



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 01:53 PM UTC

PDB ID : 2NXI / pdb_00002nxi
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 : 2.30 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

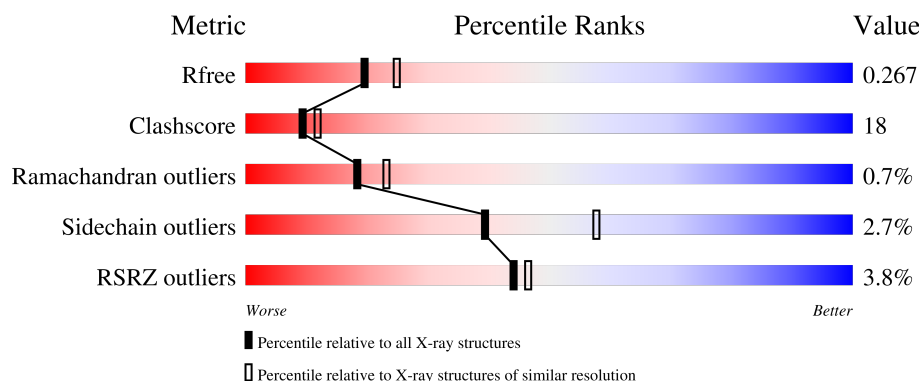
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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 $\leq 5\%$. 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	263	70% 26% ..
1	B	263	2% 73% 24% ..
1	C	263	2% 61% 35% ..
1	D	263	3% 56% 39% ..
1	E	263	6% 58% 38% ..

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Mol	Chain	Length	Quality of chain
1	F	263	
1	G	263	
1	H	263	
1	I	263	
1	J	263	
1	K	263	
1	L	263	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 25761 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
1	A	257	Total	C	N	O	S	0	0	0
			2029	1310	339	374	6			
1	B	258	Total	C	N	O	S	0	0	0
			2033	1312	340	375	6			
1	C	257	Total	C	N	O	S	0	0	0
			2025	1306	339	374	6			
1	D	256	Total	C	N	O	S	0	0	0
			2021	1304	338	373	6			
1	E	256	Total	C	N	O	S	0	0	0
			2021	1304	338	373	6			
1	F	255	Total	C	N	O	S	0	0	0
			2017	1302	337	372	6			
1	G	259	Total	C	N	O	S	0	0	0
			2041	1316	341	378	6			
1	H	256	Total	C	N	O	S	0	0	0
			2021	1304	338	373	6			
1	I	262	Total	C	N	O	S	0	0	0
			2060	1327	345	382	6			
1	J	262	Total	C	N	O	S	0	0	0
			2060	1327	345	382	6			
1	K	257	Total	C	N	O	S	0	0	0
			2029	1310	339	374	6			
1	L	256	Total	C	N	O	S	0	0	0
			2021	1304	338	373	6			

There are 24 discrepancies between the modelled and reference sequences:

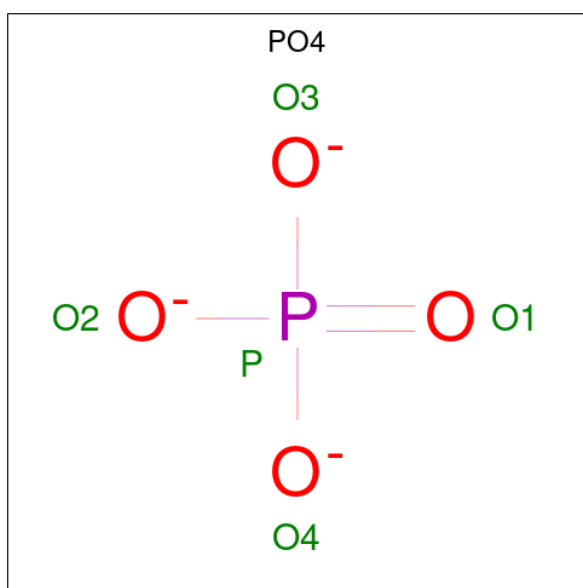
Chain	Residue	Modelled	Actual	Comment	Reference
A	10	MET	PRO	engineered mutation	UNP O66496
A	11	ASN	CYS	engineered mutation	UNP O66496
B	10	MET	PRO	engineered mutation	UNP O66496
B	11	ASN	CYS	engineered mutation	UNP O66496
C	10	MET	PRO	engineered mutation	UNP O66496

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Chain	Residue	Modelled	Actual	Comment	Reference
C	11	ASN	CYS	engineered mutation	UNP O66496
D	10	MET	PRO	engineered mutation	UNP O66496
D	11	ASN	CYS	engineered mutation	UNP O66496
E	10	MET	PRO	engineered mutation	UNP O66496
E	11	ASN	CYS	engineered mutation	UNP O66496
F	10	MET	PRO	engineered mutation	UNP O66496
F	11	ASN	CYS	engineered mutation	UNP O66496
G	10	MET	PRO	engineered mutation	UNP O66496
G	11	ASN	CYS	engineered mutation	UNP O66496
H	10	MET	PRO	engineered mutation	UNP O66496
H	11	ASN	CYS	engineered mutation	UNP O66496
I	10	MET	PRO	engineered mutation	UNP O66496
I	11	ASN	CYS	engineered mutation	UNP O66496
J	10	MET	PRO	engineered mutation	UNP O66496
J	11	ASN	CYS	engineered mutation	UNP O66496
K	10	MET	PRO	engineered mutation	UNP O66496
K	11	ASN	CYS	engineered mutation	UNP O66496
L	10	MET	PRO	engineered mutation	UNP O66496
L	11	ASN	CYS	engineered mutation	UNP O66496

