Full wwPDB X-ray Structure Validation Report (i)

Jun 12, 2024 – 09:04 PM EDT

PDB ID	:	1EYW
Title	:	THREE-DIMENSIONAL STRUCTURE OF THE ZINC-CONTAINING PHOSPHOTRIESTERASE WITH BOUND SUBSTRATE ANALOG TRI-ETHYLPHOSPHATE
Authors	:	Holden, H.M.; Benning, M.M.; Raushel, F.M.; Hong, S.-B.
Deposited on	:	2000-05-09
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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

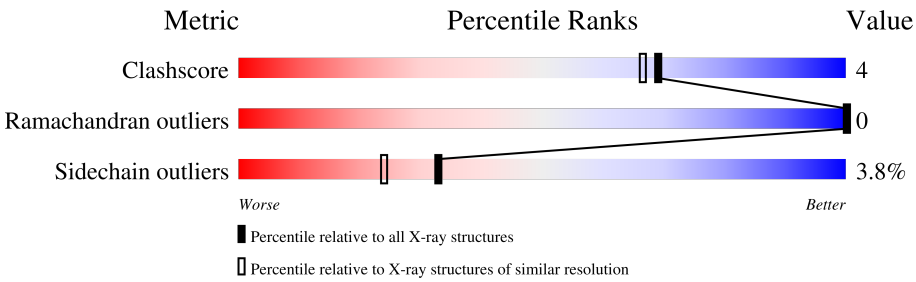
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 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))
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	331	83% 14% •

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	PEL	A	404	-	X	-	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 2768 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 PHOSPHOTRIESTERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	330	2525	1598	450	470	7	0	2	0

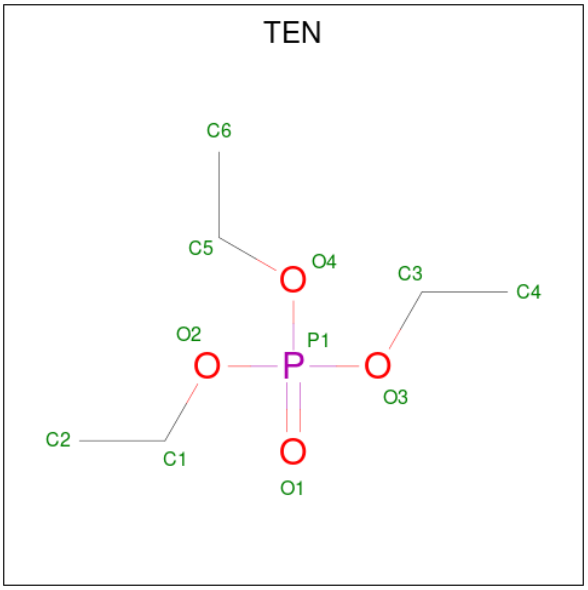
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	169	KCX	LYS	MODIFIED RESIDUE	UNP P0A434

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

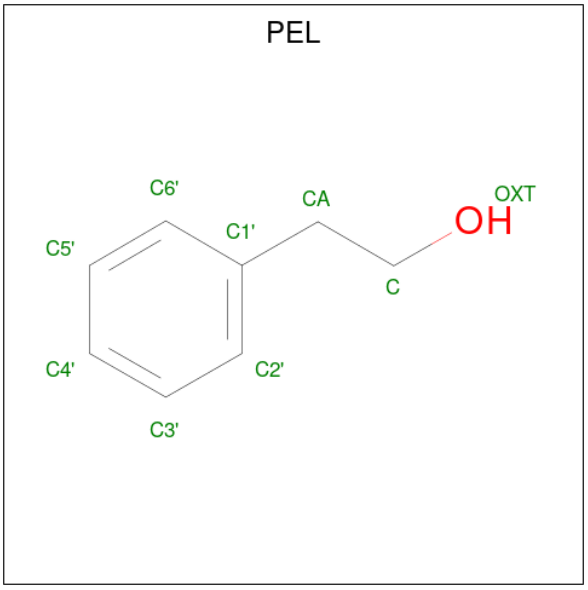
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
2	A	2	2	2	0	0

- Molecule 3 is TRIETHYL PHOSPHATE (three-letter code: TEN) (formula: $C_6H_{15}O_4P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
3	A	1	11	6	4	1	0	0

- Molecule 4 is 2-PHENYL-ETHANOL (three-letter code: PEL) (formula: $C_8H_{10}O$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	A	1	9	8	1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	221	221	221	0	0

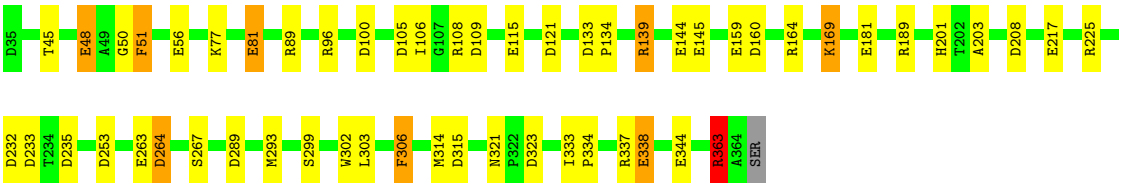
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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. 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. 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: PHOSPHOTRIESTERASE

