



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 07:17 PM GMT

PDB ID : 4OE7
Title : Crystal structure of YagE, a KDG aldolase protein, in complex with aldol condensed product of pyruvate and glyoxal
Authors : Manoj Kumar, P.; Baskar, V.; Manicka, S.; Krishnaswamy, S.
Deposited on : 2014-01-12
Resolution : 1.99 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

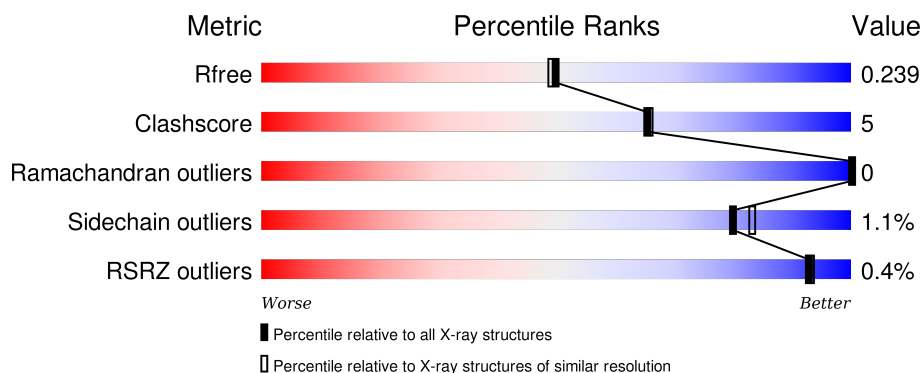
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	91344	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	343	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0; width: 100%; text-align: center;">%</div> <div style="position: absolute; top: 0; left: 0; width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 8%, green 79%, grey 13%);"></div> <div style="position: absolute; bottom: 0; left: 0; width: 100%; text-align: center;"> 79%8%13% </div> </div> </div>
1	B	343	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: 0; left: 0; width: 100%; height: 10px; background: linear-gradient(to right, green 80%, yellow 7%, orange 1%, grey 13%);"></div> <div style="position: absolute; bottom: 0; left: 0; width: 100%; text-align: center;"> 80%7%13% </div> </div> </div>
1	C	343	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: 0; left: 0; width: 100%; height: 10px; background: linear-gradient(to right, green 78%, yellow 8%, orange 1%, grey 13%);"></div> <div style="position: absolute; bottom: 0; left: 0; width: 100%; text-align: center;"> 78%8%13% </div> </div> </div>
1	D	343	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: 0; left: 0; width: 100%; height: 10px; background: linear-gradient(to right, green 81%, yellow 6%, orange 1%, grey 13%);"></div> <div style="position: absolute; bottom: 0; left: 0; width: 100%; text-align: center;"> 81%6%13% </div> </div> </div>

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	A	401	-	-	-	X
2	EDO	A	403	-	-	-	X
2	EDO	A	405	-	-	-	X
2	EDO	A	406	-	-	X	X
2	EDO	A	407	-	-	-	X
2	EDO	B	401	-	-	-	X
2	EDO	B	404	-	-	X	-
2	EDO	B	406	-	-	-	X
2	EDO	B	407	-	-	X	-
2	EDO	B	408	-	-	-	X
2	EDO	B	409	-	-	X	X
2	EDO	C	401	-	-	-	X
2	EDO	C	404	-	-	-	X
2	EDO	C	406	-	-	-	X
2	EDO	C	407	-	-	-	X
2	EDO	C	408	-	-	-	X
2	EDO	C	411	-	-	-	X
2	EDO	C	413	-	-	X	X
2	EDO	D	401	-	-	-	X
2	EDO	D	402	-	-	-	X
2	EDO	D	404	-	-	-	X
2	EDO	D	407	-	-	X	X
3	GOL	A	402	-	-	-	X
3	GOL	B	402	-	-	-	X
3	GOL	B	403	-	-	-	X
3	GOL	C	402	-	-	X	X
4	MG	C	403	-	-	-	X
5	GXT	A	409	-	-	X	X
6	PYR	A	410	-	-	-	X
6	PYR	C	412	-	-	-	X
7	GXP	B	410[A]	-	-	-	X
7	GXP	D	408[A]	-	-	-	X
8	GXS	B	411[B]	-	-	-	X
8	GXS	D	409[B]	-	-	-	X

