



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 21, 2017 – 02:41 AM EST

PDB ID : 1AMQ
Title : X-RAY CRYSTALLOGRAPHIC STUDY OF PYRIDOXAMINE 5'-
PHOSPHATE-TYPE ASPARTATE AMINOTRANSFERASES FROM
ESCHERICHIA COLI IN THREE FORMS
Authors : Miyahara, I.; Hirotsu, K.; Hayashi, H.; Kagamiyama, H.
Deposited on : unknown
Resolution : 2.20 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

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20030345

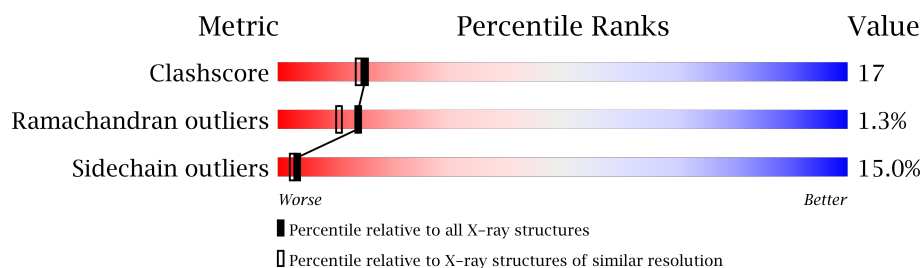
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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))
Clashscore	112137	4730 (2.20-2.20)
Ramachandran outliers	110173	4656 (2.20-2.20)
Sidechain outliers	110143	4657 (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 ≥ 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	396	

2 Entry composition [i](#)

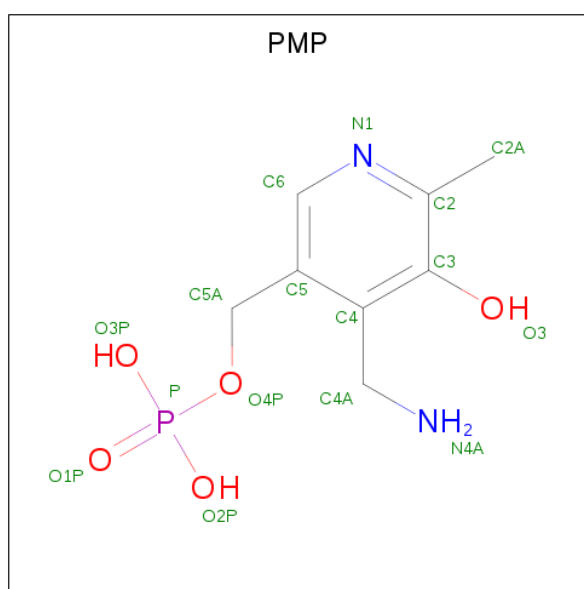
There are 3 unique types of molecules in this entry. The entry contains 3343 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	396	Total	C	N	O	S	0	0	0
			3069	1936	536	584	13			

- Molecule 2 is 4'-DEOXY-4'-AMINOPYRIDOXAL-5'-PHOSPHATE (three-letter code: PMP) (formula: C₈H₁₃N₂O₅P).



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

- Molecule 3 is water.

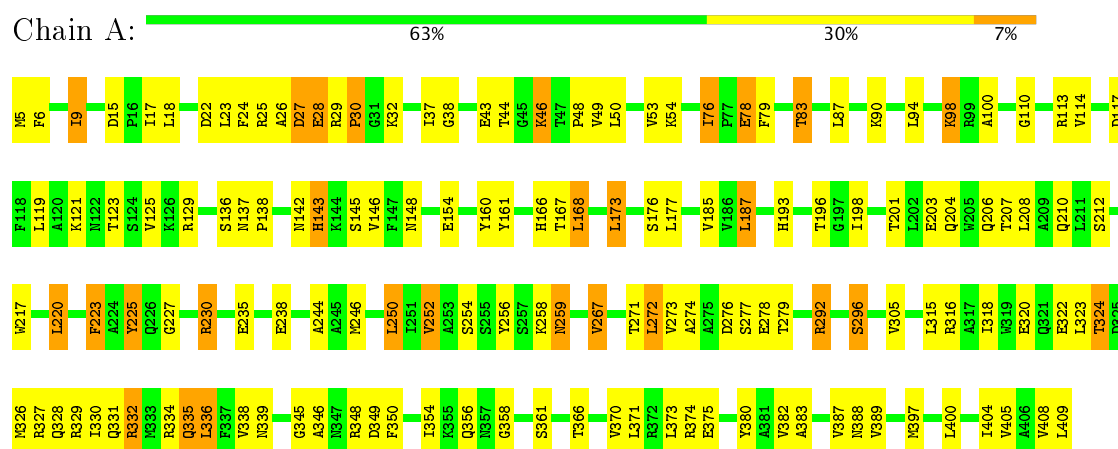
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	258	Total	O	0	0
			258	258		

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.

