



# Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 05:19 PM GMT

PDB ID : 4E3Q  
Title : PMP-bound form of Aminotransferase crystal structure from *Vibrio fluvialis*  
Authors : Midelfort, K.S.; Kumar, R.; Han, S.; Karmilowicz, M.J.; McConnell, K.; Gehlhaar, D.K.; Mistry, A.; Chang, J.S.; Anderson, M.; Vilalobos, A.; Minshull, J.; Govindarajan, S.; Wong, J.W.  
Deposited on : 2012-03-10  
Resolution : 1.90 Å(reported)

This is a full wwPDB validation 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>

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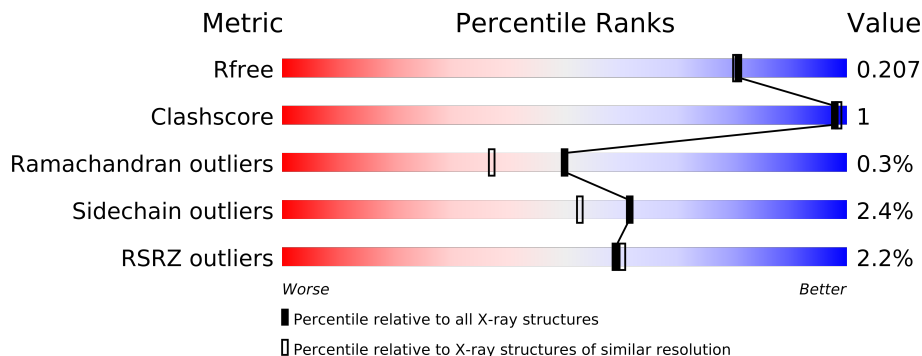
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 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 1.90 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	3684 (1.90-1.90)
Clashscore	79885	4465 (1.90-1.90)
Ramachandran outliers	78287	4413 (1.90-1.90)
Sidechain outliers	78261	4414 (1.90-1.90)
RSRZ outliers	66119	3686 (1.90-1.90)

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	473	
1	B	473	
1	C	473	
1	D	473	