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 9434 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	0	0
			2259	1446	386	421	6			
1	B	298	Total	C	N	O	S	0	0	0
			2260	1446	387	421	6			
1	C	298	Total	C	N	O	S	0	0	0
			2257	1445	385	421	6			
1	D	298	Total	C	N	O	S	0	0	0
			2261	1448	387	420	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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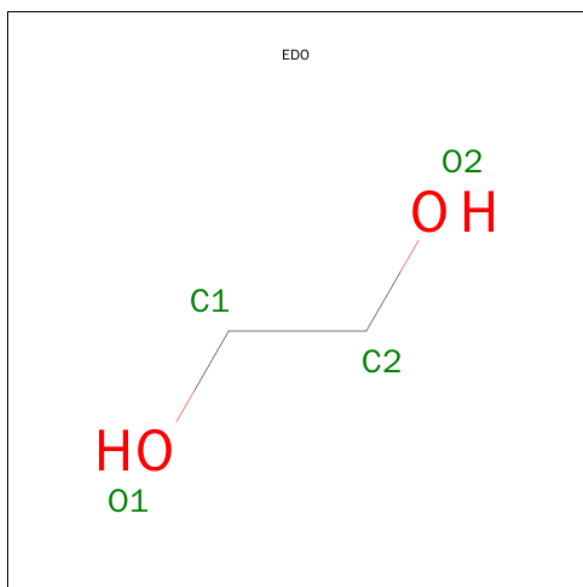
Chain	Residue	Modelled	Actual	Comment	Reference
C	6	ASP	-	EXPRESSION TAG	UNP P75682
C	7	LEU	-	EXPRESSION TAG	UNP P75682
C	310	CYS	-	EXPRESSION TAG	UNP P75682
C	311	GLY	-	EXPRESSION TAG	UNP P75682
C	312	ARG	-	EXPRESSION TAG	UNP P75682
C	313	THR	-	EXPRESSION TAG	UNP P75682
C	314	ARG	-	EXPRESSION TAG	UNP 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: C₂H₆O₂).



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

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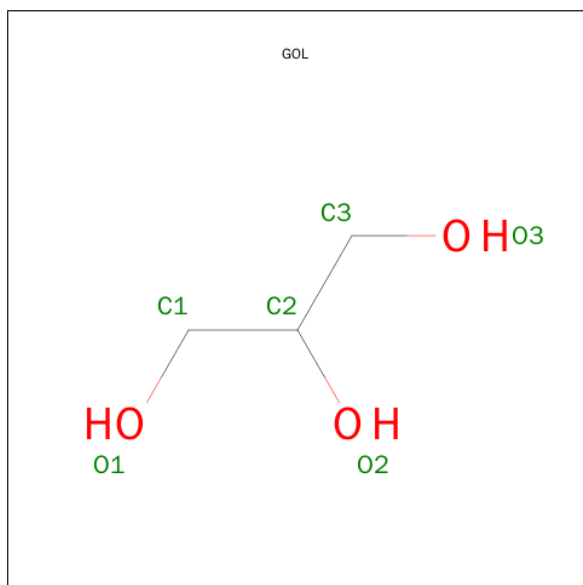
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2	A	1	Total 4	C 2	O 2	0	0
2	A	1	Total 4	C 2	O 2	0	0
2	A	1	Total 4	C 2	O 2	0	0
2	B	1	Total 4	C 2	O 2	0	0
2	B	1	Total 4	C 2	O 2	0	0
2	B	1	Total 4	C 2	O 2	0	0
2	B	1	Total 4	C 2	O 2	0	0
2	B	1	Total 4	C 2	O 2	0	0
2	B	1	Total 4	C 2	O 2	0	0
2	C	1	Total 4	C 2	O 2	0	0
2	C	1	Total 4	C 2	O 2	0	0
2	C	1	Total 4	C 2	O 2	0	0
2	C	1	Total 4	C 2	O 2	0	0
2	C	1	Total 4	C 2	O 2	0	0
2	C	1	Total 4	C 2	O 2	0	0
2	C	1	Total 4	C 2	O 2	0	0
2	C	1	Total 4	C 2	O 2	0	0
2	C	1	Total 4	C 2	O 2	0	0
2	D	1	Total 4	C 2	O 2	0	0
2	D	1	Total 4	C 2	O 2	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	D	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	0
			4	2	2		

