
B	282	MSE	MET	MODIFIED RESIDUE	UNP P96060
B	362	MSE	MET	MODIFIED RESIDUE	UNP P96060
C	23	MSE	MET	MODIFIED RESIDUE	UNP P96060
C	95	MSE	MET	MODIFIED RESIDUE	UNP P96060
C	98	MSE	MET	MODIFIED RESIDUE	UNP P96060
C	102	MSE	MET	MODIFIED RESIDUE	UNP P96060
C	137	MSE	MET	MODIFIED RESIDUE	UNP P96060
C	146	MSE	MET	MODIFIED RESIDUE	UNP P96060
C	169	MSE	MET	MODIFIED RESIDUE	UNP P96060
C	177	MSE	MET	MODIFIED RESIDUE	UNP P96060
C	232	MSE	MET	MODIFIED RESIDUE	UNP P96060
C	282	MSE	MET	MODIFIED RESIDUE	UNP P96060
C	362	MSE	MET	MODIFIED RESIDUE	UNP P96060
D	23	MSE	MET	MODIFIED RESIDUE	UNP P96060
D	95	MSE	MET	MODIFIED RESIDUE	UNP P96060
D	98	MSE	MET	MODIFIED RESIDUE	UNP P96060
D	102	MSE	MET	MODIFIED RESIDUE	UNP P96060
D	137	MSE	MET	MODIFIED RESIDUE	UNP P96060
D	146	MSE	MET	MODIFIED RESIDUE	UNP P96060
D	169	MSE	MET	MODIFIED RESIDUE	UNP P96060
D	177	MSE	MET	MODIFIED RESIDUE	UNP P96060
D	232	MSE	MET	MODIFIED RESIDUE	UNP P96060
D	282	MSE	MET	MODIFIED RESIDUE	UNP P96060
D	362	MSE	MET	MODIFIED RESIDUE	UNP P96060
E	23	MSE	MET	MODIFIED RESIDUE	UNP P96060
E	95	MSE	MET	MODIFIED RESIDUE	UNP P96060
E	98	MSE	MET	MODIFIED RESIDUE	UNP P96060
E	102	MSE	MET	MODIFIED RESIDUE	UNP P96060
E	137	MSE	MET	MODIFIED RESIDUE	UNP P96060
E	146	MSE	MET	MODIFIED RESIDUE	UNP P96060
E	169	MSE	MET	MODIFIED RESIDUE	UNP P96060
E	177	MSE	MET	MODIFIED RESIDUE	UNP P96060
E	232	MSE	MET	MODIFIED RESIDUE	UNP P96060
E	282	MSE	MET	MODIFIED RESIDUE	UNP P96060
E	362	MSE	MET	MODIFIED RESIDUE	UNP P96060
F	23	MSE	MET	MODIFIED RESIDUE	UNP P96060
F	95	MSE	MET	MODIFIED RESIDUE	UNP P96060
F	98	MSE	MET	MODIFIED RESIDUE	UNP P96060
F	102	MSE	MET	MODIFIED RESIDUE	UNP P96060

*Continued on next page...*

Continued from previous page...

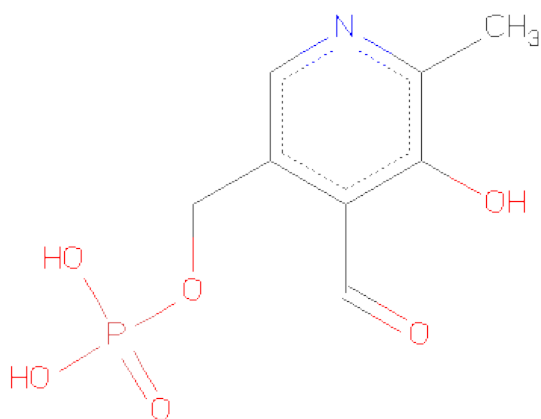
Chain	Residue	Modelled	Actual	Comment	Reference
F	137	MSE	MET	MODIFIED RESIDUE	UNP P96060
F	146	MSE	MET	MODIFIED RESIDUE	UNP P96060
F	169	MSE	MET	MODIFIED RESIDUE	UNP P96060
F	177	MSE	MET	MODIFIED RESIDUE	UNP P96060
F	232	MSE	MET	MODIFIED RESIDUE	UNP P96060
F	282	MSE	MET	MODIFIED RESIDUE	UNP P96060
F	362	MSE	MET	MODIFIED RESIDUE	UNP P96060