Note EDS was not executed.

• Molecule 1: ASPARTATE AMINOTRANSFERASE



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	155.70 Å 86.70 Å 79.60 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.20	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-2.20)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR, TOM, TOM/FRODO	Depositor
R, R_{free}	0.192 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3343	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

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: PMP

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	0.47	0/3130	0.77	1/4240 (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	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	187	LEU	CA-CB-CG	6.61	130.50	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	225	TYR	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	3069	0	3018	100	0
2	A	16	0	11	2	0
3	A	258	0	0	8	0
All	All	3343	0	3029	102	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 17.

All (102) 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:50:LEU:HB2	1:A:53:VAL:HG13	1.53	0.90
1:A:76:ILE:HD11	1:A:78:GLU:HB2	1.59	0.83
1:A:28:GLU:O	1:A:30:PRO:HD3	1.81	0.79
1:A:348:ARG:HH22	1:A:405:VAL:HG22	1.50	0.76
1:A:98:LYS:HZ2	1:A:98:LYS:HA	1.53	0.73
1:A:38:GLY:H	1:A:388:ASN:HD22	1.37	0.73
1:A:17:ILE:HG13	1:A:18:LEU:HD12	1.70	0.73
1:A:117:ASP:O	1:A:121:LYS:HG2	1.90	0.71
1:A:168:LEU:HD21	1:A:173:LEU:HD12	1.74	0.69
1:A:129:ARG:CZ	1:A:154:GLU:HG2	2.23	0.69
1:A:252:VAL:HG13	1:A:271:THR:HB	1.76	0.68
1:A:334:ARG:HH22	1:A:361:SER:HB3	1.56	0.68
1:A:335:GLN:HG3	3:A:674:HOH:O	1.94	0.67
1:A:328:GLN:O	1:A:332:ARG:HD3	1.94	0.67
1:A:37:ILE:HG13	1:A:388:ASN:ND2	2.10	0.67
1:A:94:LEU:HD11	1:A:244:ALA:HB1	1.78	0.66
1:A:227:GLY:O	1:A:327:ARG:HD3	1.97	0.65
1:A:235:GLU:O	1:A:238:GLU:HG2	1.97	0.64
1:A:37:ILE:HG13	1:A:388:ASN:HD22	1.63	0.64
1:A:185:VAL:HG11	1:A:220:LEU:HD12	1.80	0.64
1:A:373:LEU:HD11	1:A:408:VAL:HG21	1.81	0.63
1:A:27:ASP:HB3	1:A:32:LYS:HD3	1.80	0.63
1:A:256:TYR:HB2	1:A:267:VAL:HG22	1.81	0.62
1:A:43:GLU:HG2	1:A:329:ARG:HD2	1.80	0.62
1:A:346:ALA:HB3	1:A:348:ARG:CZ	2.30	0.62
1:A:346:ALA:HB3	1:A:348:ARG:NH1	2.15	0.62
1:A:79:PHE:O	1:A:83:THR:HG22	2.00	0.61
1:A:203:GLU:O	1:A:207:THR:HG23	2.00	0.61
1:A:366:THR:O	1:A:370:VAL:HG13	2.03	0.59
1:A:373:LEU:CD1	1:A:408:VAL:HG21	2.33	0.59
1:A:274:ALA:HB1	1:A:279:THR:HG23	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:THR:HB	1:A:256:TYR:OH	2.03	0.58
1:A:201:THR:HG22	1:A:204:GLN:HG3	1.87	0.57
1:A:346:ALA:HB3	1:A:348:ARG:NH2	2.20	0.57
1:A:50:LEU:HB2	1:A:53:VAL:CG1	2.33	0.56
1:A:374:ARG:HH21	1:A:375:GLU:HG2	1.70	0.55
1:A:334:ARG:NH2	1:A:361:SER:HB3	2.22	0.55
1:A:335:GLN:HA	1:A:354:ILE:CD1	2.36	0.55
1:A:98:LYS:NZ	1:A:98:LYS:HA	2.20	0.55
