



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 02:19 am 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 X-ray Structure 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/validation/2016/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	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

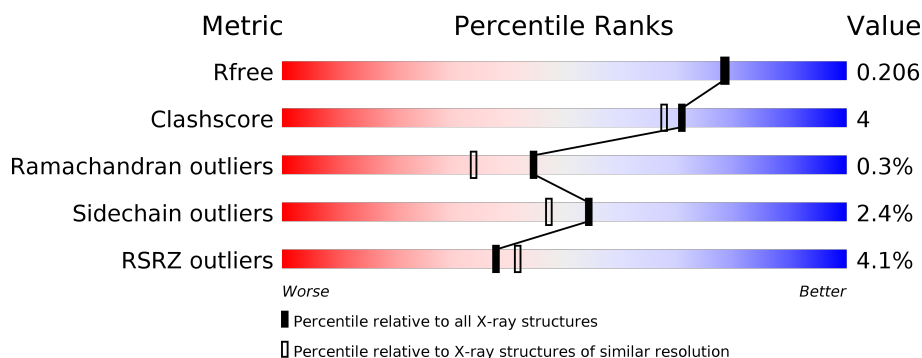
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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))
$R_{free}$	100719	5047 (1.90-1.90)
Clashscore	112137	5731 (1.90-1.90)
Ramachandran outliers	110173	5669 (1.90-1.90)
Sidechain outliers	110143	5670 (1.90-1.90)
RSRZ outliers	101464	5100 (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. 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	473	<div> <div>3%</div> <div> <div></div> <div>85%</div> <div>11%</div> <div>•</div> </div> </div>
1	B	473	<div> <div>3%</div> <div> <div></div> <div>86%</div> <div>9%</div> <div>• 5%</div> </div> </div>
1	C	473	<div> <div>5%</div> <div> <div></div> <div>87%</div> <div>8%</div> <div>5%</div> </div> </div>
1	D	473	<div> <div>4%</div> <div> <div></div> <div>85%</div> <div>10%</div> <div>• •</div> </div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	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 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 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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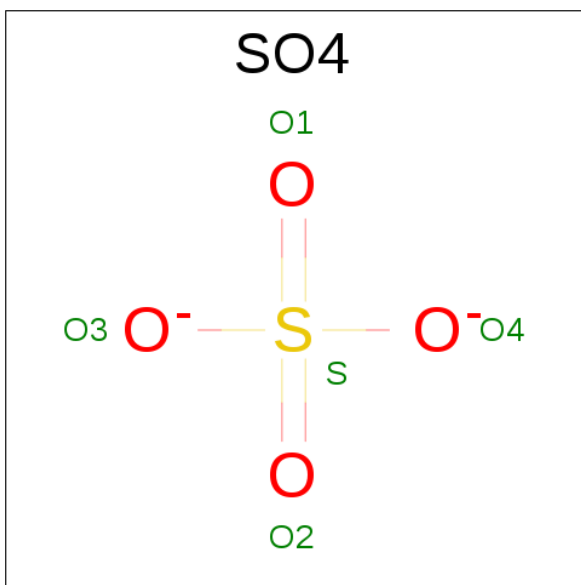
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Chain	Residue	Modelled	Actual	Comment	Reference
D	-16	SER	-	EXPRESSION TAG	UNP F2XBU9
D	-15	HIS	-	EXPRESSION TAG	UNP F2XBU9
D	-14	HIS	-	EXPRESSION TAG	UNP F2XBU9
D	-13	HIS	-	EXPRESSION TAG	UNP F2XBU9
D	-12	HIS	-	EXPRESSION TAG	UNP F2XBU9
D	-11	HIS	-	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).

