Full wwPDB X-ray Structure Validation Report (i)

Jun 22, 2024 – 11:43 AM EDT

PDB ID	:	4ONV
Title	:	Crystal structure of YagE, a KDG aldolase protein in complex with 2-Keto-3-deoxy gluconate
Authors	:	Manoj Kumar, P.; Bhaskar, V.; Manicka, S.; Krishnaswamy, S.
Deposited on	:	2014-01-29
Resolution	:	2.57 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:

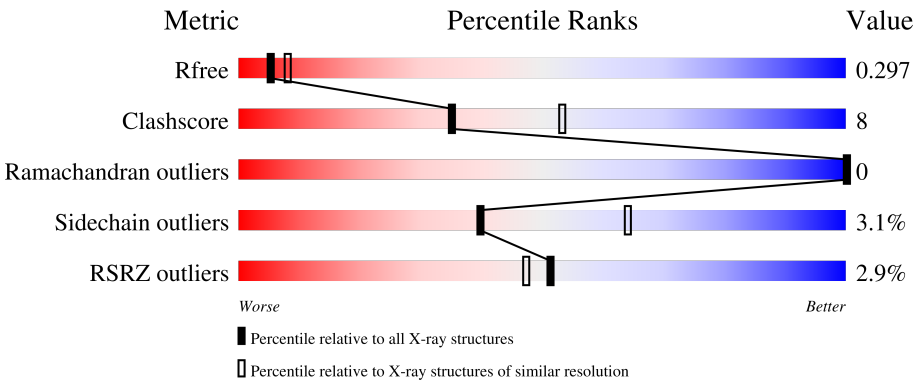
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.57 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	3676 (2.60-2.56)
Clashscore	141614	4049 (2.60-2.56)
Ramachandran outliers	138981	3979 (2.60-2.56)
Sidechain outliers	138945	3979 (2.60-2.56)
RSRZ outliers	127900	3614 (2.60-2.56)

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	3% 77% 10% • 13%
1	B	343	2% 76% 11% • 13%
1	C	343	3% 75% 12% 13%
1	D	343	2% 77% 9% 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	C	403	-	-	X	-
2	EDO	D	402	-	-	X	-
3	GOL	B	405	-	X	X	-
3	GOL	B	408	-	X	X	-
3	GOL	C	406	-	-	-	X
4	KDG	A	406	-	-	X	-
4	KDG	C	408	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 9430 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
			Total	C	N	O	S			
1	A	298	2259	1446	386	421	6	0	0	0
			Total	C	N	O	S			
1	B	298	2260	1447	387	420	6	0	0	0
			Total	C	N	O	S			
1	C	298	2268	1451	389	422	6	0	1	0
			Total	C	N	O	S			
1	D	298	2261	1447	387	421	6	0	0	0

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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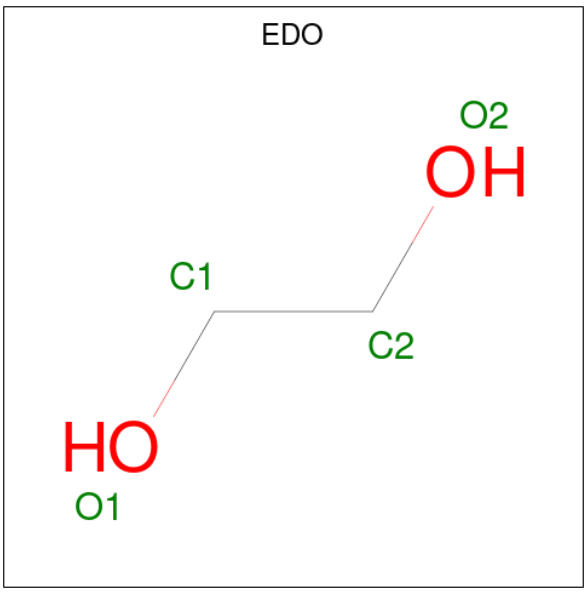
Chain	Residue	Modelled	Actual	Comment	Reference
D	7	LEU	-	EXPRESSION TAG	UNP P75682
D	310	CYS	-	EXPRESSION TAG	UNP P75682
D	311	GLY	-	EXPRESSION TAG	UNP P75682
D	312	ARG	-	EXPRESSION TAG	UNP P75682
D	313	THR	-	EXPRESSION TAG	UNP P75682
D	314	ARG	-	EXPRESSION TAG	UNP P75682
D	315	ALA	-	EXPRESSION TAG	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
			Total	C	O		
2	A	1	4	2	2	0	0
2	B	1	4	2	2	0	0
2	B	1	4	2	2	0	0