- Molecule 2 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



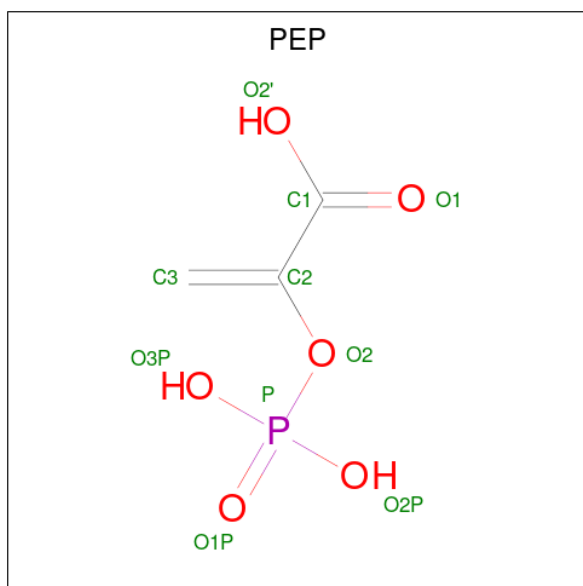
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	D	1	Total	O	P	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	E	1	Total	O	P	0	0
			5	4	1		
2	F	1	Total	O	P	0	0
			5	4	1		
2	J	1	Total	O	P	0	0
			5	4	1		
2	K	1	Total	O	P	0	0
			5	4	1		
2	L	1	Total	O	P	0	0
			5	4	1		

- Molecule 3 is PHOSPHOENOLPYRUVATE (CCD ID: PEP) (formula: $C_3H_5O_6P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	P	0	0
			10	3	6	1		
3	B	1	Total	C	O	P	0	0
			10	3	6	1		
3	B	1	Total	C	O	P	0	0
			10	3	6	1		
3	C	1	Total	C	O	P	0	0
			10	3	6	1		
3	C	1	Total	C	O	P	0	0
			10	3	6	1		
3	D	1	Total	C	O	P	0	0
			10	3	6	1		

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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	147	Total	O	0	0
			147	147		
4	B	145	Total	O	0	0
			145	145		
4	C	93	Total	O	0	0
			93	93		
4	D	60	Total	O	0	0
			60	60		
4	E	52	Total	O	0	0
			52	52		
4	F	49	Total	O	0	0
			49	49		
4	G	125	Total	O	0	0
			125	125		
4	H	132	Total	O	0	0
			132	132		

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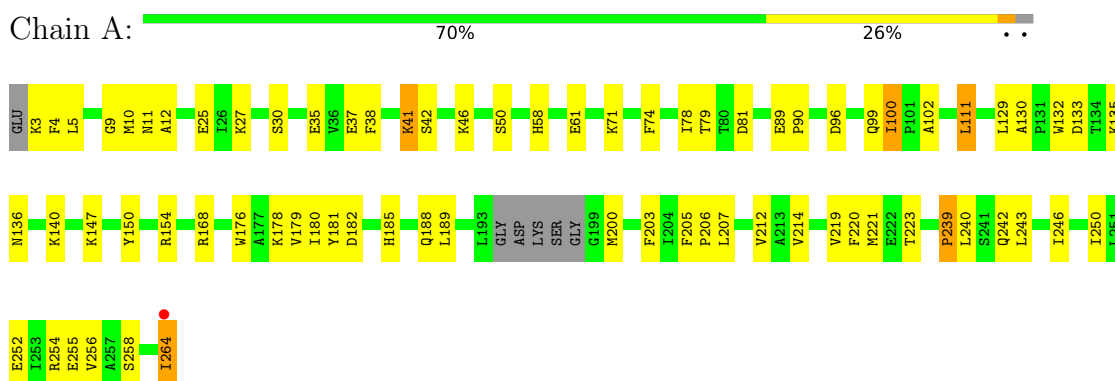
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	I	136	Total 136	O 136	0	0
4	J	136	Total 136	O 136	0	0
4	K	37	Total 37	O 37	0	0
4	L	66	Total 66	O 66	0	0