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

Mol	Type	Chain	Res	Geometry	Electron density
3	SO4	A	502	-	X
4	BEN	A	503	-	X
4	BEN	A	504	-	X
4	BEN	B	502	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 15466 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 Pyruvate transaminase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	452	Total	C	N	O	S	Se	0	0	0
			3522	2252	599	651	7	13			
1	B	450	Total	C	N	O	S	Se	0	0	0
			3505	2242	595	648	7	13			
1	C	451	Total	C	N	O	S	Se	0	0	0
			3517	2249	598	650	7	13			
1	D	452	Total	C	N	O	S	Se	0	0	0
			3522	2252	599	651	7	13			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MSE	-	EXPRESSION TAG	UNP F2XBU9
A	-18	GLY	-	EXPRESSION TAG	UNP F2XBU9
A	-17	SER	-	EXPRESSION TAG	UNP F2XBU9
A	-16	SER	-	EXPRESSION TAG	UNP F2XBU9
A	-15	HIS	-	EXPRESSION TAG	UNP F2XBU9
A	-14	HIS	-	EXPRESSION TAG	UNP F2XBU9
A	-13	HIS	-	EXPRESSION TAG	UNP F2XBU9
A	-12	HIS	-	EXPRESSION TAG	UNP F2XBU9
A	-11	HIS	-	EXPRESSION TAG	UNP F2XBU9
A	-10	HIS	-	EXPRESSION TAG	UNP F2XBU9
A	-9	SER	-	EXPRESSION TAG	UNP F2XBU9
A	-8	SER	-	EXPRESSION TAG	UNP F2XBU9
A	-7	GLY	-	EXPRESSION TAG	UNP F2XBU9
A	-6	LEU	-	EXPRESSION TAG	UNP F2XBU9
A	-5	VAL	-	EXPRESSION TAG	UNP F2XBU9
A	-4	PRO	-	EXPRESSION TAG	UNP F2XBU9
A	-3	ARG	-	EXPRESSION TAG	UNP F2XBU9
A	-2	GLY	-	EXPRESSION TAG	UNP F2XBU9
A	-1	SER	-	EXPRESSION TAG	UNP F2XBU9
A	0	HIS	-	EXPRESSION TAG	UNP F2XBU9
B	-19	MSE	-	EXPRESSION TAG	UNP F2XBU9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	GLY	-	EXPRESSION TAG	UNP F2XBU9
B	-17	SER	-	EXPRESSION TAG	UNP F2XBU9
B	-16	SER	-	EXPRESSION TAG	UNP F2XBU9
B	-15	HIS	-	EXPRESSION TAG	UNP F2XBU9
B	-14	HIS	-	EXPRESSION TAG	UNP F2XBU9
B	-13	HIS	-	EXPRESSION TAG	UNP F2XBU9
B	-12	HIS	-	EXPRESSION TAG	UNP F2XBU9
B	-11	HIS	-	EXPRESSION TAG	UNP F2XBU9
B	-10	HIS	-	EXPRESSION TAG	UNP F2XBU9
B	-9	SER	-	EXPRESSION TAG	UNP F2XBU9
B	-8	SER	-	EXPRESSION TAG	UNP F2XBU9
B	-7	GLY	-	EXPRESSION TAG	UNP F2XBU9
B	-6	LEU	-	EXPRESSION TAG	UNP F2XBU9
B	-5	VAL	-	EXPRESSION TAG	UNP F2XBU9
B	-4	PRO	-	EXPRESSION TAG	UNP F2XBU9
B	-3	ARG	-	EXPRESSION TAG	UNP F2XBU9
B	-2	GLY	-	EXPRESSION TAG	UNP F2XBU9
B	-1	SER	-	EXPRESSION TAG	UNP F2XBU9
B	0	HIS	-	EXPRESSION TAG	UNP F2XBU9
C	-19	MSE	-	EXPRESSION TAG	UNP F2XBU9
C	-18	GLY	-	EXPRESSION TAG	UNP F2XBU9
C	-17	SER	-	EXPRESSION TAG	UNP F2XBU9
C	-16	SER	-	EXPRESSION TAG	UNP F2XBU9
C	-15	HIS	-	EXPRESSION TAG	UNP F2XBU9
C	-14	HIS	-	EXPRESSION TAG	UNP F2XBU9
C	-13	HIS	-	EXPRESSION TAG	UNP F2XBU9
C	-12	HIS	-	EXPRESSION TAG	UNP F2XBU9
C	-11	HIS	-	EXPRESSION TAG	UNP F2XBU9
C	-10	HIS	-	EXPRESSION TAG	UNP F2XBU9
C	-9	SER	-	EXPRESSION TAG	UNP F2XBU9
C	-8	SER	-	EXPRESSION TAG	UNP F2XBU9
C	-7	GLY	-	EXPRESSION TAG	UNP F2XBU9
C	-6	LEU	-	EXPRESSION TAG	UNP F2XBU9
C	-5	VAL	-	EXPRESSION TAG	UNP F2XBU9
C	-4	PRO	-	EXPRESSION TAG	UNP F2XBU9
C	-3	ARG	-	EXPRESSION TAG	UNP F2XBU9
C	-2	GLY	-	EXPRESSION TAG	UNP F2XBU9
C	-1	SER	-	EXPRESSION TAG	UNP F2XBU9
C	0	HIS	-	EXPRESSION TAG	UNP F2XBU9
D	-19	MSE	-	EXPRESSION TAG	UNP F2XBU9
D	-18	GLY	-	EXPRESSION TAG	UNP F2XBU9
D	-17	SER	-	EXPRESSION TAG	UNP F2XBU9

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-16	SER	-	EXPRESSION TAG	UNP F2XBU9
D	-15	HIS	-	EXPRESSION TAG	UNP F2XBU9
D	-14	HIS	-	EXPRESSION TAG	UNP F2XBU9
D	-13	HIS	-	EXPRESSION TAG	UNP F2XBU9
D	-12	HIS	-	EXPRESSION TAG	UNP F2XBU9
D	-11	HIS	-	EXPRESSION TAG	UNP F2XBU9
D	-10	HIS	-	EXPRESSION TAG	UNP F2XBU9
D	-9	SER	-	EXPRESSION TAG	UNP F2XBU9
D	-8	SER	-	EXPRESSION TAG	UNP F2XBU9
D	-7	GLY	-	EXPRESSION TAG	UNP F2XBU9
D	-6	LEU	-	EXPRESSION TAG	UNP F2XBU9
D	-5	VAL	-	EXPRESSION TAG	UNP F2XBU9
D	-4	PRO	-	EXPRESSION TAG	UNP F2XBU9
D	-3	ARG	-	EXPRESSION TAG	UNP F2XBU9
D	-2	GLY	-	EXPRESSION TAG	UNP F2XBU9
D	-1	SER	-	EXPRESSION TAG	UNP F2XBU9
D	0	HIS	-	EXPRESSION TAG	UNP F2XBU9