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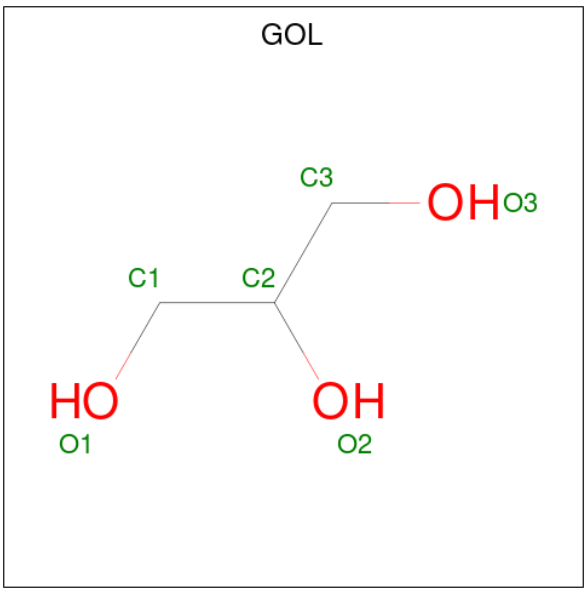
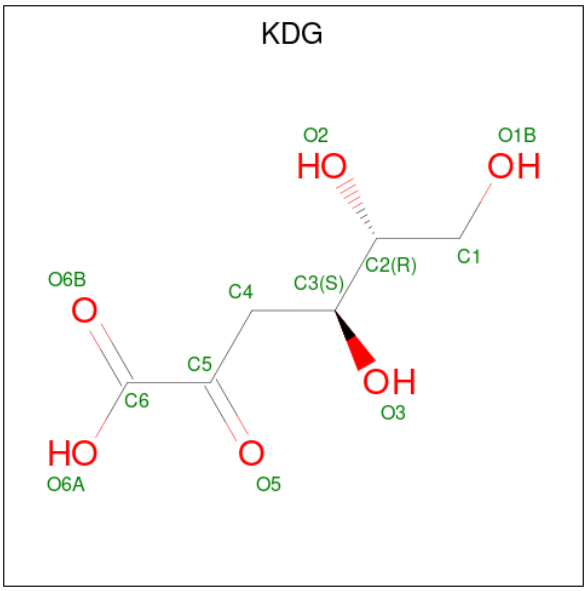
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O			
2	B	1	4	2	2		0	0
			Total	C	O			
2	B	1	4	2	2		0	0
			Total	C	O			
2	C	1	4	2	2		0	0
			Total	C	O			
2	C	1	4	2	2		0	0
			Total	C	O			
2	C	1	4	2	2		0	0
			Total	C	O			
2	C	1	4	2	2		0	0
			Total	C	O			
2	C	1	4	2	2		0	0
			Total	C	O			
2	C	1	4	2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

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 4 is 2-KETO-3-DEOXYGLUCONATE (three-letter code: KDG) (formula: $C_6H_{10}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	A	1	11	6	5	0	0
			Total	C	O		
4	B	1	11	6	5	0	0
			Total	C	O		
4	C	1	11	6	5	0	0
			Total	C	O		
4	D	1	11	6	5	0	0

- Molecule 5 is water.

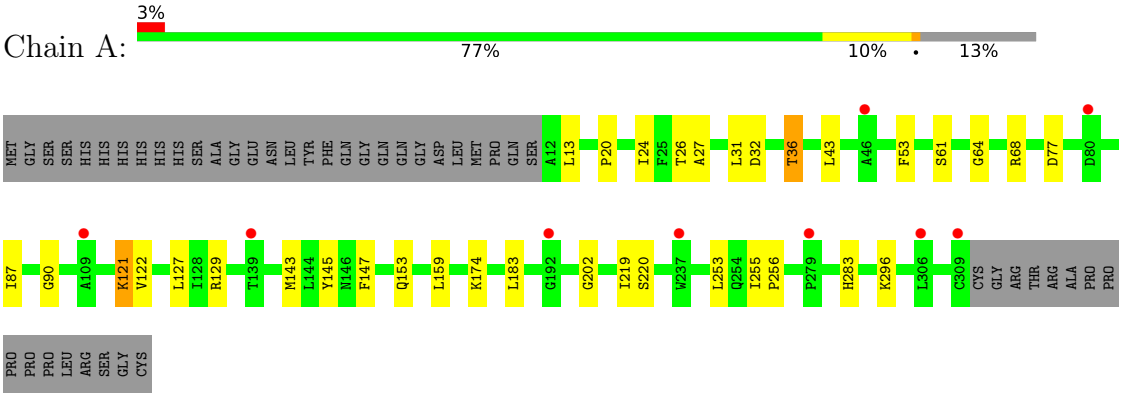
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	48	48	48	0	0
			Total	O		
5	B	59	59	59	0	0
			Total	O		
5	C	41	41	41	0	0
			Total	O		
5	D	52	52	52	0	0

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.

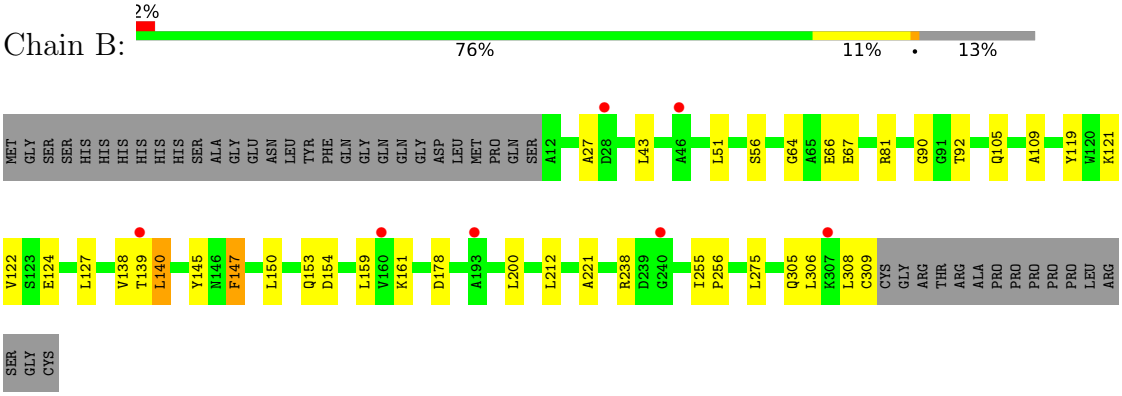
• Molecule 1: Probable 2-keto-3-deoxy-galactonate aldolase YagE

Chain A:



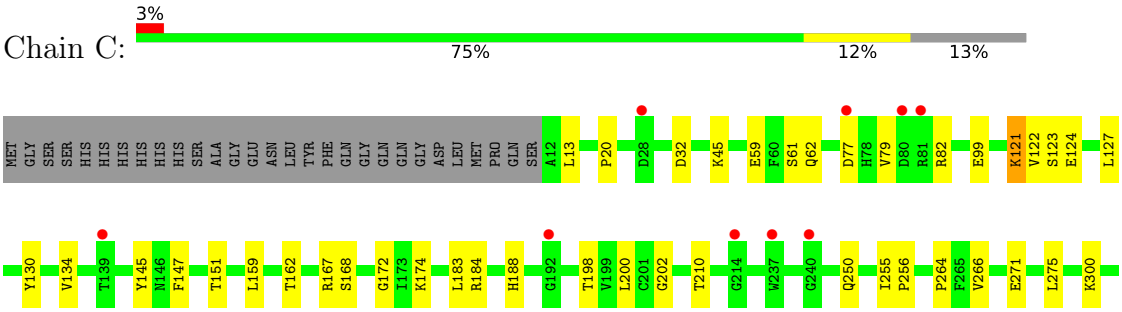
• Molecule 1: Probable 2-keto-3-deoxy-galactonate aldolase YagE

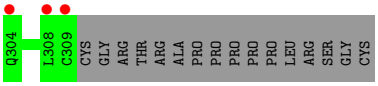
Chain B:



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

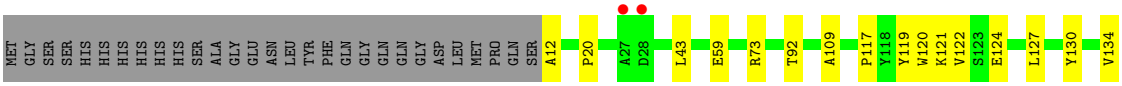
Chain C:

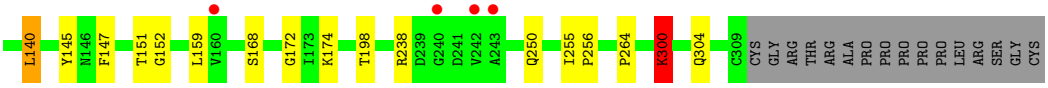




• Molecule 1: Probable 2-keto-3-deoxy-galactonate aldolase YagE

Chain D:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	141.17Å 155.41Å 55.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.79 – 2.57 19.79 – 2.57	Depositor EDS
% Data completeness (in resolution range)	98.9 (19.79-2.57) 99.2 (19.79-2.57)	Depositor EDS
R_{merge}	0.41	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.62 (at 2.56Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.247 , 0.284 0.257 , 0.297	Depositor DCC
R_{free} test set	1970 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	23.1	Xtriage
Anisotropy	0.210	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 38.8	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	0.90	EDS
Total number of atoms	9430	wwPDB-VP
Average B, all atoms (Å^2)	22.0	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 45.08 % 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 1.3923e-04. 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: KDG, EDO, GOL

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	0.58	0/2307	0.74	0/3144
1	B	0.59	0/2308	0.75	0/3145
1	C	0.59	0/2316	0.75	0/3155
1	D	0.59	0/2309	0.74	1/3147 (0.0%)
All	All	0.59	0/9240	0.74	1/12591 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	300	LYS	CA-CB-CG	6.46	127.60	113.40

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	2259	0	2272	35	0
1	B	2260	0	2283	44	0
1	C	2268	0	2286	38	0
1	D	2261	0	2280	33	0
2	A	4	0	6	2	0
2	B	16	0	24	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	24	0	36	6	0
2	D	16	0	24	7	0
3	A	24	0	32	1	0
3	B	24	0	32	14	0
3	C	6	0	8	3	0
3	D	24	0	32	5	0
4	A	11	0	9	11	0
4	B	11	0	9	5	0
4	C	11	0	9	9	0
4	D	11	0	9	2	0
5	A	48	0	0	9	0
5	B	59	0	0	12	0
5	C	41	0	0	8	0
5	D	52	0	0	10	0
All	All	9430	0	9351	153	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 8.

