



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:42 PM GMT

PDB ID : 4MFE  
Title : Structure of the carboxyl transferase domain from *Rhizobium etli* pyruvate carboxylase with 3-hydroxypyruvate  
Authors : Lietzan, A.D.; St. Maurice, M.  
Deposited on : 2013-08-27  
Resolution : 2.61 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  
<http://wwpdb.org/validation/2016/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 : 1.7 (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

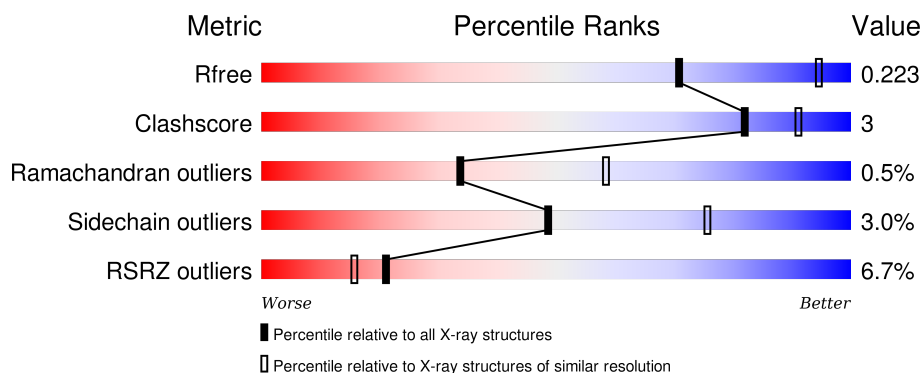
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.61 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	2700 (2.64-2.60)
Clashscore	102246	3065 (2.64-2.60)
Ramachandran outliers	100387	3015 (2.64-2.60)
Sidechain outliers	100360	3015 (2.64-2.60)
RSRZ outliers	91569	2706 (2.64-2.60)

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. 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	632	<div> <div>10%</div> <div>83% 11% 6%</div> </div>
1	B	632	<div> <div>10%</div> <div>87% 7% 6%</div> </div>
1	C	632	<div> <div>4%</div> <div>86% 9% 6%</div> </div>
1	D	632	<div> <div>11%</div> <div>83% 11% 6%</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
5	MG	B	1104	-	-	-	X

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 17744 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 PYRUVATE CARBOXYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	597	Total	C	N	O	S	0	1	0
			4497	2859	752	863	23			
1	B	594	Total	C	N	O	S	0	1	0
			4295	2720	720	832	23			
1	C	597	Total	C	N	O	S	0	2	0
			4416	2807	743	843	23			
1	D	594	Total	C	N	O	S	0	1	0
			4278	2708	727	820	23			

There are 116 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	436	MET	-	EXPRESSION TAG	UNP Q2K340
A	437	GLY	-	EXPRESSION TAG	UNP Q2K340
A	438	SER	-	EXPRESSION TAG	UNP Q2K340
A	439	SER	-	EXPRESSION TAG	UNP Q2K340
A	440	HIS	-	EXPRESSION TAG	UNP Q2K340
A	441	HIS	-	EXPRESSION TAG	UNP Q2K340
A	442	HIS	-	EXPRESSION TAG	UNP Q2K340
A	443	HIS	-	EXPRESSION TAG	UNP Q2K340
A	444	HIS	-	EXPRESSION TAG	UNP Q2K340
A	445	HIS	-	EXPRESSION TAG	UNP Q2K340
A	446	HIS	-	EXPRESSION TAG	UNP Q2K340
A	447	HIS	-	EXPRESSION TAG	UNP Q2K340
A	448	ASP	-	EXPRESSION TAG	UNP Q2K340
A	449	TYR	-	EXPRESSION TAG	UNP Q2K340
A	450	ASP	-	EXPRESSION TAG	UNP Q2K340
A	451	ILE	-	EXPRESSION TAG	UNP Q2K340
A	452	PRO	-	EXPRESSION TAG	UNP Q2K340
A	453	THR	-	EXPRESSION TAG	UNP Q2K340
A	454	SER	-	EXPRESSION TAG	UNP Q2K340
A	455	GLU	-	EXPRESSION TAG	UNP Q2K340
A	456	ASN	-	EXPRESSION TAG	UNP Q2K340

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Chain	Residue	Modelled	Actual	Comment	Reference
A	457	LEU	-	EXPRESSION TAG	UNP Q2K340
A	458	TYR	-	EXPRESSION TAG	UNP Q2K340
A	459	PHE	-	EXPRESSION TAG	UNP Q2K340
A	460	GLN	-	EXPRESSION TAG	UNP Q2K340
A	461	GLY	-	EXPRESSION TAG	UNP Q2K340
A	462	LEU	-	EXPRESSION TAG	UNP Q2K340
A	463	LEU	-	EXPRESSION TAG	UNP Q2K340
A	464	HIS	-	EXPRESSION TAG	UNP Q2K340
B	436	MET	-	EXPRESSION TAG	UNP Q2K340
B	437	GLY	-	EXPRESSION TAG	UNP Q2K340
B	438	SER	-	EXPRESSION TAG	UNP Q2K340
B	439	SER	-	EXPRESSION TAG	UNP Q2K340
B	440	HIS	-	EXPRESSION TAG	UNP Q2K340
B	441	HIS	-	EXPRESSION TAG	UNP Q2K340
B	442	HIS	-	EXPRESSION TAG	UNP Q2K340
B	443	HIS	-	EXPRESSION TAG	UNP Q2K340
B	444	HIS	-	EXPRESSION TAG	UNP Q2K340
B	445	HIS	-	EXPRESSION TAG	UNP Q2K340
B	446	HIS	-	EXPRESSION TAG	UNP Q2K340
B	447	HIS	-	EXPRESSION TAG	UNP Q2K340
B	448	ASP	-	EXPRESSION TAG	UNP Q2K340
B	449	TYR	-	EXPRESSION TAG	UNP Q2K340
B	450	ASP	-	EXPRESSION TAG	UNP Q2K340
B	451	ILE	-	EXPRESSION TAG	UNP Q2K340
B	452	PRO	-	EXPRESSION TAG	UNP Q2K340
B	453	THR	-	EXPRESSION TAG	UNP Q2K340
B	454	SER	-	EXPRESSION TAG	UNP Q2K340
B	455	GLU	-	EXPRESSION TAG	UNP Q2K340
B	456	ASN	-	EXPRESSION TAG	UNP Q2K340
B	457	LEU	-	EXPRESSION TAG	UNP Q2K340
B	458	TYR	-	EXPRESSION TAG	UNP Q2K340
B	459	PHE	-	EXPRESSION TAG	UNP Q2K340
B	460	GLN	-	EXPRESSION TAG	UNP Q2K340
B	461	GLY	-	EXPRESSION TAG	UNP Q2K340
B	462	LEU	-	EXPRESSION TAG	UNP Q2K340
B	463	LEU	-	EXPRESSION TAG	UNP Q2K340
B	464	HIS	-	EXPRESSION TAG	UNP Q2K340
C	436	MET	-	EXPRESSION TAG	UNP Q2K340
C	437	GLY	-	EXPRESSION TAG	UNP Q2K340
C	438	SER	-	EXPRESSION TAG	UNP Q2K340
C	439	SER	-	EXPRESSION TAG	UNP Q2K340
C	440	HIS	-	EXPRESSION TAG	UNP Q2K340

