



# Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 06:37 am BST

PDB ID : 4UR7  
Title : Crystal structure of keto-deoxy-D-galactarate dehydratase complexed with pyruvate  
Authors : Taberman, H.; Parkkinen, T.; Hakulinen, N.; Rouvinen, J.  
Deposited on : 2014-06-26  
Resolution : 1.50 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
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) : 2.11

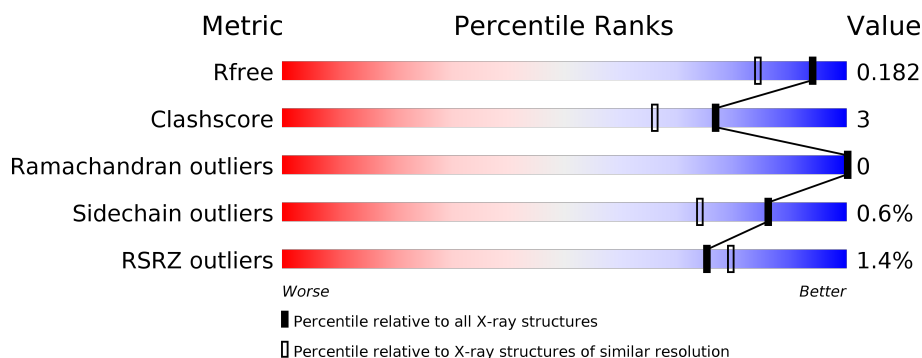
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.50 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	2936 (1.50-1.50)
Clashscore	141614	3144 (1.50-1.50)
Ramachandran outliers	138981	3066 (1.50-1.50)
Sidechain outliers	138945	3064 (1.50-1.50)
RSRZ outliers	127900	2884 (1.50-1.50)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	312	
1	B	312	
1	C	312	
1	D	312	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10972 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 KETO-DEOXY-D-GALACTARATE DEHYDRATASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	303	Total	C	N	O	S	0	5	0
			2316	1482	390	431	13			
1	B	310	Total	C	N	O	S	0	3	0
			2374	1521	400	440	13			
1	C	307	Total	C	N	O	S	0	4	0
			2348	1504	396	435	13			
1	D	301	Total	C	N	O	S	0	5	0
			2303	1474	386	430	13			

There are 40 discrepancies between the modelled and reference sequences:

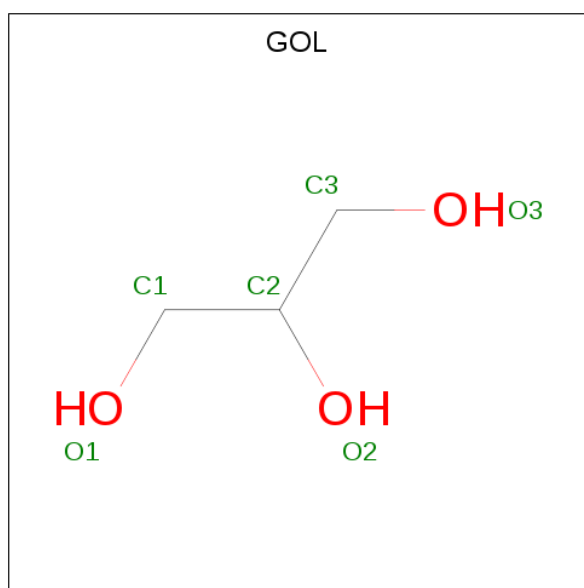
Chain	Residue	Modelled	Actual	Comment	Reference
A	2	ASP	ASN	cloning artifact	UNP Q8UB77
A	166	KPI	LYS	microheterogeneity	UNP Q8UB77
A	304	TRP	-	expression tag	UNP Q8UB77
A	305	SER	-	expression tag	UNP Q8UB77
A	306	HIS	-	expression tag	UNP Q8UB77
A	307	PRO	-	expression tag	UNP Q8UB77
A	308	GLN	-	expression tag	UNP Q8UB77
A	309	PHE	-	expression tag	UNP Q8UB77
A	310	GLU	-	expression tag	UNP Q8UB77
A	311	LYS	-	expression tag	UNP Q8UB77
B	2	ASP	ASN	cloning artifact	UNP Q8UB77
B	166	KPI	LYS	microheterogeneity	UNP Q8UB77
B	304	TRP	-	expression tag	UNP Q8UB77
B	305	SER	-	expression tag	UNP Q8UB77
B	306	HIS	-	expression tag	UNP Q8UB77
B	307	PRO	-	expression tag	UNP Q8UB77
B	308	GLN	-	expression tag	UNP Q8UB77
B	309	PHE	-	expression tag	UNP Q8UB77
B	310	GLU	-	expression tag	UNP Q8UB77
B	311	LYS	-	expression tag	UNP Q8UB77
C	2	ASP	ASN	cloning artifact	UNP Q8UB77

