wwPDB X-ray Structure Validation Summary Report (i)

Aug 20, 2023 – 04:36 PM EDT

PDB ID	:	2NXH
Title	:	Structural and mechanistic changes along an engineered path from metallo to non-metallo KDO8P synthase.
Authors	:	Kona, F.; Xu, X.; Martin, P.; Kuzmic, P.; Gatti, D.L.
Deposited on	:	2006-11-17
Resolution	:	2.11 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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:

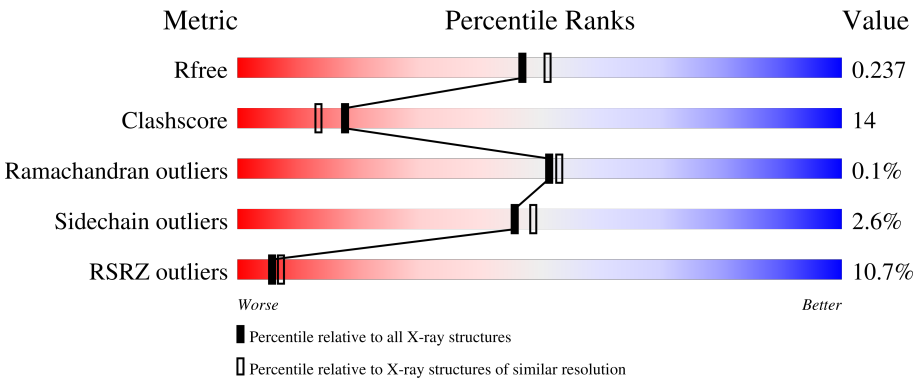
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.11 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}	130704	6241 (2.14-2.10)
Clashscore	141614	6778 (2.14-2.10)
Ramachandran outliers	138981	6705 (2.14-2.10)
Sidechain outliers	138945	6706 (2.14-2.10)
RSRZ outliers	127900	6112 (2.14-2.10)

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% 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	263	5% 79% 19% •
1	B	263	6% 78% 20% •
1	C	263	7% 73% 25% •
1	D	263	12% 69% 30% •
1	E	263	18% 65% 33% •

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Mol	Chain	Length	Quality of chain
1	F	263	27% 57% 41%
1	G	263	6% 77% 21%
1	H	263	3% 72% 24%
1	I	263	6% 78% 20%
1	J	263	3% 71% 24%
1	K	263	24% 62% 36%
1	L	263	11% 73% 25%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 26278 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 2-dehydro-3-deoxyphosphooctonate aldolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	262	2056	1327	344	380	5	0	0	0
1	B	262	2056	1327	344	380	5	0	0	0
1	C	262	2056	1327	344	380	5	0	0	0
1	D	262	2056	1327	344	380	5	0	0	0
1	E	259	2035	1315	340	375	5	0	0	0
1	F	262	2056	1327	344	380	5	0	0	0
1	G	262	2056	1327	344	380	5	0	0	0
1	H	256	2017	1304	337	371	5	0	0	0
1	I	262	2056	1327	344	380	5	0	0	0
1	J	255	2013	1302	336	370	5	0	0	0
1	K	262	2056	1327	344	380	5	0	0	0
1	L	262	2056	1327	344	380	5	0	0	0

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1011	ASN	CYS	engineered mutation	UNP O66496
A	1235	PRO	SER	engineered mutation	UNP O66496
A	1237	ALA	GLN	engineered mutation	UNP O66496
B	2011	ASN	CYS	engineered mutation	UNP O66496
B	2235	PRO	SER	engineered mutation	UNP O66496