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Chain	Residue	Modelled	Actual	Comment	Reference
C	441	HIS	-	EXPRESSION TAG	UNP Q2K340
C	442	HIS	-	EXPRESSION TAG	UNP Q2K340
C	443	HIS	-	EXPRESSION TAG	UNP Q2K340
C	444	HIS	-	EXPRESSION TAG	UNP Q2K340
C	445	HIS	-	EXPRESSION TAG	UNP Q2K340
C	446	HIS	-	EXPRESSION TAG	UNP Q2K340
C	447	HIS	-	EXPRESSION TAG	UNP Q2K340
C	448	ASP	-	EXPRESSION TAG	UNP Q2K340
C	449	TYR	-	EXPRESSION TAG	UNP Q2K340
C	450	ASP	-	EXPRESSION TAG	UNP Q2K340
C	451	ILE	-	EXPRESSION TAG	UNP Q2K340
C	452	PRO	-	EXPRESSION TAG	UNP Q2K340
C	453	THR	-	EXPRESSION TAG	UNP Q2K340
C	454	SER	-	EXPRESSION TAG	UNP Q2K340
C	455	GLU	-	EXPRESSION TAG	UNP Q2K340
C	456	ASN	-	EXPRESSION TAG	UNP Q2K340
C	457	LEU	-	EXPRESSION TAG	UNP Q2K340
C	458	TYR	-	EXPRESSION TAG	UNP Q2K340
C	459	PHE	-	EXPRESSION TAG	UNP Q2K340
C	460	GLN	-	EXPRESSION TAG	UNP Q2K340
C	461	GLY	-	EXPRESSION TAG	UNP Q2K340
C	462	LEU	-	EXPRESSION TAG	UNP Q2K340
C	463	LEU	-	EXPRESSION TAG	UNP Q2K340
C	464	HIS	-	EXPRESSION TAG	UNP Q2K340
D	436	MET	-	EXPRESSION TAG	UNP Q2K340
D	437	GLY	-	EXPRESSION TAG	UNP Q2K340
D	438	SER	-	EXPRESSION TAG	UNP Q2K340
D	439	SER	-	EXPRESSION TAG	UNP Q2K340
D	440	HIS	-	EXPRESSION TAG	UNP Q2K340
D	441	HIS	-	EXPRESSION TAG	UNP Q2K340
D	442	HIS	-	EXPRESSION TAG	UNP Q2K340
D	443	HIS	-	EXPRESSION TAG	UNP Q2K340
D	444	HIS	-	EXPRESSION TAG	UNP Q2K340
D	445	HIS	-	EXPRESSION TAG	UNP Q2K340
D	446	HIS	-	EXPRESSION TAG	UNP Q2K340
D	447	HIS	-	EXPRESSION TAG	UNP Q2K340
D	448	ASP	-	EXPRESSION TAG	UNP Q2K340
D	449	TYR	-	EXPRESSION TAG	UNP Q2K340
D	450	ASP	-	EXPRESSION TAG	UNP Q2K340
D	451	ILE	-	EXPRESSION TAG	UNP Q2K340
D	452	PRO	-	EXPRESSION TAG	UNP Q2K340
D	453	THR	-	EXPRESSION TAG	UNP Q2K340

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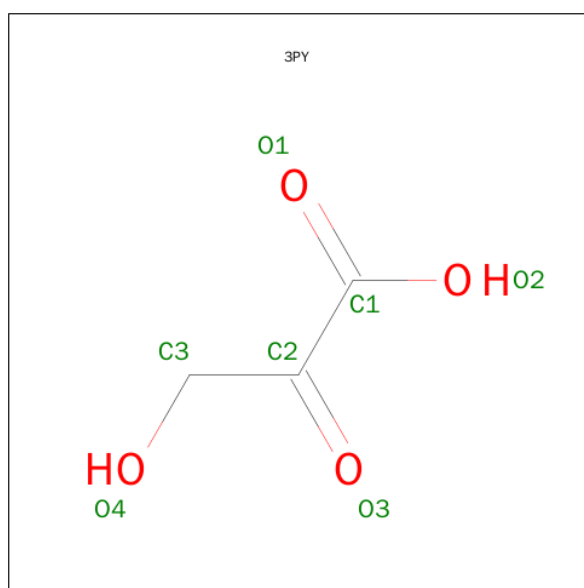
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Chain	Residue	Modelled	Actual	Comment	Reference
D	454	SER	-	EXPRESSION TAG	UNP Q2K340
D	455	GLU	-	EXPRESSION TAG	UNP Q2K340
D	456	ASN	-	EXPRESSION TAG	UNP Q2K340
D	457	LEU	-	EXPRESSION TAG	UNP Q2K340
D	458	TYR	-	EXPRESSION TAG	UNP Q2K340
D	459	PHE	-	EXPRESSION TAG	UNP Q2K340
D	460	GLN	-	EXPRESSION TAG	UNP Q2K340
D	461	GLY	-	EXPRESSION TAG	UNP Q2K340
D	462	LEU	-	EXPRESSION TAG	UNP Q2K340
D	463	LEU	-	EXPRESSION TAG	UNP Q2K340
D	464	HIS	-	EXPRESSION TAG	UNP Q2K340