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



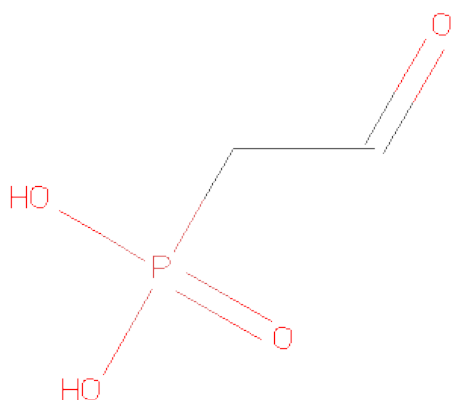
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	O	P	0	0
			5	4	1		
2	C	1	Total	O	P	0	0
			5	4	1		
2	E	1	Total	O	P	0	0
			5	4	1		
2	F	1	Total	O	P	0	0
			5	4	1		

- 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
3	A	1	Total	C	N	O	P	0	0
			14	7	1	5	1		
3	B	1	Total	C	N	O	P	0	0
			14	7	1	5	1		
3	C	1	Total	C	N	O	P	0	0
			14	7	1	5	1		
3	D	1	Total	C	N	O	P	0	0
			14	7	1	5	1		
3	E	1	Total	C	N	O	P	0	0
			14	7	1	5	1		
3	F	1	Total	C	N	O	P	0	0
			14	7	1	5	1		

- Molecule 4 is PHOSPHONOACETALDEHYDE (three-letter code: POA) (formula:  $C_2H_5O_4P$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	P	0	0
			7	2	4	1		
4	C	1	Total	C	O	P	0	0
			7	2	4	1		

- Molecule 5 is water.

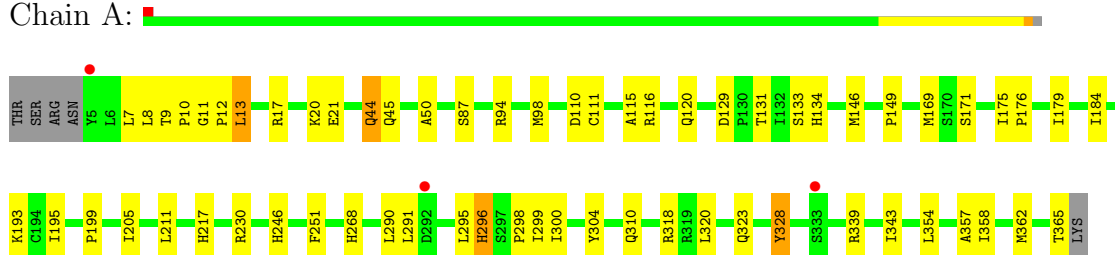
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	500	Total	O	0	1
			501	501		
5	B	506	Total	O	0	1
			507	507		
5	C	481	Total	O	0	1
			482	482		
5	D	499	Total	O	0	1
			500	500		
5	E	518	Total	O	0	1
			519	519		
5	F	530	Total	O	0	1
			531	531		

### 3 Residue-property plots

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

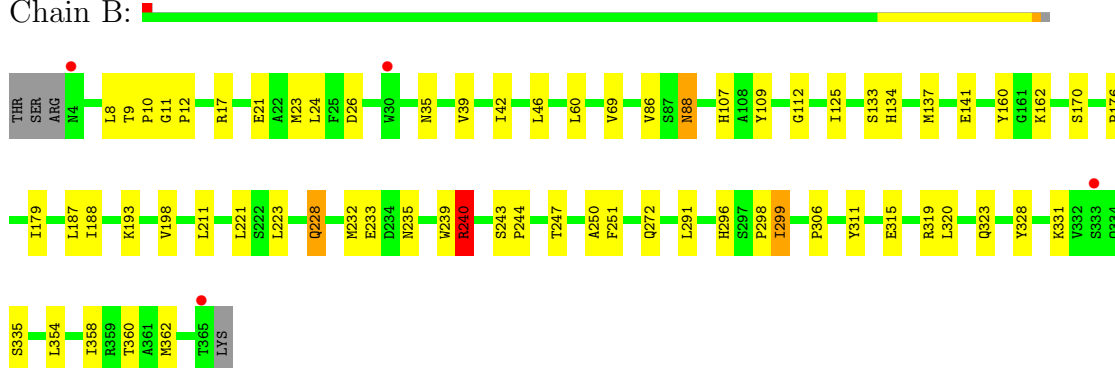
- Molecule 1: 2-aminoethylphosphonate-pyruvateaminotransferase

Chain A:



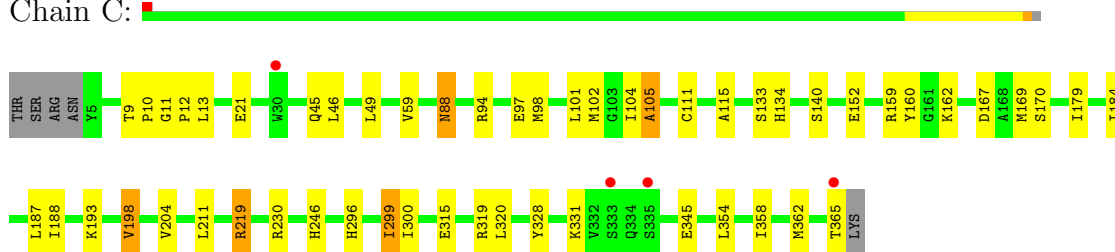
- Molecule 1: 2-aminoethylphosphonate-pyruvateaminotransferase

Chain B:



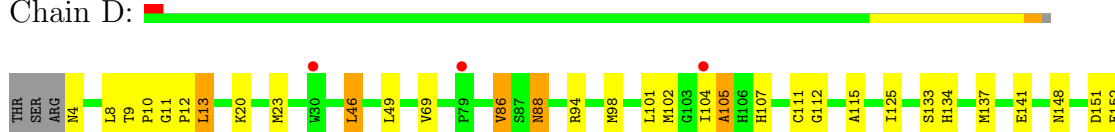
- Molecule 1: 2-aminoethylphosphonate-pyruvateaminotransferase

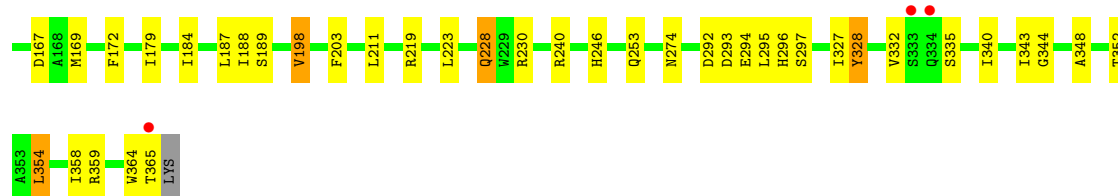
Chain C:



- Molecule 1: 2-aminoethylphosphonate-pyruvateaminotransferase

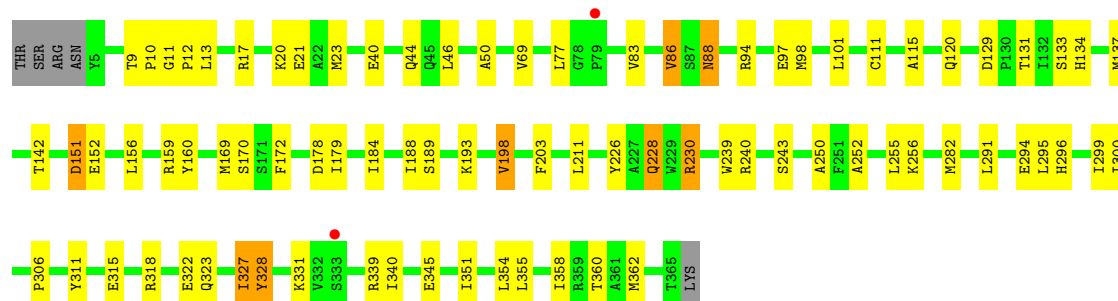
Chain D:





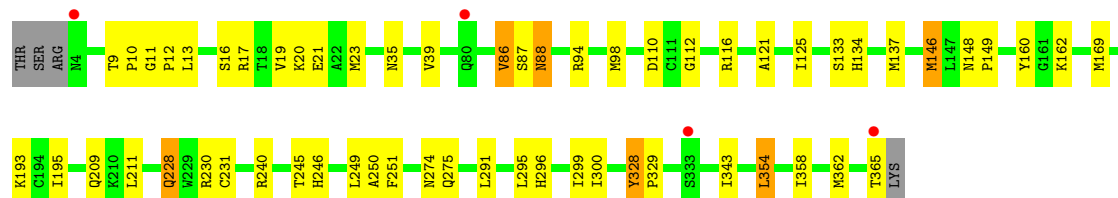
- Molecule 1: 2-aminoethylphosphonate-pyruvateaminotransferase

Chain E:



- Molecule 1: 2-aminoethylphosphonate-pyruvateaminotransferase

Chain F:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	49.60Å 155.30Å 168.60Å 90.00° 90.60° 90.00°	Depositor
Resolution (Å)	20.00 – 2.20 19.92 – 2.15	Depositor EDS
% Data completeness (in resolution range)	98.6 (20.00-2.20) 99.2 (19.92-2.15)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.88 (at 2.15Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.166 , 0.200 0.170 , 0.203	Depositor DCC
$R_{free}$ test set	12782 reflections (9.96%)	DCC
Wilson B-factor (Å <sup>2</sup> )	22.0	Xtriage
Anisotropy	0.056	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 58.4	EDS
Estimated twinning fraction	0.089 for h,-k,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 136969 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	19906	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.93% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, PLP, POA

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	0.39	0/2836	0.57	0/3832
1	B	0.46	1/2865 (0.0%)	0.62	3/3874 (0.1%)
1	C	0.40	0/2866	0.57	0/3874
1	D	0.39	0/2859	0.57	1/3864 (0.0%)
1	E	0.40	0/2835	0.56	0/3831
1	F	0.40	0/2835	0.57	0/3831
All	All	0.41	1/17096 (0.0%)	0.58	4/23106 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	235	ASN	C-N	-7.07	1.17	1.34

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	240	ARG	NE-CZ-NH1	6.98	123.79	120.30
1	B	240	ARG	NE-CZ-NH2	5.88	123.24	120.30
1	B	240	ARG	NH1-CZ-NH2	-5.85	112.97	119.40
1	D	297	SER	N-CA-C	-5.01	97.48	111.00

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit,

and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2783	0	2735	46	0
1	B	2800	0	2760	57	0
1	C	2799	0	2747	43	0
1	D	2798	0	2758	64	0
1	E	2782	0	2738	64	0
1	F	2786	0	2737	44	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	E	5	0	0	0	0
2	F	5	0	0	0	0
3	A	14	0	6	1	0
3	B	14	0	6	1	0
3	C	14	0	6	1	0
3	D	14	0	6	1	0
3	E	14	0	6	1	0
3	F	14	0	6	1	0
4	A	7	0	3	3	0
4	C	7	0	3	0	0
5	A	501	0	0	4	0
5	B	507	0	0	8	0
5	C	482	0	0	9	0
5	D	500	0	0	10	0
5	E	519	0	0	8	0
5	F	531	0	0	6	0
All	All	19906	0	16517	307	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 9.

The worst 5 of 307 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:282:MSE:HE1	1:E:358:ILE:HG13	1.25	1.14
1:B:228:GLN:NE2	1:B:240:ARG:HG3	1.84	0.91
3:E:4405:PLP:C4	5:E:5123[A]:HOH:O	2.26	0.82
1:B:221:LEU:O	1:B:240:ARG:NH2	2.12	0.81
1:B:240:ARG:HG3	1:B:240:ARG:HH11	1.42	0.80

There are no symmetry-related clashes.

## 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	360/366 (98%)	350 (97%)	10 (3%)	0	100	100
1	B	364/366 (100%)	352 (97%)	10 (3%)	2 (0%)	38	38
1	C	363/366 (99%)	348 (96%)	14 (4%)	1 (0%)	50	53
1	D	363/366 (99%)	350 (96%)	12 (3%)	1 (0%)	50	53
1	E	360/366 (98%)	346 (96%)	14 (4%)	0	100	100
1	F	360/366 (98%)	347 (96%)	13 (4%)	0	100	100
All	All	2170/2196 (99%)	2093 (96%)	73 (3%)	4 (0%)	56	62

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	105	ALA
1	D	105	ALA
1	B	335	SER
1	B	24	LEU

### 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	291/284 (102%)	282 (97%)	9 (3%)	52	63
1	B	295/284 (104%)	286 (97%)	9 (3%)	52	63
1	C	294/284 (104%)	283 (96%)	11 (4%)	45	54
1	D	294/284 (104%)	280 (95%)	14 (5%)	35	41
1	E	291/284 (102%)	277 (95%)	14 (5%)	35	41
1	F	291/284 (102%)	282 (97%)	9 (3%)	52	63

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1756/1704 (103%)	1690 (96%)	66 (4%)	47 53

5 of 66 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	4	ASN
1	D	198	VAL
1	F	146	MSE
1	D	13	LEU
1	D	86	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 52 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	127	ASN
1	D	296	HIS
1	F	274	ASN
1	D	134	HIS
1	D	228	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