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



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

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

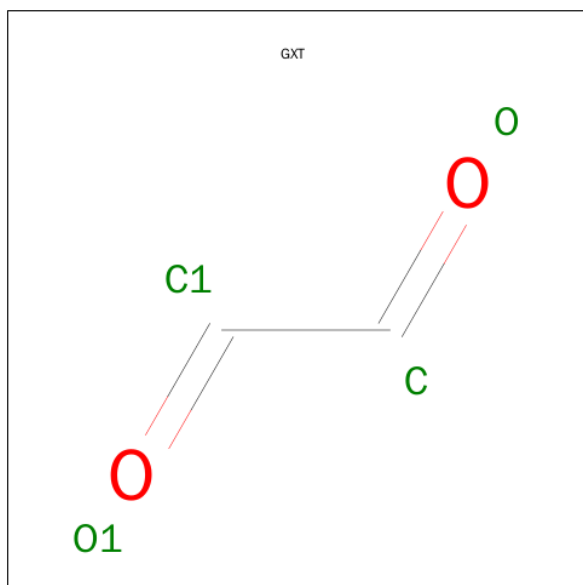
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Mg	0	0
			1	1		

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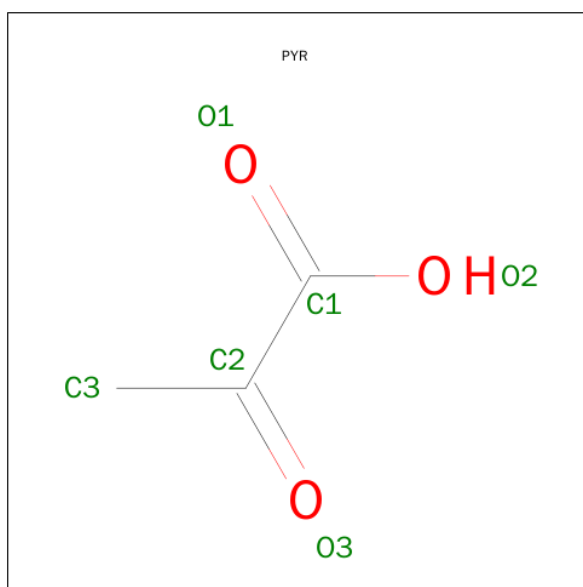
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	0
			1	1		
4	D	1	Total	Mg	0	0
			1	1		
4	C	1	Total	Mg	0	0
			1	1		

- Molecule 5 is ETHANEDIAL (three-letter code: GXT) (formula: $C_2H_2O_2$).