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

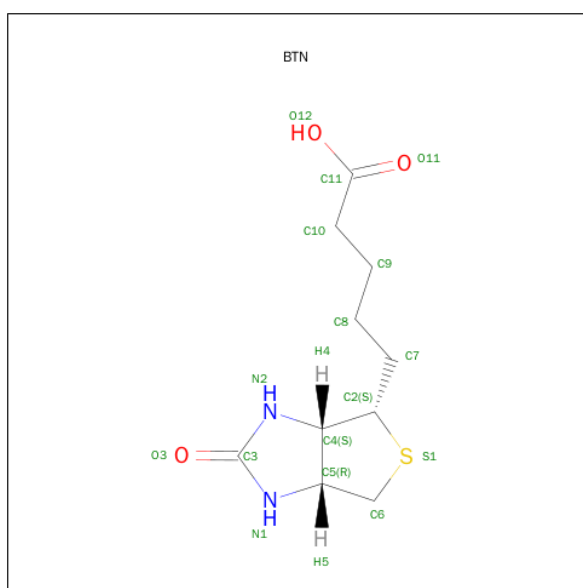
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Zn 1 1	0	0
2	A	1	Total Zn 1 1	0	0
2	D	1	Total Zn 1 1	0	0
2	C	1	Total Zn 1 1	0	0

- Molecule 3 is 3-HYDROXYPYRUVIC ACID (three-letter code: 3PY) (formula: C<sub>3</sub>H<sub>4</sub>O<sub>4</sub>).



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

- Molecule 4 is BIOTIN (three-letter code: BTN) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>2</sub>O<sub>3</sub>S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O S 9 5 2 1 1	0	0
4	B	1	Total C N O S 10 6 2 1 1	0	0
4	C	1	Total C N O S 10 6 2 1 1	0	0
4	D	1	Total C N O S 9 5 2 1 1	0	0

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total Mg 1 1	0	0
5	A	1	Total Mg 1 1	0	0

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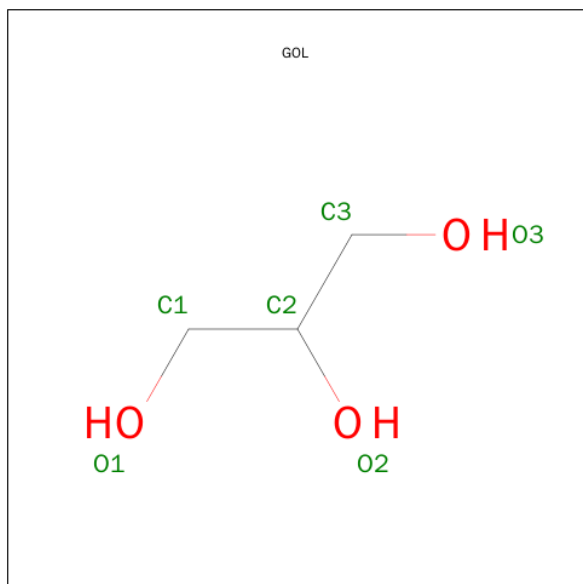
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	1	Total	Mg	0	0
			1	1		
5	C	1	Total	Mg	0	0
			1	1		

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Cl	0	0
			1	1		
6	A	1	Total	Cl	0	0
			1	1		
6	C	1	Total	Cl	0	0
			1	1		

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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

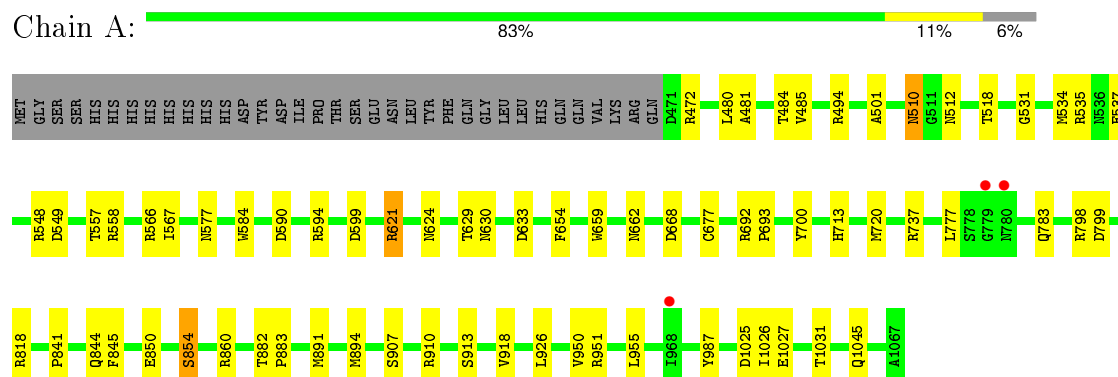
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	62	Total 62	O 62	0	0
8	B	35	Total 35	O 35	0	0
8	C	40	Total 40	O 40	0	0
8	D	32	Total 32	O 32	0	0

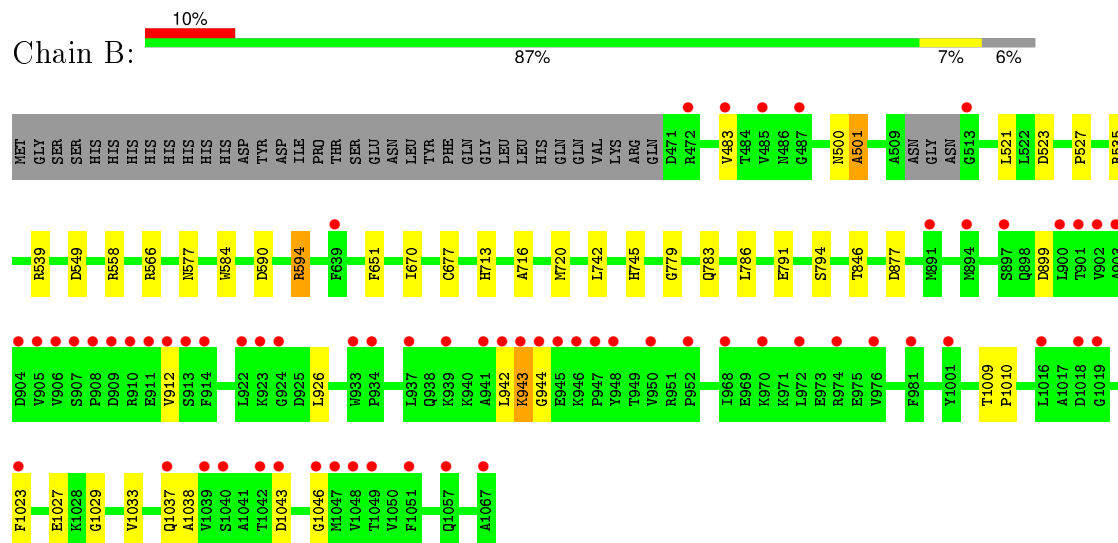
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

