Full wwPDB X-ray Structure Validation Report ⓘ

Nov 7, 2023 – 02:17 AM EST

PDB ID	:	4PTN
Title	:	Crystal Structure of YagE, a KDG aldolase protein in complex with Magnesium cation coordinated L-glyceraldehyde
Authors	:	Manoj Kumar, P.; Baskar, V.; Manicka, S.; Krishnaswamy, S.
Deposited on	:	2014-03-11
Resolution	:	1.99 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 ⓘ 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:

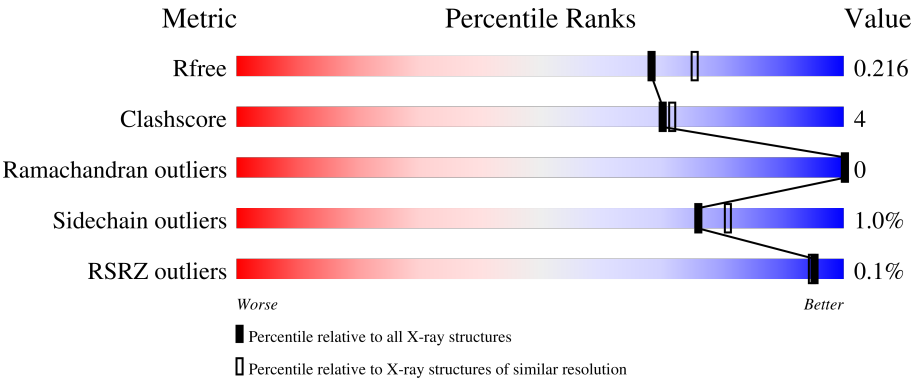
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.99 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	343	81% 6% 13%
1	B	343	78% 8% 13%
1	C	343	79% 8% 13%
1	D	343	80% 7% 13%

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
2	EDO	B	404	-	-	X	-
2	EDO	C	403	-	-	X	-
3	GXV	D	403[B]	-	X	-	-
5	GOL	B	405	-	-	X	-

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 9706 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 Probable 2-keto-3-deoxy-galactonate aldolase YagE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	298	Total	C	N	O	S	0	1	0
			2267	1451	389	421	6			
1	B	298	Total	C	N	O	S	0	0	0
			2262	1447	388	421	6			
1	C	298	Total	C	N	O	S	0	1	0
			2268	1451	390	421	6			
1	D	298	Total	C	N	O	S	0	0	0
			2262	1447	388	421	6			

There are 164 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-17	MET	-	expression tag	UNP P75682
A	-16	GLY	-	expression tag	UNP P75682
A	-15	SER	-	expression tag	UNP P75682
A	-14	SER	-	expression tag	UNP P75682
A	-13	HIS	-	expression tag	UNP P75682
A	-12	HIS	-	expression tag	UNP P75682
A	-11	HIS	-	expression tag	UNP P75682
A	-10	HIS	-	expression tag	UNP P75682
A	-9	HIS	-	expression tag	UNP P75682
A	-8	HIS	-	expression tag	UNP P75682
A	-7	SER	-	expression tag	UNP P75682
A	-6	ALA	-	expression tag	UNP P75682
A	-5	GLY	-	expression tag	UNP P75682
A	-4	GLU	-	expression tag	UNP P75682
A	-3	ASN	-	expression tag	UNP P75682
A	-2	LEU	-	expression tag	UNP P75682
A	-1	TYR	-	expression tag	UNP P75682
A	0	PHE	-	expression tag	UNP P75682
A	1	GLN	-	expression tag	UNP P75682
A	2	GLY	-	expression tag	UNP P75682
A	3	GLN	-	expression tag	UNP P75682

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Chain	Residue	Modelled	Actual	Comment	Reference
A	4	GLN	-	expression tag	UNP P75682
A	5	GLY	-	expression tag	UNP P75682
A	6	ASP	-	expression tag	UNP P75682
A	7	LEU	-	expression tag	UNP P75682
A	310	CYS	-	expression tag	UNP P75682
A	311	GLY	-	expression tag	UNP P75682
A	312	ARG	-	expression tag	UNP P75682
A	313	THR	-	expression tag	UNP P75682
A	314	ARG	-	expression tag	UNP P75682
A	315	ALA	-	expression tag	UNP P75682
A	316	PRO	-	expression tag	UNP P75682
A	317	PRO	-	expression tag	UNP P75682
A	318	PRO	-	expression tag	UNP P75682
A	319	PRO	-	expression tag	UNP P75682
A	320	PRO	-	expression tag	UNP P75682
A	321	LEU	-	expression tag	UNP P75682
A	322	ARG	-	expression tag	UNP P75682
A	323	SER	-	expression tag	UNP P75682
A	324	GLY	-	expression tag	UNP P75682
A	325	CYS	-	expression tag	UNP P75682
B	-17	MET	-	expression tag	UNP P75682
B	-16	GLY	-	expression tag	UNP P75682
B	-15	SER	-	expression tag	UNP P75682
B	-14	SER	-	expression tag	UNP P75682
B	-13	HIS	-	expression tag	UNP P75682
B	-12	HIS	-	expression tag	UNP P75682
B	-11	HIS	-	expression tag	UNP P75682
B	-10	HIS	-	expression tag	UNP P75682
B	-9	HIS	-	expression tag	UNP P75682
B	-8	HIS	-	expression tag	UNP P75682
B	-7	SER	-	expression tag	UNP P75682
B	-6	ALA	-	expression tag	UNP P75682
B	-5	GLY	-	expression tag	UNP P75682
B	-4	GLU	-	expression tag	UNP P75682
B	-3	ASN	-	expression tag	UNP P75682
B	-2	LEU	-	expression tag	UNP P75682
B	-1	TYR	-	expression tag	UNP P75682
B	0	PHE	-	expression tag	UNP P75682
B	1	GLN	-	expression tag	UNP P75682
B	2	GLY	-	expression tag	UNP P75682
B	3	GLN	-	expression tag	UNP P75682
B	4	GLN	-	expression tag	UNP P75682

