Full wwPDB X-ray Structure Validation Report ⓘ

Jan 3, 2024 – 07:46 am GMT

PDB ID	:	4UXD
Title	:	2-keto 3-deoxygluconate aldolase from Picrophilus torridus
Authors	:	Priftis, A.; Zaitsev, V.; Reher, M.; Johnsen, U.; Danson, M.J.; Taylor, G.L.; Schoenheit, P.; Crennell, S.J.
Deposited on	:	2014-08-22
Resolution	:	2.50 Å(reported)

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

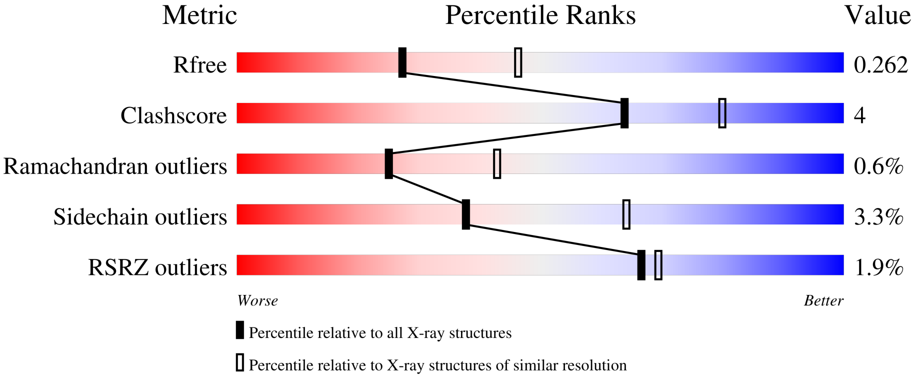
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

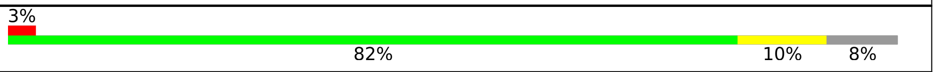
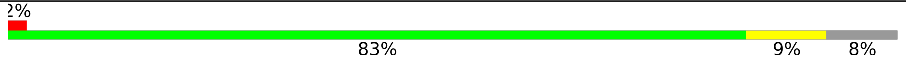
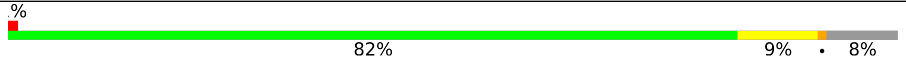
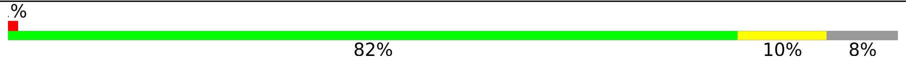
The reported resolution of this entry is 2.50 Å.

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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	297	
1	B	297	
1	C	297	
1	D	297	

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	GOL	B	1275	-	-	X	-
2	GOL	B	1276	-	-	X	-

2 Entry composition ⓘ

There are 7 unique types of molecules in this entry. The entry contains 9319 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called 2-DEHYDRO-3-DEOXY-D-GLUCONATE/2-DEHYDRO-3-DEOXY-PHOSPHOGLUCONATE ALDOLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	274	Total 2199	C 1421	N 349	O 414	S 15	0	0	0
1	B	274	Total 2209	C 1427	N 352	O 415	S 15	0	1	0
1	C	274	Total 2199	C 1421	N 349	O 414	S 15	0	0	0
1	D	274	Total 2209	C 1427	N 352	O 415	S 15	0	1	0

There are 92 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-22	MET	-	expression tag	UNP Q6KZI8
A	-21	GLY	-	expression tag	UNP Q6KZI8
A	-20	HIS	-	expression tag	UNP Q6KZI8
A	-19	HIS	-	expression tag	UNP Q6KZI8
A	-18	HIS	-	expression tag	UNP Q6KZI8
A	-17	HIS	-	expression tag	UNP Q6KZI8
A	-16	HIS	-	expression tag	UNP Q6KZI8
A	-15	HIS	-	expression tag	UNP Q6KZI8
A	-14	HIS	-	expression tag	UNP Q6KZI8
A	-13	HIS	-	expression tag	UNP Q6KZI8
A	-12	HIS	-	expression tag	UNP Q6KZI8
A	-11	HIS	-	expression tag	UNP Q6KZI8
A	-10	SER	-	expression tag	UNP Q6KZI8
A	-9	SER	-	expression tag	UNP Q6KZI8
A	-8	GLY	-	expression tag	UNP Q6KZI8
A	-7	HIS	-	expression tag	UNP Q6KZI8
A	-6	ILE	-	expression tag	UNP Q6KZI8
A	-5	ASP	-	expression tag	UNP Q6KZI8
A	-4	ASP	-	expression tag	UNP Q6KZI8
A	-3	ASP	-	expression tag	UNP Q6KZI8