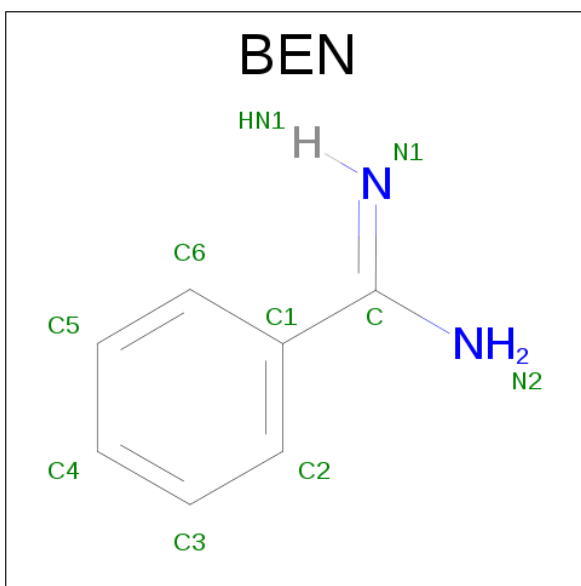
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Na 1 1	0	0
2	A	1	Total Na 1 1	0	0
2	D	1	Total Na 1 1	0	0
2	C	1	Total Na 1 1	0	0

- 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>).



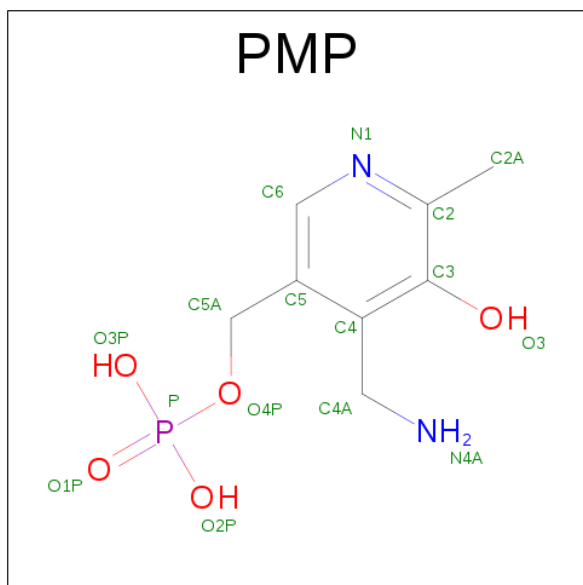
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	N	0	0
			9	7	2		
4	A	1	Total	C	N	0	0
			9	7	2		

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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:  $C_8H_{13}N_2O_5P$ ).



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.

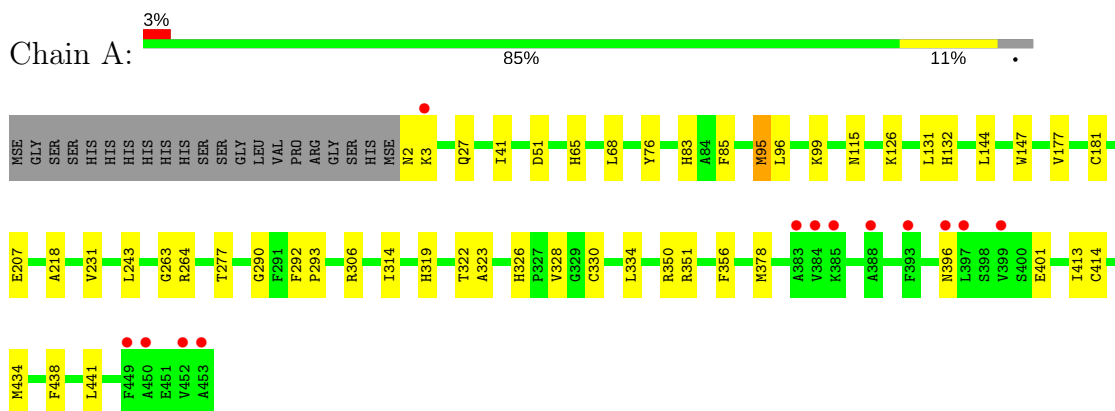
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	306	Total	O	0	0
			306	306		
6	B	339	Total	O	0	0
			339	339		
6	C	328	Total	O	0	0
			328	328		
6	D	322	Total	O	0	0
			322	322		