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Chain	Residue	Modelled	Actual	Comment	Reference
C	166	KPI	LYS	microheterogeneity	UNP Q8UB77
C	304	TRP	-	expression tag	UNP Q8UB77
C	305	SER	-	expression tag	UNP Q8UB77
C	306	HIS	-	expression tag	UNP Q8UB77
C	307	PRO	-	expression tag	UNP Q8UB77
C	308	GLN	-	expression tag	UNP Q8UB77
C	309	PHE	-	expression tag	UNP Q8UB77
C	310	GLU	-	expression tag	UNP Q8UB77
C	311	LYS	-	expression tag	UNP Q8UB77
D	2	ASP	ASN	cloning artifact	UNP Q8UB77
D	166	KPI	LYS	microheterogeneity	UNP Q8UB77
D	304	TRP	-	expression tag	UNP Q8UB77
D	305	SER	-	expression tag	UNP Q8UB77
D	306	HIS	-	expression tag	UNP Q8UB77
D	307	PRO	-	expression tag	UNP Q8UB77
D	308	GLN	-	expression tag	UNP Q8UB77
D	309	PHE	-	expression tag	UNP Q8UB77
D	310	GLU	-	expression tag	UNP Q8UB77
D	311	LYS	-	expression tag	UNP Q8UB77

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



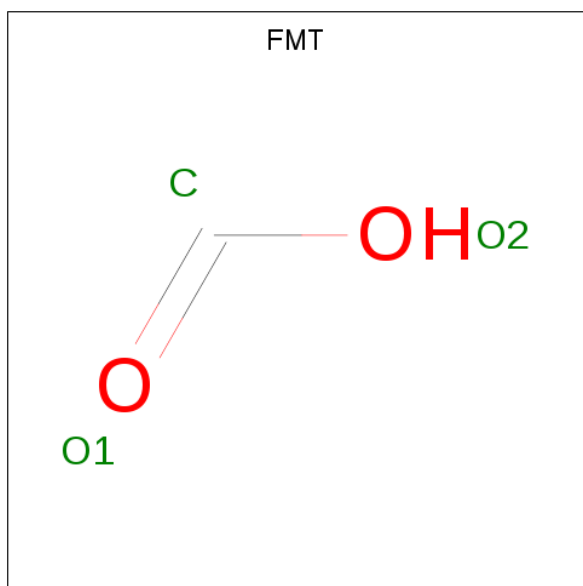
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		

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

- Molecule 3 is FORMIC ACID (three-letter code: FMT) (formula: CH<sub>2</sub>O<sub>2</sub>).



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

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

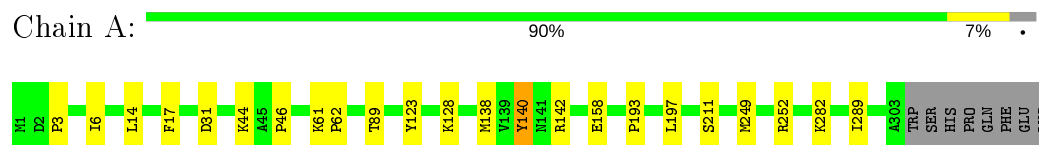
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	468	Total	O	0	0
			468	468		
4	B	406	Total	O	0	0
			406	406		
4	C	325	Total	O	0	0
			325	325		
4	D	360	Total	O	0	0
			360	360		

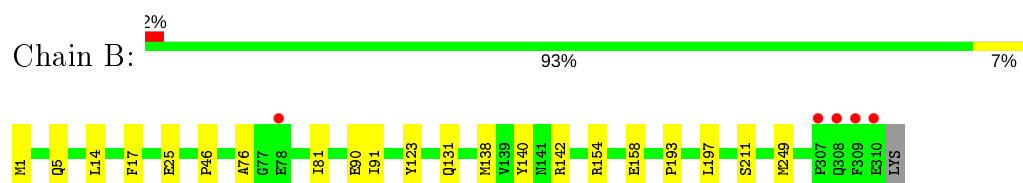
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