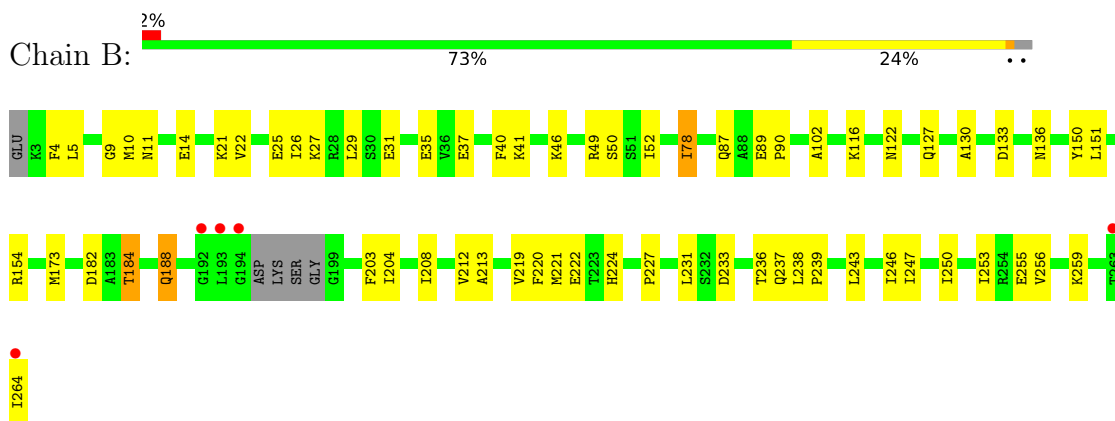
3 Residue-property plots [i](#)

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.

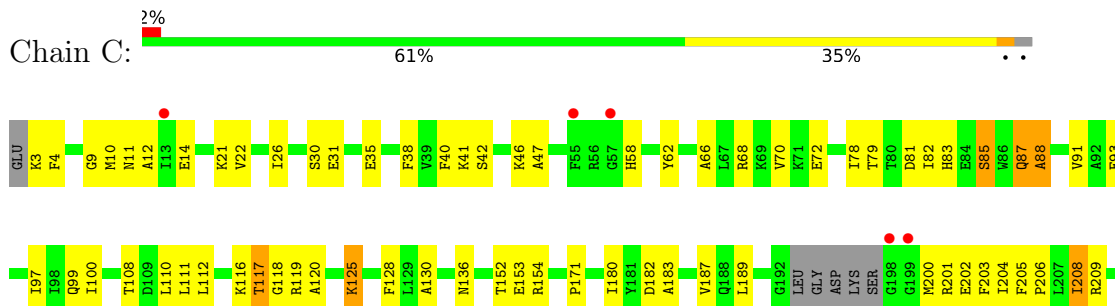
- Molecule 1: 2-dehydro-3-deoxyphosphooctonate aldolase