All (153) 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:87:ILE:HD13	5:A:528:HOH:O	1.41	1.17
1:C:61:SER:O	1:D:92:THR:HG23	1.42	1.16
1:A:53:PHE:HB2	5:A:528:HOH:O	1.56	1.03
1:A:174:LYS:HE2	4:A:406:KDG:O3	1.62	0.99
1:C:121:LYS:HE2	1:C:151:THR:O	1.71	0.91
1:C:79:VAL:O	1:C:82:ARG:HD3	1.74	0.88
1:A:20:PRO:HG3	4:A:406:KDG:H4C1	1.53	0.87
1:A:174:LYS:CE	4:A:406:KDG:O3	2.23	0.87
1:B:178:ASP:O	2:B:404:EDO:H21	1.74	0.86
1:B:64:GLY:HA3	3:B:405:GOL:H2	1.58	0.86
1:C:275:LEU:CD2	5:C:527:HOH:O	2.23	0.85
1:C:271:GLU:O	1:C:275:LEU:HD23	1.76	0.85
1:B:154:ASP:H	3:B:408:GOL:H32	1.40	0.84
1:B:238:ARG:NH2	3:B:406:GOL:O2	2.13	0.82
1:C:124:GLU:OE2	2:C:403:EDO:C1	2.28	0.82
1:D:250:GLN:HB2	5:D:529:HOH:O	1.78	0.82
1:A:121:LYS:HG3	1:A:153:GLN:HB2	1.63	0.80
1:B:66:GLU:H	3:B:405:GOL:HO2	1.26	0.79
1:C:168:SER:HB3	3:C:406:GOL:H2	1.66	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:59:GLU:HG3	5:D:524:HOH:O	1.82	0.78
1:C:124:GLU:OE2	2:C:403:EDO:H11	1.83	0.78
4:B:409:KDG:H4C1	5:B:642:HOH:O	1.86	0.76
1:B:66:GLU:N	3:B:405:GOL:O2	2.19	0.76
1:B:67:GLU:HG3	3:B:405:GOL:H11	1.69	0.75
1:A:283:HIS:HB2	5:A:508:HOH:O	1.87	0.75
1:A:32:ASP:O	1:A:36:THR:CG2	2.35	0.74
1:B:309:CYS:C	5:B:628:HOH:O	2.27	0.73
1:C:123:SER:HA	2:C:405:EDO:H12	1.71	0.73
5:C:524:HOH:O	1:D:92:THR:HG21	1.91	0.70
1:D:121:LYS:HE3	1:D:152:GLY:HA3	1.73	0.70
1:B:67:GLU:HG3	3:B:405:GOL:C1	2.22	0.69
1:A:296:LYS:HE3	3:A:403:GOL:H31	1.73	0.69
1:D:92:THR:OG1	2:D:402:EDO:H22	1.92	0.69
4:A:406:KDG:O6B	5:A:532:HOH:O	2.10	0.69
1:C:61:SER:O	1:D:92:THR:CG2	2.32	0.69
1:B:124:GLU:H	2:B:403:EDO:H21	1.57	0.68
4:A:406:KDG:H4C2	5:A:532:HOH:O	1.94	0.67
1:B:27:ALA:CB	5:B:636:HOH:O	2.41	0.67
1:B:154:ASP:H	3:B:408:GOL:C3	2.07	0.67
1:A:174:LYS:NZ	4:A:406:KDG:O3	2.27	0.67
1:A:61:SER:HB2	1:B:92:THR:HG21	1.77	0.66
1:A:202:GLY:O	4:A:406:KDG:H3	1.95	0.65
4:C:408:KDG:H4C2	5:C:533:HOH:O	1.96	0.65
4:B:409:KDG:C4	5:B:642:HOH:O	2.41	0.65
1:A:202:GLY:O	4:A:406:KDG:C3	2.45	0.64
1:B:306:LEU:O	1:B:308:LEU:HD12	1.97	0.64
1:A:32:ASP:O	1:A:36:THR:HG23	1.96	0.64
1:C:124:GLU:OE2	2:C:403:EDO:H12	1.97	0.63
1:B:90:GLY:H	2:B:402:EDO:H21	1.64	0.62
1:D:120:TRP:HB2	2:D:402:EDO:H12	1.83	0.61
1:A:32:ASP:O	1:A:36:THR:HG22	2.00	0.60
1:C:202:GLY:O	4:C:408:KDG:H3	2.01	0.59
1:D:73:ARG:HB2	3:D:408:GOL:O2	2.02	0.59
1:C:20:PRO:HG3	4:C:408:KDG:C4	2.33	0.58
1:B:67:GLU:CG	3:B:405:GOL:H11	2.33	0.58
1:D:12:ALA:N	5:D:547:HOH:O	2.37	0.58
1:B:81:ARG:HD2	5:B:632:HOH:O	2.03	0.58
1:B:124:GLU:N	2:B:403:EDO:H21	2.17	0.58
1:D:168:SER:HB3	5:D:532:HOH:O	2.03	0.57
4:C:408:KDG:O6B	5:C:533:HOH:O	2.17	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:127:LEU:HD23	1:D:159:LEU:HD21	1.87	0.57
1:A:127:LEU:HD23	1:A:159:LEU:HD21	1.86	0.56
1:B:90:GLY:H	2:B:402:EDO:C2	2.18	0.56
1:C:127:LEU:HD23	1:C:159:LEU:HD21	1.86	0.56
1:D:124:GLU:H	2:D:405:EDO:H12	1.71	0.56
1:B:153:GLN:HA	3:B:408:GOL:H31	1.87	0.56
1:B:127:LEU:HD23	1:B:159:LEU:HD21	1.88	0.55
1:B:306:LEU:HB2	1:B:308:LEU:HD13	1.87	0.55
1:D:238:ARG:NH2	3:D:407:GOL:O2	2.37	0.54
1:B:306:LEU:O	1:B:308:LEU:CD1	2.55	0.54
1:C:174:LYS:NZ	4:C:408:KDG:O3	2.40	0.54
1:D:119:TYR:HB3	2:D:402:EDO:H11	1.90	0.54
1:C:20:PRO:HG3	4:C:408:KDG:H4C1	1.89	0.54
1:C:183:LEU:HD23	1:C:210:THR:OG1	2.09	0.53
1:C:162:THR:OG1	2:C:403:EDO:O2	2.27	0.52
1:D:109:ALA:O	1:D:140:LEU:HD21	2.09	0.52
1:A:26:THR:HG22	1:A:27:ALA:N	2.23	0.52
1:A:174:LYS:HE3	1:A:219:ILE:CG2	2.40	0.52
1:D:117:PRO:HB3	2:D:402:EDO:H21	1.91	0.52
1:D:124:GLU:H	2:D:405:EDO:C1	2.22	0.52
1:B:105:GLN:NE2	1:B:139:THR:H	2.08	0.51
1:D:130:TYR:O	1:D:134:VAL:HG13	2.10	0.51