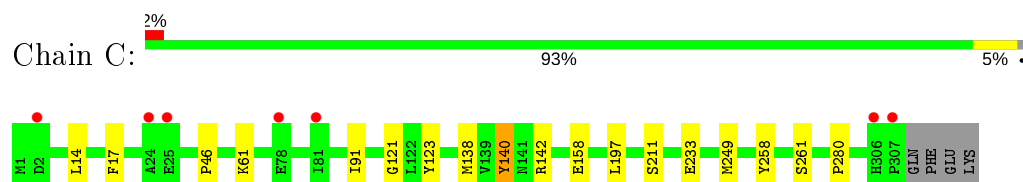
- Molecule 1: KETO-DEOXY-D-GALACTARATE DEHYDRATASE



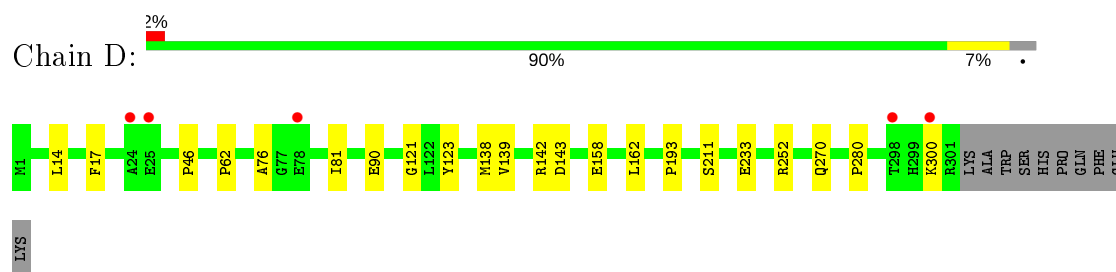
- Molecule 1: KETO-DEOXY-D-GALACTARATE DEHYDRATASE



- Molecule 1: KETO-DEOXY-D-GALACTARATE DEHYDRATASE



- Molecule 1: KETO-DEOXY-D-GALACTARATE DEHYDRATASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	169.80Å 120.14Å 74.07Å 90.00° 112.01° 90.00°	Depositor
Resolution (Å)	48.09 – 1.50 48.09 – 1.50	Depositor EDS
% Data completeness (in resolution range)	97.8 (48.09-1.50) 97.8 (48.09-1.50)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.17 (at 1.50Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, $R_{free}$	0.163 , 0.182 0.163 , 0.182	Depositor DCC
$R_{free}$ test set	10750 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	18.3	Xtriage
Anisotropy	0.536	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 41.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	10972	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.87% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, FMT, KPI

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	0.37	0/2360	0.58	0/3193
1	B	0.37	0/2417	0.56	0/3272
1	C	0.29	0/2393	0.49	0/3240
1	D	0.32	0/2347	0.51	0/3176
All	All	0.34	0/9517	0.54	0/12881

There are no bond length outliers.

There are no bond angle outliers.

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	2316	0	2316	20	0
1	B	2374	0	2357	15	0
1	C	2348	0	2339	11	0
1	D	2303	0	2298	17	0
2	A	24	0	32	0	0
2	B	18	0	24	0	0
2	C	6	0	8	0	0
2	D	12	0	16	0	0
3	A	3	0	1	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	3	0	1	0	0
3	C	3	0	1	0	0
3	D	3	0	1	0	0
4	A	468	0	0	7	1
4	B	406	0	0	5	1
4	C	325	0	0	1	0
4	D	360	0	0	5	1
All	All	10972	0	9394	57	2

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 3.