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Chain	Residue	Modelled	Actual	Comment	Reference
B	5	GLY	-	expression tag	UNP P75682
B	6	ASP	-	expression tag	UNP P75682
B	7	LEU	-	expression tag	UNP P75682
B	310	CYS	-	expression tag	UNP P75682
B	311	GLY	-	expression tag	UNP P75682
B	312	ARG	-	expression tag	UNP P75682
B	313	THR	-	expression tag	UNP P75682
B	314	ARG	-	expression tag	UNP P75682
B	315	ALA	-	expression tag	UNP P75682
B	316	PRO	-	expression tag	UNP P75682
B	317	PRO	-	expression tag	UNP P75682
B	318	PRO	-	expression tag	UNP P75682
B	319	PRO	-	expression tag	UNP P75682
B	320	PRO	-	expression tag	UNP P75682
B	321	LEU	-	expression tag	UNP P75682
B	322	ARG	-	expression tag	UNP P75682
B	323	SER	-	expression tag	UNP P75682
B	324	GLY	-	expression tag	UNP P75682
B	325	CYS	-	expression tag	UNP P75682
C	-17	MET	-	expression tag	UNP P75682
C	-16	GLY	-	expression tag	UNP P75682
C	-15	SER	-	expression tag	UNP P75682
C	-14	SER	-	expression tag	UNP P75682
C	-13	HIS	-	expression tag	UNP P75682
C	-12	HIS	-	expression tag	UNP P75682
C	-11	HIS	-	expression tag	UNP P75682
C	-10	HIS	-	expression tag	UNP P75682
C	-9	HIS	-	expression tag	UNP P75682
C	-8	HIS	-	expression tag	UNP P75682
C	-7	SER	-	expression tag	UNP P75682
C	-6	ALA	-	expression tag	UNP P75682
C	-5	GLY	-	expression tag	UNP P75682
C	-4	GLU	-	expression tag	UNP P75682
C	-3	ASN	-	expression tag	UNP P75682
C	-2	LEU	-	expression tag	UNP P75682
C	-1	TYR	-	expression tag	UNP P75682
C	0	PHE	-	expression tag	UNP P75682
C	1	GLN	-	expression tag	UNP P75682
C	2	GLY	-	expression tag	UNP P75682
C	3	GLN	-	expression tag	UNP P75682
C	4	GLN	-	expression tag	UNP P75682
C	5	GLY	-	expression tag	UNP P75682

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Chain	Residue	Modelled	Actual	Comment	Reference
C	6	ASP	-	expression tag	UNP P75682
C	7	LEU	-	expression tag	UNP P75682
C	310	CYS	-	expression tag	UNP P75682
C	311	GLY	-	expression tag	UNP P75682
C	312	ARG	-	expression tag	UNP P75682
C	313	THR	-	expression tag	UNP P75682
C	314	ARG	-	expression tag	UNP P75682
C	315	ALA	-	expression tag	UNP P75682
C	316	PRO	-	expression tag	UNP P75682
C	317	PRO	-	expression tag	UNP P75682
C	318	PRO	-	expression tag	UNP P75682
C	319	PRO	-	expression tag	UNP P75682
C	320	PRO	-	expression tag	UNP P75682
C	321	LEU	-	expression tag	UNP P75682
C	322	ARG	-	expression tag	UNP P75682
C	323	SER	-	expression tag	UNP P75682
C	324	GLY	-	expression tag	UNP P75682
C	325	CYS	-	expression tag	UNP P75682
D	-17	MET	-	expression tag	UNP P75682
D	-16	GLY	-	expression tag	UNP P75682
D	-15	SER	-	expression tag	UNP P75682
D	-14	SER	-	expression tag	UNP P75682
D	-13	HIS	-	expression tag	UNP P75682
D	-12	HIS	-	expression tag	UNP P75682
D	-11	HIS	-	expression tag	UNP P75682
D	-10	HIS	-	expression tag	UNP P75682
D	-9	HIS	-	expression tag	UNP P75682
D	-8	HIS	-	expression tag	UNP P75682
D	-7	SER	-	expression tag	UNP P75682
D	-6	ALA	-	expression tag	UNP P75682
D	-5	GLY	-	expression tag	UNP P75682
D	-4	GLU	-	expression tag	UNP P75682
D	-3	ASN	-	expression tag	UNP P75682
D	-2	LEU	-	expression tag	UNP P75682
D	-1	TYR	-	expression tag	UNP P75682
D	0	PHE	-	expression tag	UNP P75682
D	1	GLN	-	expression tag	UNP P75682
D	2	GLY	-	expression tag	UNP P75682
D	3	GLN	-	expression tag	UNP P75682
D	4	GLN	-	expression tag	UNP P75682
D	5	GLY	-	expression tag	UNP P75682
D	6	ASP	-	expression tag	UNP P75682

