



Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 04:11 am BST

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (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

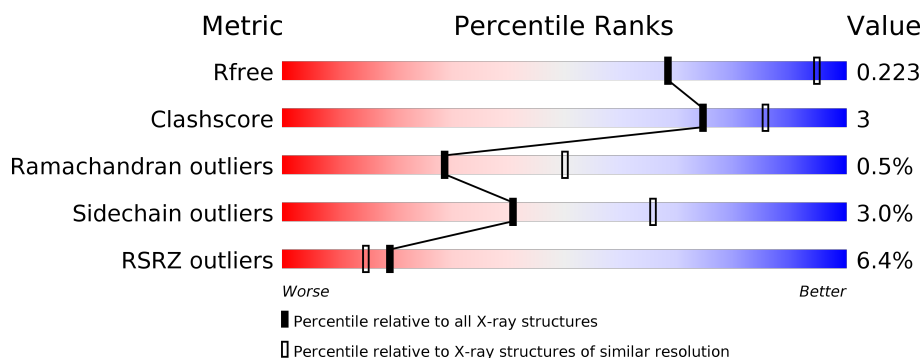
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	130704	3797 (2.64-2.60)
Clashscore	141614	4168 (2.64-2.60)
Ramachandran outliers	138981	4093 (2.64-2.60)
Sidechain outliers	138945	4093 (2.64-2.60)
RSRZ outliers	127900	3731 (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 ≥ 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	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>10%</div> <div>83% 11% 6%</div> </div>

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

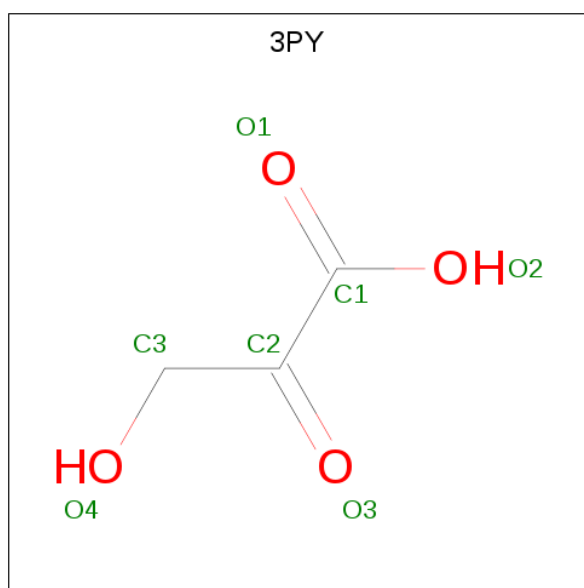
Continued from previous page...

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).

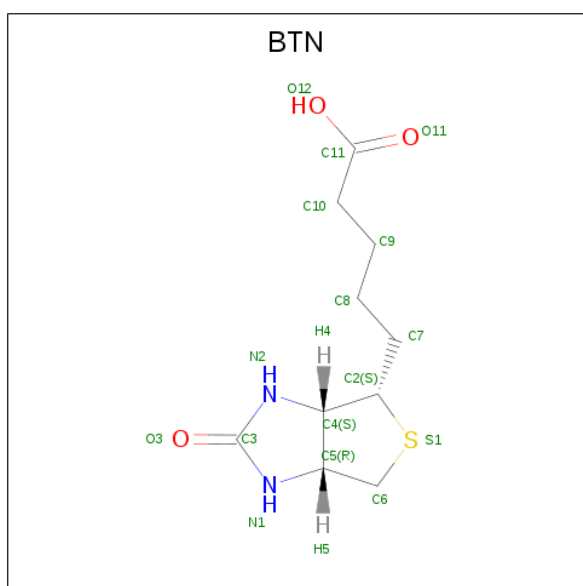
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Zn 1 1	0	0
2	A	1	Total Zn 1 1	0	0
2	D	1	Total Zn 1 1	0	0
2	C	1	Total Zn 1 1	0	0

- Molecule 3 is 3-HYDROXYPYRUVIC ACID (three-letter code: 3PY) (formula: C₃H₄O₄).



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: C₁₀H₁₆N₂O₃S).



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

Continued on next page...