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

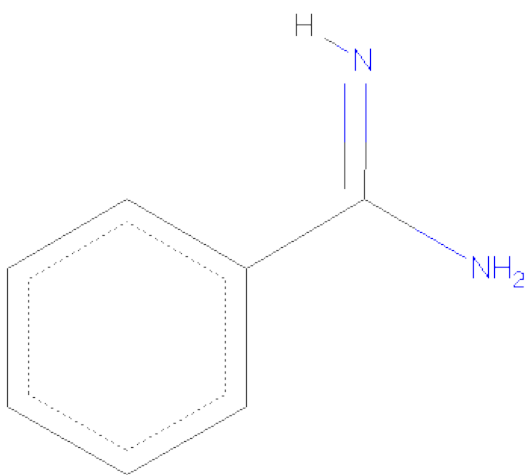
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Na 1 1	0	0
2	A	1	Total Na 1 1	0	0
2	D	1	Total Na 1 1	0	0
2	C	1	Total Na 1 1	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is BENZAMIDINE (three-letter code: BEN) (formula: C<sub>7</sub>H<sub>8</sub>N<sub>2</sub>).



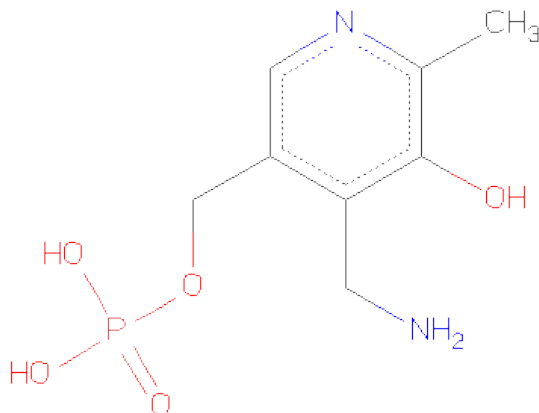
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	N	0	0
			9	7	2		
4	A	1	Total	C	N	0	0
			9	7	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	N	0	0
			9	7	2		

- Molecule 5 is 4'-DEOXY-4'-AMINOPYRIDOXAL-5'-PHOSPHATE (three-letter code: PMP) (formula: C<sub>8</sub>H<sub>13</sub>N<sub>2</sub>O<sub>5</sub>P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			16	8	2	5	1		
5	B	1	Total	C	N	O	P	0	0
			16	8	2	5	1		
5	C	1	Total	C	N	O	P	0	0
			16	8	2	5	1		
5	D	1	Total	C	N	O	P	0	0
			16	8	2	5	1		

- Molecule 6 is water.

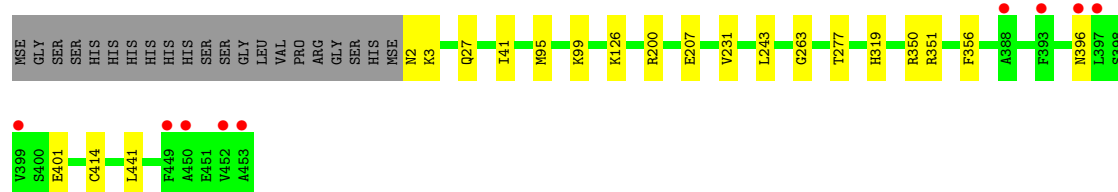
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	306	Total	O	0	0
			306	306		
6	B	339	Total	O	0	0
			339	339		
6	C	328	Total	O	0	0
			328	328		
6	D	322	Total	O	0	0
			322	322		

### 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: Pyruvate transaminase

Chain A: 