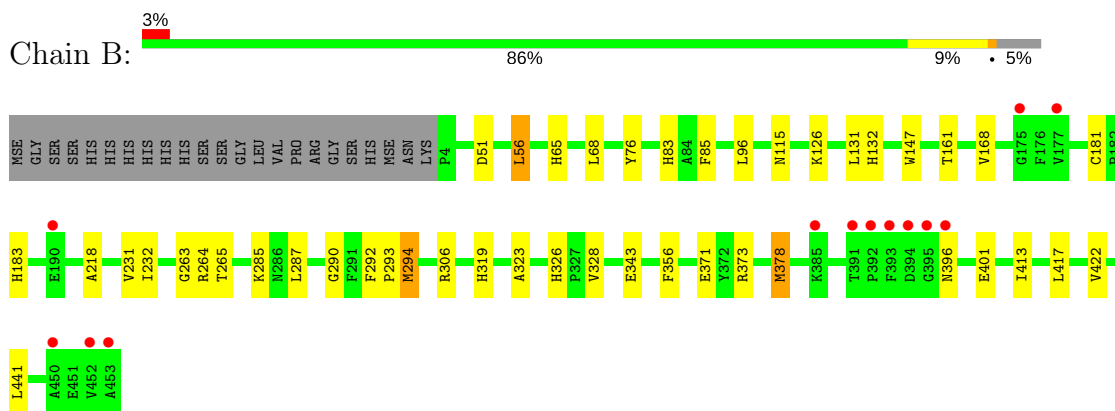
### 3 Residue-property plots [i](#)

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.

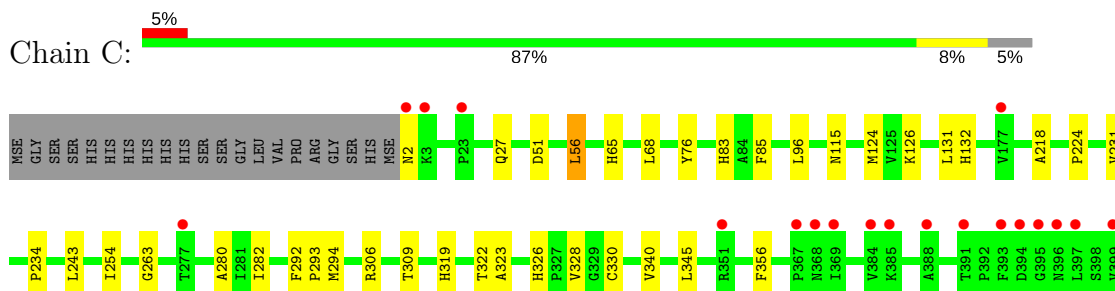
#### • Molecule 1: Pyruvate transaminase

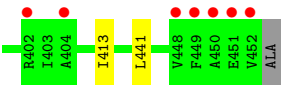


#### • Molecule 1: Pyruvate transaminase

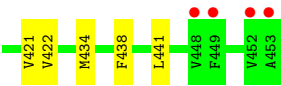
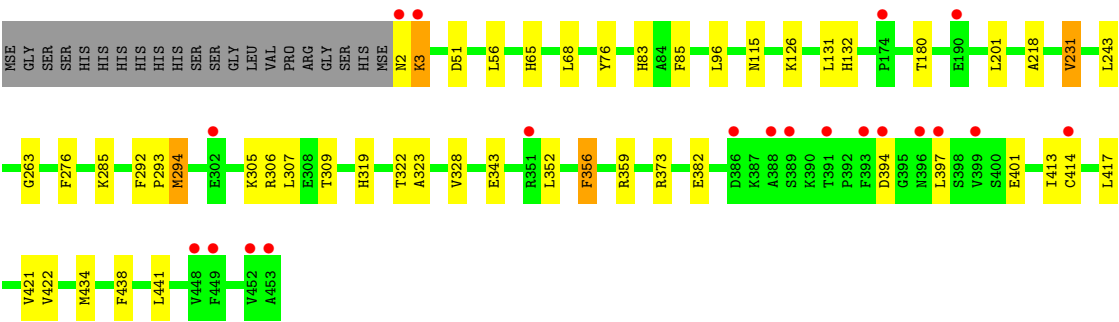
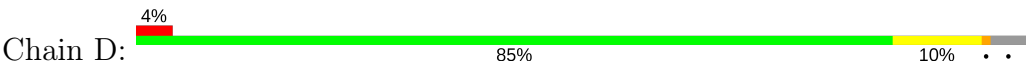


#### • Molecule 1: Pyruvate transaminase





● Molecule 1: Pyruvate transaminase



## 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) 98.9 (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 0.169 , 0.206	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> )	0.35 , 49.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	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.