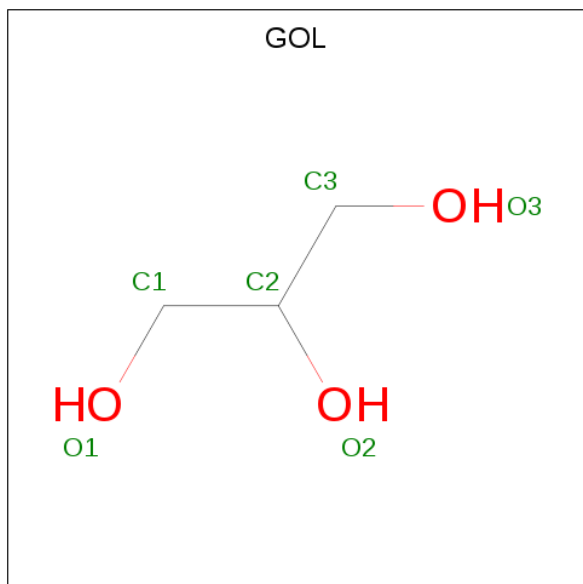
Continued from previous page...

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: C₃H₈O₃).



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		

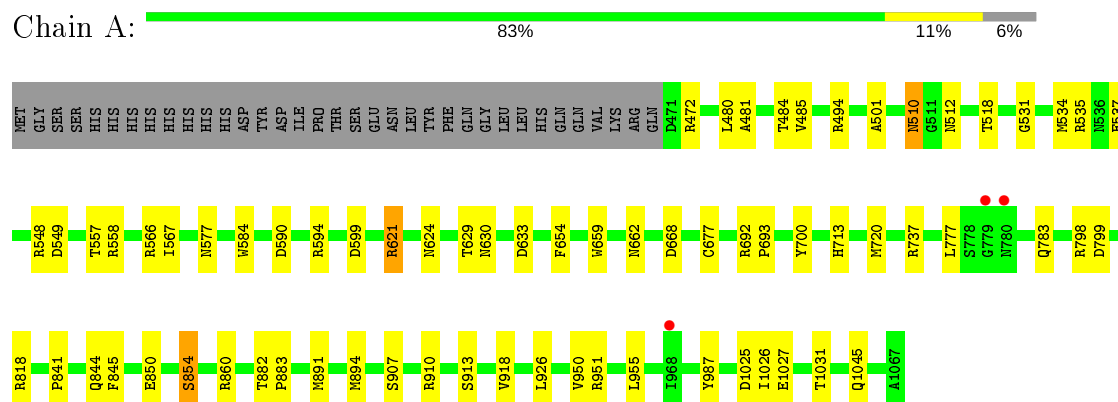
- Molecule 8 is water.