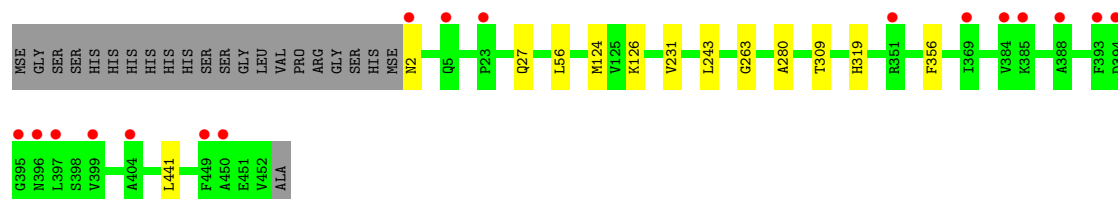
- Molecule 1: Pyruvate transaminase

Chain B: 



- Molecule 1: Pyruvate transaminase

Chain C: 



- Molecule 1: Pyruvate transaminase

Chain D: 





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	63.07Å 162.18Å 180.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.79 – 1.90 49.79 – 1.90	Depositor EDS
% Data completeness (in resolution range)	98.8 (49.79-1.90) 98.8 (49.79-1.90)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.27 (at 1.90Å)	Xtriage
Refinement program	BUSTER 2.9.5	Depositor
R, $R_{free}$	0.174 , 0.210 0.170 , 0.207	Depositor DCC
$R_{free}$ test set	7258 reflections (5.28%)	DCC
Wilson B-factor (Å <sup>2</sup> )	29.0	Xtriage
Anisotropy	0.309	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 44.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	1 of 144629 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	15466	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	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 57.28 % 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 2.4223e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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: BEN, PMP, SO4, NA

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	0.49	0/3600	0.66	1/4860 (0.0%)
1	B	0.52	1/3583 (0.0%)	0.63	1/4837 (0.0%)
1	C	0.50	0/3595	0.65	1/4853 (0.0%)
1	D	0.50	0/3600	0.65	1/4860 (0.0%)
All	All	0.51	1/14378 (0.0%)	0.65	4/19410 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	378	MSE	SE-CE	-5.13	1.65	1.95

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	263	GLY	N-CA-C	6.38	129.05	113.10
1	A	263	GLY	N-CA-C	6.06	128.26	113.10
1	D	263	GLY	N-CA-C	5.67	127.26	113.10
1	B	263	GLY	N-CA-C	5.64	127.19	113.10

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	3522	0	0	3	0
1	B	3505	0	0	2	0
1	C	3517	0	0	2	0
1	D	3522	0	0	3	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	5	0	0	0	0
3	C	5	0	0	0	0
4	A	18	0	14	0	0
4	B	9	0	7	0	0
5	A	16	0	10	0	0
5	B	16	0	10	0	0
5	C	16	0	10	0	0
5	D	16	0	10	0	0
6	A	306	0	0	2	0
6	B	339	0	0	1	0
6	C	328	0	0	0	0
6	D	322	0	0	0	0
All	All	15466	0	61	10	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 1.

All (10) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:200:ARG:NH2	6:A:894:HOH:O	2.20	0.73
1:D:373:ARG:NH2	1:D:382:GLU:OE1	2.35	0.59
1:D:414:CYS:SG	1:D:421:VAL:CG1	2.95	0.54
1:B:126:LYS:NZ	1:B:319:HIS:CD2	2.78	0.51
1:C:124:MSE:CE	1:C:280:ALA:CB	2.89	0.50
1:B:161:THR:O	6:B:929:HOH:O	2.20	0.49
1:C:126:LYS:NZ	1:C:319:HIS:CD2	2.81	0.48
1:A:126:LYS:NZ	1:A:319:HIS:CD2	2.82	0.47
1:A:350:ARG:NH2	6:A:898:HOH:O	2.51	0.44
1:D:359:ARG:NH2	1:D:442:GLU:OE1	2.51	0.43

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	450/473 (95%)	431 (96%)	18 (4%)	1 (0%)	56	44
1	B	448/473 (95%)	433 (97%)	13 (3%)	2 (0%)	43	29
1	C	449/473 (95%)	430 (96%)	18 (4%)	1 (0%)	56	44
1	D	450/473 (95%)	430 (96%)	18 (4%)	2 (0%)	43	29
All	All	1797/1892 (95%)	1724 (96%)	67 (4%)	6 (0%)	50	37

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	3	LYS
1	B	285	LYS
1	A	231	VAL
1	B	231	VAL
1	C	231	VAL
1	D	231	VAL