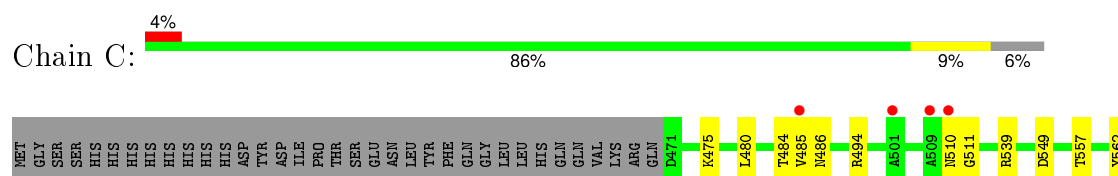
#### • Molecule 1: PYRUVATE CARBOXYLASE

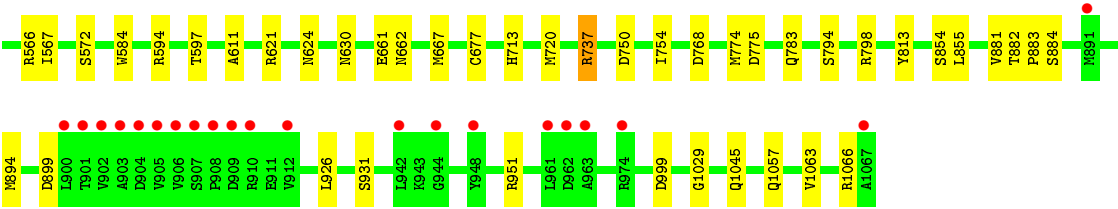


#### • Molecule 1: PYRUVATE CARBOXYLASE

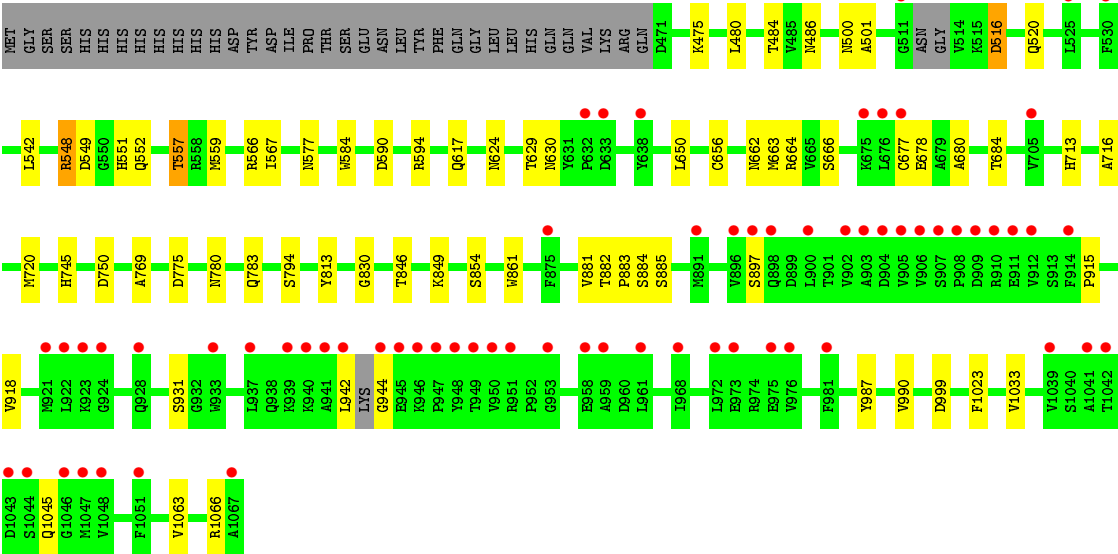
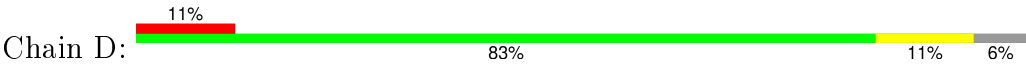


#### • Molecule 1: PYRUVATE CARBOXYLASE





● Molecule 1: PYRUVATE CARBOXYLASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	84.25Å 157.85Å 243.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.37 – 2.61 49.32 – 2.61	Depositor EDS
% Data completeness (in resolution range)	95.7 (49.37-2.61) 95.7 (49.32-2.61)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.81 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, $R_{free}$	0.177 , 0.225 0.180 , 0.223	Depositor DCC
$R_{free}$ test set	4777 reflections (5.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	63.5	Xtriage
Anisotropy	0.140	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 45.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 95679 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	17744	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.54% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: 3PY, ZN, GOL, CL, MG, BTN, KCX

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.89	4/4583 (0.1%)	0.94	9/6245 (0.1%)
1	B	0.71	1/4380 (0.0%)	0.82	6/5991 (0.1%)
1	C	0.74	0/4507	0.88	8/6156 (0.1%)
1	D	0.65	0/4362	0.76	1/5967 (0.0%)
All	All	0.75	5/17832 (0.0%)	0.85	24/24359 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	854	SER	CB-OG	-5.64	1.34	1.42
1	A	700	TYR	CE1-CZ	-5.62	1.31	1.38
1	B	791	GLU	CD-OE2	5.50	1.31	1.25
1	A	845	PHE	CB-CG	-5.46	1.42	1.51
1	A	659	TRP	CZ3-CH2	5.25	1.48	1.40

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	737	ARG	NE-CZ-NH2	12.93	126.77	120.30
1	A	737	ARG	NE-CZ-NH1	-8.58	116.01	120.30
1	C	737	ARG	NE-CZ-NH1	-7.68	116.46	120.30
1	C	594	ARG	NE-CZ-NH2	7.09	123.85	120.30
1	A	737	ARG	NE-CZ-NH2	6.75	123.67	120.30
1	A	535	ARG	NE-CZ-NH1	6.71	123.66	120.30
1	B	539	ARG	NE-CZ-NH1	6.63	123.62	120.30
1	D	750	ASP	CB-CG-OD1	6.38	124.04	118.30
1	C	594	ARG	NE-CZ-NH1	-6.37	117.11	120.30
1	C	768	ASP	CB-CG-OD2	-6.34	112.60	118.30
1	B	523	ASP	CB-CG-OD1	6.21	123.89	118.30
1	A	558	ARG	NE-CZ-NH1	-6.01	117.29	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	539	ARG	NE-CZ-NH1	5.94	123.27	120.30
1	A	558	ARG	NE-CZ-NH2	5.83	123.22	120.30
1	B	791	GLU	OE1-CD-OE2	5.82	130.28	123.30
1	A	668	ASP	CB-CG-OD2	-5.75	113.12	118.30
1	C	951	ARG	NE-CZ-NH2	5.41	123.01	120.30
1	A	599	ASP	CB-CG-OD1	5.38	123.14	118.30
1	B	558	ARG	NE-CZ-NH2	-5.24	117.68	120.30
1	A	621	ARG	NE-CZ-NH2	-5.21	117.69	120.30
1	A	537	GLU	CG-CD-OE2	-5.21	107.88	118.30
1	B	1027	GLU	N-CA-C	-5.17	97.03	111.00
1	C	798	ARG	NE-CZ-NH1	5.17	122.88	120.30
1	B	558	ARG	NE-CZ-NH1	5.12	122.86	120.30