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

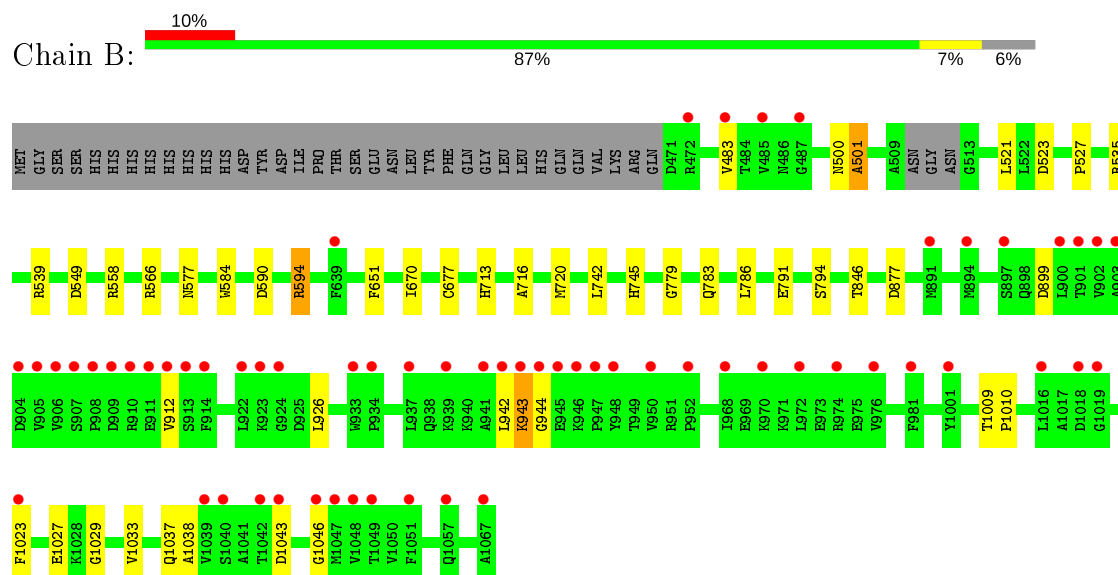
3 Residue-property plots

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

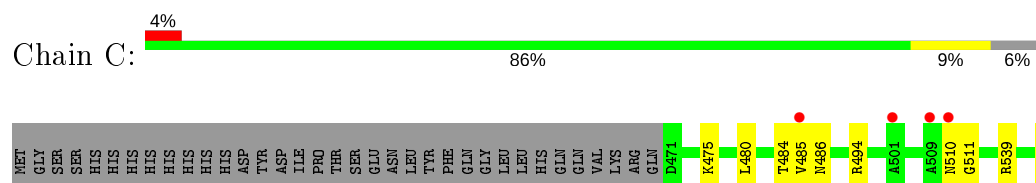
• Molecule 1: PYRUVATE CARBOXYLASE

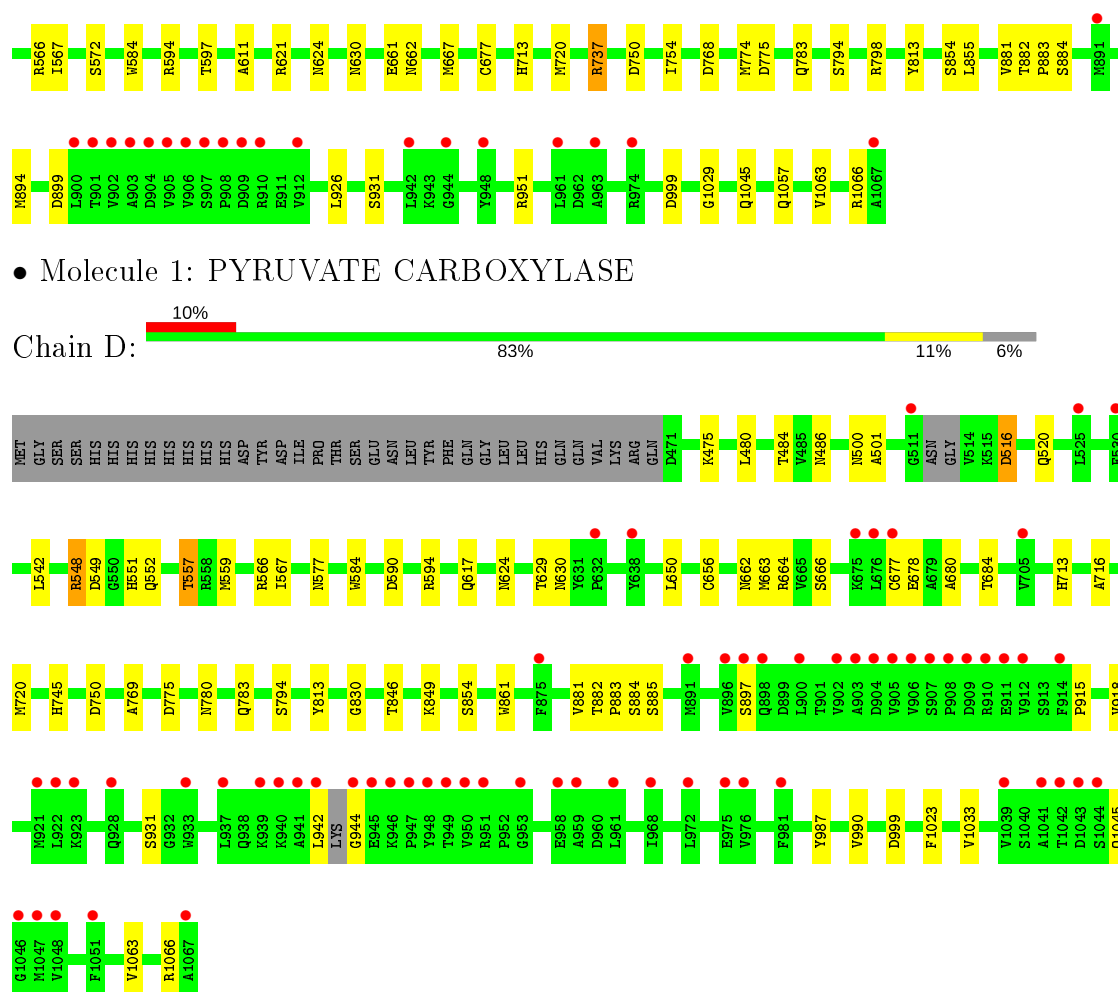


• Molecule 1: PYRUVATE CARBOXYLASE



• 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, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	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	4797 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	63.5	Xtriage
Anisotropy	0.140	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 45.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	17744	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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: 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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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:B:1023:PHE:CD1	1:B:1033:VAL:HG22	2.38	0.58
1:C:486:ASN:HD21	1:C:1066:ARG:N	2.01	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:1045:GLN:OE1	1:C:1045:GLN:N	2.39	0.55
1:C:549:ASP:HB3	1:C:783:GLN:HE22	1.70	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:C:881:VAL:O	1:C:884:SER:N	2.47	0.48
1:D:630:ASN:HD21	1:D:662:ASN:HD21	1.61	0.48
1:A:677:CYS:H	1:A:713:HIS:CD2	2.17	0.48
1:B:1037:GLN:O	1:B:1038:ALA:HB2	2.14	0.48
1:B:527:PRO:HB2	1:B:713:HIS:CE1	2.48	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

Continued on next page...

Continued from previous page...

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:A:548:ARG:C	1:A:548:ARG:HD2	2.38	0.43
1:C:475:LYS:HE2	1:C:999:ASP:O	2.17	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:C:621:ARG:O	1:C:624:ASN:HB2	2.18	0.43
1:D:745:HIS:HA	1:D:769:ALA:O	2.19	0.43
1:D:849:LYS:HG3	1:D:861:TRP:CE3	2.53	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:C:882:THR:OG1	3:C:1102:3PY:H32	2.19	0.43
1:D:678:GLU:CG	1:D:716:ALA:HB2	2.49	0.43
1:C:774:MET:O	1:C:775:ASP:C	2.56	0.43