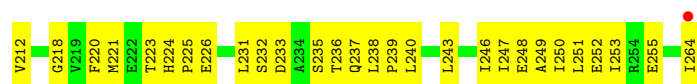


- Molecule 1: 2-dehydro-3-deoxyphosphooctonate aldolase

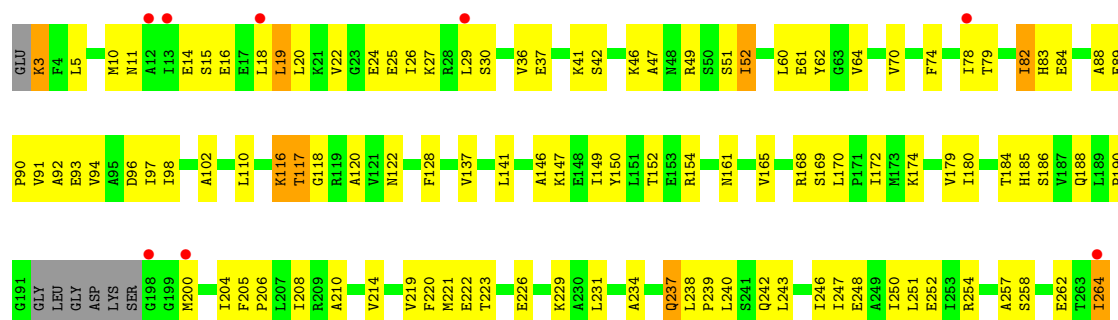


- Molecule 1: 2-dehydro-3-deoxyphosphooctonate aldolase

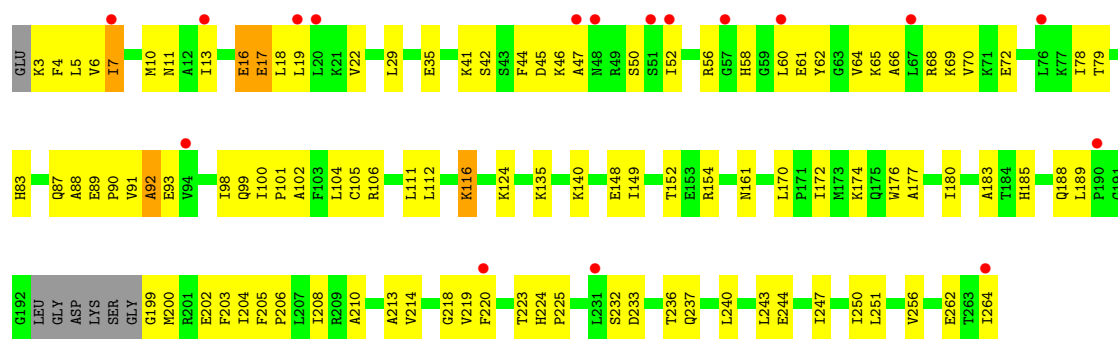




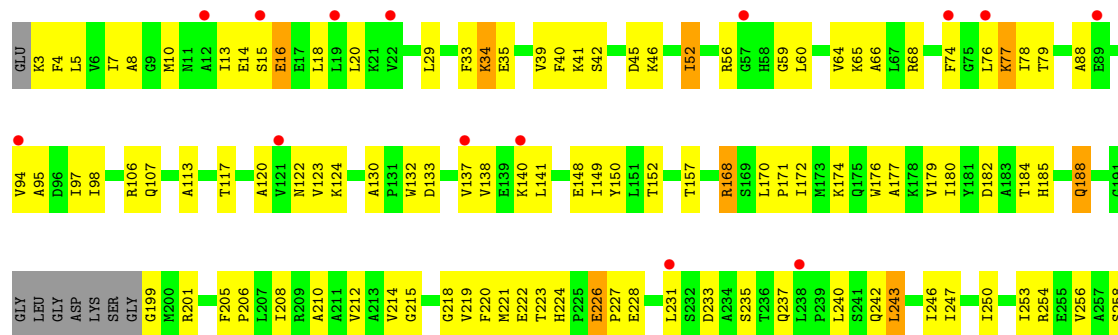
• Molecule 1: 2-dehydro-3-deoxyphosphooctonate aldolase



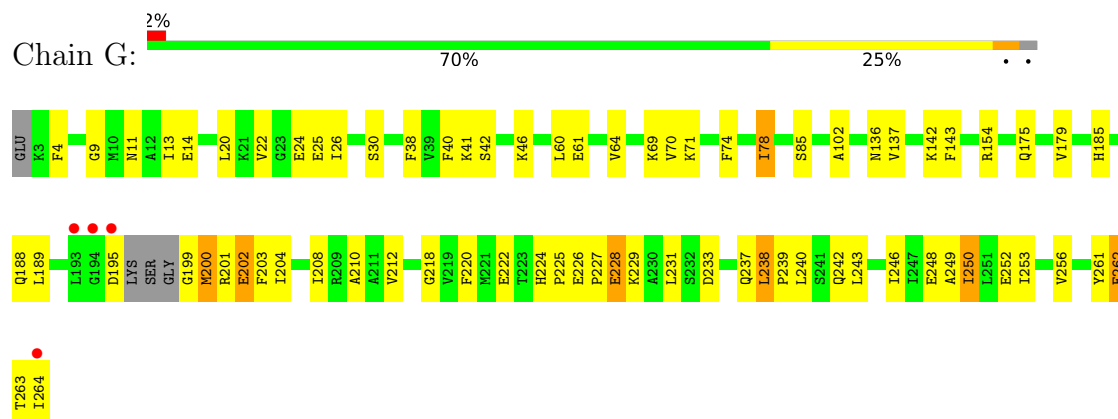
• Molecule 1: 2-dehydro-3-deoxyphosphooctonate aldolase



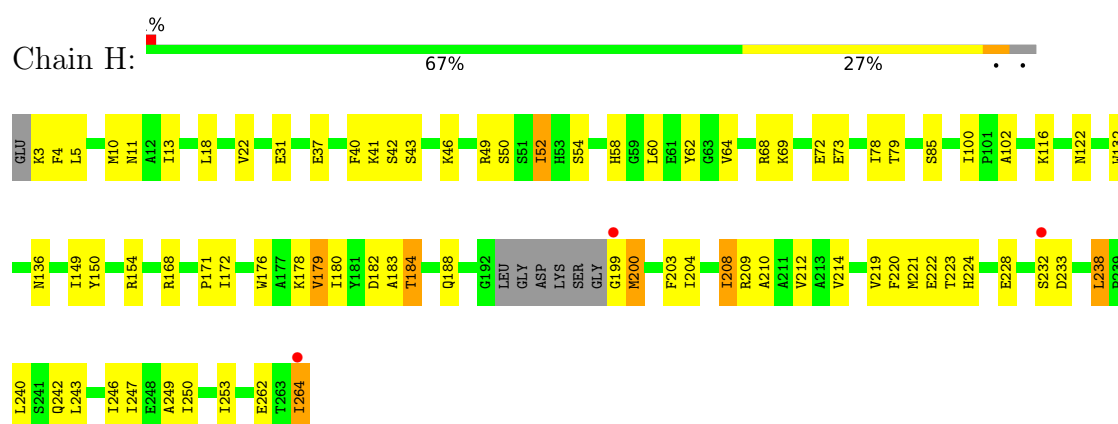
• Molecule 1: 2-dehydro-3-deoxyphosphooctonate aldolase