All (57) 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:D:123:TYR:OH	4:D:2201:HOH:O	2.05	0.75
1:D:233[B]:GLU:OE1	4:D:2291:HOH:O	2.07	0.71
1:A:289:ILE:HD11	4:A:2421:HOH:O	1.91	0.70
1:C:233:GLU:OE1	4:C:2247:HOH:O	2.11	0.68
1:A:123:TYR:OH	1:A:158:GLU:OE1	2.09	0.66
1:A:282:LYS:NZ	4:A:2437:HOH:O	2.25	0.66
1:B:158:GLU:OE2	4:B:2249:HOH:O	2.13	0.65
1:B:197:LEU:HD21	1:B:249[A]:MET:HG3	1.80	0.63
1:A:249[B]:MET:SD	1:A:252:ARG:NH1	2.71	0.63
1:D:158:GLU:HB2	4:D:2201:HOH:O	1.99	0.62
1:A:197:LEU:HD11	1:A:249[B]:MET:SD	2.42	0.60
1:A:61:LYS:HG3	1:B:90:GLU:HB3	1.84	0.58
1:B:193:PRO:HA	4:B:2287:HOH:O	2.04	0.58
1:B:123:TYR:OH	1:B:158:GLU:OE1	2.21	0.58
1:B:17:PHE:CE1	1:B:211:SER:HB3	2.39	0.58
1:C:61:LYS:HG3	1:D:90:GLU:HB3	1.89	0.54
1:B:131:GLN:NE2	4:B:2228:HOH:O	2.27	0.53
1:A:31:ASP:OD1	4:A:2079:HOH:O	2.19	0.52
1:C:123:TYR:OH	1:C:158:GLU:OE1	2.23	0.50
1:A:193:PRO:HA	4:A:2340:HOH:O	2.11	0.50
1:D:193:PRO:HA	4:D:2255:HOH:O	2.12	0.50
1:C:91:ILE:HD11	1:D:62:PRO:HD3	1.94	0.50
1:A:89:THR:HG21	1:A:128:LYS:HD3	1.94	0.49
1:C:17:PHE:CE1	1:C:211:SER:HB3	2.47	0.49
1:C:197:LEU:HD21	1:C:249[B]:MET:SD	2.53	0.49
1:A:140:TYR:CZ	1:A:142:ARG:HD2	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:17:PHE:CE1	1:A:211[A]:SER:HB3	2.48	0.49
1:B:1:MET:HG3	1:B:5:GLN:HB2	1.96	0.48
1:C:258:TYR:HA	1:C:261:SER:HB2	1.95	0.47
1:B:14:LEU:O	1:B:46:PRO:HD2	2.15	0.47
1:D:17:PHE:CE1	1:D:211[A]:SER:HB3	2.49	0.47
1:D:270:GLN:NE2	4:D:2268:HOH:O	2.48	0.47
1:B:140:TYR:CZ	1:B:142:ARG:HD2	2.50	0.46
1:A:62:PRO:HD3	1:B:91:ILE:HD11	1.97	0.46
1:A:44:LYS:NZ	4:A:2113:HOH:O	2.47	0.46
1:D:139:VAL:HG13	1:D:162:LEU:HD11	1.97	0.45
1:A:282:LYS:NZ	4:A:2417:HOH:O	2.48	0.45
1:D:193:PRO:HB2	1:D:252:ARG:NH1	2.32	0.44
1:C:140:TYR:CZ	1:C:142:ARG:HD2	2.53	0.44
1:B:76:ALA:CB	1:B:81:ILE:HD11	2.47	0.44
1:A:140:TYR:CE1	1:A:142:ARG:HD2	2.53	0.44
1:A:14:LEU:O	1:A:46:PRO:HD2	2.17	0.44
1:C:14:LEU:O	1:C:46:PRO:HD2	2.17	0.43
1:C:121:GLY:HA3	1:D:280:PRO:O	2.17	0.43
1:D:14:LEU:O	1:D:46:PRO:HD2	2.19	0.43
1:D:76:ALA:CB	1:D:81:ILE:HD11	2.49	0.43
1:A:3:PRO:HA	1:A:6:ILE:HG22	2.01	0.43
1:D:300:LYS:HE3	1:D:300:LYS:HB2	1.57	0.43
1:A:252:ARG:CZ	4:A:2396:HOH:O	2.68	0.42
1:D:142:ARG:HG2	1:D:143:ASP:OD2	2.20	0.42
1:A:197:LEU:HD11	1:A:249[B]:MET:CG	2.50	0.41
1:B:158:GLU:HG3	4:B:2249:HOH:O	2.19	0.41
1:C:280:PRO:O	1:D:121:GLY:HA3	2.20	0.41
1:D:17:PHE:CE1	1:D:211[B]:SER:HB2	2.55	0.41
1:A:17:PHE:CE1	1:A:211[B]:SER:HB2	2.55	0.41
1:B:154:ARG:HD3	4:B:2245:HOH:O	2.22	0.40
1:B:25:GLU:OE1	1:B:25:GLU:N	2.55	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:2125:HOH:O	4:D:2127:HOH:O[2_658]	1.95	0.25
4:A:2148:HOH:O	4:B:2124:HOH:O[2_557]	2.15	0.05