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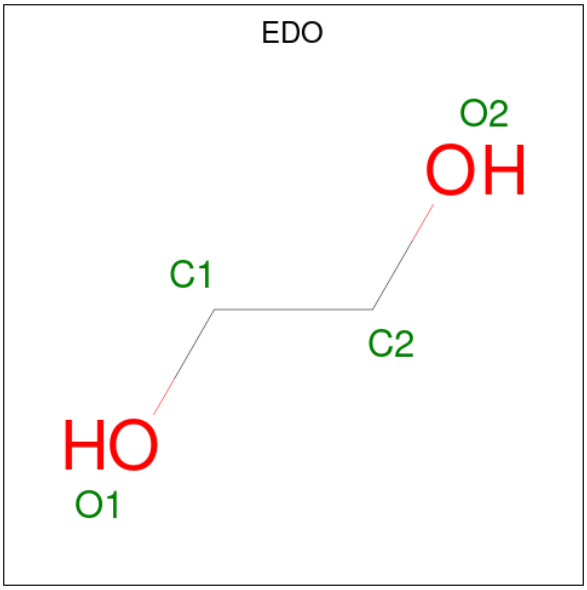
Chain	Residue	Modelled	Actual	Comment	Reference
D	7	LEU	-	expression tag	UNP P75682
D	310	CYS	-	expression tag	UNP P75682
D	311	GLY	-	expression tag	UNP P75682
D	312	ARG	-	expression tag	UNP P75682
D	313	THR	-	expression tag	UNP P75682
D	314	ARG	-	expression tag	UNP P75682
D	315	ALA	-	expression tag	UNP P75682
D	316	PRO	-	expression tag	UNP P75682
D	317	PRO	-	expression tag	UNP P75682
D	318	PRO	-	expression tag	UNP P75682
D	319	PRO	-	expression tag	UNP P75682
D	320	PRO	-	expression tag	UNP P75682
D	321	LEU	-	expression tag	UNP P75682
D	322	ARG	-	expression tag	UNP P75682
D	323	SER	-	expression tag	UNP P75682
D	324	GLY	-	expression tag	UNP P75682
D	325	CYS	-	expression tag	UNP P75682

- Molecule 2 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0

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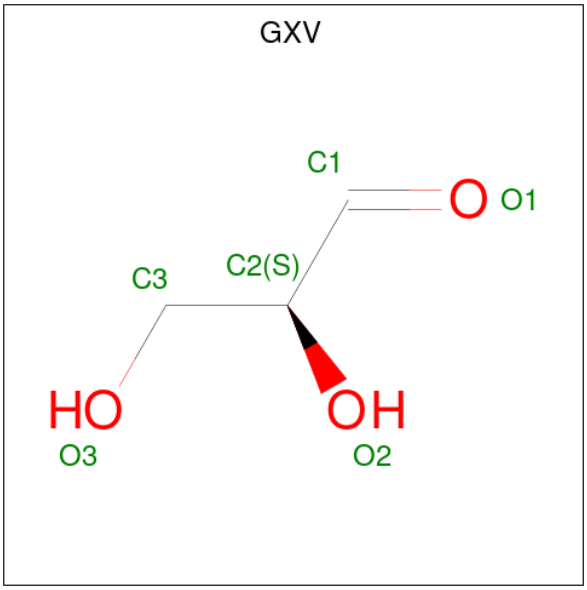
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	C	1	Total	C	O	0	0
			4	2	2		
2	C	1	Total	C	O	0	0
			4	2	2		
2	C	1	Total	C	O	0	0
			4	2	2		
2	D	1	Total	C	O	0	0
			4	2	2		
2	D	1	Total	C	O	0	1
			8	4	4		

- Molecule 3 is L-glyceraldehyde (three-letter code: GXV) (formula: $C_3H_6O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	1
			12	6	6		
3	B	1	Total	C	O	0	1
			12	6	6		
3	C	1	Total	C	O	0	1
			12	6	6		

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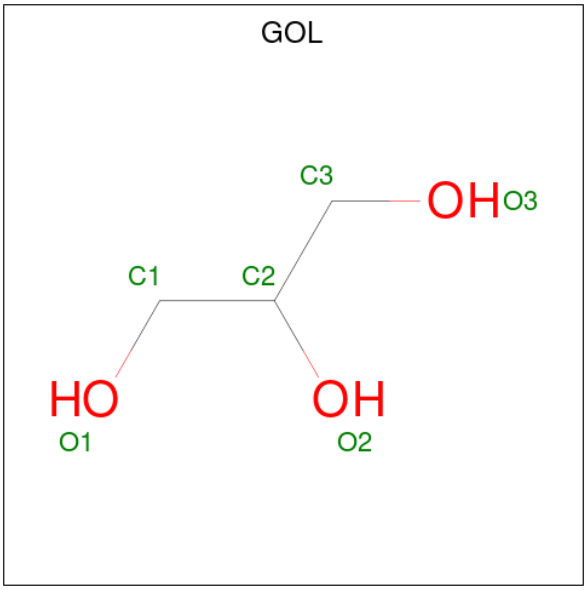
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	1	Total C O 12 6 6	0	1