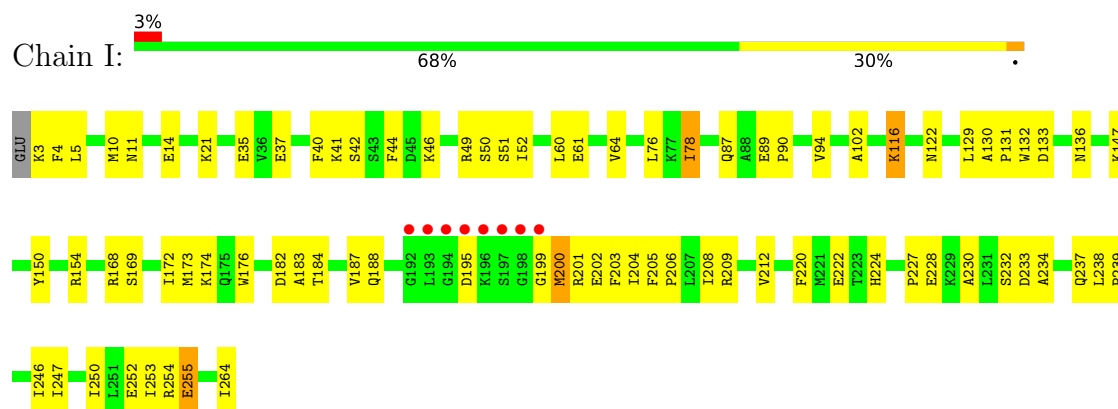
• Molecule 1: 2-dehydro-3-deoxyphosphooctonate aldolase



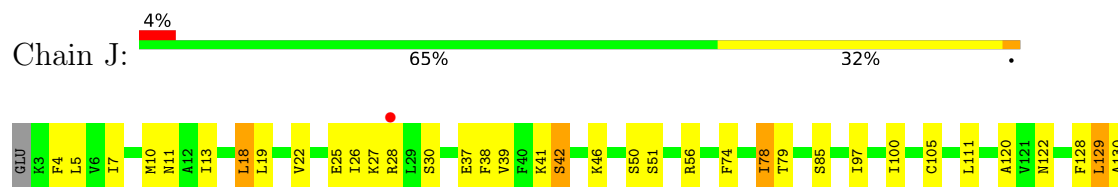
• Molecule 1: 2-dehydro-3-deoxyphosphooctonate aldolase