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	ASP	-	expression tag	UNP Q6KZI8
A	-1	LYS	-	expression tag	UNP Q6KZI8
A	0	HIS	-	expression tag	UNP Q6KZI8
B	-22	MET	-	expression tag	UNP Q6KZI8
B	-21	GLY	-	expression tag	UNP Q6KZI8
B	-20	HIS	-	expression tag	UNP Q6KZI8
B	-19	HIS	-	expression tag	UNP Q6KZI8
B	-18	HIS	-	expression tag	UNP Q6KZI8
B	-17	HIS	-	expression tag	UNP Q6KZI8
B	-16	HIS	-	expression tag	UNP Q6KZI8
B	-15	HIS	-	expression tag	UNP Q6KZI8
B	-14	HIS	-	expression tag	UNP Q6KZI8
B	-13	HIS	-	expression tag	UNP Q6KZI8
B	-12	HIS	-	expression tag	UNP Q6KZI8
B	-11	HIS	-	expression tag	UNP Q6KZI8
B	-10	SER	-	expression tag	UNP Q6KZI8
B	-9	SER	-	expression tag	UNP Q6KZI8
B	-8	GLY	-	expression tag	UNP Q6KZI8
B	-7	HIS	-	expression tag	UNP Q6KZI8
B	-6	ILE	-	expression tag	UNP Q6KZI8
B	-5	ASP	-	expression tag	UNP Q6KZI8
B	-4	ASP	-	expression tag	UNP Q6KZI8
B	-3	ASP	-	expression tag	UNP Q6KZI8
B	-2	ASP	-	expression tag	UNP Q6KZI8
B	-1	LYS	-	expression tag	UNP Q6KZI8
B	0	HIS	-	expression tag	UNP Q6KZI8
C	-22	MET	-	expression tag	UNP Q6KZI8
C	-21	GLY	-	expression tag	UNP Q6KZI8
C	-20	HIS	-	expression tag	UNP Q6KZI8
C	-19	HIS	-	expression tag	UNP Q6KZI8
C	-18	HIS	-	expression tag	UNP Q6KZI8
C	-17	HIS	-	expression tag	UNP Q6KZI8
C	-16	HIS	-	expression tag	UNP Q6KZI8
C	-15	HIS	-	expression tag	UNP Q6KZI8
C	-14	HIS	-	expression tag	UNP Q6KZI8
C	-13	HIS	-	expression tag	UNP Q6KZI8
C	-12	HIS	-	expression tag	UNP Q6KZI8
C	-11	HIS	-	expression tag	UNP Q6KZI8
C	-10	SER	-	expression tag	UNP Q6KZI8
C	-9	SER	-	expression tag	UNP Q6KZI8
C	-8	GLY	-	expression tag	UNP Q6KZI8
C	-7	HIS	-	expression tag	UNP Q6KZI8

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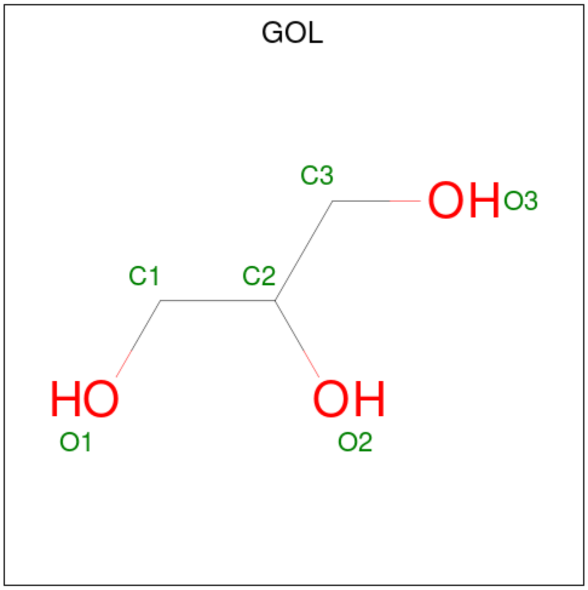
Chain	Residue	Modelled	Actual	Comment	Reference
C	-6	ILE	-	expression tag	UNP Q6KZI8
C	-5	ASP	-	expression tag	UNP Q6KZI8
C	-4	ASP	-	expression tag	UNP Q6KZI8
C	-3	ASP	-	expression tag	UNP Q6KZI8
C	-2	ASP	-	expression tag	UNP Q6KZI8
C	-1	LYS	-	expression tag	UNP Q6KZI8
C	0	HIS	-	expression tag	UNP Q6KZI8
D	-22	MET	-	expression tag	UNP Q6KZI8
D	-21	GLY	-	expression tag	UNP Q6KZI8
D	-20	HIS	-	expression tag	UNP Q6KZI8
D	-19	HIS	-	expression tag	UNP Q6KZI8
D	-18	HIS	-	expression tag	UNP Q6KZI8
D	-17	HIS	-	expression tag	UNP Q6KZI8
D	-16	HIS	-	expression tag	UNP Q6KZI8
D	-15	HIS	-	expression tag	UNP Q6KZI8
D	-14	HIS	-	expression tag	UNP Q6KZI8
D	-13	HIS	-	expression tag	UNP Q6KZI8
D	-12	HIS	-	expression tag	UNP Q6KZI8
D	-11	HIS	-	expression tag	UNP Q6KZI8
D	-10	SER	-	expression tag	UNP Q6KZI8
D	-9	SER	-	expression tag	UNP Q6KZI8
D	-8	GLY	-	expression tag	UNP Q6KZI8
D	-7	HIS	-	expression tag	UNP Q6KZI8
D	-6	ILE	-	expression tag	UNP Q6KZI8
D	-5	ASP	-	expression tag	UNP Q6KZI8
D	-4	ASP	-	expression tag	UNP Q6KZI8
D	-3	ASP	-	expression tag	UNP Q6KZI8
D	-2	ASP	-	expression tag	UNP Q6KZI8
D	-1	LYS	-	expression tag	UNP Q6KZI8
D	0	HIS	-	expression tag	UNP Q6KZI8