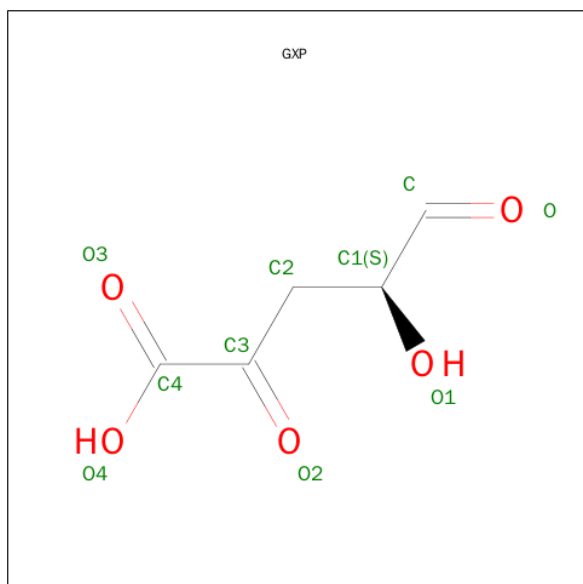
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			5	3	2		
6	C	1	Total	C	O	0	0
			5	3	2		

- Molecule 7 is (4S)-4-HYDROXY-2,5-DIOXOPENTANOIC ACID (three-letter code: GXP) (formula: C₅H₆O₅).



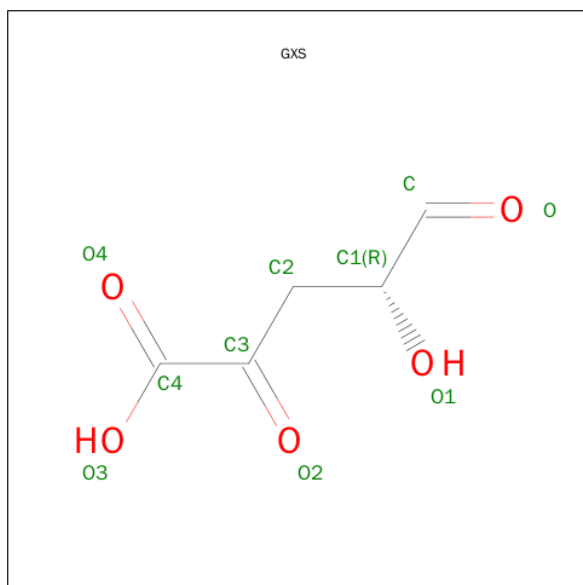
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	1
			9	5	4		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	D	1	Total	C	O	0	1
			9	5	4		

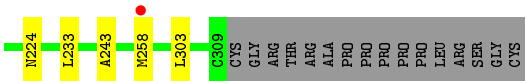
- Molecule 8 is (4R)-4-HYDROXY-2,5-DIOXOPENTANOIC ACID (three-letter code: GXS) (formula: C₅H₆O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	C	O	0	1
			9	5	4		
8	D	1	Total	C	O	0	1
			9	5	4		

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	47	Total	O	0	0
			47	47		
9	B	58	Total	O	0	0
			58	58		
9	C	45	Total	O	0	0
			45	45		
9	D	55	Total	O	0	0
			55	55		



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	141.24Å 155.14Å 55.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.06 – 1.99 48.56 – 1.99	Depositor EDS
% Data completeness (in resolution range)	98.3 (49.06-1.99) 98.3 (48.56-1.99)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.60 (at 1.98Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.198 , 0.233 0.206 , 0.239	Depositor DCC
R_{free} test set	4170 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	19.2	Xtriage
Anisotropy	0.133	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 38.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	4 of 83412 reflections (0.005%)	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9434	wwPDB-VP
Average B, all atoms (Å ²)	19.0	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 50.13 % 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 6.7587e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: GOL, MG, PYR, EDO, GXT, GXP, GXS

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	1.00	4/2307 (0.2%)	1.02	9/3143 (0.3%)
1	B	1.13	8/2308 (0.3%)	0.96	7/3146 (0.2%)
1	C	1.01	4/2305 (0.2%)	1.02	8/3141 (0.3%)
1	D	1.08	7/2309 (0.3%)	0.96	6/3145 (0.2%)
All	All	1.06	23/9229 (0.2%)	0.99	30/12575 (0.2%)

The worst 5 of 23 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	129	ARG	CZ-NH1	-15.30	1.13	1.33
1	A	129	ARG	CZ-NH1	-15.25	1.13	1.33
1	B	145	TYR	CE1-CZ	-14.76	1.19	1.38
1	B	145	TYR	CG-CD2	-12.97	1.22	1.39
1	D	145	TYR	CE1-CZ	-12.03	1.23	1.38