## 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	304/312 (97%)	300 (99%)	4 (1%)	0	100	100
1	B	309/312 (99%)	305 (99%)	4 (1%)	0	100	100
1	C	307/312 (98%)	302 (98%)	5 (2%)	0	100	100
1	D	302/312 (97%)	296 (98%)	6 (2%)	0	100	100
All	All	1222/1248 (98%)	1203 (98%)	19 (2%)	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	234/238 (98%)	232 (99%)	2 (1%)	78	61
1	B	239/238 (100%)	238 (100%)	1 (0%)	91	82
1	C	237/238 (100%)	235 (99%)	2 (1%)	81	66
1	D	233/238 (98%)	232 (100%)	1 (0%)	91	82
All	All	943/952 (99%)	937 (99%)	6 (1%)	86	74

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	138	MET
1	A	140	TYR

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Mol	Chain	Res	Type
1	B	138	MET
1	C	138	MET
1	C	140	TYR
1	D	138	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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	$\# Z  > 2$
1	KPI	C	166[A]	1	10,13,14	2.83	1 (10%)	6,15,17	3.80	3 (50%)
1	KPI	B	166[A]	1	10,13,14	2.72	1 (10%)	6,15,17	3.09	3 (50%)
1	KPI	D	166[A]	1	10,13,14	2.94	1 (10%)	6,15,17	2.23	2 (33%)
1	KPI	A	166[A]	1	10,13,14	2.81	1 (10%)	6,15,17	2.22	3 (50%)

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
1	KPI	C	166[A]	1	-	0/9/14/16	-
1	KPI	B	166[A]	1	-	0/9/14/16	-
1	KPI	D	166[A]	1	-	0/9/14/16	-
1	KPI	A	166[A]	1	-	0/9/14/16	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	166[A]	KPI	CX2-CX1	-8.75	1.38	1.52
1	C	166[A]	KPI	CX2-CX1	-8.52	1.39	1.52
1	A	166[A]	KPI	CX2-CX1	-8.51	1.39	1.52
1	B	166[A]	KPI	CX2-CX1	-8.33	1.39	1.52

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	166[A]	KPI	CE-NZ-CX1	7.32	141.46	121.77
1	B	166[A]	KPI	CE-NZ-CX1	5.91	137.67	121.77
1	C	166[A]	KPI	C1-CX1-NZ	-4.45	112.03	123.12
1	D	166[A]	KPI	CE-NZ-CX1	4.19	133.03	121.77
1	A	166[A]	KPI	CE-NZ-CX1	3.76	131.89	121.77
1	C	166[A]	KPI	CD-CE-NZ	3.34	116.73	110.66
1	B	166[A]	KPI	C1-CX1-NZ	-3.27	114.96	123.12
1	D	166[A]	KPI	CD-CE-NZ	3.11	116.32	110.66
1	B	166[A]	KPI	CD-CE-NZ	2.98	116.08	110.66
1	A	166[A]	KPI	C1-CX1-CX2	2.60	120.80	117.92
1	A	166[A]	KPI	CD-CE-NZ	2.33	114.89	110.66