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

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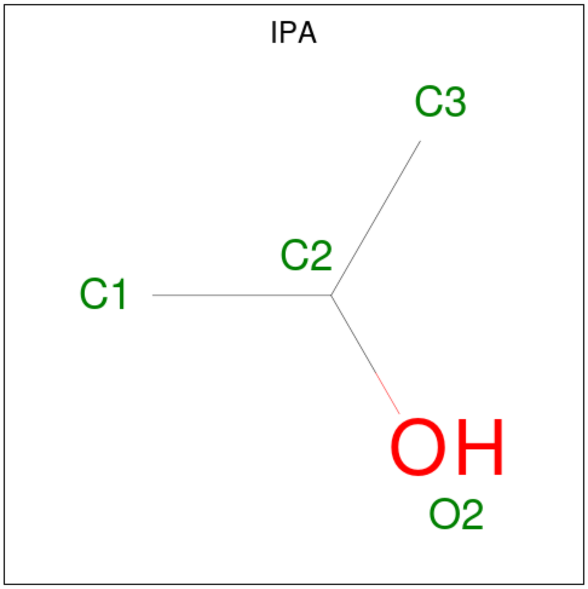
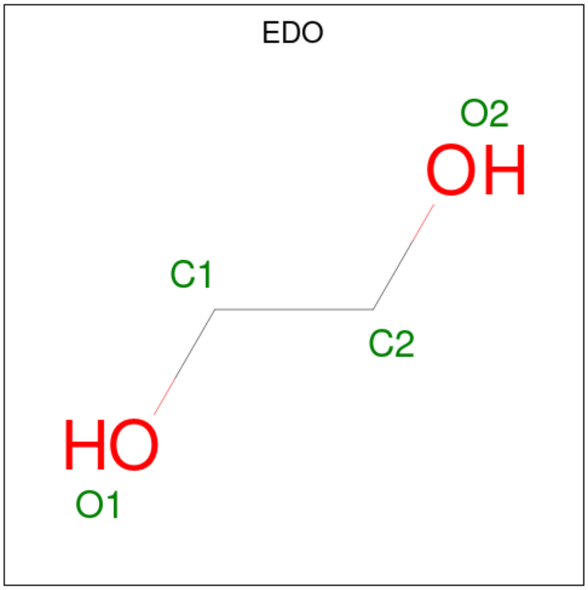
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	1	Total C O 6 3 3	0	0
2	D	1	Total C O 6 3 3	0	0
2	D	1	Total C O 6 3 3	0	0
2	D	1	Total C O 6 3 3	0	0
2	D	1	Total C O 6 3 3	0	0

- Molecule 3 is ISOPROPYL ALCOHOL (three-letter code: IPA) (formula: C_3H_8O).



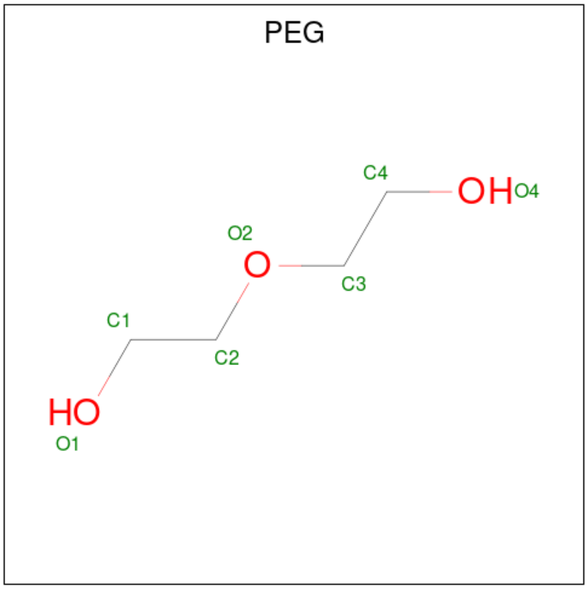
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 4 3 1	0	0
3	B	1	Total C O 4 3 1	0	0
3	D	1	Total C O 4 3 1	0	0

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



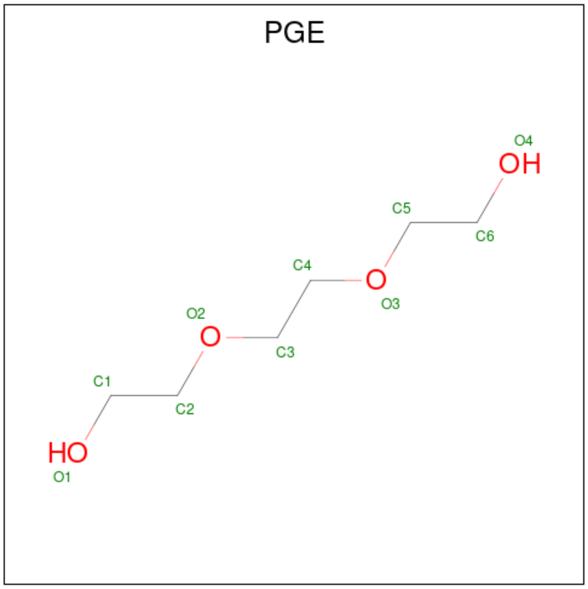
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C O 7 4 3	0	0

- Molecule 6 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	C	1	Total C O 10 6 4	0	0

- Molecule 7 is water.