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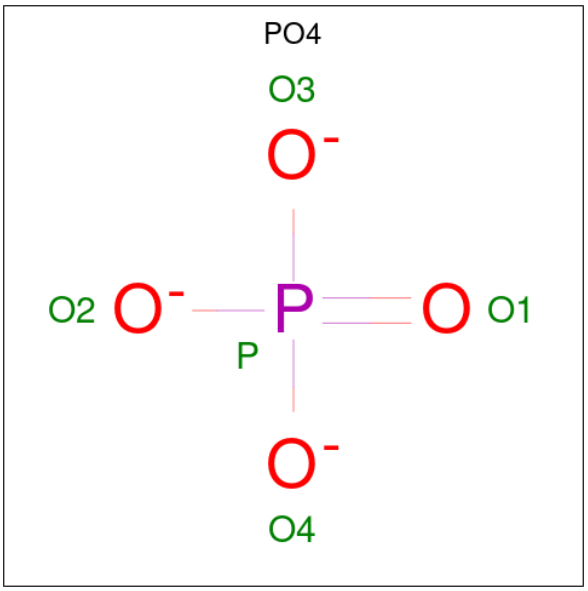
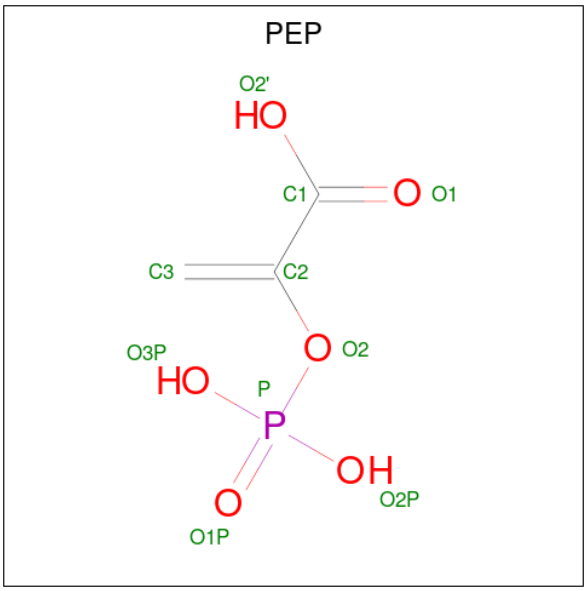
Chain	Residue	Modelled	Actual	Comment	Reference
B	2237	ALA	GLN	engineered mutation	UNP O66496
C	3011	ASN	CYS	engineered mutation	UNP O66496
C	3235	PRO	SER	engineered mutation	UNP O66496
C	3237	ALA	GLN	engineered mutation	UNP O66496
D	4011	ASN	CYS	engineered mutation	UNP O66496
D	4235	PRO	SER	engineered mutation	UNP O66496
D	4237	ALA	GLN	engineered mutation	UNP O66496
E	1011	ASN	CYS	engineered mutation	UNP O66496
E	1235	PRO	SER	engineered mutation	UNP O66496
E	1237	ALA	GLN	engineered mutation	UNP O66496
F	2011	ASN	CYS	engineered mutation	UNP O66496
F	2235	PRO	SER	engineered mutation	UNP O66496
F	2237	ALA	GLN	engineered mutation	UNP O66496
G	3011	ASN	CYS	engineered mutation	UNP O66496
G	3235	PRO	SER	engineered mutation	UNP O66496
G	3237	ALA	GLN	engineered mutation	UNP O66496
H	4011	ASN	CYS	engineered mutation	UNP O66496
H	4235	PRO	SER	engineered mutation	UNP O66496
H	4237	ALA	GLN	engineered mutation	UNP O66496
I	1011	ASN	CYS	engineered mutation	UNP O66496
I	1235	PRO	SER	engineered mutation	UNP O66496
I	1237	ALA	GLN	engineered mutation	UNP O66496
J	2011	ASN	CYS	engineered mutation	UNP O66496
J	2235	PRO	SER	engineered mutation	UNP O66496
J	2237	ALA	GLN	engineered mutation	UNP O66496
K	3011	ASN	CYS	engineered mutation	UNP O66496
K	3235	PRO	SER	engineered mutation	UNP O66496
K	3237	ALA	GLN	engineered mutation	UNP O66496
L	4011	ASN	CYS	engineered mutation	UNP O66496
L	4235	PRO	SER	engineered mutation	UNP O66496
L	4237	ALA	GLN	engineered mutation	UNP O66496

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	P		
2	A	1	5	4	1	0	0
2	B	1	5	4	1	0	0
2	C	1	5	4	1	0	0
2	D	1	5	4	1	0	0
2	E	1	5	4	1	0	0
2	F	1	5	4	1	0	0
2	G	1	5	4	1	0	0
2	H	1	5	4	1	0	0
2	I	1	5	4	1	0	0
2	J	1	5	4	1	0	0
2	K	1	5	4	1	0	0
2	L	1	5	4	1	0	0

- Molecule 3 is PHOSPHOENOLPYRUVATE (three-letter code: PEP) (formula: $C_3H_5O_6P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
3	A	1	10	3	6	1	0	0
3	B	1	10	3	6	1	0	0
3	C	1	10	3	6	1	0	0
3	D	1	10	3	6	1	0	0
3	E	1	10	3	6	1	0	0
3	F	1	10	3	6	1	0	0
3	G	1	10	3	6	1	0	0
3	H	1	10	3	6	1	0	0
3	I	1	10	3	6	1	0	0
3	J	1	10	3	6	1	0	0
3	K	1	10	3	6	1	0	0
3	L	1	10	3	6	1	0	0

- Molecule 4 is water.

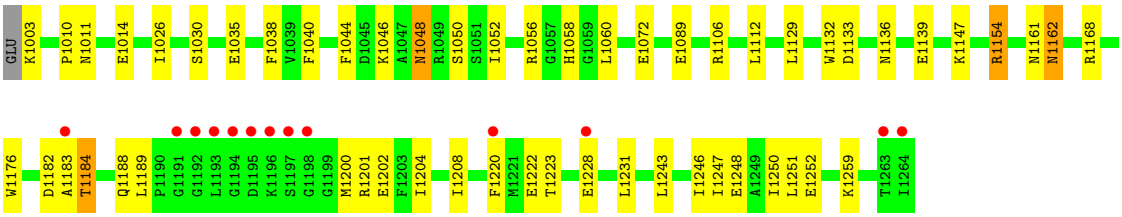
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	185	185	185	0	0
			Total	O		
4	B	190	190	190	0	0
			Total	O		
4	C	107	107	107	0	0
			Total	O		
4	D	75	75	75	0	0
			Total	O		
4	E	64	64	64	0	0
			Total	O		
4	F	54	54	54	0	0
			Total	O		
4	G	178	178	178	0	0
			Total	O		
4	H	170	170	170	0	0
			Total	O		
4	I	185	185	185	0	0
			Total	O		
4	J	172	172	172	0	0
			Total	O		
4	K	50	50	50	0	0
			Total	O		
4	L	99	99	99	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 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.