<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 ⓘ

### 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 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	3522	0	3447	31	0
1	B	3505	0	3429	34	0
1	C	3517	0	3442	30	0
1	D	3522	0	3447	30	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	1	0
6	A	306	0	0	2	0
6	B	339	0	0	2	0
6	C	328	0	0	2	0
6	D	322	0	0	0	0
All	All	15466	0	13826	115	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 4.

All (115) 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:A:83:HIS:HD2	1:A:85:PHE:H	1.17	0.93
1:C:83:HIS:HD2	1:C:85:PHE:H	1.24	0.85
1:C:65:HIS:HD2	1:C:68:LEU:H	1.25	0.83
1:B:83:HIS:HD2	1:B:85:PHE:H	1.23	0.82
1:A:65:HIS:HD2	1:A:68:LEU:H	1.30	0.80
1:B:65:HIS:HD2	1:B:68:LEU:H	1.27	0.79
1:C:124:MSE:HE1	1:C:280:ALA:HB1	1.64	0.78
1:D:65:HIS:HD2	1:D:68:LEU:H	1.35	0.73
1:D:414:CYS:SG	1:D:421:VAL:HG13	2.31	0.70
1:B:126:LYS:NZ	1:B:319:HIS:HD2	1.90	0.69
1:B:126:LYS:HZ3	1:B:319:HIS:HD2	1.40	0.69
1:D:83:HIS:HD2	1:D:85:PHE:H	1.41	0.69
1:B:265:THR:HG22	1:B:378:MSE:HE1	1.77	0.67
1:A:264:ARG:CD	1:A:378:MSE:HG3	2.25	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:126:LYS:NZ	1:C:319:HIS:HD2	1.93	0.66
1:A:126:LYS:NZ	1:A:319:HIS:HD2	1.94	0.64
1:B:264:ARG:HG2	1:B:378:MSE:HE2	1.80	0.63
1:A:126:LYS:HZ3	1:A:319:HIS:HD2	1.49	0.60
1:A:115:ASN:HD21	1:A:323:ALA:HB3	1.67	0.60
1:B:265:THR:CG2	1:B:378:MSE:HE1	2.30	0.59
1:D:394:ASP:HB2	1:D:397:LEU:HD23	1.84	0.59
1:C:126:LYS:HZ3	1:C:319:HIS:HD2	1.50	0.58
1:C:56:LEU:HD23	1:D:322:THR:HA	1.86	0.58
1:D:231:VAL:O	1:D:373:ARG:HD2	2.04	0.57
1:D:373:ARG:NH2	1:D:382:GLU:OE1	2.35	0.56
1:D:126:LYS:NZ	1:D:319:HIS:HD2	2.04	0.54
1:D:414:CYS:SG	1:D:421:VAL:CG1	2.95	0.54
1:D:352:LEU:HB3	1:D:434:MSE:HE1	1.88	0.54
1:B:115:ASN:HD21	1:B:323:ALA:HB3	1.73	0.53
1:C:254:ILE:HD12	1:C:280:ALA:HB3	1.90	0.53
1:A:434:MSE:HE3	1:A:438:PHE:HE2	1.72	0.53
1:C:124:MSE:HE1	1:C:280:ALA:CB	2.35	0.53
1:C:326:HIS:HD2	1:C:328:VAL:H	1.57	0.52
1:C:294:MSE:HE2	6:C:623:HOH:O	2.08	0.52
1:C:124:MSE:CE	1:C:280:ALA:HB1	2.38	0.51
1:C:124:MSE:HE2	1:C:282:ILE:HD11	1.92	0.51
1:B:76:TYR:CE2	1:B:328:VAL:HG11	2.45	0.51
1:D:131:LEU:HD11	1:D:306:ARG:HB3	1.93	0.50
1:C:124:MSE:CE	1:C:280:ALA:CB	2.89	0.50
1:D:115:ASN:HD21	1:D:323:ALA:HB3	1.76	0.50
1:A:83:HIS:CD2	1:A:85:PHE:H	2.10	0.50
1:A:51:ASP:HA	1:A:413:ILE:HB	1.93	0.50
1:D:76:TYR:CE2	1:D:328:VAL:HG11	2.47	0.50
1:B:326:HIS:HD2	1:B:328:VAL:H	1.59	0.50
1:A:264:ARG:HD3	1:A:378:MSE:HG3	1.91	0.49
1:D:126:LYS:HZ3	1:D:319:HIS:HD2	1.59	0.49
1:A:132:HIS:HD2	6:A:762:HOH:O	1.95	0.49
1:A:290:GLY:O	1:B:326:HIS:HE1	1.95	0.49
1:A:76:TYR:CE2	1:A:328:VAL:HG11	2.47	0.49
1:B:264:ARG:CG	1:B:378:MSE:HE2	2.41	0.49
1:B:161:THR:O	6:B:929:HOH:O	2.20	0.49
1:C:131:LEU:HD11	1:C:306:ARG:HB3	1.95	0.49