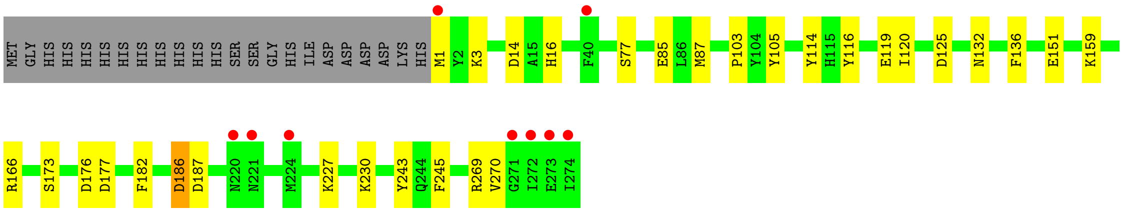
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	92	Total O 92 92	0	0
7	B	74	Total O 74 74	0	0
7	C	84	Total O 84 84	0	0
7	D	90	Total O 90 90	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

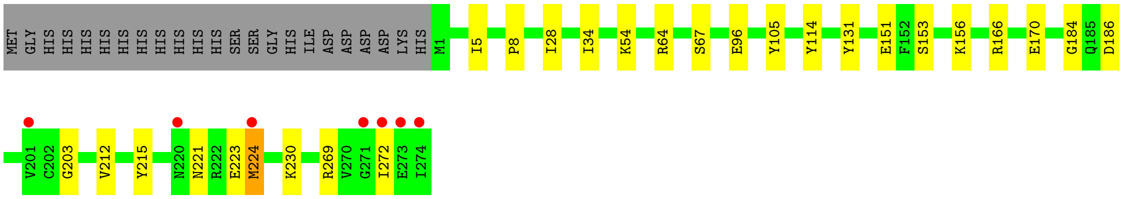
- Molecule 1: 2-DEHYDRO-3-DEOXY-D-GLUCONATE/2-DEHYDRO-3-DEOXY-PHOSPHO GLUCONATE ALDOLASE

Chain A:



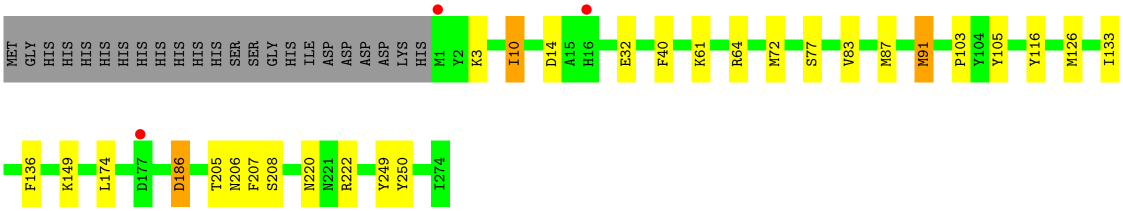
- Molecule 1: 2-DEHYDRO-3-DEOXY-D-GLUCONATE/2-DEHYDRO-3-DEOXY-PHOSPHO GLUCONATE ALDOLASE

Chain B:



- Molecule 1: 2-DEHYDRO-3-DEOXY-D-GLUCONATE/2-DEHYDRO-3-DEOXY-PHOSPHO GLUCONATE ALDOLASE

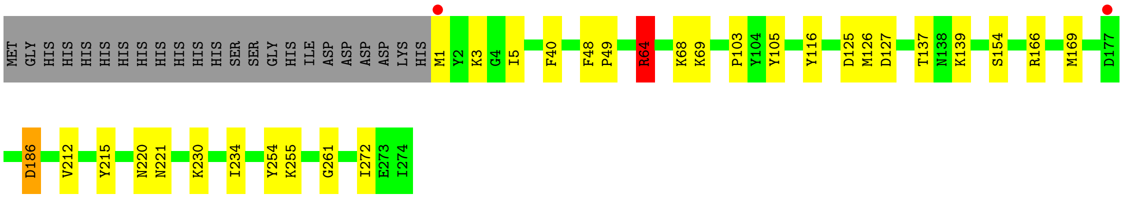
Chain C:



- Molecule 1: 2-DEHYDRO-3-DEOXY-D-GLUCONATE/2-DEHYDRO-3-DEOXY-PHOSPHO GLUCONATE ALDOLASE

Chain D:


%
82%
10%
8%


MET
GLY
HIS
HIS
HIS
HIS
HIS
HIS
HIS
HIS
HIS
HIS
SER
SER
GLY
HIS
ILE
ASP
ASP
ASP
ASP
LYS
HIS
M1
Y2
K3
G4
I5
F40
F48
P49
R64
K68
K69
P103
Y104
Y105
Y116
D125
M126
D127
T137
N138
K139
S154
R166
M169
D177
D186
V212
Y215
N220
N221
K230
I234
Y254
K255
G261
I272
E273
I274