1:A:123:THR:OG1	1:A:125:VAL:HG13	2.08	0.54
1:A:404:ILE:O	1:A:409:LEU:HD13	2.09	0.53
1:A:76:ILE:CD1	1:A:78:GLU:HB2	2.35	0.53
1:A:345:GLY:HA2	3:A:677:HOH:O	2.10	0.52
1:A:316:ARG:O	1:A:320:GLU:HG3	2.10	0.52
1:A:273:VAL:HG11	3:A:569:HOH:O	2.09	0.52
1:A:46:LYS:O	1:A:48:PRO:HD3	2.11	0.51
1:A:318:ILE:HG23	3:A:561:HOH:O	2.11	0.50
1:A:370:VAL:HG21	1:A:383:ALA:HA	1.93	0.50
1:A:206:GLN:HG2	3:A:635:HOH:O	2.11	0.50
2:A:413:PMP:H4A2	2:A:413:PMP:O4P	2.11	0.50
1:A:136:SER:OG	1:A:193:HIS:HE1	1.94	0.49
1:A:142:ASN:O	1:A:146:VAL:HG23	2.12	0.49
1:A:76:ILE:O	1:A:79:PHE:HB3	2.13	0.49
1:A:110:GLY:O	1:A:114:VAL:HG13	2.13	0.49
1:A:161:TYR:CE1	1:A:166:HIS:HA	2.48	0.49
1:A:334:ARG:NH1	1:A:358:GLY:O	2.45	0.49
1:A:320:GLU:O	1:A:324:THR:HG23	2.13	0.49
1:A:335:GLN:HA	1:A:354:ILE:HD12	1.95	0.48
2:A:413:PMP:N4A	2:A:413:PMP:O3	2.47	0.48
1:A:331:GLN:O	1:A:335:GLN:NE2	2.46	0.48
1:A:143:HIS:CE1	1:A:187:LEU:HD11	2.49	0.47
1:A:334:ARG:HH22	1:A:361:SER:CB	2.25	0.47
1:A:276:ASP:OD1	1:A:279:THR:HG22	2.14	0.47
1:A:274:ALA:CB	1:A:279:THR:HG23	2.44	0.47
1:A:168:LEU:CD2	1:A:173:LEU:HD12	2.43	0.47
1:A:292:ARG:HA	1:A:296:SER:HA	1.96	0.47
1:A:23:LEU:HB3	1:A:380:TYR:HE2	1.79	0.46
1:A:338:VAL:HG21	1:A:354:ILE:HG12	1.96	0.46
1:A:193:HIS:HD2	1:A:196:THR:H	1.63	0.46
1:A:225:TYR:CE1	1:A:258:LYS:HG3	2.50	0.46
1:A:15:ASP:HB3	1:A:18:LEU:HB2	1.96	0.46
1:A:373:LEU:HD12	1:A:408:VAL:HG11	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:336:LEU:HD13	1:A:397:MET:HG2	1.98	0.46
1:A:230:ARG:HH11	1:A:235:GLU:HB3	1.80	0.46
1:A:76:ILE:O	1:A:76:ILE:HG13	2.16	0.45
1:A:330:ILE:O	1:A:334:ARG:HG3	2.17	0.45
1:A:100:ALA:HA	1:A:272:LEU:O	2.16	0.45
1:A:404:ILE:O	1:A:408:VAL:HG22	2.17	0.45
1:A:250:LEU:HD21	3:A:569:HOH:O	2.16	0.44
1:A:346:ALA:HB2	1:A:405:VAL:HG13	2.00	0.44
1:A:212:SER:HA	1:A:217:TRP:CD1	2.53	0.44
1:A:201:THR:HG22	1:A:204:GLN:CG	2.47	0.44
1:A:334:ARG:HG2	1:A:389:VAL:HG11	2.00	0.44
1:A:256:TYR:HA	1:A:259:ASN:HD21	1.83	0.43
1:A:113:ARG:NH2	3:A:494:HOH:O	2.52	0.43
1:A:356:GLN:HE21	1:A:361:SER:HB3	1.83	0.43
1:A:76:ILE:HG13	1:A:79:PHE:H	1.83	0.43
1:A:24:PHE:O	1:A:32:LYS:NZ	2.46	0.43
1:A:22:ASP:HA	1:A:25:ARG:HG2	2.00	0.42
1:A:336:LEU:HD22	1:A:336:LEU:O	2.19	0.42
1:A:6:PHE:O	1:A:9:ILE:HB	2.20	0.42
1:A:137:ASN:HA	1:A:138:PRO:HA	1.77	0.42
1:A:223:PHE:HD1	1:A:223:PHE:HA	1.77	0.42
1:A:348:ARG:HB2	1:A:350:PHE:CD1	2.55	0.42
1:A:223:PHE:O	1:A:254:SER:HA	2.19	0.42
1:A:278:GLU:HB2	3:A:658:HOH:O	2.20	0.42
1:A:201:THR:HG23	1:A:203:GLU:H	1.84	0.41
1:A:322:GLU:O	1:A:326:MET:HG3	2.20	0.41
1:A:79:PHE:O	1:A:83:THR:CG2	2.67	0.41
1:A:227:GLY:HA3	1:A:323:LEU:HD21	2.02	0.41
1:A:53:VAL:HB	1:A:305:VAL:HG11	2.02	0.40
1:A:348:ARG:NH2	1:A:405:VAL:HG22	2.28	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	394/396 (100%)	368 (93%)	21 (5%)	5 (1%)	14	11