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

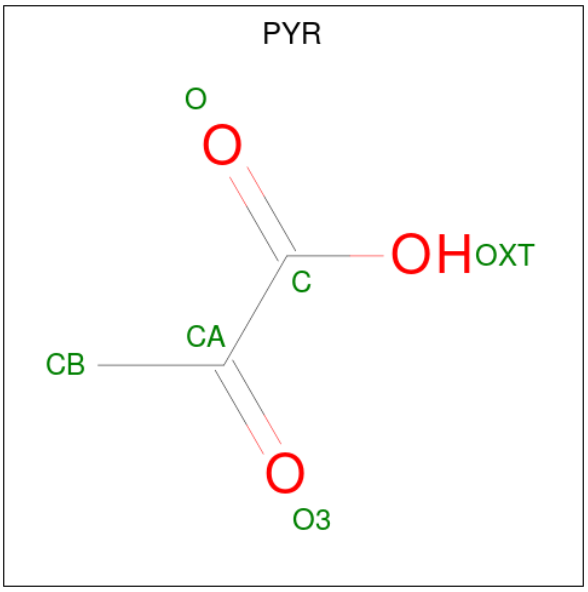
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Mg 2 2	0	1
4	B	1	Total Mg 2 2	0	1
4	C	1	Total Mg 2 2	0	1
4	D	1	Total Mg 2 2	0	1

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C O 6 3 3	0	0

- Molecule 6 is PYRUVIC ACID (three-letter code: PYR) (formula: $C_3H_4O_3$).



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

- Molecule 7 is water.

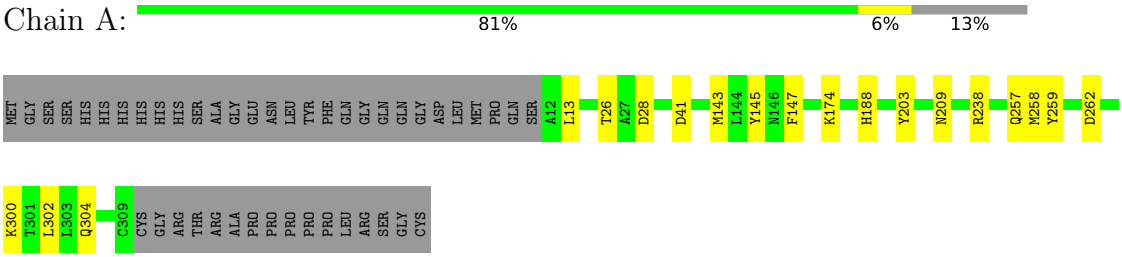
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	112	Total O 112 112	0	0
7	B	145	Total O 145 145	0	0
7	C	125	Total O 125 125	0	0
7	D	143	Total O 143 143	0	0

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.

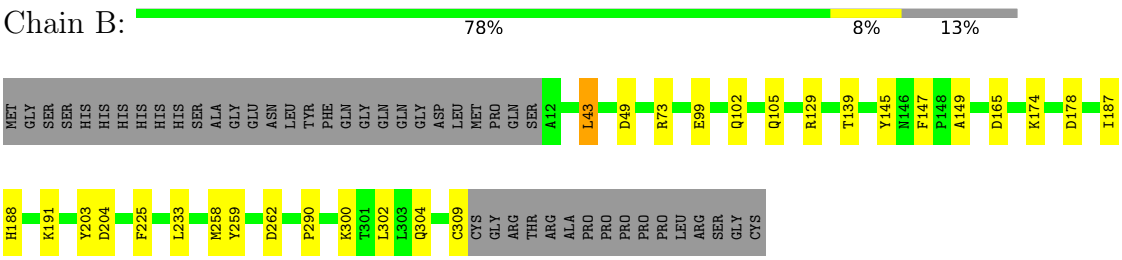
• Molecule 1: Probable 2-keto-3-deoxy-galactonate aldolase YagE

Chain A:



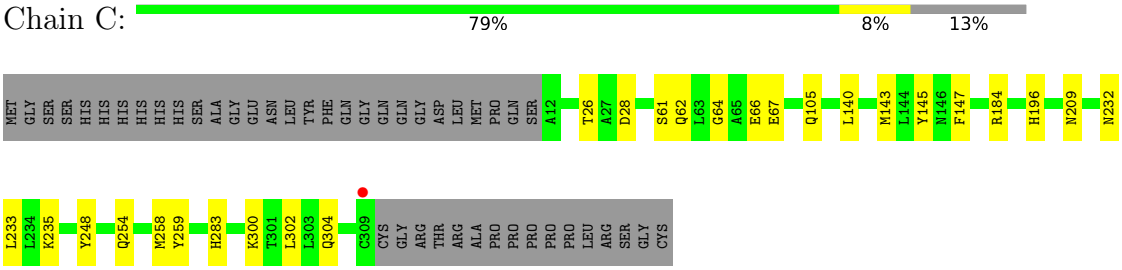
• Molecule 1: Probable 2-keto-3-deoxy-galactonate aldolase YagE

Chain B:



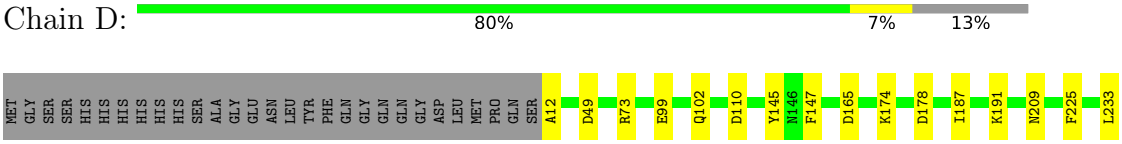
• Molecule 1: Probable 2-keto-3-deoxy-galactonate aldolase YagE