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α, β, γ	77.95Å 100.16Å 154.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.58 – 2.50 28.58 – 2.50	Depositor EDS
% Data completeness (in resolution range)	86.1 (28.58-2.50) 75.5 (28.58-2.50)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.91 (at 2.51Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.175 , 0.260 0.184 , 0.262	Depositor DCC
R_{free} test set	1894 reflections (5.13%)	wwPDB-VP
Wilson B-factor (Å^2)	28.5	Xtriage
Anisotropy	0.451	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 50.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	9319	wwPDB-VP
Average B, all atoms (Å^2)	34.0	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 69.92 % 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 3.4133e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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[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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, PGE, IPA, PEG, EDO

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	$\#\lvert Z\rvert > 5$	RMSZ	$\#\lvert Z\rvert > 5$
1	A	0.42	0/2249	0.55	0/3033
1	B	0.43	0/2260	0.57	0/3048
1	C	0.44	0/2249	0.55	0/3033
1	D	0.45	0/2260	0.59	2/3048 (0.1%)
All	All	0.43	0/9018	0.56	2/12162 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	64	ARG	NE-CZ-NH1	6.14	123.37	120.30
1	D	64	ARG	CG-CD-NE	5.78	123.94	111.80

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	2199	0	2185	20	0
1	B	2209	0	2191	19	0
1	C	2199	0	2185	16	0
1	D	2209	0	2191	19	0
2	A	36	0	48	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	30	0	40	9	0
2	C	18	0	24	2	0
2	D	30	0	40	2	0
3	A	4	0	8	3	0
3	B	4	0	8	0	0
3	D	4	0	8	1	0
4	A	4	0	6	1	0
4	C	4	0	6	0	0
4	D	12	0	18	0	0
5	B	7	0	10	1	0
6	C	10	0	14	0	0
7	A	92	0	0	3	0
7	B	74	0	0	0	0
7	C	84	0	0	2	0
7	D	90	0	0	1	0
All	All	9319	0	8982	75	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 (75) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:221:ASN:ND2	1:B:224:MET:SD	2.45	0.89
1:D:255:LYS:NZ	1:D:272:ILE:O	2.15	0.80
2:B:1275:GOL:O2	2:B:1276:GOL:O1	2.10	0.70
1:A:136:PHE:CZ	3:A:1277:IPA:H13	2.28	0.69
1:C:14:ASP:OD2	7:C:2006:HOH:O	2.11	0.69
1:C:32:GLU:OE2	7:C:2015:HOH:O	2.11	0.68
1:B:114:TYR:OH	1:B:151:GLU:OE1	2.13	0.66
1:B:96:GLU:OE1	1:B:96:GLU:N	2.31	0.63
1:D:139:LYS:H	3:D:1283:IPA:H12	1.65	0.62
1:A:114:TYR:OH	1:A:151:GLU:OE1	2.18	0.61
1:D:64:ARG:HG3	1:D:64:ARG:HH11	1.66	0.60
1:A:14:ASP:OD2	4:A:1278:EDO:O2	2.20	0.60
1:B:170:GLU:OE2	2:B:1280:GOL:O2	2.20	0.59
1:A:85:GLU:OE1	7:A:2046:HOH:O	2.17	0.56
1:B:166:ARG:NH1	5:B:1281:PEG:O1	2.32	0.56
1:B:184:GLY:O	2:B:1276:GOL:O1	2.17	0.56
1:A:1:MET:N	7:A:2002:HOH:O	2.38	0.55
1:A:176:ASP:OD1	1:A:177:ASP:N	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:PHE:HZ	3:A:1277:IPA:H13	1.73	0.54
1:D:186:ASP:N	1:D:186:ASP:OD1	2.41	0.54
1:C:186:ASP:OD1	1:C:186:ASP:N	2.40	0.54
1:D:5:ILE:HD13	1:D:212:VAL:HA	1.89	0.54
1:C:10:ILE:HD11	1:C:249:TYR:HB3	1.93	0.51
1:A:227:LYS:HA	1:A:230:LYS:HG2	1.95	0.49
1:A:166:ARG:NH2	7:A:2075:HOH:O	2.40	0.48
1:A:245:PHE:CE2	3:A:1277:IPA:H11	2.48	0.48
1:A:132:ASN:HD21	2:A:1282:GOL:C3	2.26	0.48
1:D:64:ARG:NH2	1:D:69:LYS:O	2.47	0.48
1:D:137:THR:HA	2:D:1282:GOL:C1	2.44	0.48
1:D:64:ARG:NH1	1:D:64:ARG:O	2.46	0.47
1:C:10:ILE:HG23	1:C:250:TYR:CE2	2.50	0.47
1:C:91:MET:HG3	1:C:126:MET:HB3	1.96	0.47
1:D:137:THR:HA	2:D:1282:GOL:H12	1.96	0.47
1:A:187:ASP:OD1	1:A:187:ASP:N	2.47	0.47
1:B:153:SER:O	1:B:156:LYS:NZ	2.47	0.47
1:A:132:ASN:HD21	2:A:1282:GOL:H31	1.80	0.46
1:A:14:ASP:OD1	1:A:16:HIS:N	2.44	0.46
1:D:5:ILE:CD1	1:D:212:VAL:HA	2.45	0.46
1:D:64:ARG:HH11	1:D:64:ARG:CG	2.29	0.46
1:B:5:ILE:CD1	1:B:212:VAL:HA	2.46	0.45
1:A:87:MET:HE2	1:A:120:ILE:CG2	2.47	0.45
1:B:5:ILE:HD11	1:B:215:TYR:CB	2.47	0.45
1:D:5:ILE:HD11	1:D:215:TYR:CB	2.46	0.44
1:D:254:TYR:CZ	1:D:261:GLY:HA3	2.52	0.44
1:D:127:ASP:OD1	7:D:2044:HOH:O	2.21	0.44
1:A:243:TYR:CG	1:A:270:VAL:HG11	2.52	0.43
1:D:166:ARG:HA	1:D:169:MET:HE3	2.00	0.43
1:B:28:ILE:HG21	1:B:67:SER:HB2	2.00	0.43
1:B:131:TYR:CZ	2:B:1275:GOL:H31	2.53	0.43
1:B:131:TYR:CZ	2:B:1275:GOL:C3	3.02	0.43
1:C:40:PHE:CE2	2:C:1275:GOL:H31	2.54	0.43
1:D:48:PHE:CG	1:D:49:PRO:HD3	2.53	0.43
1:C:87:MET:HB2	1:C:87:MET:HE3	1.82	0.42
1:C:10:ILE:HD12	1:C:206:ASN:CG	2.39	0.42
1:A:186:ASP:OD1	1:A:186:ASP:N	2.52	0.42
1:B:34:ILE:O	1:B:212:VAL:HG11	2.18	0.42
1:D:103:PRO:HD3	1:D:116:TYR:CE1	2.53	0.42
1:A:159:LYS:HG2	1:A:182:PHE:HB2	2.01	0.42
1:B:105:TYR:H	2:B:1279:GOL:H31	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:126:MET:O	1:D:154:SER:OG	2.37	0.42
1:B:203:GLY:H	2:B:1276:GOL:H12	1.83	0.42
1:C:40:PHE:HE2	2:C:1275:GOL:H31	1.85	0.41
1:A:103:PRO:HG3	1:A:116:TYR:CZ	2.55	0.41
1:B:8:PRO:HD2	1:B:203:GLY:HA2	2.02	0.41
2:A:1281:GOL:C1	1:D:234:ILE:HG21	2.51	0.41
1:B:131:TYR:CE1	2:B:1275:GOL:H32	2.54	0.41
1:B:203:GLY:H	2:B:1276:GOL:C1	2.34	0.41
1:C:133:ILE:HD11	1:C:136:PHE:CD2	2.56	0.41
1:A:87:MET:HE2	1:A:120:ILE:HG23	2.03	0.41
1:C:83:VAL:HG12	1:C:87:MET:HE2	2.02	0.41
1:C:103:PRO:HG3	1:C:116:TYR:CZ	2.56	0.41
1:B:28:ILE:CG2	1:B:67:SER:HB2	2.51	0.40
1:C:149:LYS:NZ	1:C:174:LEU:O	2.53	0.40
1:C:205:THR:HA	1:C:208:SER:O	2.22	0.40
1:C:40:PHE:HA	1:C:72:MET:O	2.22	0.40