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	4497	0	4328	35	0
1	B	4295	0	3918	21	0
1	C	4416	0	4162	24	0
1	D	4278	0	3903	29	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	7	0	3	0	0
3	B	7	0	3	0	0
3	C	7	0	3	1	0
3	D	7	0	3	0	0
4	A	9	0	6	0	0
4	B	10	0	7	0	0
4	C	10	0	7	0	0
4	D	9	0	6	0	0
5	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
7	A	6	0	8	3	0
7	D	6	0	8	1	0
8	A	62	0	0	0	0
8	B	35	0	0	2	0
8	C	40	0	0	0	0
8	D	32	0	0	0	0
All	All	17744	0	16365	110	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 3.

All (110) 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:481:ALA:O	1:A:485:VAL:HG23	1.46	1.15
1:B:500:ASN:OD1	1:B:501:ALA:N	1.94	1.00
1:A:480:LEU:O	1:A:484:THR:OG1	1.79	0.99
1:C:480:LEU:O	1:C:484:THR:OG1	1.91	0.88
1:D:942:LEU:C	1:D:944:GLY:N	2.26	0.88
1:A:891[B]:MET:HE1	1:A:918:VAL:HG11	1.58	0.85
1:A:677:CYS:H	1:A:713:HIS:HD2	1.27	0.83
1:A:472:ARG:HB3	1:A:1026:ILE:HD11	1.61	0.83
1:B:677:CYS:H	1:B:713:HIS:HD2	1.27	0.80
1:C:677:CYS:H	1:C:713:HIS:HD2	1.31	0.76
1:A:630:ASN:HD21	1:A:662:ASN:HD21	1.32	0.75
1:A:472:ARG:CB	1:A:1026:ILE:HD11	2.19	0.72
1:C:486:ASN:HD21	1:C:1066:ARG:H	1.36	0.71
1:D:549:ASP:HB3	1:D:783:GLN:HE22	1.58	0.67
1:C:677:CYS:H	1:C:713:HIS:CD2	2.13	0.66
1:D:480:LEU:O	1:D:484:THR:OG1	2.08	0.66
1:A:891[B]:MET:CE	1:A:918:VAL:HG11	2.27	0.64
1:B:677:CYS:H	1:B:713:HIS:CD2	2.13	0.62
1:B:549:ASP:HB3	1:B:783:GLN:HE22	1.64	0.62
1:B:590:ASP:OD1	1:B:594:ARG:NH2	2.32	0.61
1:A:894:MET:HE1	1:A:913:SER:O	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:486:ASN:ND2	1:C:1066:ARG:H	1.99	0.60
1:B:942:LEU:O	1:B:943:LYS:C	2.39	0.59
1:A:1025:ASP:OD2	1:A:1031:THR:OG1	2.20	0.59
1:C:486:ASN:HD21	1:C:1066:ARG:N	2.01	0.58
1:B:1023:PHE:CD1	1:B:1033:VAL:HG22	2.38	0.58
1:A:1045:GLN:OE1	1:A:1045:GLN:N	2.39	0.56
1:A:566:ARG:HG3	1:A:566:ARG:HH11	1.71	0.56
1:C:549:ASP:HB3	1:C:783:GLN:HE22	1.70	0.55
1:C:1045:GLN:OE1	1:C:1045:GLN:N	2.39	0.55
1:B:677:CYS:N	1:B:713:HIS:HD2	2.02	0.54
1:D:678:GLU:HG2	1:D:716:ALA:HB2	1.90	0.54
1:A:472:ARG:HB3	1:A:1026:ILE:CD1	2.36	0.53
1:D:677:CYS:H	1:D:713:HIS:HD2	1.58	0.51
1:A:633:ASP:OD1	1:A:951:ARG:NH1	2.43	0.51
1:A:549:ASP:HB3	1:A:783:GLN:HE22	1.73	0.51
1:A:624:ASN:HD22	1:A:629:THR:C	2.12	0.51
1:B:942:LEU:O	1:B:944:GLY:N	2.44	0.51
1:B:577:ASN:HB2	8:B:1213:HOH:O	2.12	0.50
1:A:907:SER:HB3	1:A:910:ARG:HB3	1.92	0.50
1:D:881:VAL:O	1:D:884:SER:N	2.45	0.49
1:A:894:MET:CE	1:A:913:SER:O	2.60	0.49
1:D:475:LYS:HD3	1:D:999:ASP:O	2.12	0.49
1:C:630:ASN:HD21	1:C:662:ASN:HD21	1.60	0.49
1:A:590:ASP:OD1	1:A:594:ARG:NH2	2.46	0.49
1:C:667:MET:HG2	1:C:677:CYS:SG	2.53	0.48
1:D:630:ASN:HD21	1:D:662:ASN:HD21	1.61	0.48
1:C:881:VAL:O	1:C:884:SER:N	2.47	0.48
1:A:677:CYS:H	1:A:713:HIS:CD2	2.17	0.48
1:B:527:PRO:HB2	1:B:713:HIS:CE1	2.48	0.48
1:B:1037:GLN:O	1:B:1038:ALA:HB2	2.14	0.48
1:B:651:PHE:HB2	1:B:670:ILE:HD13	1.95	0.48
7:A:1106:GOL:H11	8:B:1218:HOH:O	2.13	0.47
1:B:716:ALA:HA	1:B:745:HIS:O	2.14	0.47
1:D:516:ASP:HB3	1:D:520:GLN:HG2	1.96	0.47
1:D:551:HIS:CE1	1:D:559:MET:HB3	2.48	0.47
1:D:987:TYR:HB3	1:D:990:VAL:HB	1.95	0.47
1:D:780:ASN:OD1	1:D:830:GLY:HA2	2.14	0.47
1:A:510:ASN:HD22	1:A:512:ASN:H	1.63	0.47
1:A:1026:ILE:HG23	1:A:1027:GLU:N	2.30	0.46
1:C:754:ILE:O	1:C:754:ILE:HG13	2.15	0.46
7:A:1106:GOL:H12	1:B:779:GLY:HA3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:590:ASP:OD2	1:D:594:ARG:NH2	2.50	0.45
1:D:617:GLN:HA	1:D:650:LEU:O	2.16	0.45
1:A:950:VAL:HG21	1:A:955:LEU:HD21	1.98	0.44
1:A:590:ASP:HB2	1:A:987:TYR:CZ	2.53	0.44
1:A:692:ARG:N	1:A:693:PRO:CD	2.81	0.44
1:A:841:PRO:HD2	1:A:844:GLN:OE1	2.18	0.44
1:C:475:LYS:HE2	1:C:999:ASP:O	2.17	0.43
1:A:548:ARG:C	1:A:548:ARG:HD2	2.38	0.43
1:D:548:ARG:HE	1:D:548:ARG:HB3	1.66	0.43
1:D:1023:PHE:CE1	1:D:1033:VAL:HG22	2.53	0.43
1:D:1045:GLN:N	1:D:1045:GLN:OE1	2.51	0.43
1:D:849:LYS:HG3	1:D:861:TRP:CE3	2.53	0.43
1:D:745:HIS:HA	1:D:769:ALA:O	2.19	0.43
1:C:621:ARG:O	1:C:624:ASN:HB2	2.18	0.43
1:A:621:ARG:HG2	1:A:654:PHE:CZ	2.53	0.43
1:C:562:TYR:CE2	1:C:566:ARG:HD2	2.53	0.43
1:D:678:GLU:CG	1:D:716:ALA:HB2	2.49	0.43
1:C:882:THR:OG1	3:C:1102:3PY:H32	2.19	0.43
1:D:915:PRO:HD2	1:D:918:VAL:CB	2.49	0.43
1:C:774:MET:O	1:C:775:ASP:C	2.56	0.43
1:B:483:VAL:O	1:B:483:VAL:HG22	2.19	0.42
1:A:472:ARG:HB2	1:A:1026:ILE:HD11	1.99	0.42
7:A:1106:GOL:H12	1:B:779:GLY:CA	2.49	0.42
1:D:882:THR:HA	1:D:883:PRO:HA	1.82	0.42
1:A:531:GLY:O	1:A:534:MET:HB2	2.19	0.42
1:A:567:ILE:HD12	1:A:567:ILE:HA	1.87	0.42
1:D:552:GLN:HG3	1:D:557:THR:OG1	2.20	0.42
1:C:882:THR:HA	1:C:883:PRO:HA	1.89	0.42
1:A:882:THR:HA	1:A:883:PRO:HA	1.85	0.41
1:A:798:ARG:O	1:A:799:ASP:C	2.58	0.41
1:D:567:ILE:HB	1:D:813:TYR:CE2	2.55	0.41
1:A:894:MET:HE3	1:A:894:MET:HB2	1.90	0.41
1:B:786:LEU:O	1:B:786:LEU:HD12	2.20	0.41
1:C:750:ASP:OD2	7:D:1101:GOL:O3	2.30	0.41
1:D:624:ASN:HD22	1:D:629:THR:C	2.23	0.41
1:C:485:VAL:HG21	1:C:1063:VAL:CG2	2.51	0.41
1:A:777:LEU:CD2	1:A:818:ARG:HD2	2.50	0.41
1:D:663:MET:O	1:D:664:ARG:C	2.59	0.41
1:B:535:ARG:NH1	1:B:742:LEU:O	2.54	0.41
1:C:677:CYS:N	1:C:713:HIS:HD2	2.08	0.40
1:D:680:ALA:HA	1:D:716:ALA:HB3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:572:SER:HB2	1:C:611:ALA:HA	2.03	0.40
1:D:486:ASN:HD21	1:D:1066:ARG:H	1.68	0.40
1:C:894:MET:HB2	1:C:894:MET:HE3	1.96	0.40
1:B:1009:THR:HB	1:B:1010:PRO:HD3	2.03	0.40
1:B:1043:ASP:OD1	1:B:1046:GLY:N	2.55	0.40
1:D:656:CYS:HA	1:D:881:VAL:CG1	2.52	0.40
1:C:567:ILE:HB	1:C:813:TYR:CE2	2.57	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	595/632 (94%)	573 (96%)	21 (4%)	1 (0%)	52	76
1	B	590/632 (93%)	556 (94%)	29 (5%)	5 (1%)	24	44
1	C	596/632 (94%)	557 (94%)	35 (6%)	4 (1%)	26	49
1	D	588/632 (93%)	558 (95%)	28 (5%)	2 (0%)	46	70
All	All	2369/2528 (94%)	2244 (95%)	113 (5%)	12 (0%)	34	58