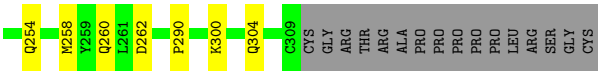
Chain C:



• Molecule 1: Probable 2-keto-3-deoxy-galactonate aldolase YagE

Chain D:




Q254
M258
Y259
Q260
L261
D262
P290
K300
Q304
C309
CYS
GLY
ARG
THR
ARG
ALA
PRO
PRO
PRO
PRO
PRO
LEU
ARG
SER
GLY
CYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	141.20Å 155.07Å 55.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.94 – 1.99 48.94 – 1.99	Depositor EDS
% Data completeness (in resolution range)	99.0 (48.94-1.99) 99.0 (48.94-1.99)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.82 (at 1.98Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.174 , 0.203 0.185 , 0.216	Depositor DCC
R_{free} test set	4194 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	16.8	Xtriage
Anisotropy	0.106	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 45.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	9706	wwPDB-VP
Average B, all atoms (Å^2)	16.0	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 48.85 % 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 8.1141e-05. 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: GOL, PYR, EDO, MG, GXV

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	0.89	0/2318	0.90	5/3159 (0.2%)
1	B	0.95	1/2310 (0.0%)	0.89	7/3147 (0.2%)
1	C	0.90	0/2319	0.89	2/3160 (0.1%)
1	D	0.93	1/2310 (0.0%)	0.90	7/3147 (0.2%)
All	All	0.92	2/9257 (0.0%)	0.90	21/12613 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	99	GLU	CD-OE2	6.15	1.32	1.25
1	D	99	GLU	CD-OE2	5.69	1.31	1.25

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	238	ARG	NE-CZ-NH1	8.11	124.35	120.30
1	D	165	ASP	CB-CG-OD1	6.58	124.22	118.30
1	B	165	ASP	CB-CG-OD1	6.22	123.90	118.30
1	B	204	ASP	CB-CG-OD1	6.11	123.80	118.30
1	B	165	ASP	CB-CG-OD2	-6.10	112.81	118.30
1	D	262	ASP	CB-CG-OD2	5.93	123.63	118.30
1	D	49	ASP	CB-CG-OD1	5.74	123.47	118.30
1	D	73	ARG	NE-CZ-NH2	-5.52	117.54	120.30
1	D	165	ASP	CB-CG-OD2	-5.49	113.36	118.30
1	B	43	LEU	CB-CG-CD1	5.45	120.27	111.00
1	B	262	ASP	CB-CG-OD2	5.41	123.17	118.30
1	B	73	ARG	NE-CZ-NH2	-5.24	117.68	120.30
1	C	184	ARG	NE-CZ-NH1	-5.15	117.72	120.30
1	D	110	ASP	CB-CG-OD2	5.13	122.92	118.30
1	C	143	MET	CG-SD-CE	-5.12	92.00	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	262	ASP	CB-CG-OD2	5.12	122.91	118.30
1	A	257	GLN	CB-CA-C	-5.11	100.19	110.40
1	D	73	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	A	41	ASP	CB-CG-OD1	5.07	122.86	118.30
1	B	49	ASP	CB-CG-OD1	5.05	122.85	118.30
1	A	143	MET	CG-SD-CE	-5.01	92.19	100.20