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	272/297 (92%)	264 (97%)	6 (2%)	2 (1%)	22	39
1	B	273/297 (92%)	260 (95%)	13 (5%)	0	100	100
1	C	272/297 (92%)	257 (94%)	12 (4%)	3 (1%)	14	26
1	D	273/297 (92%)	263 (96%)	9 (3%)	1 (0%)	34	54
All	All	1090/1188 (92%)	1044 (96%)	40 (4%)	6 (1%)	25	43

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	105	TYR
1	C	105	TYR
1	D	105	TYR
1	C	77	SER
1	C	207	PHE
1	A	77	SER

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	243/264 (92%)	237 (98%)	6 (2%)	47	73
1	B	244/264 (92%)	236 (97%)	8 (3%)	38	64
1	C	243/264 (92%)	235 (97%)	8 (3%)	38	64
1	D	244/264 (92%)	234 (96%)	10 (4%)	30	55
All	All	974/1056 (92%)	942 (97%)	32 (3%)	38	64

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LYS
1	A	119	GLU
1	A	125	ASP
1	A	173	SER
1	A	186	ASP
1	A	269	ARG
1	B	54	LYS
1	B	64	ARG
1	B	186	ASP
1	B	223	GLU
1	B	224	MET
1	B	230	LYS
1	B	269	ARG
1	B	272	ILE
1	C	3	LYS
1	C	10	ILE

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Mol	Chain	Res	Type
1	C	61	LYS
1	C	64	ARG
1	C	91	MET
1	C	186	ASP
1	C	220	ASN
1	C	222	ARG
1	D	1	MET
1	D	3	LYS
1	D	40	PHE
1	D	64	ARG
1	D	68	LYS
1	D	125	ASP
1	D	186	ASP
1	D	220	ASN
1	D	221	ASN
1	D	230	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	124	ASN