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	510	ASN
1	D	501	ALA
1	A	501	ALA
1	B	501	ALA
1	C	511	GLY
1	C	854	SER
1	C	1029	GLY
1	B	943	LYS

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Mol	Chain	Res	Type
1	D	897	SER
1	B	912	VAL
1	B	877	ASP
1	B	1029	GLY

### 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	451/519 (87%)	440 (98%)	11 (2%)	57	81
1	B	401/519 (77%)	392 (98%)	9 (2%)	60	83
1	C	430/519 (83%)	417 (97%)	13 (3%)	48	75
1	D	397/519 (76%)	379 (96%)	18 (4%)	34	61
All	All	1679/2076 (81%)	1628 (97%)	51 (3%)	48	75

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	494	ARG
1	A	510	ASN
1	A	518	THR
1	A	557	THR
1	A	577	ASN
1	A	584	TRP
1	A	720	MET
1	A	850	GLU
1	A	854	SER
1	A	860	ARG
1	A	926	LEU
1	B	521	LEU
1	B	566	ARG
1	B	584	TRP
1	B	594	ARG
1	B	720	MET
1	B	794	SER

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Mol	Chain	Res	Type
1	B	846	THR
1	B	899	ASP
1	B	926	LEU
1	C	494	ARG
1	C	557	THR
1	C	584	TRP
1	C	597	THR
1	C	661	GLU
1	C	720	MET
1	C	737	ARG
1	C	794	SER
1	C	855	LEU
1	C	899	ASP
1	C	926	LEU
1	C	931	SER
1	C	1057	GLN
1	D	500	ASN
1	D	516	ASP
1	D	542	LEU
1	D	548	ARG
1	D	557	THR
1	D	566	ARG
1	D	577	ASN
1	D	584	TRP
1	D	666	SER
1	D	684	THR
1	D	720	MET
1	D	775	ASP
1	D	794	SER
1	D	846	THR
1	D	854	SER
1	D	885	SER
1	D	931	SER
1	D	1063	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	486	ASN
1	A	510	ASN
1	A	624	ASN
1	A	630	ASN