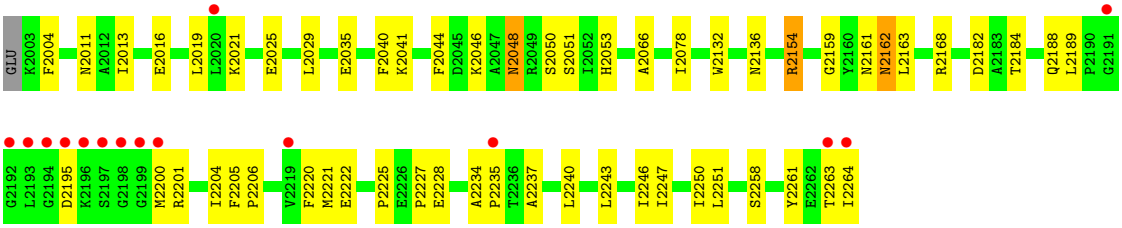
• Molecule 1: 2-dehydro-3-deoxyphosphooctonate aldolase

Chain A:



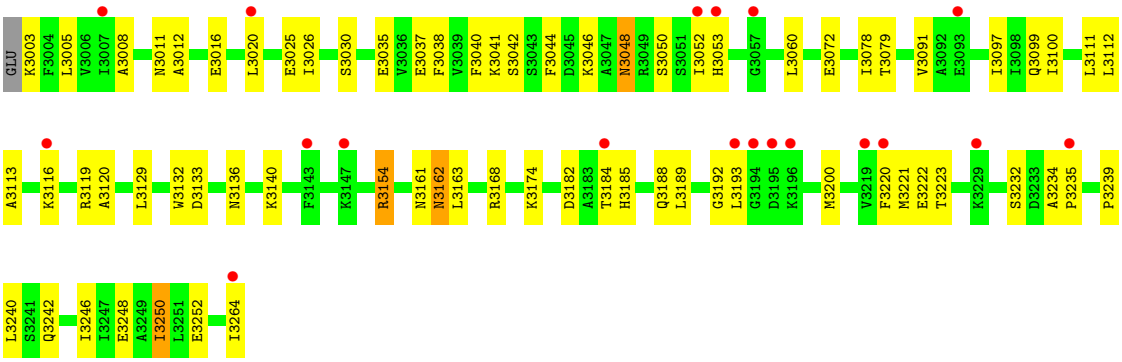
• Molecule 1: 2-dehydro-3-deoxyphosphooctonate aldolase

Chain B:



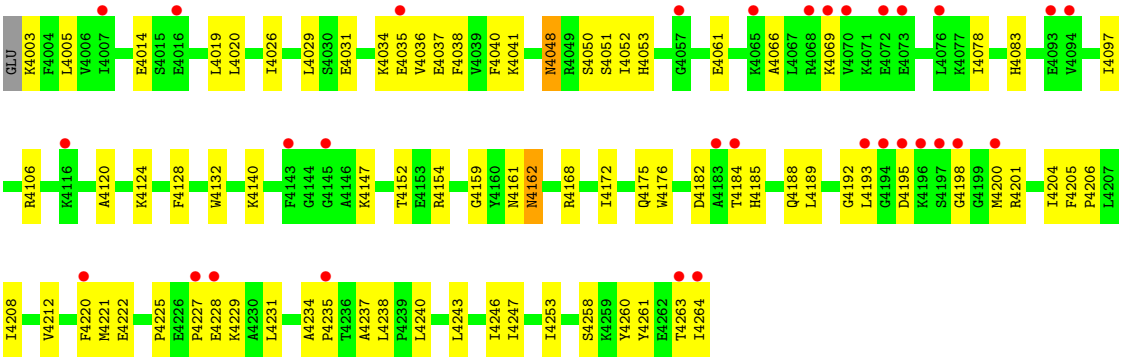
• Molecule 1: 2-dehydro-3-deoxyphosphooctonate aldolase

Chain C:



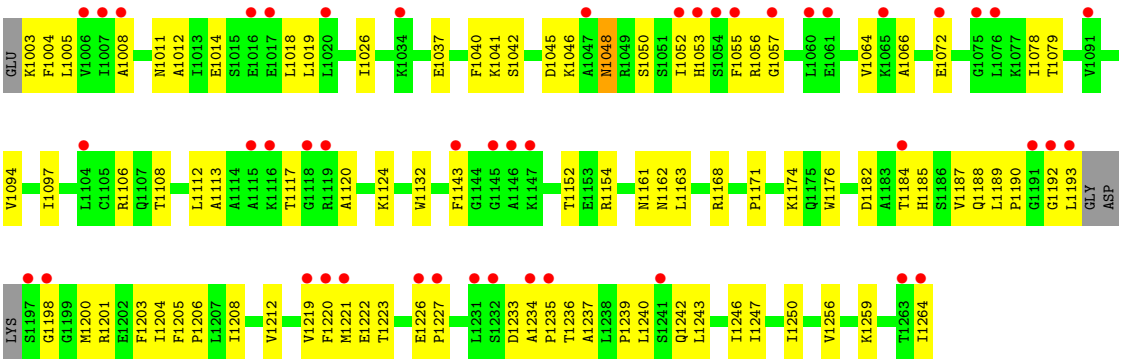
• Molecule 1: 2-dehydro-3-deoxyphosphooctonate aldolase