1:B:81:ARG:NH1	5:B:622:HOH:O	2.43	0.51
3:D:404:GOL:C1	5:D:543:HOH:O	2.60	0.50
1:A:53:PHE:CB	5:A:528:HOH:O	2.35	0.50
1:C:130:TYR:O	1:C:134:VAL:HG13	2.12	0.50
1:C:183:LEU:CD2	1:C:210:THR:OG1	2.60	0.50
1:D:174:LYS:NZ	4:D:409:KDG:O3	2.45	0.50
1:A:31:LEU:CD1	1:A:36:THR:HG21	2.42	0.49
1:C:188:HIS:CE1	5:C:522:HOH:O	2.63	0.49
1:B:109:ALA:O	1:B:140:LEU:HD21	2.11	0.49
1:B:27:ALA:HB2	5:B:636:HOH:O	2.09	0.49
1:B:122:VAL:HG12	1:B:127:LEU:HB2	1.94	0.49
1:B:154:ASP:N	3:B:408:GOL:H32	2.18	0.49
1:D:122:VAL:HB	5:D:539:HOH:O	2.11	0.49
1:D:152:GLY:HA3	5:D:536:HOH:O	2.13	0.49
1:A:202:GLY:O	4:A:406:KDG:C2	2.61	0.49
1:B:122:VAL:HB	5:B:603:HOH:O	2.11	0.49
1:B:27:ALA:HB3	5:B:636:HOH:O	2.07	0.48
1:C:13:LEU:HD12	1:C:13:LEU:N	2.29	0.48
1:D:122:VAL:HG12	1:D:127:LEU:HB2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:122:VAL:HG12	1:C:127:LEU:HB2	1.95	0.47
1:B:67:GLU:HG3	3:B:405:GOL:H12	1.97	0.47
1:A:20:PRO:HG3	4:A:406:KDG:C4	2.35	0.47
1:B:221:ALA:HB2	4:B:409:KDG:H1C1	1.96	0.47
1:B:105:GLN:HE22	1:B:139:THR:H	1.63	0.46
1:B:67:GLU:CD	3:B:405:GOL:H11	2.36	0.46
1:D:121:LYS:HE3	1:D:151:THR:O	2.15	0.46
1:D:20:PRO:HG3	4:D:409:KDG:H4C1	1.97	0.46
1:D:255:ILE:N	1:D:256:PRO:CD	2.80	0.45
1:B:275:LEU:HG	5:B:629:HOH:O	2.16	0.45
1:C:167:ARG:HA	3:C:406:GOL:H12	1.99	0.45
1:D:300:LYS:HE3	1:D:304:GLN:NE2	2.31	0.45
1:C:122:VAL:HB	5:C:526:HOH:O	2.16	0.45
1:C:174:LYS:HE2	4:C:408:KDG:O3	2.16	0.45
1:A:13:LEU:HD12	1:A:13:LEU:N	2.32	0.45
1:D:92:THR:OG1	2:D:402:EDO:C2	2.63	0.45
1:C:59:GLU:HG3	1:C:266:VAL:HG21	1.99	0.44
4:B:409:KDG:H4C2	5:B:642:HOH:O	2.14	0.44
1:C:122:VAL:HG22	1:D:264:PRO:HD3	1.99	0.44
1:B:147:PHE:CE1	1:B:150:LEU:HD12	2.52	0.44
1:A:253:LEU:O	1:C:184:ARG:HD3	2.17	0.44
1:A:255:ILE:N	1:A:256:PRO:CD	2.80	0.44
1:B:306:LEU:CB	1:B:308:LEU:HD13	2.48	0.44
1:B:255:ILE:N	1:B:256:PRO:CD	2.81	0.44
1:A:24:ILE:HB	1:A:36:THR:HG22	1.99	0.43
1:B:56:SER:N	4:B:409:KDG:O6B	2.51	0.43
1:B:119:TYR:O	1:B:121:LYS:HE3	2.18	0.43
1:C:255:ILE:N	1:C:256:PRO:CD	2.82	0.43
1:A:31:LEU:HD11	1:A:36:THR:HG21	2.01	0.43
1:A:77:ASP:HA	5:A:526:HOH:O	2.19	0.43
1:C:202:GLY:O	4:C:408:KDG:H2	2.18	0.43
1:D:172:GLY:HA3	1:D:198:THR:HG22	2.01	0.42
1:A:90:GLY:HA3	2:A:401:EDO:O1	2.18	0.42
1:A:220:SER:HA	4:A:406:KDG:H3	2.02	0.42
1:A:68:ARG:NE	5:A:507:HOH:O	2.45	0.42
1:A:174:LYS:HE3	1:A:219:ILE:HG22	2.01	0.42
1:C:174:LYS:CE	4:C:408:KDG:O3	2.67	0.42
1:A:53:PHE:HD2	5:A:528:HOH:O	2.02	0.42
1:B:212:LEU:CD2	5:D:529:HOH:O	2.67	0.42
1:C:62:GLN:HG2	5:C:510:HOH:O	2.19	0.42
1:C:172:GLY:HA3	1:C:198:THR:HG22	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:264:PRO:HD3	1:D:122:VAL:HG22	2.02	0.42
1:A:64:GLY:HA2	5:B:634:HOH:O	2.20	0.41
1:A:90:GLY:N	2:A:401:EDO:O1	2.54	0.41
1:C:32:ASP:CG	2:C:407:EDO:HO1	2.23	0.41
1:B:66:GLU:HB2	3:B:405:GOL:O2	2.19	0.41
1:C:300:LYS:HB3	5:C:530:HOH:O	2.20	0.41
3:D:404:GOL:H12	5:D:543:HOH:O	2.20	0.40
1:C:168:SER:H	3:C:406:GOL:C1	2.35	0.40
1:D:152:GLY:CA	5:D:536:HOH:O	2.67	0.40
1:B:105:GLN:HE21	1:B:138:VAL:HB	1.86	0.40
1:D:168:SER:HB2	3:D:406:GOL:H32	2.04	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	296/343 (86%)	290 (98%)	6 (2%)	0	100	100
1	B	296/343 (86%)	289 (98%)	7 (2%)	0	100	100
1	C	297/343 (87%)	290 (98%)	7 (2%)	0	100	100
1	D	296/343 (86%)	289 (98%)	7 (2%)	0	100	100
All	All	1185/1372 (86%)	1158 (98%)	27 (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	240/280 (86%)	231 (96%)	9 (4%)	33	57
1	B	242/280 (86%)	234 (97%)	8 (3%)	38	61
1	C	242/280 (86%)	234 (97%)	8 (3%)	38	61
1	D	242/280 (86%)	237 (98%)	5 (2%)	53	75
All	All	966/1120 (86%)	936 (97%)	30 (3%)	40	64