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	129	ARG	NE-CZ-NH2	14.47	127.53	120.30
1	C	129	ARG	NE-CZ-NH2	14.24	127.42	120.30
1	C	129	ARG	NH1-CZ-NH2	-11.89	106.32	119.40
1	C	129	ARG	NE-CZ-NH1	11.81	126.21	120.30
1	A	129	ARG	NH1-CZ-NH2	-11.56	106.68	119.40

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	2259	0	2274	19	0
1	B	2260	0	2278	29	0
1	C	2257	0	2267	22	0
1	D	2261	0	2283	17	0
2	A	24	0	33	13	0
2	B	24	0	35	22	0
2	C	40	0	57	17	0
2	D	20	0	29	8	0
3	A	6	0	8	0	0
3	B	12	0	16	4	0
3	C	6	0	8	5	0
3	D	6	0	8	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	4	0	2	4	0
6	A	5	0	3	2	0
6	C	5	0	3	1	0
7	B	9	0	5	0	0
7	D	9	0	5	1	0
8	B	9	0	5	0	0
8	D	9	0	5	1	0
9	A	47	0	0	0	0
9	B	58	0	0	0	0
9	C	45	0	0	3	0
9	D	55	0	0	2	0
All	All	9434	0	9324	93	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 5.

The worst 5 of 93 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:100:LEU:HD22	2:C:404:EDO:H11	1.53	0.87
7:D:408[A]:GXP:H1	9:D:537:HOH:O	1.78	0.84
1:C:280:VAL:HA	2:C:407:EDO:H11	1.61	0.82
1:A:117:PRO:HB3	2:A:406:EDO:H12	1.62	0.81
1:A:117:PRO:CB	2:A:406:EDO:H12	2.12	0.80

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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%)	292 (99%)	4 (1%)	0	100	100
1	B	296/343 (86%)	293 (99%)	3 (1%)	0	100	100
1	C	296/343 (86%)	292 (99%)	4 (1%)	0	100	100
1	D	296/343 (86%)	292 (99%)	4 (1%)	0	100	100
All	All	1184/1372 (86%)	1169 (99%)	15 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	241/280 (86%)	238 (99%)	3 (1%)	78	81
1	B	242/280 (86%)	238 (98%)	4 (2%)	68	71

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	240/280 (86%)	238 (99%)	2 (1%)	86	89
1	D	242/280 (86%)	240 (99%)	2 (1%)	86	89
All	All	965/1120 (86%)	954 (99%)	11 (1%)	80	83

5 of 11 residues with a non-rotameric sidechain are listed below:

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

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	62	GLN
1	A	283	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 43 ligands modelled in this entry, 4 are monoatomic - leaving 39 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	A	401	-	3,3,3	0.54	0	2,2,2	0.49	0
3	GOL	A	402	-	5,5,5	0.57	0	5,5,5	0.76	0
2	EDO	A	403	-	3,3,3	0.72	0	2,2,2	0.62	0
2	EDO	A	405	-	3,3,3	1.32	0	2,2,2	0.92	0
2	EDO	A	406	-	3,3,3	1.15	0	2,2,2	0.95	0
2	EDO	A	407	-	3,3,3	0.36	0	2,2,2	0.89	0
2	EDO	A	408	-	3,3,3	0.60	0	2,2,2	1.41	0
5	GXT	A	409	4	3,3,3	0.51	0	2,2,2	3.14	2 (100%)
6	PYR	A	410	1,4	1,4,5	0.55	0	0,4,6	0.00	-
2	EDO	B	401	-	3,3,3	0.59	0	2,2,2	0.98	0
3	GOL	B	402	-	5,5,5	1.15	0	5,5,5	1.35	0
3	GOL	B	403	-	5,5,5	0.82	0	5,5,5	1.25	1 (20%)
2	EDO	B	404	-	3,3,3	0.90	0	2,2,2	0.96	0
2	EDO	B	406	-	3,3,3	0.42	0	2,2,2	0.94	0
2	EDO	B	407	-	3,3,3	0.48	0	2,2,2	0.25	0
2	EDO	B	408	-	3,3,3	0.45	0	2,2,2	0.92	0
2	EDO	B	409	-	3,3,3	1.04	0	2,2,2	1.01	0
7	GXP	B	410[A]	1,4	5,8,9	1.82	1 (20%)	6,9,11	1.60	2 (33%)
8	GXS	B	411[B]	1,4	5,8,9	0.97	0	6,9,11	0.87	0
2	EDO	C	401	-	3,3,3	0.64	0	2,2,2	0.35	0
3	GOL	C	402	-	5,5,5	0.46	0	5,5,5	1.06	1 (20%)
2	EDO	C	404	-	3,3,3	0.82	0	2,2,2	0.59	0
2	EDO	C	405	-	3,3,3	0.82	0	2,2,2	1.22	0
2	EDO	C	406	-	3,3,3	0.44	0	2,2,2	0.78	0
2	EDO	C	407	-	3,3,3	0.49	0	2,2,2	0.63	0
2	EDO	C	408	-	3,3,3	1.04	0	2,2,2	1.52	1 (50%)
2	EDO	C	409	-	3,3,3	0.59	0	2,2,2	0.37	0
2	EDO	C	410	-	3,3,3	0.47	0	2,2,2	0.94	0
2	EDO	C	411	-	3,3,3	0.40	0	2,2,2	0.66	0
6	PYR	C	412	1,4	1,4,5	0.64	0	0,4,6	0.00	-
2	EDO	C	413	-	3,3,3	0.63	0	2,2,2	0.33	0
2	EDO	D	401	-	3,3,3	0.38	0	2,2,2	1.06	0
2	EDO	D	402	-	3,3,3	0.54	0	2,2,2	0.79	0
2	EDO	D	403	-	3,3,3	0.71	0	2,2,2	1.18	0
2	EDO	D	404	-	3,3,3	0.84	0	2,2,2	0.89	0
3	GOL	D	405	-	5,5,5	0.58	0	5,5,5	0.49	0
2	EDO	D	407	-	3,3,3	0.79	0	2,2,2	0.91	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	GXP	D	408[A]	1,4	5,8,9	1.04	1 (20%)	6,9,11	0.93	0
8	GXS	D	409[B]	1,4	5,8,9	1.59	1 (20%)	6,9,11	1.07	1 (16%)