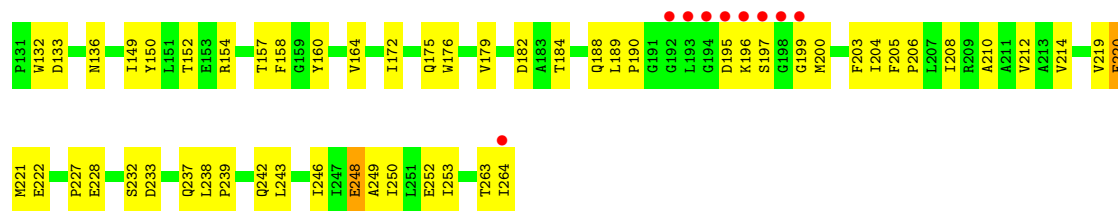


• Molecule 1: 2-dehydro-3-deoxyphosphooctonate aldolase

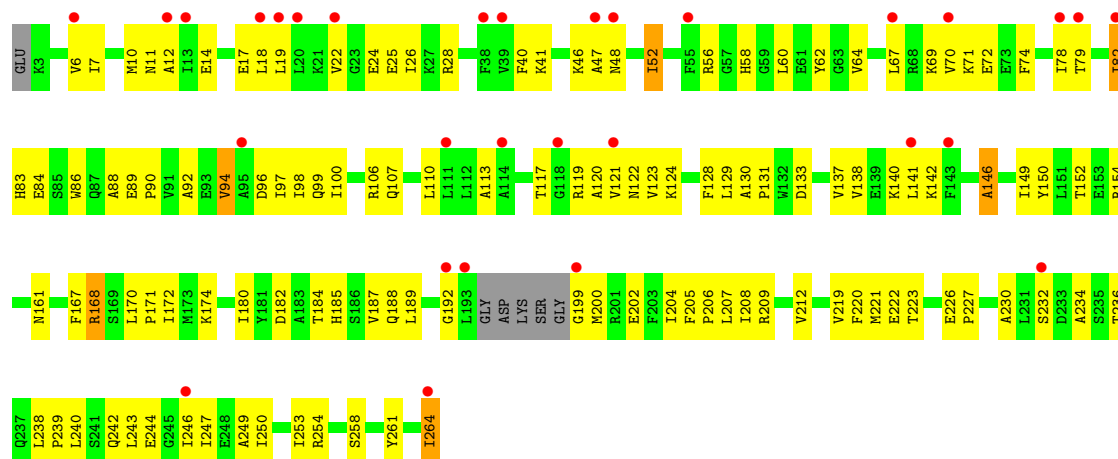


• Molecule 1: 2-dehydro-3-deoxyphosphooctonate aldolase

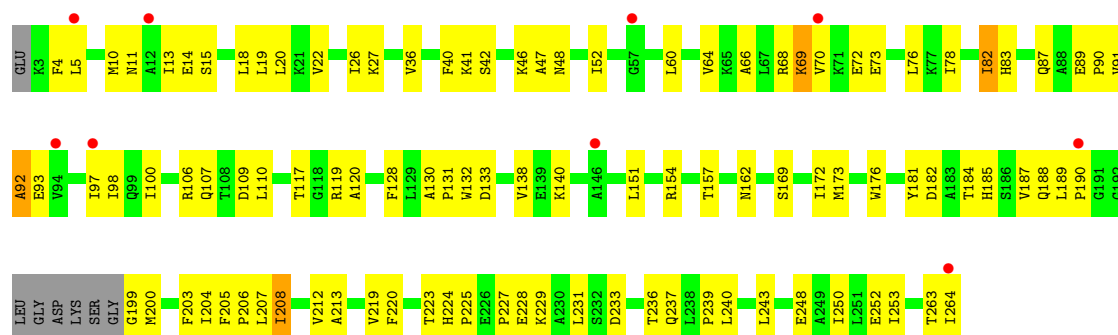




• Molecule 1: 2-dehydro-3-deoxyphosphooctonate aldolase



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	75.88Å 197.47Å 124.87Å 90.00° 93.84° 90.00°	Depositor
Resolution (Å)	25.00 – 2.30 25.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	76.3 (25.00-2.30) 76.2 (25.00-2.30)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.28 (at 2.22Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.207 , 0.267 0.207 , 0.267	Depositor DCC
R_{free} test set	6337 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	30.0	Xtriage
Anisotropy	0.743	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 46.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	25761	wwPDB-VP
Average B, all atoms (Å ²)	55.0	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 21.62 % 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 6.7524e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical 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: PEP, PO4

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	0/2068	0.96	6/2786 (0.2%)
1	B	0.49	0/2072	0.92	3/2791 (0.1%)
1	C	0.42	0/2064	0.88	4/2780 (0.1%)
1	D	0.38	0/2060	0.90	2/2775 (0.1%)
1	E	0.39	0/2060	0.82	0/2775
1	F	0.38	0/2056	0.87	5/2770 (0.2%)
1	G	0.46	0/2080	0.91	3/2802 (0.1%)
1	H	0.49	0/2060	0.95	7/2775 (0.3%)
1	I	0.46	0/2100	0.91	1/2829 (0.0%)
1	J	0.47	0/2100	0.94	3/2829 (0.1%)
1	K	0.37	0/2068	0.84	1/2786 (0.0%)
1	L	0.39	0/2060	0.85	1/2775 (0.0%)
All	All	0.43	0/24848	0.90	36/33473 (0.1%)

There are no bond length outliers.

The worst 5 of 36 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	100	ILE	CA-C-N	7.20	127.23	119.89
1	H	100	ILE	C-N-CA	7.20	127.23	119.89
1	I	78	ILE	N-CA-C	6.80	118.40	108.53
1	F	179	VAL	N-CA-C	6.71	117.50	108.11
1	J	149	ILE	N-CA-C	6.69	118.11	108.48

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	2029	0	2069	64	0
1	B	2033	0	2072	53	0
1	C	2025	0	2061	81	0
1	D	2021	0	2058	95	0
1	E	2021	0	2058	84	0
1	F	2017	0	2055	92	0
1	G	2041	0	2076	59	0
1	H	2021	0	2058	72	0
1	I	2060	0	2098	68	0
1	J	2060	0	2098	63	0
1	K	2029	0	2069	119	0
1	L	2021	0	2058	85	0
2	A	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	J	5	0	0	1	0
2	K	5	0	0	0	0
2	L	5	0	0	0	0
3	A	10	0	2	0	0
3	B	20	0	4	5	0
3	C	20	0	4	0	0
3	D	10	0	2	1	0
3	E	10	0	2	1	0
3	F	10	0	2	2	0
3	G	20	0	4	0	0
3	H	20	0	4	4	0
3	I	20	0	4	2	0
3	J	10	0	2	1	0
3	K	10	0	2	0	0
3	L	10	0	2	1	0
4	A	147	0	0	5	0
4	B	145	0	0	3	0
4	C	93	0	0	9	0
4	D	60	0	0	6	0
4	E	52	0	0	3	0
4	F	49	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	G	125	0	0	8	0
4	H	132	0	0	3	0
4	I	136	0	0	6	0
4	J	136	0	0	1	0
4	K	37	0	0	5	0
4	L	66	0	0	7	0
All	All	25761	0	24864	891	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 18.

The worst 5 of 891 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:B:184:THR:HG21	1:B:222:GLU:H	1.21	1.06
1:H:184:THR:HG21	1:H:222:GLU:H	1.20	1.04
1:D:146:ALA:HB1	1:D:149:ILE:HD11	1.37	1.00
1:K:188:GLN:HA	1:K:199:GLY:HA3	1.44	0.99
1:C:238:LEU:HD12	1:C:239:PRO:HD2	1.50	0.94

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	253/263 (96%)	241 (95%)	12 (5%)	0	100	100
1	B	254/263 (97%)	245 (96%)	9 (4%)	0	100	100
1	C	253/263 (96%)	234 (92%)	15 (6%)	4 (2%)	7	7
1	D	252/263 (96%)	230 (91%)	17 (7%)	5 (2%)	6	5
1	E	252/263 (96%)	227 (90%)	22 (9%)	3 (1%)	10	12