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	2267	0	2289	10	0
1	B	2262	0	2286	24	0
1	C	2268	0	2294	18	0
1	D	2262	0	2286	13	0
2	A	8	0	12	1	0
2	B	16	0	24	4	0
2	C	12	0	17	5	0
2	D	12	0	18	0	0
3	A	12	0	0	1	0
3	B	12	0	0	1	0
3	C	12	0	0	0	0
3	D	12	0	0	2	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
4	D	2	0	0	0	0
5	B	6	0	8	4	0
6	B	6	0	0	3	0
6	D	6	0	0	3	0
7	A	112	0	0	1	0
7	B	145	0	0	10	0
7	C	125	0	0	3	0
7	D	143	0	0	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	9706	0	9234	67	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 (67) 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:C:235:LYS:HE2	7:C:623:HOH:O	1.49	1.12
6:D:405:PYR:CA	7:D:609:HOH:O	2.11	0.97
1:B:309:CYS:C	7:B:642:HOH:O	2.02	0.96
1:B:259:TYR:HD2	7:B:644:HOH:O	1.48	0.95
1:B:259:TYR:CD2	7:B:644:HOH:O	2.20	0.91
1:C:66:GLU:HB2	2:C:403:EDO:H21	1.53	0.90
1:C:283:HIS:HB2	7:C:620:HOH:O	1.73	0.87
1:B:178:ASP:O	5:B:405:GOL:H2	1.77	0.84
6:B:408:PYR:CA	7:B:600:HOH:O	2.25	0.83
1:C:26:THR:OG1	1:C:28:ASP:OD1	1.97	0.83
5:B:405:GOL:H11	1:D:178:ASP:O	1.80	0.80
1:B:203:TYR:OH	2:B:404:EDO:O2	1.98	0.79
1:A:26:THR:OG1	1:A:28:ASP:OD1	2.00	0.79
1:B:105:GLN:HE22	1:B:139:THR:H	1.29	0.79
1:C:196:HIS:HD2	7:C:624:HOH:O	1.66	0.78
1:B:129:ARG:HD2	7:B:643:HOH:O	1.84	0.76
6:D:405:PYR:C	7:D:609:HOH:O	2.32	0.72
1:B:105:GLN:NE2	1:B:139:THR:H	1.95	0.65
3:D:403[B]:GXV:C2	7:D:643:HOH:O	2.46	0.64
6:B:408:PYR:C	7:B:600:HOH:O	2.46	0.63
1:B:102:GLN:NE2	7:B:598:HOH:O	2.33	0.59
1:B:178:ASP:O	5:B:405:GOL:C2	2.49	0.59
1:B:188:HIS:HE1	1:D:254:GLN:OE1	1.87	0.57
1:C:67:GLU:HG3	2:C:403:EDO:O2	2.05	0.57
1:C:66:GLU:CB	2:C:403:EDO:H21	2.33	0.56
1:B:178:ASP:O	5:B:405:GOL:C3	2.55	0.55
1:D:225:PHE:CZ	1:D:258:MET:HE1	2.43	0.54
1:A:209:ASN:HD21	1:C:209:ASN:HD21	1.57	0.53
1:A:13:LEU:HD12	1:A:13:LEU:N	2.28	0.49
1:B:105:GLN:HE22	1:B:139:THR:N	2.05	0.49
1:B:174:LYS:HZ1	3:B:406[A]:GXV:C1	2.27	0.48
1:B:225:PHE:CZ	1:B:258:MET:HE1	2.48	0.48
1:D:209:ASN:ND2	7:D:625:HOH:O	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:300:LYS:HE2	1:D:304:GLN:NE2	2.30	0.47
1:B:309:CYS:CB	7:B:642:HOH:O	2.62	0.47
2:B:404:EDO:H22	7:B:511:HOH:O	2.15	0.46
1:C:258:MET:HG3	1:C:259:TYR:CD1	2.51	0.45
1:B:300:LYS:HE2	1:B:304:GLN:NE2	2.32	0.44
1:D:290:PRO:O	6:D:405:PYR:CB	2.65	0.44
1:A:258:MET:HG3	1:A:259:TYR:CD1	2.53	0.44
1:C:61:SER:OG	1:C:62:GLN:NE2	2.51	0.44
1:B:149:ALA:HB2	2:B:404:EDO:H22	2.00	0.44
1:C:66:GLU:H	2:C:403:EDO:C2	2.30	0.43
1:D:187:ILE:O	1:D:191:LYS:HB2	2.18	0.43
1:D:233:LEU:C	1:D:233:LEU:HD23	2.39	0.43
1:A:188:HIS:HB3	7:A:612:HOH:O	2.18	0.43
1:B:259:TYR:CE2	7:B:644:HOH:O	2.64	0.43
1:C:105:GLN:HA	1:C:140:LEU:HD11	2.00	0.42
1:A:203:TYR:CG	2:A:402:EDO:H21	2.54	0.42
1:D:260:GLN:NE2	7:D:545:HOH:O	2.51	0.42
1:C:233:LEU:C	1:C:233:LEU:HD23	2.40	0.42
1:D:102:GLN:NE2	7:D:605:HOH:O	2.42	0.42
1:B:188:HIS:CE1	1:D:254:GLN:OE1	2.69	0.41
1:C:258:MET:HB3	1:C:302:LEU:HD23	2.02	0.41
1:A:188:HIS:CE1	1:C:254:GLN:OE1	2.73	0.41
1:C:64:GLY:C	2:C:403:EDO:H22	2.41	0.41
1:A:258:MET:HB3	1:A:302:LEU:HD23	2.03	0.41
1:A:300:LYS:HE2	1:A:304:GLN:NE2	2.36	0.41
1:B:149:ALA:HB2	2:B:404:EDO:C2	2.51	0.41
1:B:290:PRO:O	6:B:408:PYR:CB	2.69	0.41
1:C:300:LYS:HE2	1:C:304:GLN:NE2	2.36	0.41
1:D:174:LYS:HZ1	3:D:403[B]:GXV:C1	2.33	0.41
1:B:233:LEU:HD23	1:B:233:LEU:C	2.42	0.40
1:A:174:LYS:HZ1	3:A:403[A]:GXV:C1	2.33	0.40
1:C:232:ASN:HB3	1:C:248:TYR:CE1	2.56	0.40
1:B:187:ILE:O	1:B:191:LYS:HB2	2.22	0.40
1:D:12:ALA:N	7:D:642:HOH:O	2.53	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	297/343 (87%)	294 (99%)	3 (1%)	0	100	100
1	B	296/343 (86%)	292 (99%)	4 (1%)	0	100	100
1	C	297/343 (87%)	294 (99%)	3 (1%)	0	100	100
1	D	296/343 (86%)	293 (99%)	3 (1%)	0	100	100
All	All	1186/1372 (86%)	1173 (99%)	13 (1%)	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	242/280 (86%)	240 (99%)	2 (1%)	81	86
1	B	243/280 (87%)	239 (98%)	4 (2%)	62	67
1	C	243/280 (87%)	241 (99%)	2 (1%)	81	86
1	D	242/280 (86%)	240 (99%)	2 (1%)	81	86
All	All	970/1120 (87%)	960 (99%)	10 (1%)	76	81