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	THR
1	A	43	LEU
1	A	121	LYS
1	A	122	VAL
1	A	129	ARG
1	A	143	MET
1	A	145	TYR
1	A	147	PHE
1	A	183	LEU
1	B	43	LEU
1	B	51	LEU
1	B	140	LEU
1	B	145	TYR
1	B	147	PHE
1	B	161	LYS
1	B	200	LEU
1	B	305	GLN
1	C	45	LYS
1	C	77	ASP
1	C	99	GLU
1	C	121	LYS
1	C	145	TYR
1	C	147	PHE
1	C	200	LEU
1	C	250	GLN
1	D	43	LEU
1	D	140	LEU
1	D	145	TYR
1	D	147	PHE
1	D	300	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	62	GLN
1	A	188	HIS
1	B	62	GLN
1	B	105	GLN
1	B	188	HIS
1	C	62	GLN
1	D	126	ASN
1	D	257	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

32 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	GOL	B	408	-	5,5,5	0.62	0	5,5,5	1.68	2 (40%)
2	EDO	A	401	-	3,3,3	0.31	0	2,2,2	0.47	0
3	GOL	B	407	-	5,5,5	0.62	0	5,5,5	0.71	0
3	GOL	A	405	-	5,5,5	0.73	0	5,5,5	0.87	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	GOL	A	404	-	5,5,5	0.63	0	5,5,5	0.45	0
4	KDG	A	406	1	10,10,11	0.90	0	11,12,14	1.30	1 (9%)
2	EDO	B	403	-	3,3,3	0.59	0	2,2,2	0.63	0
2	EDO	D	405	-	3,3,3	0.72	0	2,2,2	0.24	0
2	EDO	B	401	-	3,3,3	0.58	0	2,2,2	0.40	0
4	KDG	B	409	1	10,10,11	0.86	0	11,12,14	1.42	3 (27%)
4	KDG	C	408	1	10,10,11	0.80	0	11,12,14	1.60	2 (18%)
3	GOL	A	402	-	5,5,5	0.57	0	5,5,5	0.49	0
3	GOL	D	406	-	5,5,5	0.66	0	5,5,5	0.67	0
2	EDO	B	402	-	3,3,3	0.24	0	2,2,2	1.12	0
3	GOL	B	405	-	5,5,5	0.51	0	5,5,5	1.55	2 (40%)
3	GOL	D	408	-	5,5,5	0.59	0	5,5,5	0.79	0
3	GOL	B	406	-	5,5,5	0.40	0	5,5,5	0.26	0
2	EDO	C	404	-	3,3,3	0.58	0	2,2,2	0.23	0
4	KDG	D	409	1	10,10,11	0.91	0	11,12,14	1.06	1 (9%)
2	EDO	D	402	-	3,3,3	0.44	0	2,2,2	0.45	0
2	EDO	C	401	-	3,3,3	0.38	0	2,2,2	0.24	0
3	GOL	C	406	-	5,5,5	0.60	0	5,5,5	0.82	0
2	EDO	C	407	-	3,3,3	0.46	0	2,2,2	0.39	0
3	GOL	D	407	-	5,5,5	0.55	0	5,5,5	0.76	0
2	EDO	B	404	-	3,3,3	0.55	0	2,2,2	0.27	0
2	EDO	C	403	-	3,3,3	0.48	0	2,2,2	0.08	0
2	EDO	C	405	-	3,3,3	0.74	0	2,2,2	0.03	0
2	EDO	D	401	-	3,3,3	0.59	0	2,2,2	0.62	0
2	EDO	D	403	-	3,3,3	0.29	0	2,2,2	0.42	0
3	GOL	D	404	-	5,5,5	0.54	0	5,5,5	0.62	0
3	GOL	A	403	-	5,5,5	0.92	0	5,5,5	1.31	0
2	EDO	C	402	-	3,3,3	0.62	0	2,2,2	0.25	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
3	GOL	B	408	-	-	4/4/4/4	-
2	EDO	A	401	-	-	1/1/1/1	-
3	GOL	B	407	-	-	2/4/4/4	-
3	GOL	A	405	-	-	4/4/4/4	-
3	GOL	A	404	-	-	4/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	KDG	A	406	1	-	3/11/11/14	-
2	EDO	B	403	-	-	1/1/1/1	-
2	EDO	D	405	-	-	1/1/1/1	-
2	EDO	B	401	-	-	1/1/1/1	-
4	KDG	B	409	1	-	5/11/11/14	-
4	KDG	C	408	1	-	8/11/11/14	-
3	GOL	A	402	-	-	4/4/4/4	-
3	GOL	D	406	-	-	4/4/4/4	-
2	EDO	B	402	-	-	1/1/1/1	-
3	GOL	B	405	-	-	4/4/4/4	-
3	GOL	D	408	-	-	3/4/4/4	-
3	GOL	B	406	-	-	4/4/4/4	-
2	EDO	C	404	-	-	1/1/1/1	-
4	KDG	D	409	1	-	7/11/11/14	-
2	EDO	D	402	-	-	1/1/1/1	-
2	EDO	C	401	-	-	1/1/1/1	-
3	GOL	C	406	-	-	4/4/4/4	-
2	EDO	C	407	-	-	1/1/1/1	-
3	GOL	D	407	-	-	0/4/4/4	-
2	EDO	B	404	-	-	1/1/1/1	-
2	EDO	C	403	-	-	1/1/1/1	-
2	EDO	C	405	-	-	1/1/1/1	-
2	EDO	D	401	-	-	1/1/1/1	-
2	EDO	D	403	-	-	1/1/1/1	-
3	GOL	D	404	-	-	0/4/4/4	-
3	GOL	A	403	-	-	2/4/4/4	-
2	EDO	C	402	-	-	1/1/1/1	-