Chain D:



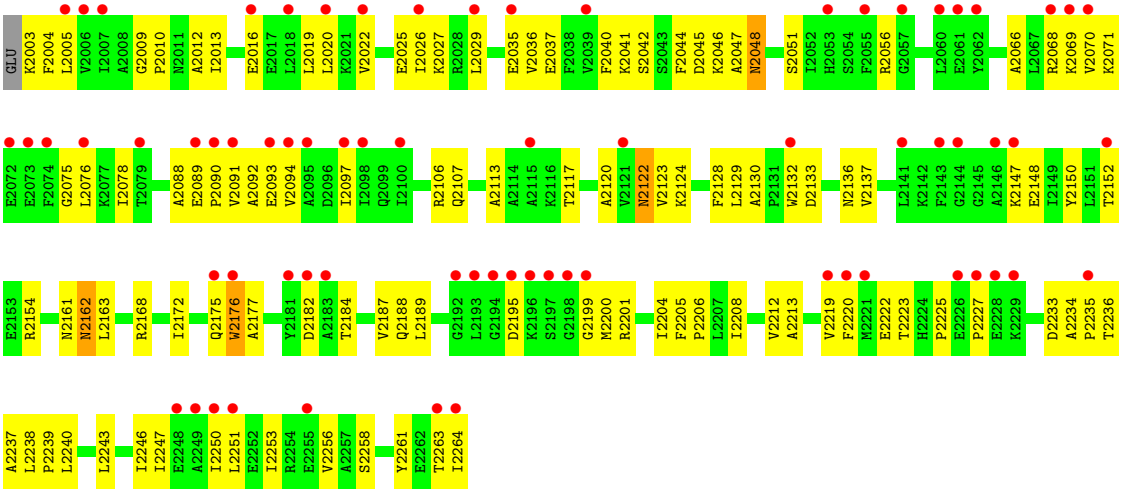
- Molecule 1: 2-dehydro-3-deoxyphosphooctonate aldolase

Chain E:



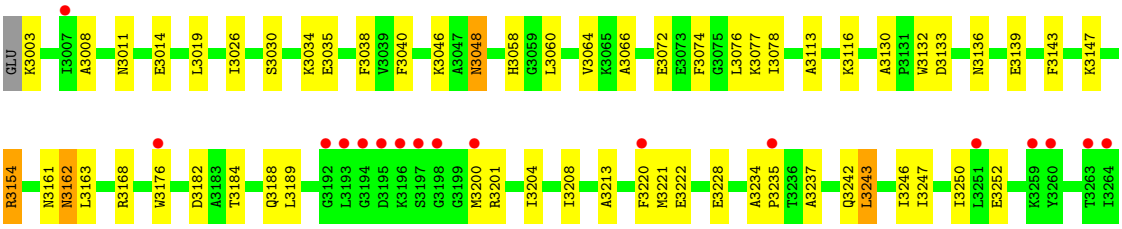
- Molecule 1: 2-dehydro-3-deoxyphosphooctonate aldolase

Chain F:



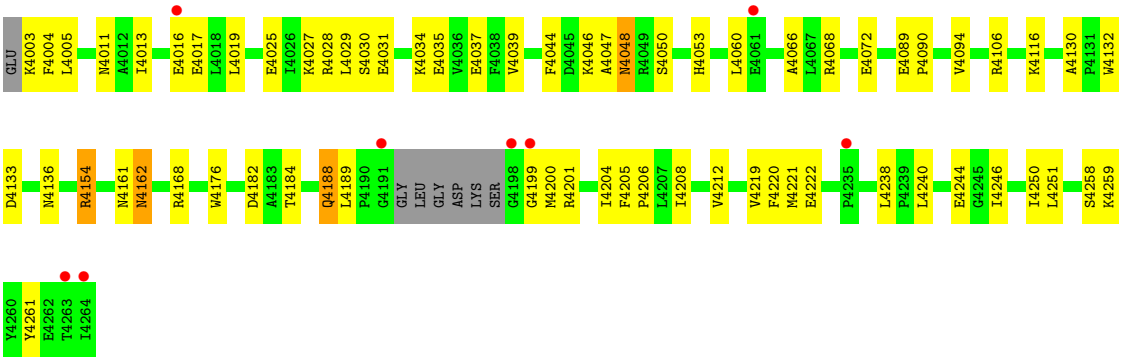
- Molecule 1: 2-dehydro-3-deoxyphosphooctonate aldolase