1:D:132:HIS:HE1	1:D:218:ALA:O	1.96	0.48
1:C:76:TYR:CE2	1:C:328:VAL:HG11	2.49	0.48
1:A:147:TRP:O	1:A:181:CYS:HB2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:326:HIS:HD2	1:A:328:VAL:H	1.62	0.48
1:C:293:PRO:HD3	1:D:292:PHE:CZ	2.47	0.48
1:A:131:LEU:HD11	1:A:306:ARG:HB3	1.96	0.48
1:D:243:LEU:HD22	1:D:276:PHE:HB2	1.94	0.47
1:C:292:PHE:CZ	1:D:293:PRO:HD3	2.49	0.47
1:B:287:LEU:HD21	1:B:294:MSE:HE2	1.97	0.47
1:A:314:ILE:HD13	1:B:168:VAL:HG11	1.97	0.47
1:A:95:MSE:HG3	1:A:334:LEU:HD11	1.96	0.46
1:A:434:MSE:HE3	1:A:438:PHE:CE2	2.49	0.46
1:B:132:HIS:HE1	1:B:218:ALA:O	1.99	0.46
1:A:132:HIS:HE1	1:A:218:ALA:O	1.99	0.46
1:C:322:THR:HA	1:D:56:LEU:HD23	1.98	0.46
1:C:51:ASP:HA	1:C:413:ILE:HB	1.96	0.46
1:B:126:LYS:NZ	1:B:319:HIS:CD2	2.78	0.46
1:C:115:ASN:HD21	1:C:323:ALA:HB3	1.80	0.45
1:D:305:LYS:O	1:D:309:THR:HG23	2.17	0.45
1:C:132:HIS:HE1	1:C:218:ALA:O	1.99	0.45
1:A:326:HIS:HE1	1:B:290:GLY:O	2.00	0.45
1:C:326:HIS:CD2	1:C:328:VAL:H	2.33	0.44
1:C:132:HIS:HD2	6:C:770:HOH:O	1.99	0.44
1:D:359:ARG:HG2	1:D:438:PHE:CG	2.52	0.44
1:B:126:LYS:HZ3	1:B:319:HIS:CD2	2.28	0.44
1:A:350:ARG:NH2	6:A:898:HOH:O	2.51	0.44
1:B:183:HIS:HB2	1:B:232:ILE:HG21	2.00	0.44
1:C:83:HIS:CD2	1:C:85:PHE:H	2.16	0.44
1:D:417:LEU:HD12	1:D:422:VAL:HG21	2.00	0.44
1:B:131:LEU:HD11	1:B:306:ARG:HB3	1.99	0.43
1:D:294:MSE:HE2	1:D:294:MSE:HB3	1.78	0.43
1:A:144:LEU:HD23	1:A:177:VAL:HB	2.01	0.43
1:A:65:HIS:CD2	1:A:68:LEU:H	2.21	0.43
1:C:65:HIS:CD2	1:C:68:LEU:H	2.17	0.43
1:D:51:ASP:HA	1:D:413:ILE:HB	2.00	0.43
1:C:126:LYS:NZ	1:C:319:HIS:CD2	2.81	0.43
1:A:293:PRO:HD3	1:B:292:PHE:CZ	2.53	0.42
1:D:65:HIS:HE1	1:D:343:GLU:OE2	2.02	0.42
1:B:294:MSE:HE2	1:B:294:MSE:HB3	1.81	0.42
1:B:378:MSE:HE3	1:B:378:MSE:HB2	1.64	0.42
1:D:65:HIS:CD2	1:D:68:LEU:H	2.25	0.42
1:C:96:LEU:HD22	1:C:330:CYS:HA	2.00	0.42
1:B:417:LEU:HD12	1:B:422:VAL:HG21	2.00	0.42
1:B:132:HIS:HD2	6:B:647:HOH:O	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:356:PHE:CD1	1:D:434:MSE:HE2	2.55	0.42
1:C:124:MSE:HE2	1:C:282:ILE:CD1	2.50	0.41
1:D:96:LEU:HD21	1:D:294:MSE:HE1	2.02	0.41
1:C:340:VAL:HA	1:C:345:LEU:HB2	2.02	0.41
1:A:292:PHE:CZ	1:B:293:PRO:HD3	2.55	0.41
1:B:96:LEU:HD21	1:B:294:MSE:HE1	2.02	0.41
1:D:285:LYS:HE2	5:D:502:PMP:H4A2	2.02	0.41
1:A:322:THR:HA	1:B:56:LEU:HD23	2.03	0.41
1:A:126:LYS:NZ	1:A:319:HIS:CD2	2.82	0.41
1:C:224:PRO:O	1:C:234:PRO:HD3	2.20	0.41
1:A:96:LEU:HD22	1:A:330:CYS:HA	2.02	0.41
1:B:51:ASP:HA	1:B:413:ILE:HB	2.01	0.41
1:A:126:LYS:HZ3	1:A:319:HIS:CD2	2.34	0.41
1:B:65:HIS:HE1	1:B:343:GLU:OE2	2.04	0.41
1:B:147:TRP:O	1:B:181:CYS:HB2	2.21	0.41
1:A:264:ARG:HG2	1:A:378:MSE:HG3	2.04	0.40
1:B:287:LEU:HD21	1:B:294:MSE:CE	2.51	0.40
1:B:371:GLU:OE1	1:B:373:ARG:HD3	2.21	0.40
1:D:180:THR:HB	1:D:201:LEU:HD23	2.03	0.40