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	251/263 (95%)	228 (91%)	23 (9%)	0	100	100
1	G	255/263 (97%)	245 (96%)	9 (4%)	1 (0%)	30	38
1	H	252/263 (96%)	242 (96%)	10 (4%)	0	100	100
1	I	260/263 (99%)	249 (96%)	11 (4%)	0	100	100
1	J	260/263 (99%)	245 (94%)	15 (6%)	0	100	100
1	K	253/263 (96%)	217 (86%)	31 (12%)	5 (2%)	6	5
1	L	252/263 (96%)	226 (90%)	23 (9%)	3 (1%)	10	12
All	All	3047/3156 (96%)	2829 (93%)	197 (6%)	21 (1%)	18	23

5 of 21 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	262	GLU
1	K	94	VAL
1	C	85	SER
1	K	146	ALA
1	C	88	ALA

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	216/220 (98%)	212 (98%)	4 (2%)	50	69
1	B	216/220 (98%)	209 (97%)	7 (3%)	34	51
1	C	215/220 (98%)	213 (99%)	2 (1%)	70	84
1	D	215/220 (98%)	206 (96%)	9 (4%)	26	40
1	E	215/220 (98%)	209 (97%)	6 (3%)	38	56
1	F	215/220 (98%)	209 (97%)	6 (3%)	38	56
1	G	217/220 (99%)	207 (95%)	10 (5%)	24	36
1	H	215/220 (98%)	210 (98%)	5 (2%)	44	63
1	I	219/220 (100%)	213 (97%)	6 (3%)	39	58

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	J	219/220 (100%)	211 (96%)	8 (4%)	30	45
1	K	216/220 (98%)	212 (98%)	4 (2%)	50	69
1	L	215/220 (98%)	211 (98%)	4 (2%)	50	69
All	All	2593/2640 (98%)	2522 (97%)	71 (3%)	39	58

5 of 71 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	J	78	ILE
1	J	220	PHE
1	K	124	LYS
1	E	17	GLU
1	E	16	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 51 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	237	GLN
1	I	188	GLN
1	L	185	HIS
1	H	11	ASN
1	H	188	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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
3	PEP	D	268	-	9,9,9	0.93	0	11,13,13	1.42	1 (9%)
3	PEP	G	269	-	9,9,9	1.25	1 (11%)	11,13,13	1.81	3 (27%)
3	PEP	H	268	-	9,9,9	0.84	0	11,13,13	1.73	4 (36%)
3	PEP	H	269	-	9,9,9	0.98	0	11,13,13	1.41	2 (18%)
3	PEP	I	268	-	9,9,9	0.90	0	11,13,13	1.96	3 (27%)
3	PEP	F	268	-	9,9,9	1.08	0	11,13,13	1.88	3 (27%)
3	PEP	E	268	-	9,9,9	1.11	0	11,13,13	2.26	5 (45%)
2	PO4	K	269	-	4,4,4	1.68	0	6,6,6	0.47	0
2	PO4	D	269	-	4,4,4	1.66	0	6,6,6	0.45	0
3	PEP	K	268	-	9,9,9	1.02	0	11,13,13	1.10	1 (9%)
2	PO4	L	269	-	4,4,4	1.66	0	6,6,6	0.46	0
2	PO4	F	269	-	4,4,4	1.65	0	6,6,6	0.46	0
2	PO4	E	269	-	4,4,4	1.72	0	6,6,6	0.47	0
3	PEP	B	268	-	9,9,9	0.96	0	11,13,13	2.07	3 (27%)
3	PEP	J	268	-	9,9,9	0.94	0	11,13,13	1.76	2 (18%)
3	PEP	G	268	-	9,9,9	1.17	0	11,13,13	2.15	3 (27%)
3	PEP	L	268	-	9,9,9	0.96	0	11,13,13	1.67	3 (27%)
2	PO4	A	269	-	4,4,4	1.63	0	6,6,6	0.48	0
2	PO4	J	269	-	4,4,4	1.80	2 (50%)	6,6,6	0.46	0
3	PEP	C	269	-	9,9,9	1.08	0	11,13,13	1.71	3 (27%)
3	PEP	C	268	-	9,9,9	1.04	0	11,13,13	1.26	1 (9%)
3	PEP	B	269	-	9,9,9	1.48	2 (22%)	11,13,13	1.85	3 (27%)
3	PEP	A	268	-	9,9,9	0.93	0	11,13,13	1.92	2 (18%)
3	PEP	I	269	-	9,9,9	1.00	0	11,13,13	2.61	3 (27%)

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	B	268	-	-	4/9/9/9	-
3	PEP	C	269	-	-	6/9/9/9	-
3	PEP	D	268	-	-	4/9/9/9	-
3	PEP	G	269	-	-	4/9/9/9	-
3	PEP	J	268	-	-	5/9/9/9	-
3	PEP	K	268	-	-	4/9/9/9	-
3	PEP	G	268	-	-	0/9/9/9	-
3	PEP	H	268	-	-	0/9/9/9	-
3	PEP	H	269	-	-	4/9/9/9	-
3	PEP	I	268	-	-	4/9/9/9	-
3	PEP	C	268	-	-	4/9/9/9	-
3	PEP	L	268	-	-	4/9/9/9	-
3	PEP	F	268	-	-	4/9/9/9	-
3	PEP	E	268	-	-	0/9/9/9	-
3	PEP	B	269	-	-	0/9/9/9	-
3	PEP	A	268	-	-	0/9/9/9	-
3	PEP	I	269	-	-	4/9/9/9	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	269	PEP	C2-C1	3.06	1.52	1.49
3	G	269	PEP	C2-C1	2.32	1.51	1.49
2	J	269	PO4	P-O4	-2.19	1.48	1.54
3	B	269	PEP	O1-C1	2.10	1.27	1.22
2	J	269	PO4	P-O3	-2.03	1.48	1.54