Chain G:



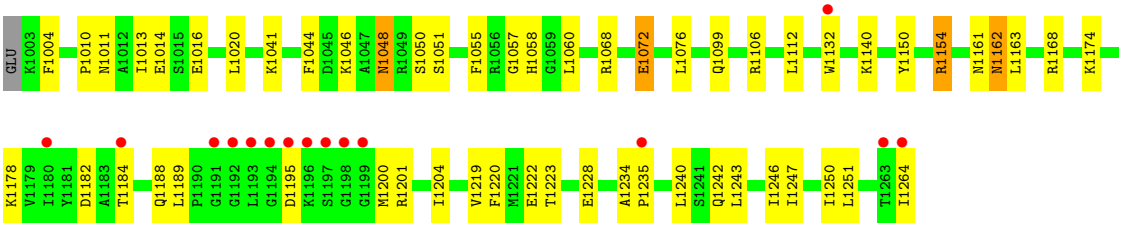
- Molecule 1: 2-dehydro-3-deoxyphosphooctonate aldolase

Chain H:



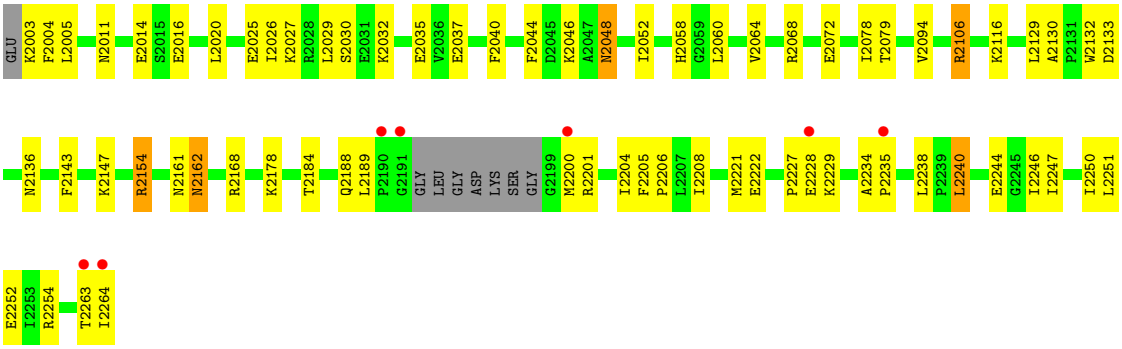
- Molecule 1: 2-dehydro-3-deoxyphosphooctonate aldolase

Chain I:



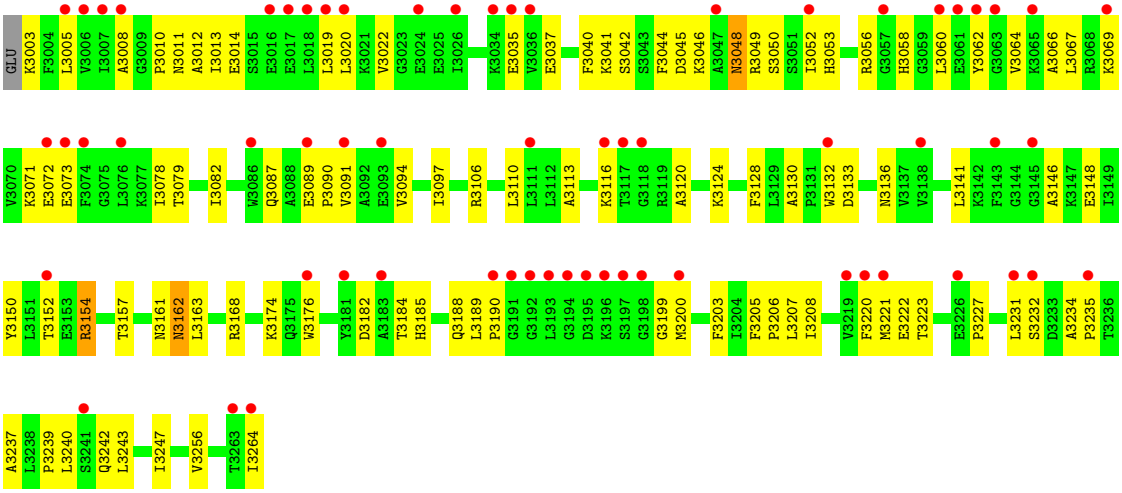
- Molecule 1: 2-dehydro-3-deoxyphosphooctonate aldolase

Chain J:



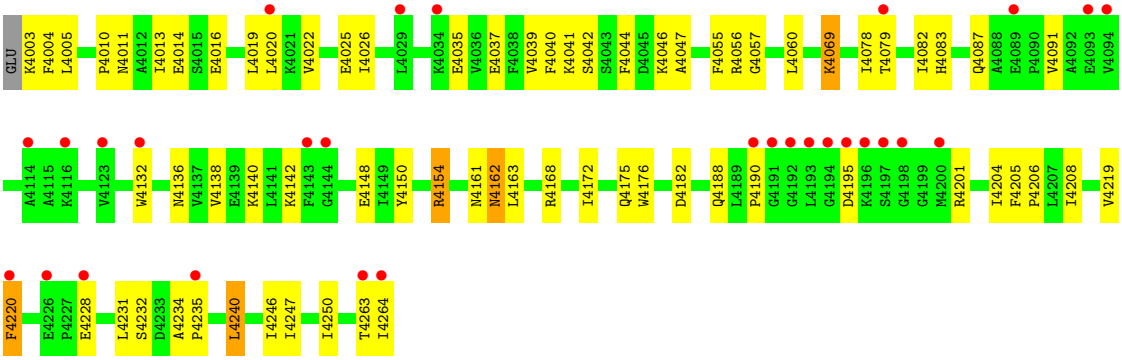
• Molecule 1: 2-dehydro-3-deoxyphosphooctonate aldolase

Chain K:



• Molecule 1: 2-dehydro-3-deoxyphosphooctonate aldolase

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	76.21Å 198.63Å 125.52Å 90.00° 94.28° 90.00°	Depositor
Resolution (Å)	30.18 – 2.11 30.18 – 2.11	Depositor EDS
% Data completeness (in resolution range)	91.7 (30.18-2.11) 91.5 (30.18-2.11)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
$< I/\sigma(I) >$ [1]	1.94 (at 2.12Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.206 , 0.245 0.198 , 0.237	Depositor DCC
R_{free} test set	19281 reflections (9.37%)	wwPDB-VP
Wilson B-factor (Å^2)	27.7	Xtriage
Anisotropy	0.581	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 55.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	26278	wwPDB-VP
Average B, all atoms (Å^2)	38.0	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 20.05 % 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 9.4622e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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: PO4, PEP

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	0.40	1/2098 (0.0%)	0.60	0/2830
1	B	0.37	0/2098	0.60	0/2830
1	C	0.35	1/2098 (0.0%)	0.53	0/2830
1	D	0.31	0/2098	0.53	0/2830
1	E	0.34	1/2076 (0.0%)	0.52	0/2800
1	F	0.30	0/2098	0.49	0/2830
1	G	0.38	1/2098 (0.0%)	0.59	0/2830
1	H	0.37	0/2058	0.59	0/2776
1	I	0.40	1/2098 (0.0%)	0.60	0/2830
1	J	0.36	0/2054	0.60	0/2771
1	K	0.33	1/2098 (0.0%)	0.50	0/2830
1	L	0.31	0/2098	0.53	0/2830
All	All	0.35	6/25070 (0.0%)	0.56	0/33817

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1072	GLU	CD-OE2	7.41	1.33	1.25
1	G	3072	GLU	CD-OE2	7.40	1.33	1.25
1	E	1072	GLU	CD-OE2	7.16	1.33	1.25
1	K	3072	GLU	CD-OE2	7.08	1.33	1.25
1	I	1072	GLU	CD-OE2	6.91	1.33	1.25

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	2056	0	2095	48	0
1	B	2056	0	2095	54	0
1	C	2056	0	2095	62	0
1	D	2056	0	2095	57	0
1	E	2035	0	2074	64	0
1	F	2056	0	2095	82	0
1	G	2056	0	2095	48	0
1	H	2017	0	2055	63	0
1	I	2056	0	2095	52	0
1	J	2013	0	2052	68	0
1	K	2056	0	2095	70	0
1	L	2056	0	2095	61	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
2	E	5	0	0	0	0
2	F	5	0	0	0	0
2	G	5	0	0	0	0
2	H	5	0	0	0	0
2	I	5	0	0	0	0
2	J	5	0	0	0	0
2	K	5	0	0	0	0
2	L	5	0	0	0	0
3	A	10	0	2	0	0
3	B	10	0	2	0	0
3	C	10	0	2	0	0
3	D	10	0	2	0	0
3	E	10	0	2	0	0
3	F	10	0	2	0	0
3	G	10	0	2	0	0
3	H	10	0	2	0	0
3	I	10	0	2	0	0
3	J	10	0	2	0	0
3	K	10	0	2	0	0
3	L	10	0	2	0	0
4	A	185	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	190	0	0	2	0
4	C	107	0	0	2	0
4	D	75	0	0	2	0
4	E	64	0	0	5	0
4	F	54	0	0	3	0
4	G	178	0	0	4	0
4	H	170	0	0	7	0
4	I	185	0	0	4	0
4	J	172	0	0	6	0
4	K	50	0	0	3	0
4	L	99	0	0	3	0
All	All	26278	0	25060	676	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 14.