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%)	51	41
1	B	448/473 (95%)	433 (97%)	13 (3%)	2 (0%)	38	26
1	C	449/473 (95%)	430 (96%)	18 (4%)	1 (0%)	51	41
1	D	450/473 (95%)	430 (96%)	18 (4%)	2 (0%)	38	26
All	All	1797/1892 (95%)	1724 (96%)	67 (4%)	6 (0%)	44	34



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%)	35	24
1	B	366/371 (99%)	360 (98%)	6 (2%)	68	65
1	C	368/371 (99%)	361 (98%)	7 (2%)	62	57
1	D	368/371 (99%)	361 (98%)	7 (2%)	62	57
All	All	1470/1484 (99%)	1435 (98%)	35 (2%)	54	47

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

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Mol	Chain	Res	Type
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. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2	ASN
1	A	53	ASN
1	A	65	HIS
1	A	83	HIS
1	A	115	ASN
1	A	121	ASN
1	A	132	HIS
1	A	148	ASN
1	A	267	ASN
1	A	319	HIS
1	A	326	HIS
1	B	53	ASN
1	B	65	HIS
1	B	83	HIS
1	B	115	ASN
1	B	121	ASN
1	B	132	HIS

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Mol	Chain	Res	Type
1	B	267	ASN
1	B	319	HIS
1	B	326	HIS
1	B	396	ASN
1	C	53	ASN
1	C	65	HIS
1	C	83	HIS
1	C	115	ASN
1	C	121	ASN
1	C	132	HIS
1	C	319	HIS
1	C	326	HIS
1	D	2	ASN
1	D	53	ASN
1	D	65	HIS
1	D	83	HIS
1	D	115	ASN
1	D	121	ASN
1	D	132	HIS
1	D	267	ASN
1	D	319	HIS
1	D	368	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](#)