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	408	KDG	C4-C5-C6	3.14	120.84	112.51
4	C	408	KDG	O6A-C6-C5	2.49	122.02	114.03
4	B	409	KDG	O2-C2-C3	2.47	114.79	109.72
3	B	405	GOL	C3-C2-C1	2.42	121.11	111.70
3	B	408	GOL	O3-C3-C2	2.34	121.41	110.20
3	B	408	GOL	O1-C1-C2	2.34	121.40	110.20
4	A	406	KDG	C4-C5-C6	2.17	118.26	112.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	409	KDG	O2-C2-C3	2.09	114.01	109.72
4	B	409	KDG	C1-C2-C3	-2.07	108.62	113.11
4	B	409	KDG	O6A-C6-C5	2.06	120.65	114.03
3	B	405	GOL	O1-C1-C2	2.01	119.82	110.20

There are no chirality outliers.

All (77) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	402	GOL	C1-C2-C3-O3
3	A	402	GOL	O2-C2-C3-O3
3	A	404	GOL	C1-C2-C3-O3
3	A	405	GOL	O1-C1-C2-C3
3	B	405	GOL	C1-C2-C3-O3
3	B	406	GOL	O1-C1-C2-C3
3	B	406	GOL	C1-C2-C3-O3
3	B	408	GOL	O1-C1-C2-C3
3	C	406	GOL	O1-C1-C2-O2
3	C	406	GOL	O1-C1-C2-C3
3	D	406	GOL	O1-C1-C2-C3
3	D	406	GOL	C1-C2-C3-O3
3	D	408	GOL	O1-C1-C2-C3
4	A	406	KDG	O3-C3-C4-C5
4	A	406	KDG	C3-C4-C5-C6
4	B	409	KDG	O3-C3-C4-C5
4	C	408	KDG	C1-C2-C3-O3
4	C	408	KDG	C1-C2-C3-C4
4	C	408	KDG	O2-C2-C3-C4
4	C	408	KDG	O3-C3-C4-C5
4	D	409	KDG	C1-C2-C3-C4
4	D	409	KDG	O2-C2-C3-C4
4	D	409	KDG	O3-C3-C4-C5
4	D	409	KDG	C3-C4-C5-C6
4	D	409	KDG	O1B-C1-C2-O2
4	D	409	KDG	O1B-C1-C2-C3
3	A	402	GOL	O1-C1-C2-O2
3	A	405	GOL	O2-C2-C3-O3
3	C	406	GOL	O2-C2-C3-O3
3	D	406	GOL	O2-C2-C3-O3
3	D	408	GOL	O1-C1-C2-O2
4	C	408	KDG	C2-C3-C4-C5
3	A	402	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
3	A	403	GOL	C1-C2-C3-O3
3	A	404	GOL	O1-C1-C2-C3
3	A	405	GOL	C1-C2-C3-O3
3	B	405	GOL	O1-C1-C2-C3
3	C	406	GOL	C1-C2-C3-O3
3	D	408	GOL	C1-C2-C3-O3
3	A	403	GOL	O2-C2-C3-O3
3	A	404	GOL	O2-C2-C3-O3
3	B	405	GOL	O1-C1-C2-O2
3	B	406	GOL	O1-C1-C2-O2
3	D	406	GOL	O1-C1-C2-O2
2	B	401	EDO	O1-C1-C2-O2
2	B	403	EDO	O1-C1-C2-O2
2	C	403	EDO	O1-C1-C2-O2
2	C	404	EDO	O1-C1-C2-O2
2	C	405	EDO	O1-C1-C2-O2
2	D	402	EDO	O1-C1-C2-O2
3	A	404	GOL	O1-C1-C2-O2
3	B	405	GOL	O2-C2-C3-O3
2	A	401	EDO	O1-C1-C2-O2
4	C	408	KDG	O2-C2-C3-O3
4	A	406	KDG	C2-C3-C4-C5
4	B	409	KDG	C1-C2-C3-O3
3	B	406	GOL	O2-C2-C3-O3
3	B	408	GOL	O1-C1-C2-O2
2	B	404	EDO	O1-C1-C2-O2
2	D	403	EDO	O1-C1-C2-O2
4	C	408	KDG	O1B-C1-C2-O2
3	B	408	GOL	O2-C2-C3-O3
3	B	407	GOL	C1-C2-C3-O3
4	B	409	KDG	O1B-C1-C2-O2
4	B	409	KDG	C3-C4-C5-C6
3	A	405	GOL	O1-C1-C2-O2
4	D	409	KDG	C2-C3-C4-C5
2	C	401	EDO	O1-C1-C2-O2
3	B	408	GOL	C1-C2-C3-O3
3	B	407	GOL	O2-C2-C3-O3
2	B	402	EDO	O1-C1-C2-O2
2	D	401	EDO	O1-C1-C2-O2
4	B	409	KDG	C2-C3-C4-C5
2	C	402	EDO	O1-C1-C2-O2
2	C	407	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
2	D	405	EDO	O1-C1-C2-O2
4	C	408	KDG	C3-C4-C5-C6

There are no ring outliers.