Chain A:



4 Data and refinement statistics (i)

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	128.62Å 92.33Å 69.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.90	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-1.90)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT	Depositor
R, R_{free}	0.148 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2768	wwPDB-VP
Average B, all atoms (Å^2)	21.0	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: PEL, ZN, KCX, TEN

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	23.66	18/2570 (0.7%)	2.94	38/3490 (1.1%)

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

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	363	ARG	NE-CZ	819.49	11.98	1.33
1	A	363	ARG	CD-NE	734.18	13.94	1.46
1	A	363	ARG	CG-CD	380.85	11.04	1.51
1	A	363	ARG	CB-CG	174.42	6.23	1.52
1	A	363	ARG	CZ-NH1	173.00	3.58	1.33
1	A	363	ARG	CZ-NH2	146.13	3.23	1.33
1	A	338	GLU	CD-OE2	6.17	1.32	1.25
1	A	56	GLU	CD-OE2	6.01	1.32	1.25
1	A	81	GLU	CD-OE2	5.88	1.32	1.25
1	A	344	GLU	CD-OE2	5.79	1.32	1.25
1	A	144	GLU	CD-OE2	5.67	1.31	1.25
1	A	263	GLU	CD-OE2	5.57	1.31	1.25
1	A	48	GLU	CD-OE2	5.55	1.31	1.25
1	A	115	GLU	CD-OE2	5.50	1.31	1.25
1	A	159	GLU	CD-OE2	5.49	1.31	1.25
1	A	145	GLU	CD-OE2	5.31	1.31	1.25
1	A	181	GLU	CD-OE2	5.24	1.31	1.25
1	A	217	GLU	CD-OE2	5.20	1.31	1.25

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	363	ARG	NE-CZ-NH1	-113.30	63.65	120.30
1	A	363	ARG	CD-NE-CZ	-75.19	18.34	123.60
1	A	363	ARG	CA-CB-CG	-42.44	20.04	113.40
1	A	363	ARG	NH1-CZ-NH2	39.32	162.65	119.40
1	A	363	ARG	CB-CG-CD	-39.26	9.53	111.60
1	A	363	ARG	CG-CD-NE	-32.25	44.08	111.80
1	A	363	ARG	NE-CZ-NH2	18.97	129.79	120.30
1	A	164	ARG	NE-CZ-NH1	10.92	125.76	120.30
1	A	225	ARG	NE-CZ-NH1	9.90	125.25	120.30
1	A	225	ARG	NE-CZ-NH2	-7.53	116.54	120.30
1	A	108	ARG	NE-CZ-NH1	7.02	123.81	120.30
1	A	109	ASP	CB-CG-OD2	-6.97	112.03	118.30
1	A	100	ASP	CB-CG-OD1	6.97	124.57	118.30
1	A	315	ASP	CB-CG-OD2	-6.76	112.21	118.30
1	A	264	ASP	CB-CG-OD2	-6.73	112.25	118.30
1	A	109	ASP	CB-CG-OD1	6.70	124.33	118.30
1	A	203	ALA	N-CA-C	-6.69	92.94	111.00
1	A	160	ASP	CB-CG-OD2	-6.64	112.32	118.30
1	A	160	ASP	CB-CG-OD1	6.59	124.23	118.30
1	A	164	ARG	NE-CZ-NH2	-6.56	117.02	120.30
1	A	139	ARG	NE-CZ-NH1	6.31	123.46	120.30
1	A	323	ASP	CB-CG-OD1	5.99	123.69	118.30
1	A	253	ASP	CB-CG-OD1	5.78	123.50	118.30
1	A	315	ASP	CB-CG-OD1	5.77	123.49	118.30
1	A	105	ASP	CB-CG-OD1	5.64	123.38	118.30
1	A	232	ASP	CB-CG-OD2	-5.64	113.22	118.30
1	A	189	ARG	NE-CZ-NH2	-5.48	117.56	120.30
1	A	121	ASP	CB-CG-OD1	5.45	123.21	118.30
1	A	100	ASP	CB-CG-OD2	-5.44	113.40	118.30
1	A	289	ASP	CB-CG-OD2	-5.40	113.44	118.30
1	A	133	ASP	CB-CG-OD1	5.37	123.13	118.30
1	A	235	ASP	CB-CG-OD2	-5.27	113.56	118.30
1	A	233	ASP	CB-CG-OD1	5.23	123.01	118.30
1	A	121	ASP	CB-CG-OD2	-5.18	113.64	118.30
1	A	208	ASP	CB-CG-OD2	-5.18	113.64	118.30
1	A	232	ASP	CB-CG-OD1	5.07	122.86	118.30
1	A	208	ASP	CB-CG-OD1	5.06	122.86	118.30
1	A	289	ASP	CB-CG-OD1	5.03	122.83	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	363	ARG	Sidechain