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

Mol	Chain	Res	Type
1	A	145	TYR
1	A	147	PHE

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Mol	Chain	Res	Type
1	B	43	LEU
1	B	145	TYR
1	B	147	PHE
1	B	302	LEU
1	C	145	TYR
1	C	147	PHE
1	D	145	TYR
1	D	147	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	62	GLN
1	A	102	GLN
1	A	188	HIS
1	B	62	GLN
1	B	105	GLN
1	B	188	HIS
1	C	62	GLN
1	C	102	GLN
1	C	257	GLN
1	C	305	GLN
1	D	62	GLN
1	D	102	GLN
1	D	126	ASN
1	D	257	GLN
1	D	260	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 31 ligands modelled in this entry, 8 are monoatomic - leaving 23 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	$\#\|Z\| > 2$
2	EDO	C	403	-	3,3,3	0.70	0	2,2,2	1.53	1 (50%)
2	EDO	B	404	-	3,3,3	0.38	0	2,2,2	1.21	0
3	GXV	B	406[A]	4	4,5,5	3.62	2 (50%)	4,5,5	1.26	0
2	EDO	B	401	-	3,3,3	0.32	0	2,2,2	1.77	1 (50%)
3	GXV	A	403[B]	-	4,5,5	1.14	0	4,5,5	1.65	1 (25%)
3	GXV	A	403[A]	4	4,5,5	3.17	1 (25%)	4,5,5	2.19	1 (25%)
3	GXV	D	403[B]	4	4,5,5	3.53	2 (50%)	4,5,5	3.00	2 (50%)
2	EDO	B	403	-	3,3,3	1.09	0	2,2,2	1.42	0
3	GXV	C	404[B]	-	4,5,5	0.88	0	4,5,5	2.68	2 (50%)
3	GXV	D	403[A]	-	4,5,5	0.41	0	4,5,5	1.46	1 (25%)
2	EDO	B	402	-	3,3,3	0.72	0	2,2,2	0.26	0
3	GXV	C	404[A]	4	4,5,5	3.24	1 (25%)	4,5,5	1.09	0
5	GOL	B	405	-	5,5,5	0.87	0	5,5,5	1.19	0
2	EDO	A	401	-	3,3,3	0.16	0	2,2,2	1.22	0
6	PYR	D	405	-	5,5,5	3.80	4 (80%)	3,6,6	2.05	1 (33%)
2	EDO	D	401	-	3,3,3	0.44	0	2,2,2	0.59	0
2	EDO	A	402	-	3,3,3	0.39	0	2,2,2	0.51	0
2	EDO	D	402[B]	-	3,3,3	0.34	0	2,2,2	0.12	0
2	EDO	C	401	-	3,3,3	0.95	0	2,2,2	1.31	0
2	EDO	D	402[A]	-	3,3,3	0.37	0	2,2,2	0.68	0
2	EDO	C	402	-	3,3,3	0.53	0	2,2,2	0.30	0
6	PYR	B	408	-	5,5,5	3.80	4 (80%)	3,6,6	1.15	0
3	GXV	B	406[B]	-	4,5,5	0.48	0	4,5,5	1.44	1 (25%)

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	EDO	C	403	-	-	1/1/1/1	-
2	EDO	B	404	-	-	1/1/1/1	-
3	GXV	B	406[A]	4	-	0/3/4/4	-
2	EDO	B	401	-	-	0/1/1/1	-
3	GXV	A	403[B]	-	-	2/3/4/4	-
3	GXV	A	403[A]	4	-	1/3/4/4	-
3	GXV	D	403[B]	4	-	2/3/4/4	-
2	EDO	B	403	-	-	1/1/1/1	-
3	GXV	C	404[B]	-	-	2/3/4/4	-
3	GXV	D	403[A]	-	-	2/3/4/4	-
2	EDO	B	402	-	-	0/1/1/1	-
3	GXV	C	404[A]	4	-	1/3/4/4	-
5	GOL	B	405	-	-	0/4/4/4	-
2	EDO	A	401	-	-	0/1/1/1	-
6	PYR	D	405	-	-	0/4/4/4	-
2	EDO	D	401	-	-	0/1/1/1	-
2	EDO	A	402	-	-	1/1/1/1	-
2	EDO	D	402[B]	-	-	0/1/1/1	-
2	EDO	C	401	-	-	0/1/1/1	-
2	EDO	D	402[A]	-	-	0/1/1/1	-
2	EDO	C	402	-	-	1/1/1/1	-
6	PYR	B	408	-	-	0/4/4/4	-
3	GXV	B	406[B]	-	-	2/3/4/4	-

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	404[A]	GXV	O1-C1	6.43	1.45	1.19
3	B	406[A]	GXV	O1-C1	6.31	1.45	1.19
3	D	403[B]	GXV	O1-C1	6.26	1.44	1.19
3	A	403[A]	GXV	O1-C1	5.98	1.43	1.19
6	D	405	PYR	O3-CA	5.97	1.36	1.23
6	B	408	PYR	O3-CA	5.67	1.35	1.23
6	B	408	PYR	O-C	4.87	1.35	1.22
6	D	405	PYR	O-C	4.52	1.34	1.22
3	B	406[A]	GXV	C3-C2	3.33	1.55	1.50
6	B	408	PYR	CB-CA	3.02	1.56	1.50
6	D	405	PYR	CB-CA	2.80	1.55	1.50
3	D	403[B]	GXV	C3-C2	2.65	1.54	1.50
6	B	408	PYR	CA-C	-2.27	1.46	1.54
6	D	405	PYR	CA-C	-2.17	1.46	1.54