22 monomers are involved in 70 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	408	GOL	4	0
2	A	401	EDO	2	0
4	A	406	KDG	11	0
2	B	403	EDO	2	0
2	D	405	EDO	2	0
4	B	409	KDG	5	0
4	C	408	KDG	9	0
3	D	406	GOL	1	0
2	B	402	EDO	2	0
3	B	405	GOL	9	0
3	D	408	GOL	1	0
3	B	406	GOL	1	0
4	D	409	KDG	2	0
2	D	402	EDO	5	0
3	C	406	GOL	3	0
2	C	407	EDO	1	0
3	D	407	GOL	1	0
2	B	404	EDO	1	0
2	C	403	EDO	4	0
2	C	405	EDO	1	0
3	D	404	GOL	2	0
3	A	403	GOL	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 (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	298/343 (86%)	0.37	9 (3%)	50	46	14, 23, 37, 43	0
1	B	298/343 (86%)	0.25	7 (2%)	60	57	13, 20, 32, 45	0
1	C	298/343 (86%)	0.32	12 (4%)	38	34	12, 22, 38, 57	0
1	D	298/343 (86%)	0.30	6 (2%)	65	62	12, 21, 34, 47	0
All	All	1192/1372 (86%)	0.31	34 (2%)	51	47	12, 21, 36, 57	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	192	GLY	3.7
1	C	139	THR	3.2
1	D	240	GLY	3.1
1	B	46	ALA	2.9
1	A	192	GLY	2.9
1	D	243	ALA	2.7
1	B	240	GLY	2.7
1	C	309	CYS	2.7
1	B	139	THR	2.6
1	C	214	GLY	2.6
1	C	28	ASP	2.5
1	C	81	ARG	2.5
1	A	139	THR	2.5
1	C	304	GLN	2.4
1	A	309	CYS	2.4
1	A	306	LEU	2.4
1	D	28	ASP	2.4
1	C	240	GLY	2.4
1	C	237	TRP	2.4
1	B	28	ASP	2.3
1	A	237	TRP	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	46	ALA	2.3
1	C	77	ASP	2.2
1	D	27	ALA	2.2
1	C	80	ASP	2.2
1	B	193	ALA	2.2
1	B	160	VAL	2.2
1	D	242	VAL	2.2
1	D	160	VAL	2.1
1	A	279	PRO	2.1
1	A	80	ASP	2.1
1	B	307	LYS	2.1
1	A	109	ALA	2.0
1	C	308	LEU	2.0

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
3	GOL	A	403	6/6	0.58	0.39	29,31,32,32	0
3	GOL	B	407	6/6	0.63	0.37	40,41,42,43	0
3	GOL	D	406	6/6	0.63	0.28	35,37,40,40	0
3	GOL	D	404	6/6	0.66	0.33	36,39,41,42	0
3	GOL	D	408	6/6	0.66	0.31	37,43,43,46	0
3	GOL	B	405	6/6	0.72	0.40	25,31,31,33	0
3	GOL	D	407	6/6	0.73	0.28	31,35,38,40	0
3	GOL	C	406	6/6	0.73	0.45	32,33,34,34	0
3	GOL	A	404	6/6	0.75	0.34	28,31,34,35	0
3	GOL	A	402	6/6	0.75	0.25	37,39,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	EDO	C	403	4/4	0.77	0.31	31,32,32,33	0
2	EDO	D	405	4/4	0.78	0.28	19,19,19,20	0
2	EDO	B	403	4/4	0.79	0.29	25,26,27,28	0
4	KDG	A	406	11/12	0.80	0.33	15,17,18,18	11
4	KDG	C	408	11/12	0.80	0.29	17,19,20,20	11
3	GOL	A	405	6/6	0.81	0.33	35,37,39,39	0
4	KDG	B	409	11/12	0.83	0.22	30,35,39,42	0
2	EDO	D	401	4/4	0.83	0.36	25,25,26,27	0
2	EDO	C	404	4/4	0.84	0.20	31,34,35,35	0
2	EDO	C	405	4/4	0.84	0.25	24,24,25,26	0
2	EDO	B	404	4/4	0.84	0.16	33,34,35,36	0
4	KDG	D	409	11/12	0.84	0.21	25,29,31,33	0
2	EDO	C	407	4/4	0.85	0.18	32,33,35,36	0
2	EDO	C	402	4/4	0.85	0.38	19,19,20,20	0
3	GOL	B	408	6/6	0.86	0.30	20,20,21,21	0
3	GOL	B	406	6/6	0.86	0.19	29,31,35,37	0
2	EDO	D	402	4/4	0.87	0.31	18,19,19,19	0
2	EDO	B	402	4/4	0.90	0.23	16,17,17,18	0
2	EDO	B	401	4/4	0.91	0.13	27,27,28,28	0
2	EDO	D	403	4/4	0.93	0.23	24,24,26,29	0
2	EDO	A	401	4/4	0.94	0.18	26,27,28,28	0
2	EDO	C	401	4/4	0.95	0.12	23,23,23,25	0

6.5 Other polymers (i)

There are no such residues in this entry.