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	A	401	-	-	0/1/1/1	0/0/0/0
3	GOL	A	402	-	-	0/4/4/4	0/0/0/0
2	EDO	A	403	-	-	0/1/1/1	0/0/0/0
2	EDO	A	405	-	-	0/1/1/1	0/0/0/0
2	EDO	A	406	-	-	0/1/1/1	0/0/0/0
2	EDO	A	407	-	-	0/1/1/1	0/0/0/0
2	EDO	A	408	-	-	0/1/1/1	0/0/0/0
5	GXT	A	409	4	-	0/0/1/1	0/0/0/0
6	PYR	A	410	1,4	-	0/0/2/4	0/0/0/0
2	EDO	B	401	-	-	0/1/1/1	0/0/0/0
3	GOL	B	402	-	-	0/4/4/4	0/0/0/0
3	GOL	B	403	-	-	0/4/4/4	0/0/0/0
2	EDO	B	404	-	-	0/1/1/1	0/0/0/0
2	EDO	B	406	-	-	0/1/1/1	0/0/0/0
2	EDO	B	407	-	-	0/1/1/1	0/0/0/0
2	EDO	B	408	-	-	0/1/1/1	0/0/0/0
2	EDO	B	409	-	-	0/1/1/1	0/0/0/0
7	GXP	B	410[A]	1,4	-	0/3/7/10	0/0/0/0
8	GXS	B	411[B]	1,4	-	0/3/7/10	0/0/0/0
2	EDO	C	401	-	-	0/1/1/1	0/0/0/0
3	GOL	C	402	-	-	0/4/4/4	0/0/0/0
2	EDO	C	404	-	-	0/1/1/1	0/0/0/0
2	EDO	C	405	-	-	0/1/1/1	0/0/0/0
2	EDO	C	406	-	-	0/1/1/1	0/0/0/0
2	EDO	C	407	-	-	0/1/1/1	0/0/0/0
2	EDO	C	408	-	-	0/1/1/1	0/0/0/0
2	EDO	C	409	-	-	0/1/1/1	0/0/0/0
2	EDO	C	410	-	-	0/1/1/1	0/0/0/0
2	EDO	C	411	-	-	0/1/1/1	0/0/0/0
6	PYR	C	412	1,4	-	0/0/2/4	0/0/0/0
2	EDO	C	413	-	-	0/1/1/1	0/0/0/0
2	EDO	D	401	-	-	0/1/1/1	0/0/0/0
2	EDO	D	402	-	-	0/1/1/1	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	D	403	-	-	0/1/1/1	0/0/0/0
2	EDO	D	404	-	-	0/1/1/1	0/0/0/0
3	GOL	D	405	-	-	0/4/4/4	0/0/0/0
2	EDO	D	407	-	-	0/1/1/1	0/0/0/0
7	GXP	D	408[A]	1,4	-	0/3/7/10	0/0/0/0
8	GXS	D	409[B]	1,4	-	0/3/7/10	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	D	408[A]	GXP	C1-C	2.00	1.53	1.50
8	D	409[B]	GXS	C1-C	2.99	1.55	1.50
7	B	410[A]	GXP	C1-C	3.01	1.55	1.50

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	409	GXT	O1-C1-C	-3.54	119.16	123.69
5	A	409	GXT	O-C-C1	-2.67	120.27	123.69
2	C	408	EDO	O1-C1-C2	-2.07	97.71	112.54
3	C	402	GOL	O3-C3-C2	2.00	119.91	110.18
7	B	410[A]	GXP	O1-C1-C2	2.14	112.50	108.85

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

27 monomers are involved in 76 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	403	EDO	2	0
2	A	405	EDO	2	0
2	A	406	EDO	6	0
2	A	407	EDO	1	0
2	A	408	EDO	2	0
5	A	409	GXT	4	0
6	A	410	PYR	2	0
3	B	402	GOL	2	0
3	B	403	GOL	2	0
2	B	404	EDO	4	0
2	B	406	EDO	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	407	EDO	7	0
2	B	408	EDO	1	0
2	B	409	EDO	7	0
3	C	402	GOL	5	0
2	C	404	EDO	3	0
2	C	405	EDO	2	0
2	C	406	EDO	1	0
2	C	407	EDO	3	0
2	C	410	EDO	2	0
6	C	412	PYR	1	0
2	C	413	EDO	6	0
2	D	403	EDO	3	0
2	D	404	EDO	1	0
2	D	407	EDO	4	0
7	D	408[A]	GXP	1	0
8	D	409[B]	GXS	1	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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%)	0.07	2 (0%) 89 89	11, 19, 33, 52	0
1	B	298/343 (86%)	-0.03	1 (0%) 94 94	10, 15, 28, 41	0
1	C	298/343 (86%)	0.03	1 (0%) 94 94	12, 18, 31, 47	0
1	D	298/343 (86%)	0.02	1 (0%) 94 94	10, 17, 28, 40	0
All	All	1192/1372 (86%)	0.02	5 (0%) 93 93	10, 17, 30, 52	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	258	MET	2.7
1	B	309	CYS	2.5
1	C	196	HIS	2.2
1	A	12	ALA	2.1
1	A	196	HIS	2.1

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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains.