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Mol	Chain	Res	Type
1	A	713	HIS
1	A	783	GLN
1	A	898	GLN
1	B	486	ASN
1	B	577	ASN
1	B	624	ASN
1	B	630	ASN
1	B	642	GLN
1	B	713	HIS
1	B	783	GLN
1	B	873	GLN
1	C	486	ASN
1	C	577	ASN
1	C	624	ASN
1	C	662	ASN
1	C	713	HIS
1	C	783	GLN
1	D	486	ASN
1	D	500	ASN
1	D	577	ASN
1	D	624	ASN
1	D	630	ASN
1	D	713	HIS
1	D	783	GLN
1	D	820	GLN

### 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	KCX	A	718	1,2	7,11,12	0.89	1 (14%)	7,12,14	2.61	2 (28%)
1	KCX	B	718	1,2	7,11,12	0.46	0	7,12,14	1.22	0
1	KCX	C	718	1,2	7,11,12	0.80	0	7,12,14	1.03	0
1	KCX	D	718	1,2	7,11,12	0.54	0	7,12,14	3.70	2 (28%)

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	KCX	A	718	1,2	-	0/6/10/12	0/0/0/0
1	KCX	B	718	1,2	-	0/6/10/12	0/0/0/0
1	KCX	C	718	1,2	-	0/6/10/12	0/0/0/0
1	KCX	D	718	1,2	-	0/6/10/12	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	718	KCX	CB-CA	2.03	1.55	1.53

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	718	KCX	CD-CE-NZ	2.85	119.18	111.46
1	D	718	KCX	CD-CE-NZ	4.40	123.38	111.46
1	A	718	KCX	CE-NZ-CX	5.79	130.05	123.49
1	D	718	KCX	CE-NZ-CX	8.49	133.11	123.49

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 ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 21 ligands modelled in this entry, 11 are monoatomic - leaving 10 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$
3	3PY	A	1102	-	2,6,6	0.25	0	2,7,7	1.06	0
4	BTN	A	1103	-	8,10,17	1.17	2 (25%)	7,14,23	1.58	1 (14%)
7	GOL	A	1106	-	5,5,5	0.28	0	5,5,5	0.99	0
3	3PY	B	1102	-	2,6,6	0.17	0	2,7,7	2.10	1 (50%)
4	BTN	B	1103	-	9,11,17	0.61	0	8,16,23	0.97	0
3	3PY	C	1102	-	2,6,6	0.25	0	2,7,7	1.53	0
4	BTN	C	1103	-	9,11,17	0.97	0	8,16,23	1.36	2 (25%)
7	GOL	D	1101	-	5,5,5	0.47	0	5,5,5	1.46	1 (20%)
3	3PY	D	1103	-	2,6,6	0.78	0	2,7,7	0.24	0
4	BTN	D	1104	-	8,10,17	0.89	0	7,14,23	0.88	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	3PY	A	1102	-	-	0/2/6/6	0/0/0/0
4	BTN	A	1103	-	-	0/0/18/28	0/2/2/2
7	GOL	A	1106	-	-	0/4/4/4	0/0/0/0
3	3PY	B	1102	-	-	0/2/6/6	0/0/0/0
4	BTN	B	1103	-	-	0/0/21/28	0/2/2/2
3	3PY	C	1102	-	-	0/2/6/6	0/0/0/0
4	BTN	C	1103	-	-	0/0/21/28	0/2/2/2
7	GOL	D	1101	-	-	0/4/4/4	0/0/0/0
3	3PY	D	1103	-	-	0/2/6/6	0/0/0/0
4	BTN	D	1104	-	-	0/0/18/28	0/2/2/2

All (2) bond length outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1103	BTN	C6-S1	-2.45	1.75	1.81
4	A	1103	BTN	C3-N1	-2.09	1.32	1.35

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1102	3PY	O4-C3-C2	-2.76	106.04	112.33
4	C	1103	BTN	C5-C4-N2	-2.11	100.39	102.52
7	D	1101	GOL	O2-C2-C1	2.10	118.30	108.65
4	C	1103	BTN	C4-N2-C3	2.22	114.78	112.66
4	A	1103	BTN	C4-N2-C3	2.53	114.38	112.49

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	1106	GOL	3	0
3	C	1102	3PY	1	0
7	D	1101	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

### 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	596/632 (94%)	-0.21	3 (0%) <span>91</span> <span>90</span>	34, 56, 84, 138	13 (2%)
1	B	593/632 (93%)	0.41	64 (10%) <span>8</span> <span>4</span>	40, 86, 160, 212	5 (0%)
1	C	596/632 (94%)	0.03	25 (4%) <span>40</span> <span>33</span>	45, 70, 120, 158	10 (1%)
1	D	593/632 (93%)	0.37	67 (11%) <span>7</span> <span>4</span>	45, 88, 146, 188	8 (1%)
All	All	2378/2528 (94%)	0.15	159 (6%) <span>21</span> <span>16</span>	34, 72, 140, 212	36 (1%)

All (159) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	912	VAL	7.4
1	D	944	GLY	6.9
1	D	907	SER	6.0
1	D	941	ALA	5.8
1	D	908	PRO	5.5
1	B	911	GLU	5.5
1	B	1048	VAL	5.4
1	D	942	LEU	5.3
1	D	947	PRO	5.2
1	B	909	ASP	5.0
1	B	1047	MET	5.0
1	D	909	ASP	5.0
1	B	905	VAL	4.9
1	D	961	LEU	4.8
1	B	902	VAL	4.7
1	D	1046	GLY	4.7
1	C	944	GLY	4.7
1	B	1051	PHE	4.7
1	B	907	SER	4.6
1	B	906	VAL	4.5
1	C	902	VAL	4.5