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	349	ASP
1	A	26	ALA
1	A	27	ASP
1	A	30	PRO
1	A	160	TYR

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	320/320 (100%)	272 (85%)	48 (15%)	3	2

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	MET
1	A	9	ILE
1	A	28	GLU
1	A	29	ARG
1	A	44	THR
1	A	46	LYS
1	A	49	VAL
1	A	54	LYS
1	A	76	ILE
1	A	78	GLU
1	A	83	THR
1	A	87	LEU
1	A	90	LYS
1	A	98	LYS

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Mol	Chain	Res	Type
1	A	119	LEU
1	A	143	HIS
1	A	145	SER
1	A	148	ASN
1	A	167	THR
1	A	168	LEU
1	A	173	LEU
1	A	176	SER
1	A	177	LEU
1	A	198	ILE
1	A	208	LEU
1	A	210	GLN
1	A	220	LEU
1	A	223	PHE
1	A	230	ARG
1	A	246	MET
1	A	250	LEU
1	A	252	VAL
1	A	259	ASN
1	A	267	VAL
1	A	272	LEU
1	A	277	SER
1	A	292	ARG
1	A	296	SER
1	A	315	LEU
1	A	324	THR
1	A	332	ARG
1	A	335	GLN
1	A	336	LEU
1	A	339	ASN
1	A	371	LEU
1	A	382	VAL
1	A	387	VAL
1	A	400	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	58	GLN
1	A	69	ASN
1	A	84	GLN
1	A	96	ASN

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Mol	Chain	Res	Type
1	A	148	ASN
1	A	166	HIS
1	A	193	HIS
1	A	206	GLN
1	A	226	GLN
1	A	247	HIS
1	A	259	ASN
1	A	328	GLN
1	A	356	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

1 ligand is 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	$\# Z > 2$
2	PMP	A	413	-	16,16,16	2.12	3 (18%)	20,23,23	2.10	7 (35%)

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
2	PMP	A	413	-	-	0/8/8/8	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	413	PMP	C3-C2	-7.21	1.35	1.40
2	A	413	PMP	P-O2P	-2.38	1.45	1.54
2	A	413	PMP	C5A-C5	2.04	1.56	1.50

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	413	PMP	O3P-P-O1P	-2.64	100.17	110.50
2	A	413	PMP	O2P-P-O4P	-2.57	99.89	106.73
2	A	413	PMP	C5-C6-N1	-2.36	119.87	123.87
2	A	413	PMP	O2P-P-O1P	2.20	119.12	110.50
2	A	413	PMP	O3P-P-O2P	2.83	119.04	107.61
2	A	413	PMP	O4P-P-O1P	3.34	115.85	106.47
2	A	413	PMP	O4P-C5A-C5	5.29	119.95	109.32

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	413	PMP	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

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.