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	LLDF	B-factors(Å ²)	Q<0.9
5	GXT	A	409	4/4	0.74	0.42	30.47	27,29,29,30	4
2	EDO	A	406	4/4	0.95	0.30	19.63	17,17,22,23	0
2	EDO	C	406	4/4	0.88	0.25	18.14	28,30,31,35	0
2	EDO	C	408	4/4	0.90	0.24	13.03	21,24,28,37	0
3	GOL	A	402	6/6	0.90	0.33	11.71	25,36,41,44	0
2	EDO	A	405	4/4	0.92	0.28	11.34	23,24,24,24	0
2	EDO	C	404	4/4	0.96	0.26	10.46	19,20,22,23	0
2	EDO	C	413	4/4	0.93	0.26	10.33	22,27,29,31	0
2	EDO	C	407	4/4	0.88	0.32	10.32	26,39,40,46	0
2	EDO	D	401	4/4	0.88	0.18	9.91	27,27,28,31	0
8	GXS	B	411[B]	9/10	0.75	0.28	9.52	22,24,25,26	9
2	EDO	A	407	4/4	0.93	0.21	9.18	36,36,37,42	0
6	PYR	C	412	5/6	0.90	0.21	8.87	20,24,28,28	0
3	GOL	B	402	6/6	0.83	0.21	8.58	34,37,39,39	0
2	EDO	D	404	4/4	0.81	0.31	8.34	30,32,32,35	0
8	GXS	D	409[B]	9/10	0.79	0.23	8.01	24,29,33,34	9
7	GXP	D	408[A]	9/10	0.82	0.22	7.44	28,34,41,42	9
3	GOL	C	402	6/6	0.86	0.35	7.33	31,35,37,44	0
2	EDO	B	401	4/4	0.94	0.18	7.28	16,20,21,26	0
6	PYR	A	410	5/6	0.92	0.18	7.07	22,23,26,27	0
7	GXP	B	410[A]	9/10	0.82	0.23	6.98	22,32,46,46	9
2	EDO	D	407	4/4	0.90	0.21	6.69	18,24,28,36	0
3	GOL	B	403	6/6	0.66	0.28	6.42	42,46,47,47	0
2	EDO	A	401	4/4	0.92	0.15	6.10	21,23,24,25	0
2	EDO	A	403	4/4	0.83	0.31	5.11	26,31,32,37	0
2	EDO	B	409	4/4	0.95	0.23	5.01	18,21,21,22	0
2	EDO	B	406	4/4	0.93	0.19	4.95	17,25,29,33	0
2	EDO	B	408	4/4	0.90	0.20	3.54	28,29,30,33	0
2	EDO	D	402	4/4	0.95	0.15	3.26	17,20,21,24	0
4	MG	C	403	1/1	0.96	0.14	3.07	29,29,29,29	0
2	EDO	C	411	4/4	0.95	0.16	2.84	29,30,31,33	0
2	EDO	C	401	4/4	0.90	0.13	2.44	21,21,24,24	0
2	EDO	C	409	4/4	0.93	0.13	0.61	26,32,37,39	0
4	MG	A	404	1/1	0.97	0.11	0.49	27,27,27,27	0
2	EDO	B	407	4/4	0.87	0.23	-	32,33,33,34	0
2	EDO	C	410	4/4	0.80	0.32	-	27,31,33,36	0
2	EDO	B	404	4/4	0.70	0.27	-	32,35,36,40	0
4	MG	D	406	1/1	0.89	0.14	-	25,25,25,25	0
2	EDO	A	408	4/4	0.91	0.27	-	17,27,30,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	EDO	D	403	4/4	0.88	0.31	-	21,28,33,36	0
2	EDO	C	405	4/4	0.93	0.22	-	18,22,28,33	0
4	MG	B	405	1/1	0.81	0.22	-	26,26,26,26	0
3	GOL	D	405	6/6	0.81	0.23	-	26,32,35,36	0

6.5 Other polymers [i](#)

There are no such residues in this entry.