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

14 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	A	1307	-	5,5,5	0.27	0	5,5,5	0.35	0
2	GOL	A	1308	-	5,5,5	0.35	0	5,5,5	0.44	0
2	GOL	B	1312	-	5,5,5	0.31	0	5,5,5	0.36	0
2	GOL	B	1313	-	5,5,5	0.36	0	5,5,5	0.13	0
3	FMT	D	1304	-	0,2,2	0.00	-	0,1,1	0.00	-
2	GOL	A	1305	-	5,5,5	0.29	0	5,5,5	0.13	0
2	GOL	B	1314	-	5,5,5	0.28	0	5,5,5	0.37	0
2	GOL	D	1303	-	5,5,5	0.39	0	5,5,5	0.14	0
3	FMT	A	1306	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	B	1315	-	0,2,2	0.00	-	0,1,1	0.00	-
2	GOL	A	1309	-	5,5,5	0.37	0	5,5,5	0.31	0
3	FMT	C	1310	-	0,2,2	0.00	-	0,1,1	0.00	-
2	GOL	C	1309	-	5,5,5	0.38	0	5,5,5	0.21	0
2	GOL	D	1305	-	5,5,5	0.41	0	5,5,5	0.57	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	A	1307	-	-	0/4/4/4	-
2	GOL	A	1308	-	-	2/4/4/4	-
2	GOL	B	1312	-	-	0/4/4/4	-
2	GOL	C	1309	-	-	0/4/4/4	-
2	GOL	A	1305	-	-	0/4/4/4	-
2	GOL	B	1314	-	-	0/4/4/4	-
2	GOL	D	1303	-	-	0/4/4/4	-
2	GOL	A	1309	-	-	0/4/4/4	-
2	GOL	B	1313	-	-	0/4/4/4	-
2	GOL	D	1305	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1308	GOL	C1-C2-C3-O3
2	D	1305	GOL	O1-C1-C2-C3
2	A	1308	GOL	O2-C2-C3-O3
2	D	1305	GOL	O1-C1-C2-O2

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	302/312 (96%)	-0.27	0 <b>100</b> <b>100</b>	12, 17, 26, 42	0
1	B	309/312 (99%)	-0.06	5 (1%) <b>72</b> <b>77</b>	12, 18, 28, 55	0
1	C	306/312 (98%)	0.05	7 (2%) <b>60</b> <b>65</b>	18, 24, 36, 53	0
1	D	300/312 (96%)	-0.08	5 (1%) <b>70</b> <b>75</b>	16, 22, 34, 53	0
All	All	1217/1248 (97%)	-0.09	17 (1%) <b>75</b> <b>79</b>	12, 21, 33, 55	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	309	PHE	7.6
1	C	307	PRO	7.2
1	B	310	GLU	4.7
1	C	24	ALA	4.0
1	B	308	GLN	3.6
1	C	306	HIS	3.4
1	D	78	GLU	3.3
1	D	24	ALA	3.3
1	D	300	LYS	3.1
1	B	78	GLU	2.8
1	D	298	THR	2.7
1	C	78	GLU	2.6
1	D	25	GLU	2.5
1	C	2	ASP	2.4
1	B	307	PRO	2.4
1	C	81	ILE	2.4
1	C	25	GLU	2.1

## 6.2 Non-standard residues in protein, DNA, RNA chains [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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
1	KPI	B	166[A]	14/15	0.94	0.14	14,16,22,23	14
1	KPI	A	166[A]	14/15	0.94	0.13	13,14,17,21	14
1	KPI	D	166[A]	14/15	0.95	0.13	15,18,24,27	14
1	KPI	C	166[A]	14/15	0.95	0.11	17,19,27,28	14

## 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. The B-factors column lists the minimum, median, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
2	GOL	A	1309	6/6	0.76	0.32	28,40,45,47	0
3	FMT	C	1310	3/3	0.77	0.16	34,34,40,45	0
3	FMT	A	1306	3/3	0.79	0.15	32,32,32,38	0
3	FMT	D	1304	3/3	0.82	0.14	33,33,37,45	0
2	GOL	D	1305	6/6	0.89	0.20	25,31,37,40	0
2	GOL	B	1314	6/6	0.90	0.15	24,26,32,32	0
2	GOL	A	1307	6/6	0.91	0.16	22,24,30,34	0
3	FMT	B	1315	3/3	0.92	0.10	28,28,31,41	0
2	GOL	A	1308	6/6	0.94	0.08	17,20,22,28	0
2	GOL	C	1309	6/6	0.95	0.08	20,23,26,28	0
2	GOL	B	1313	6/6	0.96	0.07	16,17,17,20	0
2	GOL	D	1303	6/6	0.96	0.07	17,19,22,23	0
2	GOL	A	1305	6/6	0.97	0.07	15,16,16,19	0
2	GOL	B	1312	6/6	0.98	0.06	15,16,18,18	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.