12 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	A	4401	-	14,14,16	216.02	3 (21%)	16,20,23	2.19	4 (25%)
4	POA	A	4601	-	6,6,6	2.04	1 (16%)	8,8,8	0.86	0
3	PLP	B	4402	-	14,14,16	184.16	4 (28%)	16,20,23	2.23	4 (25%)
2	PO4	B	4602	-	4,4,4	0.87	0	6,6,6	0.31	0
3	PLP	C	4403	-	14,14,16	204.90	4 (28%)	16,20,23	2.17	5 (31%)
4	POA	C	4603	-	6,6,6	2.22	2 (33%)	8,8,8	1.00	0
2	PO4	C	4604	-	4,4,4	0.87	0	6,6,6	0.31	0
3	PLP	D	4404	-	14,14,16	205.49	4 (28%)	16,20,23	2.16	5 (31%)
3	PLP	E	4405	-	14,14,16	196.67	3 (21%)	16,20,23	2.21	5 (31%)
2	PO4	E	4605	-	4,4,4	0.89	0	6,6,6	0.31	0
3	PLP	F	4406	-	14,14,16	205.86	4 (28%)	16,20,23	2.20	5 (31%)
2	PO4	F	4606	-	4,4,4	0.88	0	6,6,6	0.31	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	A	4401	-	-	0/6/6/8	0/1/1/1
4	POA	A	4601	-	-	0/3/4/4	0/0/0/0
3	PLP	B	4402	-	-	0/6/6/8	0/1/1/1
2	PO4	B	4602	-	-	0/0/0/0	0/0/0/0
3	PLP	C	4403	-	-	0/6/6/8	0/1/1/1
4	POA	C	4603	-	-	0/3/4/4	0/0/0/0
2	PO4	C	4604	-	-	0/0/0/0	0/0/0/0
3	PLP	D	4404	-	-	0/6/6/8	0/1/1/1
3	PLP	E	4405	-	-	0/6/6/8	0/1/1/1
2	PO4	E	4605	-	-	0/0/0/0	0/0/0/0
3	PLP	F	4406	-	-	0/6/6/8	0/1/1/1
2	PO4	F	4606	-	-	0/0/0/0	0/0/0/0

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	4401	PLP	C4-C5	783.21	1.43	1.39

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	4404	PLP	C4-C5	751.66	1.43	1.39
3	F	4406	PLP	C4-C5	733.75	1.42	1.39
3	C	4403	PLP	C4-C5	716.57	1.42	1.39
3	E	4405	PLP	C4-C5	710.79	1.42	1.39

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	4406	PLP	O4P-C5A-C5	5.88	120.68	109.26
3	B	4402	PLP	O4P-C5A-C5	5.82	120.57	109.26
3	E	4405	PLP	O4P-C5A-C5	5.73	120.40	109.26
3	D	4404	PLP	O4P-C5A-C5	5.56	120.06	109.26
3	A	4401	PLP	O4P-C5A-C5	5.55	120.03	109.26

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å <sup>2</sup> )	Q<0.9
1	A	361/366 (98%)	-0.54	3 (0%)	83 85	9, 16, 30, 40	7 (1%)
1	B	362/366 (98%)	-0.43	4 (1%)	77 78	11, 19, 29, 37	9 (2%)
1	C	361/366 (98%)	-0.46	4 (1%)	77 78	10, 19, 30, 40	11 (3%)
1	D	362/366 (98%)	-0.38	6 (1%)	67 68	12, 19, 31, 38	3 (0%)
1	E	361/366 (98%)	-0.43	2 (0%)	86 88	11, 19, 29, 39	4 (1%)
1	F	362/366 (98%)	-0.52	4 (1%)	77 78	10, 18, 29, 37	5 (1%)
All	All	2169/2196 (98%)	-0.46	23 (1%)	77 78	9, 18, 30, 40	39 (1%)

The worst 5 of 23 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	333	SER	4.6
1	D	365	THR	3.7
1	C	333	SER	3.6
1	B	333	SER	3.3
1	D	334	GLN	3.2

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	PO4	B	4602	5/5	0.29	6.54	91,91,91,91	0
4	POA	A	4601	7/7	0.32	3.97	63,65,65,65	0
4	POA	C	4603	7/7	0.23	3.10	57,58,59,59	0
2	PO4	C	4604	5/5	0.24	2.83	64,64,65,65	0
2	PO4	E	4605	5/5	0.17	2.24	72,72,72,72	0
3	PLP	F	4406	14/16	0.13	2.18	19,22,23,23	0
3	PLP	D	4404	14/16	0.11	2.11	20,22,23,24	0
2	PO4	F	4606	5/5	0.18	1.89	69,69,69,69	0
3	PLP	E	4405	14/16	0.12	1.51	21,23,24,24	0
3	PLP	A	4401	14/16	0.12	1.12	17,21,22,22	0
3	PLP	C	4403	14/16	0.10	1.09	20,22,23,23	0
3	PLP	B	4402	14/16	0.10	0.87	20,25,26,26	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.