The worst 5 of 45 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	269	PEP	O2'-C1-C2	6.47	124.94	113.91
3	I	268	PEP	O2'-C1-C2	4.93	122.33	113.91
3	G	268	PEP	O2'-C1-C2	4.82	122.14	113.91
3	J	268	PEP	O2'-C1-C2	4.49	121.57	113.91
3	I	269	PEP	O1-C1-C2	-4.22	115.42	121.79

There are no chirality outliers.

5 of 51 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	268	PEP	O1-C1-C2-C3
3	B	268	PEP	O2'-C1-C2-C3
3	B	268	PEP	O2'-C1-C2-O2
3	C	268	PEP	O1-C1-C2-C3
3	C	268	PEP	O2'-C1-C2-C3

There are no ring outliers.

12 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	268	PEP	1	0
3	H	268	PEP	1	0
3	H	269	PEP	3	0
3	I	268	PEP	1	0
3	F	268	PEP	2	0
3	E	268	PEP	1	0
3	B	268	PEP	2	0
3	J	268	PEP	1	0
3	L	268	PEP	1	0
2	J	269	PO4	1	0
3	B	269	PEP	3	0
3	I	269	PEP	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, 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	257/263 (97%)	-0.27	1 (0%) 88 89	25, 38, 58, 80	0
1	B	258/263 (98%)	-0.21	5 (1%) 66 68	23, 38, 58, 94	0
1	C	257/263 (97%)	0.34	6 (2%) 61 63	31, 58, 82, 92	0
1	D	256/263 (97%)	0.54	8 (3%) 51 53	32, 65, 84, 92	0
1	E	256/263 (97%)	0.62	17 (6%) 24 26	35, 72, 100, 107	0
1	F	255/263 (96%)	0.88	15 (5%) 28 30	40, 75, 97, 102	0
1	G	259/263 (98%)	-0.15	4 (1%) 72 73	26, 41, 66, 109	0
1	H	256/263 (97%)	-0.15	3 (1%) 76 77	28, 40, 62, 84	0
1	I	262/263 (99%)	-0.10	8 (3%) 51 53	24, 40, 64, 97	0
1	J	262/263 (99%)	-0.07	10 (3%) 44 46	28, 42, 73, 101	0
1	K	257/263 (97%)	1.04	30 (11%) 9 10	40, 86, 108, 118	0
1	L	256/263 (97%)	0.58	9 (3%) 47 49	38, 65, 88, 97	0
All	All	3091/3156 (97%)	0.25	116 (3%) 44 46	23, 51, 93, 118	0

The worst 5 of 116 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	264	ILE	4.9
1	B	194	GLY	4.5
1	F	94	VAL	4.5
1	I	197	SER	4.5
1	I	198	GLY	4.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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	269	5/5	0.55	0.11	122,123,123,123	0
2	PO4	E	269	5/5	0.78	0.10	97,98,98,99	0
2	PO4	F	269	5/5	0.79	0.10	90,90,90,91	0
2	PO4	L	269	5/5	0.83	0.09	103,103,104,104	0
3	PEP	C	269	10/10	0.84	0.14	88,88,89,89	0
3	PEP	H	269	10/10	0.86	0.15	62,67,73,73	0
2	PO4	D	269	5/5	0.87	0.10	80,80,80,81	0
3	PEP	G	269	10/10	0.88	0.12	67,71,76,77	0
2	PO4	A	269	5/5	0.90	0.08	53,55,55,58	0
3	PEP	F	268	10/10	0.91	0.09	72,76,77,79	0
3	PEP	K	268	10/10	0.91	0.11	76,79,81,82	0
3	PEP	B	269	10/10	0.92	0.11	52,59,65,65	0
3	PEP	I	269	10/10	0.92	0.11	55,62,70,71	0
2	PO4	J	269	5/5	0.92	0.09	61,63,64,64	0
3	PEP	E	268	10/10	0.94	0.10	66,68,71,71	0
3	PEP	C	268	10/10	0.94	0.09	53,56,59,60	0
3	PEP	D	268	10/10	0.94	0.08	50,55,60,60	0
3	PEP	L	268	10/10	0.94	0.09	69,73,74,74	0
3	PEP	B	268	10/10	0.98	0.06	31,34,36,42	0
3	PEP	I	268	10/10	0.98	0.06	30,35,38,39	0
3	PEP	G	268	10/10	0.98	0.06	33,39,44,46	0
3	PEP	J	268	10/10	0.98	0.06	32,38,44,45	0
3	PEP	A	268	10/10	0.98	0.05	32,35,38,39	0
3	PEP	H	268	10/10	0.98	0.06	28,34,38,38	0

6.5 Other polymers [i](#)

There are no such residues in this entry.