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	0.47	0	6,6,6	0.32	0
4	BEN	A	503	-	9,9,9	2.09	4 (44%)	9,11,11	1.22	1 (11%)
4	BEN	A	504	-	9,9,9	1.85	3 (33%)	9,11,11	0.67	0
5	PMP	A	505	-	16,16,16	1.55	4 (25%)	20,23,23	1.30	2 (10%)
4	BEN	B	502	-	9,9,9	1.91	3 (33%)	9,11,11	0.57	0
5	PMP	B	503	-	16,16,16	1.37	1 (6%)	20,23,23	1.73	5 (25%)
3	SO4	C	502	-	4,4,4	0.50	0	6,6,6	0.26	0
5	PMP	C	503	-	16,16,16	1.71	6 (37%)	20,23,23	1.52	6 (30%)
5	PMP	D	502	-	16,16,16	1.51	2 (12%)	20,23,23	1.28	3 (15%)

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
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 (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	503	PMP	O3-C3	-2.97	1.30	1.37
4	A	503	BEN	C5-C4	2.04	1.43	1.38
5	C	503	PMP	C6-C5	2.05	1.42	1.37
4	A	504	BEN	C-N2	2.18	1.38	1.33
4	B	502	BEN	C-N2	2.31	1.39	1.33
5	D	502	PMP	C6-N1	2.36	1.39	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	505	PMP	C3-C2	2.38	1.42	1.40
5	C	503	PMP	C3-C4	2.38	1.43	1.40
5	C	503	PMP	C2A-C2	2.38	1.54	1.50
5	A	505	PMP	C5-C4	2.45	1.43	1.40
5	A	505	PMP	C2A-C2	2.53	1.55	1.50
4	A	504	BEN	C6-C1	2.58	1.43	1.39
5	C	503	PMP	P-O4P	2.67	1.68	1.60
4	A	504	BEN	C1-C	2.67	1.51	1.47
4	A	503	BEN	C2-C1	2.75	1.43	1.39
4	A	503	BEN	C6-C1	2.80	1.43	1.39
5	A	505	PMP	C3-C4	2.80	1.44	1.40
4	B	502	BEN	C2-C1	2.99	1.44	1.39
4	B	502	BEN	C6-C1	3.06	1.44	1.39
5	C	503	PMP	C6-N1	3.20	1.41	1.34
4	A	503	BEN	C-N2	3.32	1.41	1.33
5	D	502	PMP	C3-C4	3.87	1.46	1.40
5	B	503	PMP	C3-C4	3.98	1.46	1.40

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	503	PMP	C5-C6-N1	-2.83	119.09	123.87
5	B	503	PMP	O4P-C5A-C5	-2.80	103.67	109.32
5	C	503	PMP	C5-C6-N1	-2.25	120.06	123.87
5	C	503	PMP	O4P-C5A-C5	-2.19	104.90	109.32
5	D	502	PMP	C5-C6-N1	-2.19	120.16	123.87
5	C	503	PMP	C3-C4-C5	-2.16	116.58	118.71
5	D	502	PMP	C3-C4-C5	-2.11	116.62	118.71
5	C	503	PMP	C3-C2-N1	-2.02	118.09	120.75
5	A	505	PMP	C6-N1-C2	2.24	123.58	119.26
5	C	503	PMP	C2A-C2-N1	2.27	122.43	117.89
5	D	502	PMP	C6-C5-C4	2.37	119.89	118.13
5	A	505	PMP	C4A-C4-C3	2.66	124.44	120.44
5	C	503	PMP	C6-C5-C4	2.66	120.11	118.13
5	B	503	PMP	C6-N1-C2	2.76	124.57	119.26
5	B	503	PMP	C4A-C4-C3	3.02	125.00	120.44
5	B	503	PMP	C6-C5-C4	3.03	120.38	118.13
4	A	503	BEN	C1-C-N2	3.28	123.16	118.12

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	502	PMP	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 ⓘ