### 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	368/371 (99%)	353 (96%)	15 (4%)	41	28
1	B	366/371 (99%)	360 (98%)	6 (2%)	75	70
1	C	368/371 (99%)	361 (98%)	7 (2%)	69	63
1	D	368/371 (99%)	361 (98%)	7 (2%)	69	63
All	All	1470/1484 (99%)	1435 (98%)	35 (2%)	61	53

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ASN
1	A	3	LYS
1	A	27	GLN
1	A	41	ILE
1	A	95	MSE
1	A	99	LYS
1	A	207	GLU
1	A	243	LEU
1	A	277	THR
1	A	351	ARG
1	A	356	PHE
1	A	396	ASN
1	A	401	GLU
1	A	414	CYS
1	A	441	LEU
1	B	56	LEU
1	B	294	MSE
1	B	356	PHE
1	B	396	ASN
1	B	401	GLU
1	B	441	LEU
1	C	2	ASN
1	C	27	GLN
1	C	56	LEU
1	C	243	LEU
1	C	309	THR
1	C	356	PHE
1	C	441	LEU
1	D	2	ASN
1	D	3	LYS
1	D	294	MSE
1	D	307	LEU
1	D	356	PHE
1	D	401	GLU
1	D	441	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 ⓘ

Of 13 ligands modelled in this entry, 4 are monoatomic - leaving 9 for Mogul analysis.

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	SO4	A	502	-	4,4,4	1.13	0	6,6,6	0.41	0
4	BEN	A	503	-	9,9,9	2.06	3 (33%)	11,11,11	1.25	1 (9%)
4	BEN	A	504	-	9,9,9	1.80	3 (33%)	11,11,11	0.69	0
5	PMP	A	505	-	16,16,16	1.48	4 (25%)	23,23,23	1.27	2 (8%)
4	BEN	B	502	-	9,9,9	1.92	3 (33%)	11,11,11	0.55	0
5	PMP	B	503	-	16,16,16	1.28	1 (6%)	23,23,23	1.67	6 (26%)
3	SO4	C	502	-	4,4,4	1.04	0	6,6,6	0.31	0
5	PMP	C	503	-	16,16,16	1.61	5 (31%)	23,23,23	1.55	6 (26%)
5	PMP	D	502	-	16,16,16	1.41	2 (12%)	23,23,23	1.28	3 (13%)

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	SO4	A	502	-	-	0/0/0/0	0/0/0/0
4	BEN	A	503	-	-	0/4/4/4	0/1/1/1
4	BEN	A	504	-	-	0/4/4/4	0/1/1/1
5	PMP	A	505	-	-	0/8/8/8	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	BEN	B	502	-	-	0/4/4/4	0/1/1/1
5	PMP	B	503	-	-	0/8/8/8	0/1/1/1
3	SO4	C	502	-	-	0/0/0/0	0/0/0/0
5	PMP	C	503	-	-	0/8/8/8	0/1/1/1
5	PMP	D	502	-	-	0/8/8/8	0/1/1/1

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	503	BEN	C-N2	3.66	1.41	1.34
5	B	503	PMP	C3-C4	3.61	1.46	1.40
5	D	502	PMP	C3-C4	3.51	1.46	1.40
5	C	503	PMP	C6-N1	3.04	1.41	1.34
4	B	502	BEN	C6-C1	2.93	1.44	1.39
4	B	502	BEN	C2-C1	2.87	1.44	1.39
5	C	503	PMP	O3-C3	-2.85	1.30	1.37
4	A	503	BEN	C6-C1	2.68	1.43	1.39
4	A	504	BEN	C1-C	2.65	1.51	1.49
4	A	503	BEN	C2-C1	2.63	1.43	1.39
5	A	505	PMP	C3-C4	2.54	1.44	1.40
5	C	503	PMP	P-O4P	2.52	1.68	1.60
4	A	504	BEN	C6-C1	2.47	1.43	1.39
4	B	502	BEN	C-N2	2.45	1.39	1.34
5	A	505	PMP	C2A-C2	2.33	1.55	1.50
5	A	505	PMP	C5-C4	2.30	1.43	1.40
4	A	504	BEN	C-N2	2.29	1.38	1.34
5	A	505	PMP	C3-C2	2.27	1.42	1.40
5	D	502	PMP	C6-N1	2.24	1.39	1.34
5	C	503	PMP	C2A-C2	2.19	1.54	1.50
5	C	503	PMP	C3-C4	2.16	1.43	1.40