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 ⓘ

29 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	GOL	B	1276	-	5,5,5	0.40	0	5,5,5	0.45	0
2	GOL	A	1281	-	5,5,5	0.49	0	5,5,5	0.64	0
2	GOL	D	1282	-	5,5,5	0.42	0	5,5,5	0.60	0
3	IPA	A	1277	-	3,3,3	0.54	0	3,3,3	0.38	0
2	GOL	A	1276	-	5,5,5	0.33	0	5,5,5	0.30	0
2	GOL	C	1279	-	5,5,5	0.35	0	5,5,5	0.22	0
2	GOL	B	1280	-	5,5,5	0.52	0	5,5,5	0.94	0
2	GOL	B	1279	-	5,5,5	0.42	0	5,5,5	0.70	0
2	GOL	C	1278	-	5,5,5	0.49	0	5,5,5	0.22	0
2	GOL	A	1282	-	5,5,5	0.55	0	5,5,5	0.52	0
2	GOL	A	1280	-	5,5,5	0.35	0	5,5,5	0.33	0
2	GOL	B	1278	-	5,5,5	0.37	0	5,5,5	0.22	0
2	GOL	B	1275	-	5,5,5	0.57	0	5,5,5	0.43	0
4	EDO	D	1279	-	3,3,3	0.45	0	2,2,2	0.32	0
3	IPA	B	1277	-	3,3,3	0.59	0	3,3,3	0.17	0
6	PGE	C	1277	-	9,9,9	0.38	0	8,8,8	0.50	0
5	PEG	B	1281	-	6,6,6	0.39	0	5,5,5	0.47	0
4	EDO	A	1278	-	3,3,3	0.55	0	2,2,2	0.22	0
4	EDO	D	1276	-	3,3,3	0.63	0	2,2,2	0.14	0
2	GOL	D	1277	-	5,5,5	0.44	0	5,5,5	0.38	0
4	EDO	C	1276	-	3,3,3	0.53	0	2,2,2	0.03	0
2	GOL	D	1281	-	5,5,5	0.33	0	5,5,5	0.38	0
2	GOL	D	1280	-	5,5,5	0.36	0	5,5,5	0.36	0
2	GOL	D	1275	-	5,5,5	0.65	0	5,5,5	0.50	0
2	GOL	A	1279	-	5,5,5	0.40	0	5,5,5	0.27	0
4	EDO	D	1278	-	3,3,3	0.61	0	2,2,2	0.08	0
3	IPA	D	1283	-	3,3,3	0.67	0	3,3,3	0.23	0
2	GOL	C	1275	-	5,5,5	0.27	0	5,5,5	0.81	0
2	GOL	A	1275	-	5,5,5	0.66	0	5,5,5	0.75	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
2	GOL	B	1276	-	-	2/4/4/4	-
2	GOL	A	1281	-	-	2/4/4/4	-
2	GOL	D	1282	-	-	0/4/4/4	-
2	GOL	A	1276	-	-	0/4/4/4	-
2	GOL	C	1279	-	-	2/4/4/4	-
2	GOL	B	1280	-	-	4/4/4/4	-
2	GOL	B	1279	-	-	4/4/4/4	-
2	GOL	C	1278	-	-	2/4/4/4	-
2	GOL	A	1282	-	-	2/4/4/4	-
2	GOL	A	1280	-	-	0/4/4/4	-
2	GOL	B	1278	-	-	4/4/4/4	-
2	GOL	B	1275	-	-	0/4/4/4	-
4	EDO	D	1279	-	-	1/1/1/1	-
6	PGE	C	1277	-	-	4/7/7/7	-
5	PEG	B	1281	-	-	4/4/4/4	-
4	EDO	A	1278	-	-	0/1/1/1	-
4	EDO	D	1276	-	-	1/1/1/1	-
2	GOL	D	1277	-	-	2/4/4/4	-
4	EDO	C	1276	-	-	1/1/1/1	-
2	GOL	D	1281	-	-	0/4/4/4	-
2	GOL	D	1280	-	-	2/4/4/4	-
2	GOL	D	1275	-	-	2/4/4/4	-
2	GOL	A	1279	-	-	2/4/4/4	-
4	EDO	D	1278	-	-	0/1/1/1	-
2	GOL	C	1275	-	-	2/4/4/4	-
2	GOL	A	1275	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (47) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1275	GOL	O1-C1-C2-O2
2	A	1275	GOL	O1-C1-C2-C3
2	A	1275	GOL	C1-C2-C3-O3
2	A	1275	GOL	O2-C2-C3-O3
2	A	1279	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
2	A	1281	GOL	O1-C1-C2-O2
2	A	1281	GOL	O1-C1-C2-C3
2	A	1282	GOL	O1-C1-C2-O2
2	A	1282	GOL	O1-C1-C2-C3
2	B	1278	GOL	C1-C2-C3-O3
2	B	1279	GOL	O1-C1-C2-C3
2	B	1280	GOL	C1-C2-C3-O3
2	C	1275	GOL	C1-C2-C3-O3
2	C	1278	GOL	O1-C1-C2-O2
2	C	1278	GOL	O1-C1-C2-C3
2	C	1279	GOL	C1-C2-C3-O3
2	C	1279	GOL	O2-C2-C3-O3
2	A	1279	GOL	O1-C1-C2-O2
2	B	1278	GOL	O2-C2-C3-O3
2	D	1275	GOL	O2-C2-C3-O3
5	B	1281	PEG	O1-C1-C2-O2
5	B	1281	PEG	O2-C3-C4-O4
6	C	1277	PGE	O1-C1-C2-O2
6	C	1277	PGE	C6-C5-O3-C4
2	B	1276	GOL	C1-C2-C3-O3
2	B	1278	GOL	O1-C1-C2-C3
2	B	1279	GOL	C1-C2-C3-O3
2	B	1280	GOL	O1-C1-C2-C3
2	D	1275	GOL	C1-C2-C3-O3
2	D	1277	GOL	C1-C2-C3-O3
2	D	1280	GOL	C1-C2-C3-O3
2	B	1279	GOL	O1-C1-C2-O2
2	B	1280	GOL	O1-C1-C2-O2
2	B	1280	GOL	O2-C2-C3-O3
2	D	1280	GOL	O2-C2-C3-O3
6	C	1277	PGE	O3-C5-C6-O4
2	B	1278	GOL	O1-C1-C2-O2
2	C	1275	GOL	O2-C2-C3-O3
2	D	1277	GOL	O2-C2-C3-O3
6	C	1277	PGE	C3-C4-O3-C5
4	D	1279	EDO	O1-C1-C2-O2
2	B	1279	GOL	O2-C2-C3-O3
4	D	1276	EDO	O1-C1-C2-O2
4	C	1276	EDO	O1-C1-C2-O2
2	B	1276	GOL	O2-C2-C3-O3
5	B	1281	PEG	C1-C2-O2-C3
5	B	1281	PEG	C4-C3-O2-C2