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2525	0	2549	19	0
2	A	2	0	0	0	0
3	A	11	0	15	1	0
4	A	9	0	10	2	0
5	A	221	0	0	2	0
All	All	2768	0	2574	19	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 (19) 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:51:PHE:HD2	4:A:404:PEL:HA1	1.32	0.92
1:A:51:PHE:H	1:A:96:ARG:NE	1.83	0.77
1:A:50:GLY:HA3	1:A:96:ARG:HD2	1.77	0.66
1:A:51:PHE:H	1:A:96:ARG:HE	1.43	0.66
1:A:333:ILE:HB	1:A:334:PRO:HD3	1.85	0.58
1:A:51:PHE:CD2	4:A:404:PEL:HA1	2.25	0.57
1:A:45:THR:OG1	1:A:48:GLU:HG3	2.08	0.53
1:A:306:PHE:HZ	3:A:403:TEN:H12	1.78	0.48
1:A:51:PHE:HB2	1:A:96:ARG:HH21	1.77	0.48
1:A:302:TRP:CH2	1:A:321:ASN:HB3	2.48	0.47
1:A:106:ILE:O	1:A:106:ILE:HG22	2.16	0.46
1:A:89:ARG:HD2	5:A:581:HOH:O	2.17	0.44
1:A:50:GLY:HA3	1:A:96:ARG:CD	2.45	0.43
1:A:77:LYS:O	1:A:81:GLU:HG3	2.19	0.43
1:A:134:PRO:O	1:A:139:ARG:HD3	2.21	0.41
1:A:293:MET:HB3	5:A:465:HOH:O	2.21	0.41
1:A:51:PHE:CD1	1:A:51:PHE:C	2.93	0.41
1:A:51:PHE:C	1:A:51:PHE:HD1	2.25	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:169:KCX:OQ1	1:A:201:HIS:HB2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	329/331 (99%)	322 (98%)	7 (2%)	0	100 100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	265/265 (100%)	255 (96%)	10 (4%)	33 24

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	PHE
1	A	264	ASP
1	A	267	SER
1	A	299	SER
1	A	303	LEU

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Mol	Chain	Res	Type
1	A	306	PHE
1	A	314	MET
1	A	337	ARG
1	A	338	GLU
1	A	363	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	212	GLN
1	A	290	GLN
1	A	312	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)

1 non-standard protein/DNA/RNA residue 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	$\#\|Z\| > 2$
1	KCX	A	169	2,1	9,11,12	1.98	1 (11%)	5,12,14	0.80	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
1	KCX	A	169	2,1	-	0/9/10/12	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	169	KCX	CX-NZ	5.48	1.44	1.35

There are no bond angle outliers.

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
1	A	169	KCX	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	TEN	A	403	-	10,10,10	0.61	0	12,12,12	1.76	3 (25%)
4	PEL	A	404	-	9,9,9	2.54	4 (44%)	10,10,10	3.51	7 (70%)

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	TEN	A	403	-	-	4/12/12/12	-
4	PEL	A	404	-	-	3/3/3/3	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	404	PEL	C3'-C2'	5.45	1.50	1.38
4	A	404	PEL	C5'-C4'	3.04	1.46	1.38
4	A	404	PEL	CA-C	2.91	1.65	1.50
4	A	404	PEL	C5'-C6'	2.45	1.44	1.38

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	404	PEL	C6'-C1'-C2'	6.85	128.93	118.17
4	A	404	PEL	C3'-C2'-C1'	-4.81	113.25	120.63
4	A	404	PEL	CA-C1'-C2'	-4.09	110.89	121.23
4	A	404	PEL	C5'-C6'-C1'	-3.88	114.68	120.63
3	A	403	TEN	P1-O4-C5	-3.45	107.42	121.67
3	A	403	TEN	P1-O3-C3	-3.35	107.82	121.67
4	A	404	PEL	C4'-C3'-C2'	2.74	124.36	120.19
3	A	403	TEN	P1-O2-C1	-2.65	110.72	121.67
4	A	404	PEL	C5'-C4'-C3'	-2.56	115.16	119.93
4	A	404	PEL	C4'-C5'-C6'	2.25	123.62	120.19

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	403	TEN	C1-O2-P1-O1
4	A	404	PEL	OXT-C-CA-C1'
3	A	403	TEN	C5-O4-P1-O3
3	A	403	TEN	C1-O2-P1-O3
3	A	403	TEN	C5-O4-P1-O1
4	A	404	PEL	C2'-C1'-CA-C
4	A	404	PEL	C6'-C1'-CA-C

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	403	TEN	1	0
4	A	404	PEL	2	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.