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	503	BEN	C1-C-N2	3.27	123.16	117.99
5	B	503	PMP	C6-C5-C4	3.00	120.38	118.10
5	B	503	PMP	C4A-C4-C3	2.99	125.00	120.38
5	C	503	PMP	P-O4P-C5A	-2.99	110.46	121.22
5	B	503	PMP	O4P-C5A-C5	-2.75	103.67	109.26
5	C	503	PMP	C6-C5-C4	2.65	120.11	118.10
5	B	503	PMP	C5-C6-N1	-2.65	119.09	123.86
5	A	505	PMP	C4A-C4-C3	2.63	124.44	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	503	PMP	C6-N1-C2	2.47	124.57	119.28
5	D	502	PMP	C6-C5-C4	2.36	119.89	118.10
5	D	502	PMP	P-O4P-C5A	-2.24	113.14	121.22
5	C	503	PMP	O4P-C5A-C5	-2.14	104.90	109.26
5	C	503	PMP	C5-C6-N1	-2.11	120.06	123.86
5	B	503	PMP	P-O4P-C5A	-2.07	113.76	121.22
5	C	503	PMP	C2A-C2-N1	2.05	122.43	117.93
5	D	502	PMP	C5-C6-N1	-2.05	120.16	123.86
5	C	503	PMP	C3-C4-C5	-2.04	116.58	118.74
5	A	505	PMP	C6-N1-C2	2.01	123.58	119.28

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	452/473 (95%)	-0.22	9 (1%) 62 63	21, 29, 55, 106	0
1	B	450/473 (95%)	-0.28	4 (0%) 81 83	20, 29, 47, 86	0
1	C	451/473 (95%)	-0.12	17 (3%) 38 40	22, 33, 58, 81	0
1	D	452/473 (95%)	-0.20	9 (1%) 62 63	22, 30, 51, 88	0
All	All	1805/1892 (95%)	-0.20	39 (2%) 59 60	20, 30, 53, 106	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	452	VAL	5.9
1	B	452	VAL	4.9
1	C	397	LEU	4.6
1	C	450	ALA	4.2
1	D	452	VAL	4.1
1	A	397	LEU	4.1
1	D	453	ALA	3.9
1	C	2	ASN	3.8
1	C	396	ASN	3.8
1	D	397	LEU	3.7
1	A	449	PHE	3.6
1	C	385	LYS	3.5
1	A	396	ASN	3.5
1	D	393	PHE	3.5
1	D	2	ASN	3.5
1	A	450	ALA	3.4
1	C	399	VAL	3.4
1	C	394	ASP	3.4
1	A	393	PHE	3.3
1	A	453	ALA	3.1
1	A	399	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	395	GLY	3.0
1	D	394	ASP	3.0
1	C	449	PHE	3.0
1	D	396	ASN	2.9
1	B	453	ALA	2.8
1	C	388	ALA	2.8
1	C	384	VAL	2.6
1	B	396	ASN	2.5
1	C	404	ALA	2.5
1	C	351	ARG	2.5
1	C	369	ILE	2.4
1	B	385	LYS	2.3
1	C	23	PRO	2.3
1	D	399	VAL	2.2
1	C	393	PHE	2.2
1	A	388	ALA	2.1
1	D	449	PHE	2.1
1	C	5	GLN	2.0

## 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
4	BEN	A	504	9/9	0.23	10.33	39,40,41,43	0
3	SO4	A	502	5/5	0.30	3.41	79,83,84,85	0
4	BEN	B	502	9/9	0.13	2.87	32,33,34,36	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	BEN	A	503	9/9	0.13	2.82	37,38,39,42	0
3	SO4	C	502	5/5	0.28	1.44	75,80,81,81	0
5	PMP	D	502	16/16	0.11	0.59	22,25,28,31	0
5	PMP	C	503	16/16	0.10	0.36	22,25,28,32	0
2	NA	C	501	1/1	0.11	0.23	35,35,35,35	0
5	PMP	A	505	16/16	0.10	0.14	20,23,27,28	0
2	NA	B	501	1/1	0.10	0.08	31,31,31,31	0
5	PMP	B	503	16/16	0.11	-0.00	21,23,27,31	0
2	NA	D	501	1/1	0.07	-0.45	35,35,35,35	0
2	NA	A	501	1/1	0.07	-0.45	33,33,33,33	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.