The worst 5 of 676 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:I:1184:THR:HG21	1:I:1222:GLU:H	1.25	1.01
1:A:1154:ARG:HH22	1:A:1188:GLN:HE22	1.08	1.00
1:B:2184:THR:HG21	1:B:2222:GLU:H	1.20	1.00
1:I:1154:ARG:HH22	1:I:1188:GLN:HE22	1.07	0.99
1:L:4154:ARG:HH22	1:L:4188:GLN:HE22	1.04	0.95

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	260/263 (99%)	252 (97%)	8 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	260/263 (99%)	251 (96%)	8 (3%)	1 (0%)	34	32
1	C	260/263 (99%)	249 (96%)	11 (4%)	0	100	100
1	D	260/263 (99%)	249 (96%)	11 (4%)	0	100	100
1	E	255/263 (97%)	234 (92%)	21 (8%)	0	100	100
1	F	260/263 (99%)	239 (92%)	20 (8%)	1 (0%)	34	32
1	G	260/263 (99%)	252 (97%)	8 (3%)	0	100	100
1	H	252/263 (96%)	247 (98%)	5 (2%)	0	100	100
1	I	260/263 (99%)	254 (98%)	6 (2%)	0	100	100
1	J	251/263 (95%)	243 (97%)	8 (3%)	0	100	100
1	K	260/263 (99%)	246 (95%)	14 (5%)	0	100	100
1	L	260/263 (99%)	246 (95%)	14 (5%)	0	100	100
All	All	3098/3156 (98%)	2962 (96%)	134 (4%)	2 (0%)	51	53

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	2092	ALA
1	B	2235	PRO

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	218/219 (100%)	209 (96%)	9 (4%)	30	30
1	B	218/219 (100%)	211 (97%)	7 (3%)	39	40
1	C	218/219 (100%)	213 (98%)	5 (2%)	50	53
1	D	218/219 (100%)	213 (98%)	5 (2%)	50	53
1	E	216/219 (99%)	212 (98%)	4 (2%)	57	61
1	F	218/219 (100%)	212 (97%)	6 (3%)	43	46
1	G	218/219 (100%)	212 (97%)	6 (3%)	43	46

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	214/219 (98%)	208 (97%)	6 (3%)	43	46
1	I	218/219 (100%)	213 (98%)	5 (2%)	50	53
1	J	214/219 (98%)	208 (97%)	6 (3%)	43	46
1	K	218/219 (100%)	214 (98%)	4 (2%)	59	63
1	L	218/219 (100%)	212 (97%)	6 (3%)	43	46
All	All	2606/2628 (99%)	2537 (97%)	69 (3%)	46	49

5 of 69 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	J	2162	ASN
1	K	3048	ASN
1	L	4162	ASN
1	D	4162	ASN
1	D	4154	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 104 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	3011	ASN
1	H	4162	ASN
1	L	4099	GLN
1	G	3053	HIS
1	H	4048	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

24 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	$\#\|Z\| > 2$
2	PO4	A	1280	-	4,4,4	1.61	1 (25%)	6,6,6	0.43	0
2	PO4	H	1287	-	4,4,4	1.59	0	6,6,6	0.43	0
3	PEP	H	1275	-	9,9,9	0.95	0	11,13,13	1.27	2 (18%)
3	PEP	E	1272	-	9,9,9	1.11	0	11,13,13	1.68	2 (18%)
3	PEP	A	1268	-	9,9,9	0.88	0	11,13,13	1.56	1 (9%)
3	PEP	I	1276	-	9,9,9	0.87	0	11,13,13	1.28	1 (9%)
2	PO4	I	1288	-	4,4,4	1.62	0	6,6,6	0.44	0
2	PO4	J	1289	-	4,4,4	1.66	0	6,6,6	0.42	0
3	PEP	D	1271	-	9,9,9	0.98	0	11,13,13	1.71	2 (18%)
3	PEP	B	1269	-	9,9,9	1.08	1 (11%)	11,13,13	1.58	2 (18%)
3	PEP	G	1274	-	9,9,9	1.09	1 (11%)	11,13,13	1.60	1 (9%)
2	PO4	K	1290	-	4,4,4	1.69	0	6,6,6	0.45	0
3	PEP	F	1273	-	9,9,9	1.15	0	11,13,13	1.52	2 (18%)
2	PO4	C	1282	-	4,4,4	1.65	0	6,6,6	0.44	0
2	PO4	L	1291	-	4,4,4	1.62	0	6,6,6	0.44	0
3	PEP	J	1277	-	9,9,9	0.84	0	11,13,13	1.48	3 (27%)
2	PO4	G	1286	-	4,4,4	1.59	0	6,6,6	0.45	0
2	PO4	F	1285	-	4,4,4	1.64	0	6,6,6	0.44	0
2	PO4	B	1281	-	4,4,4	1.63	0	6,6,6	0.43	0
2	PO4	E	1284	-	4,4,4	1.64	0	6,6,6	0.44	0
3	PEP	C	1270	-	9,9,9	1.16	0	11,13,13	1.65	2 (18%)
2	PO4	D	1283	-	4,4,4	1.65	0	6,6,6	0.45	0
3	PEP	L	1279	-	9,9,9	1.09	0	11,13,13	1.49	2 (18%)
3	PEP	K	1278	-	9,9,9	1.13	0	11,13,13	1.40	2 (18%)