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Mol	Chain	Res	Type	RSRZ
1	B	910	ARG	4.5
1	C	509	ALA	4.5
1	C	900	LEU	4.3
1	C	905	VAL	4.1
1	D	906	VAL	4.1
1	D	950	VAL	4.1
1	B	939	LYS	4.1
1	B	914	PHE	4.0
1	B	908	PRO	4.0
1	B	942	LEU	3.9
1	B	950	VAL	3.9
1	B	922	LEU	3.9
1	B	924	GLY	3.8
1	D	914	PHE	3.8
1	B	913	SER	3.8
1	B	944	GLY	3.8
1	B	1046	GLY	3.8
1	D	910	ARG	3.7
1	D	1051	PHE	3.7
1	D	1044	SER	3.7
1	D	921	MET	3.7
1	D	875	PHE	3.7
1	D	705	VAL	3.6
1	C	906	VAL	3.6
1	B	947	PRO	3.5
1	C	909	ASP	3.5
1	D	676	LEU	3.5
1	D	891[A]	MET	3.4
1	C	912	VAL	3.3
1	D	905	VAL	3.3
1	D	638	TYR	3.3
1	B	968	ILE	3.2
1	D	976	VAL	3.2
1	B	948	TYR	3.2
1	D	959	ALA	3.1
1	D	675	LYS	3.1
1	C	485	VAL	3.1
1	D	933	TRP	3.1
1	B	903	ALA	3.0
1	C	907	SER	3.0
1	D	923	LYS	3.0
1	B	981	PHE	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	908	PRO	2.9
1	D	1047	MET	2.9
1	B	976	VAL	2.9
1	B	894	MET	2.9
1	C	963	ALA	2.9
1	B	639	PHE	2.9
1	B	941	ALA	2.8
1	B	933	TRP	2.8
1	B	943	LYS	2.8
1	B	972	LEU	2.8
1	B	1019	GLY	2.8
1	B	974	ARG	2.8
1	D	911	GLU	2.8
1	D	912	VAL	2.8
1	B	1018	ASP	2.8
1	D	898	GLN	2.8
1	C	501	ALA	2.8
1	C	1067	ALA	2.8
1	D	1043	ASP	2.8
1	B	904	ASP	2.7
1	B	1042	THR	2.7
1	B	952	PRO	2.7
1	C	510	ASN	2.6
1	B	1049	THR	2.6
1	D	904	ASP	2.6
1	D	968	ILE	2.6
1	D	525	LEU	2.5
1	D	928	GLN	2.5
1	B	1067	ALA	2.5
1	B	1023	PHE	2.5
1	D	1067	ALA	2.5
1	D	948	TYR	2.5
1	C	901	THR	2.5
1	D	939	LYS	2.5
1	D	922	LEU	2.4
1	C	942	LEU	2.4
1	D	981	PHE	2.4
1	B	901	THR	2.4
1	D	953	GLY	2.4
1	C	904	ASP	2.4
1	D	975	GLU	2.4
1	D	902	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	1048	VAL	2.4
1	B	485	VAL	2.4
1	D	1041	ALA	2.4
1	D	632	PRO	2.4
1	A	968	ILE	2.4
1	D	951	ARG	2.4
1	B	891[A]	MET	2.3
1	C	974	ARG	2.3
1	D	530	PHE	2.3
1	C	910	ARG	2.3
1	D	677	CYS	2.3
1	D	900	LEU	2.3
1	C	891[A]	MET	2.3
1	C	903	ALA	2.3
1	B	1001	TYR	2.3
1	D	946	LYS	2.3
1	B	923	LYS	2.3
1	B	472	ARG	2.3
1	D	949	THR	2.3
1	D	1042	THR	2.3
1	A	780	ASN	2.3
1	C	961	LEU	2.2
1	D	897	SER	2.2
1	B	1043	ASP	2.2
1	B	934	PRO	2.2
1	B	970	LYS	2.2
1	D	940	LYS	2.2
1	B	1057	GLN	2.2
1	D	903	ALA	2.2
1	D	958	GLU	2.2
1	B	937	LEU	2.2
1	B	897	SER	2.2
1	D	511	GLY	2.2
1	B	483	VAL	2.2
1	B	1039	VAL	2.2
1	B	1040	SER	2.2
1	B	900	LEU	2.1
1	D	896	VAL	2.1
1	D	972	LEU	2.1
1	B	945	GLU	2.1
1	B	487	GLY	2.1
1	C	948	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	946	LYS	2.1
1	D	937	LEU	2.1
1	D	945	GLU	2.1
1	D	1039	VAL	2.1
1	A	779	GLY	2.1
1	D	973	GLU	2.1
1	B	1016	LEU	2.1
1	C	962	ASP	2.0
1	B	513	GLY	2.0
1	D	924	GLY	2.0
1	B	1037	GLN	2.0
1	D	633	ASP	2.0

## 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. 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, 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
1	KCX	D	718	12/13	0.96	0.19	-	68,72,87,90	0
1	KCX	A	718	12/13	0.99	0.18	-	40,42,44,46	0
1	KCX	C	718	12/13	0.97	0.22	-	48,51,61,62	0
1	KCX	B	718	12/13	0.96	0.17	-	59,60,65,68	0

## 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, 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
5	MG	B	1104	1/1	0.92	0.18	2.59	60,60,60,60	0
7	GOL	D	1101	6/6	0.92	0.28	1.66	53,62,68,68	0
7	GOL	A	1106	6/6	0.95	0.31	1.10	58,63,67,72	0
5	MG	D	1105	1/1	0.78	0.21	1.02	66,66,66,66	0
4	BTN	D	1104	9/16	0.91	0.22	1.00	76,81,86,89	0
3	3PY	A	1102	7/7	0.97	0.21	0.97	44,48,52,62	0
3	3PY	C	1102	7/7	0.97	0.20	0.68	53,59,60,68	0
4	BTN	B	1103	10/16	0.89	0.29	0.40	82,94,104,106	0
4	BTN	A	1103	9/16	0.96	0.16	-0.06	58,70,73,77	0
3	3PY	D	1103	7/7	0.97	0.17	-0.21	74,82,88,92	0
4	BTN	C	1103	10/16	0.96	0.15	-0.67	67,77,81,87	0
3	3PY	B	1102	7/7	0.95	0.14	-1.29	64,70,72,78	0
2	ZN	A	1101	1/1	0.99	0.17	-1.51	44,44,44,44	0
2	ZN	C	1101	1/1	1.00	0.17	-2.07	54,54,54,54	0
5	MG	A	1104	1/1	0.92	0.05	-2.53	58,58,58,58	0
2	ZN	D	1102	1/1	0.96	0.17	-2.75	69,69,69,69	0
2	ZN	B	1101	1/1	1.00	0.13	-2.98	61,61,61,61	0
5	MG	C	1104	1/1	0.84	0.07	-4.86	61,61,61,61	0
6	CL	C	1105	1/1	0.87	0.18	-	80,80,80,80	0
6	CL	B	1105	1/1	0.94	0.06	-	89,89,89,89	0
6	CL	A	1105	1/1	0.97	0.16	-	61,61,61,61	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.