### 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	439/473 (92%)	-0.07	13 (2%) 51 54	21, 29, 55, 106	0
1	B	437/473 (92%)	-0.14	13 (2%) 51 54	20, 29, 48, 86	0
1	C	438/473 (92%)	0.10	26 (5%) 23 26	22, 33, 58, 81	0
1	D	439/473 (92%)	-0.01	20 (4%) 33 37	22, 30, 51, 88	0
All	All	1753/1892 (92%)	-0.03	72 (4%) 38 42	20, 30, 54, 106	0

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	452	VAL	8.2
1	B	452	VAL	6.1
1	D	452	VAL	6.0
1	C	397	LEU	5.4
1	C	450	ALA	5.3
1	A	397	LEU	5.0
1	A	393	PHE	4.5
1	D	397	LEU	4.5
1	D	453	ALA	4.5
1	A	449	PHE	4.5
1	D	2	ASN	4.3
1	C	388	ALA	4.3
1	D	393	PHE	4.3
1	C	396	ASN	4.2
1	C	385	LYS	4.2
1	C	384	VAL	4.1
1	C	399	VAL	4.0
1	C	449	PHE	3.9
1	C	369	ILE	3.8
1	A	396	ASN	3.7
1	A	450	ALA	3.7

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Mol	Chain	Res	Type	RSRZ
1	D	396	ASN	3.6
1	C	394	ASP	3.5
1	C	404	ALA	3.5
1	A	399	VAL	3.4
1	B	453	ALA	3.3
1	B	396	ASN	3.3
1	C	2	ASN	3.3
1	C	395	GLY	3.3
1	C	351	ARG	3.1
1	B	393	PHE	3.1
1	D	394	ASP	3.1
1	C	393	PHE	3.0
1	D	399	VAL	3.0
1	B	395	GLY	3.0
1	D	414	CYS	3.0
1	B	190	GLU	2.9
1	D	449	PHE	2.9
1	C	368	ASN	2.9
1	B	385	LYS	2.9
1	D	388	ALA	2.9
1	A	384	VAL	2.8
1	A	453	ALA	2.6
1	A	388	ALA	2.6
1	B	394	ASP	2.6
1	D	391	THR	2.6
1	C	367	PRO	2.5
1	C	452	VAL	2.5
1	C	3	LYS	2.5
1	D	389	SER	2.5
1	C	277	THR	2.4
1	C	402	ARG	2.4
1	B	450	ALA	2.3
1	C	451	GLU	2.3
1	D	302	GLU	2.3
1	D	190	GLU	2.3
1	D	3	LYS	2.3
1	B	175	GLY	2.3
1	C	448	VAL	2.3
1	A	385	LYS	2.3
1	B	391	THR	2.2
1	A	383	ALA	2.2
1	D	351	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	177	VAL	2.2
1	D	386	ASP	2.2
1	C	23	PRO	2.2
1	C	177	VAL	2.1
1	C	391	THR	2.1
1	D	174	PRO	2.0
1	B	392	PRO	2.0
1	D	448	VAL	2.0
1	A	3	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 [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. 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	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	BEN	A	504	9/9	0.88	0.23	9.32	39,40,41,43	0
3	SO4	A	502	5/5	0.82	0.29	5.14	79,83,84,85	0
4	BEN	B	502	9/9	0.91	0.14	3.37	32,33,34,36	0
4	BEN	A	503	9/9	0.87	0.15	3.16	37,38,39,42	0
2	NA	C	501	1/1	0.96	0.16	1.35	35,35,35,35	0
3	SO4	C	502	5/5	0.95	0.24	0.60	75,80,81,81	0
2	NA	A	501	1/1	0.99	0.10	0.42	33,33,33,33	0
5	PMP	D	502	16/16	0.98	0.11	0.42	22,25,28,31	0
2	NA	B	501	1/1	0.97	0.12	0.34	31,31,31,31	0
2	NA	D	501	1/1	0.97	0.10	-0.12	35,35,35,35	0
5	PMP	C	503	16/16	0.97	0.10	-0.21	22,25,28,32	0
5	PMP	A	505	16/16	0.98	0.10	-0.43	20,23,27,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
5	PMP	B	503	16/16	0.99	0.10	-0.52	21,23,27,31	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.