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	403[B]	GXV	O2-C2-C3	4.20	117.88	109.22
3	D	403[B]	GXV	O2-C2-C1	-4.09	101.10	109.17
3	A	403[A]	GXV	O2-C2-C1	-3.86	101.57	109.17
3	C	404[B]	GXV	O3-C3-C2	-3.57	107.19	112.40
3	C	404[B]	GXV	O2-C2-C1	3.06	115.19	109.17
3	A	403[B]	GXV	O3-C3-C2	2.76	116.43	112.40
6	D	405	PYR	O3-CA-CB	2.57	125.42	119.73
3	D	403[A]	GXV	O2-C2-C3	-2.39	104.29	109.22
2	B	401	EDO	O2-C2-C1	-2.32	95.23	111.91
3	B	406[B]	GXV	O2-C2-C3	-2.08	104.92	109.22
2	C	403	EDO	O1-C1-C2	-2.05	97.13	111.91

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	403[B]	GXV	O2-C2-C3-O3
3	A	403[B]	GXV	C1-C2-C3-O3
3	B	406[B]	GXV	O2-C2-C3-O3
3	C	404[B]	GXV	O2-C2-C3-O3
3	C	404[B]	GXV	C1-C2-C3-O3
3	D	403[A]	GXV	O2-C2-C3-O3
3	D	403[B]	GXV	O2-C2-C3-O3
3	A	403[A]	GXV	C1-C2-C3-O3
3	B	406[B]	GXV	C1-C2-C3-O3
3	D	403[A]	GXV	C1-C2-C3-O3
2	B	404	EDO	O1-C1-C2-O2
3	C	404[A]	GXV	O2-C2-C3-O3
2	A	402	EDO	O1-C1-C2-O2
2	B	403	EDO	O1-C1-C2-O2
2	C	402	EDO	O1-C1-C2-O2
2	C	403	EDO	O1-C1-C2-O2
3	D	403[B]	GXV	C1-C2-C3-O3

There are no ring outliers.

9 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	403	EDO	5	0
2	B	404	EDO	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	406[A]	GXV	1	0
3	A	403[A]	GXV	1	0
3	D	403[B]	GXV	2	0
5	B	405	GOL	4	0
6	D	405	PYR	3	0
2	A	402	EDO	1	0
6	B	408	PYR	3	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^{th} 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	298/343 (86%)	-0.16	0 100 100	9, 16, 31, 46	0
1	B	298/343 (86%)	-0.25	0 100 100	8, 13, 25, 37	0
1	C	298/343 (86%)	-0.23	1 (0%) 94 93	10, 15, 29, 46	0
1	D	298/343 (86%)	-0.31	0 100 100	9, 14, 27, 38	0
All	All	1192/1372 (86%)	-0.24	1 (0%) 95 95	8, 14, 28, 46	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	309	CYS	3.2

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

There are no monosaccharides in this entry.

6.4 Ligands

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, 95^{th} 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
5	GOL	B	405	6/6	0.73	0.23	33,37,38,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	EDO	B	403	4/4	0.79	0.24	35,39,40,44	0
6	PYR	B	408	6/6	0.79	0.22	25,28,30,31	0
6	PYR	D	405	6/6	0.81	0.22	24,28,30,32	0
2	EDO	C	402	4/4	0.88	0.18	27,28,29,32	0
3	GXV	A	403[B]	6/6	0.89	0.26	14,19,20,25	6
3	GXV	A	403[A]	6/6	0.89	0.26	13,13,14,14	6
2	EDO	C	401	4/4	0.90	0.14	17,19,21,24	0
3	GXV	C	404[A]	6/6	0.90	0.28	11,12,13,13	6
3	GXV	C	404[B]	6/6	0.90	0.28	15,19,21,21	6
2	EDO	A	401	4/4	0.91	0.14	18,22,23,25	0
3	GXV	B	406[B]	6/6	0.93	0.26	19,24,25,27	6
3	GXV	B	406[A]	6/6	0.93	0.26	14,16,17,18	6
2	EDO	C	403	4/4	0.94	0.32	29,29,31,33	0
3	GXV	D	403[A]	6/6	0.94	0.25	18,26,26,28	6
3	GXV	D	403[B]	6/6	0.94	0.25	14,16,17,18	6
2	EDO	D	402[B]	4/4	0.95	0.17	17,17,18,18	4
2	EDO	B	404	4/4	0.95	0.18	14,23,27,33	0
2	EDO	B	401	4/4	0.95	0.13	14,21,22,25	0
2	EDO	B	402	4/4	0.95	0.12	18,18,20,22	0
2	EDO	A	402	4/4	0.95	0.19	23,28,30,34	0
2	EDO	D	402[A]	4/4	0.95	0.17	10,10,11,11	4
2	EDO	D	401	4/4	0.96	0.11	20,21,23,25	0
4	MG	A	404[C]	1/1	0.98	0.19	11,11,11,11	1
4	MG	A	404[A]	1/1	0.98	0.19	12,12,12,12	1
4	MG	C	405[B]	1/1	0.99	0.15	11,11,11,11	1
4	MG	D	404[A]	1/1	0.99	0.14	10,10,10,10	0
4	MG	D	404[B]	1/1	0.99	0.14	15,15,15,15	1
4	MG	B	407[A]	1/1	0.99	0.14	9,9,9,9	0
4	MG	B	407[B]	1/1	0.99	0.14	11,11,11,11	1
4	MG	C	405[A]	1/1	0.99	0.15	9,9,9,9	1

6.5 Other polymers (i)

There are no such residues in this entry.