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	PEP	L	1279	-	-	0/9/9/9	-
3	PEP	J	1277	-	-	0/9/9/9	-
3	PEP	H	1275	-	-	0/9/9/9	-
3	PEP	D	1271	-	-	0/9/9/9	-
3	PEP	E	1272	-	-	1/9/9/9	-
3	PEP	B	1269	-	-	0/9/9/9	-
3	PEP	G	1274	-	-	0/9/9/9	-
3	PEP	C	1270	-	-	0/9/9/9	-
3	PEP	F	1273	-	-	0/9/9/9	-
3	PEP	A	1268	-	-	0/9/9/9	-
3	PEP	K	1278	-	-	4/9/9/9	-
3	PEP	I	1276	-	-	0/9/9/9	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1269	PEP	P-O2	2.21	1.62	1.59
2	A	1280	PO4	P-O3	-2.00	1.48	1.54
3	G	1274	PEP	P-O2	2.00	1.62	1.59

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	1271	PEP	O2'-C1-C2	4.37	121.37	113.91
3	G	1274	PEP	O2'-C1-C2	4.32	121.27	113.91
3	C	1270	PEP	O2'-C1-C2	4.30	121.25	113.91
3	B	1269	PEP	O2'-C1-C2	4.07	120.85	113.91
3	A	1268	PEP	O2'-C1-C2	3.71	120.23	113.91

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	1272	PEP	C2-O2-P-O1P
3	K	1278	PEP	O2'-C1-C2-C3
3	K	1278	PEP	O2'-C1-C2-O2
3	K	1278	PEP	O1-C1-C2-O2
3	K	1278	PEP	O1-C1-C2-C3

There are no ring outliers.

No monomer is involved in short contacts.

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)

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, 95th 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^2)	Q<0.9
1	A	262/263 (99%)	0.21	13 (4%)	28	34	15, 24, 46, 69	0
1	B	262/263 (99%)	0.37	15 (5%)	23	28	13, 24, 47, 78	0
1	C	262/263 (99%)	0.56	19 (7%)	15	19	19, 41, 57, 67	0
1	D	262/263 (99%)	0.96	31 (11%)	4	5	21, 44, 65, 79	0
1	E	259/263 (98%)	1.08	47 (18%)	1	1	23, 52, 71, 79	0
1	F	262/263 (99%)	1.58	71 (27%)	0	0	25, 57, 75, 83	0
1	G	262/263 (99%)	0.38	17 (6%)	18	23	17, 29, 59, 77	0
1	H	256/263 (97%)	0.20	8 (3%)	49	55	15, 26, 47, 79	0
1	I	262/263 (99%)	0.31	15 (5%)	23	28	15, 25, 47, 73	0
1	J	255/263 (96%)	0.20	7 (2%)	54	60	14, 27, 49, 75	0
1	K	262/263 (99%)	1.36	63 (24%)	0	0	26, 56, 73, 77	0
1	L	262/263 (99%)	0.85	29 (11%)	5	6	22, 45, 62, 79	0
All	All	3128/3156 (99%)	0.67	335 (10%)	6	7	13, 36, 68, 83	0

The worst 5 of 335 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	2193	LEU	11.4
1	G	3264	ILE	10.0
1	F	2264	ILE	9.5
1	H	4264	ILE	9.4
1	I	1193	LEU	9.0

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 monosaccharides 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. The B-factors column lists the minimum, median, 95th 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	B-factors(Å^2)	Q<0.9
2	PO4	K	1290	5/5	0.88	0.14	61,61,62,62	0
2	PO4	L	1291	5/5	0.89	0.15	60,60,61,61	0
2	PO4	D	1283	5/5	0.91	0.12	57,58,60,61	0
2	PO4	F	1285	5/5	0.92	0.14	62,63,64,64	0
2	PO4	E	1284	5/5	0.93	0.15	70,70,71,71	0
2	PO4	C	1282	5/5	0.93	0.10	47,50,51,51	0
2	PO4	B	1281	5/5	0.95	0.10	32,36,38,38	0
2	PO4	G	1286	5/5	0.96	0.10	35,37,39,39	0
3	PEP	F	1273	10/10	0.96	0.14	40,46,48,48	0
3	PEP	K	1278	10/10	0.96	0.18	40,45,49,50	0
2	PO4	I	1288	5/5	0.97	0.10	33,35,37,38	0
3	PEP	C	1270	10/10	0.97	0.16	28,35,37,39	0
3	PEP	D	1271	10/10	0.97	0.20	29,35,40,42	0
3	PEP	E	1272	10/10	0.97	0.18	42,46,50,50	0
2	PO4	J	1289	5/5	0.97	0.10	38,40,42,43	0
2	PO4	A	1280	5/5	0.97	0.08	31,33,35,37	0
3	PEP	G	1274	10/10	0.98	0.16	18,23,25,26	0
3	PEP	J	1277	10/10	0.98	0.18	16,20,22,22	0
2	PO4	H	1287	5/5	0.98	0.07	37,39,40,41	0
3	PEP	L	1279	10/10	0.98	0.11	32,37,41,43	0
3	PEP	I	1276	10/10	0.99	0.23	17,21,22,23	0
3	PEP	B	1269	10/10	0.99	0.18	14,17,22,26	0
3	PEP	A	1268	10/10	0.99	0.17	15,19,23,23	0
3	PEP	H	1275	10/10	0.99	0.16	15,21,23,24	0

6.5 Other polymers (i)

There are no such residues in this entry.