There are no ring outliers.

12 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1276	GOL	4	0
2	A	1281	GOL	1	0
2	D	1282	GOL	2	0
3	A	1277	IPA	3	0
2	B	1280	GOL	1	0
2	B	1279	GOL	1	0
2	A	1282	GOL	2	0
2	B	1275	GOL	4	0
5	B	1281	PEG	1	0
4	A	1278	EDO	1	0
3	D	1283	IPA	1	0
2	C	1275	GOL	2	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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	274/297 (92%)	-0.23	9 (3%)	46	50	17, 32, 63, 105	0
1	B	274/297 (92%)	-0.17	7 (2%)	56	59	18, 33, 63, 104	0
1	C	274/297 (92%)	-0.31	3 (1%)	80	82	15, 31, 56, 76	0
1	D	274/297 (92%)	-0.42	2 (0%)	87	89	14, 29, 51, 78	0
All	All	1096/1188 (92%)	-0.28	21 (1%)	66	69	14, 31, 58, 105	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	272	ILE	6.8
1	A	274	ILE	5.7
1	A	272	ILE	5.0
1	A	273	GLU	4.6
1	A	271	GLY	4.0
1	B	274	ILE	3.8
1	B	273	GLU	3.8
1	B	220	ASN	3.8
1	D	1	MET	3.7
1	B	224	MET	3.1
1	C	1	MET	2.6
1	D	177	ASP	2.4
1	A	221	ASN	2.3
1	A	1	MET	2.3
1	B	271	GLY	2.3
1	C	16	HIS	2.2
1	A	40	PHE	2.2
1	A	220	ASN	2.2
1	A	224	MET	2.1
1	C	177	ASP	2.1
1	B	201	VAL	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 monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	GOL	A	1281	6/6	0.85	0.32	32,33,47,47	0
2	GOL	A	1279	6/6	0.86	0.13	32,47,52,58	0
4	EDO	A	1278	4/4	0.86	0.32	36,39,46,46	0
2	GOL	B	1280	6/6	0.87	0.20	33,44,52,52	0
2	GOL	C	1278	6/6	0.88	0.23	19,43,46,48	0
3	IPA	D	1283	4/4	0.88	0.32	34,38,40,52	0
2	GOL	B	1278	6/6	0.88	0.16	37,45,51,59	0
6	PGE	C	1277	10/10	0.88	0.19	39,47,53,53	0
2	GOL	D	1277	6/6	0.89	0.18	37,37,43,45	0
2	GOL	D	1280	6/6	0.89	0.27	34,41,45,46	0
4	EDO	D	1278	4/4	0.89	0.22	32,36,37,46	0
2	GOL	D	1282	6/6	0.89	0.22	35,37,45,55	0
2	GOL	B	1275	6/6	0.90	0.35	29,41,44,52	0
2	GOL	D	1281	6/6	0.91	0.21	23,34,49,53	0
2	GOL	B	1279	6/6	0.92	0.14	29,39,40,40	0
3	IPA	B	1277	4/4	0.92	0.21	26,47,51,51	0
2	GOL	A	1275	6/6	0.92	0.28	27,33,45,50	0
3	IPA	A	1277	4/4	0.93	0.19	38,38,41,46	0
4	EDO	D	1276	4/4	0.93	0.30	28,34,42,48	0
2	GOL	A	1276	6/6	0.93	0.21	25,37,40,52	0
4	EDO	D	1279	4/4	0.93	0.20	35,37,42,43	0
2	GOL	A	1280	6/6	0.93	0.16	27,34,44,53	0
2	GOL	D	1275	6/6	0.94	0.34	17,41,45,45	0
4	EDO	C	1276	4/4	0.94	0.19	21,25,35,40	0
5	PEG	B	1281	7/7	0.94	0.24	28,32,38,40	0
2	GOL	B	1276	6/6	0.94	0.30	30,32,47,49	0
2	GOL	C	1275	6/6	0.95	0.41	28,44,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
2	GOL	C	1279	6/6	0.96	0.16	26,39,45,55	0
2	GOL	A	1282	6/6	0.97	0.20	24,28,31,34	0

6.5 Other polymers

There are no such residues in this entry.