1:D:915:PRO:HD2	1:D:918:VAL:CB	2.49	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:798:ARG:O	1:A:799:ASP:C	2.58	0.41
1:A:882:THR:HA	1:A:883:PRO:HA	1.85	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:B:535:ARG:NH1	1:B:742:LEU:O	2.54	0.41
1:D:663:MET:O	1:D:664:ARG:C	2.59	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

Continued on next page...

Continued from previous page...

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:C:894:MET:HB2	1:C:894:MET:HE3	1.96	0.40
1:D:486:ASN:HD21	1:D:1066:ARG:H	1.68	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%)	47	69
1	B	590/632 (93%)	556 (94%)	29 (5%)	5 (1%)	19	36
1	C	596/632 (94%)	557 (94%)	35 (6%)	4 (1%)	22	41
1	D	588/632 (93%)	558 (95%)	28 (5%)	2 (0%)	41	62
All	All	2369/2528 (94%)	2244 (95%)	113 (5%)	12 (0%)	29	50

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

Continued on next page...

Continued from previous page...

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%)	49	72
1	B	401/519 (77%)	392 (98%)	9 (2%)	52	74
1	C	430/519 (83%)	417 (97%)	13 (3%)	41	66
1	D	397/519 (76%)	379 (96%)	18 (4%)	27	50
All	All	1679/2076 (81%)	1628 (97%)	51 (3%)	41	66

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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	D	718	1,2	7,11,12	0.63	0	4,12,14	3.75	2 (50%)
1	KCX	A	718	1,2	7,11,12	0.77	0	4,12,14	2.64	2 (50%)
1	KCX	C	718	1,2	7,11,12	0.80	0	4,12,14	0.63	0
1	KCX	B	718	1,2	7,11,12	0.45	0	4,12,14	1.24	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
1	KCX	D	718	1,2	-	1/7/10/12	-
1	KCX	A	718	1,2	-	1/7/10/12	-
1	KCX	C	718	1,2	-	0/7/10/12	-
1	KCX	B	718	1,2	-	2/7/10/12	-

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	718	KCX	CE-NZ-CX	6.00	133.11	122.95
1	D	718	KCX	CD-CE-NZ	4.42	123.38	111.49
1	A	718	KCX	CE-NZ-CX	4.19	130.05	122.95
1	A	718	KCX	CD-CE-NZ	2.86	119.18	111.49

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	718	KCX	O-C-CA-CB
1	B	718	KCX	O-C-CA-CB
1	D	718	KCX	CG-CD-CE-NZ
1	B	718	KCX	CD-CE-NZ-CX

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](#)

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	$\# Z > 2$
4	BTN	C	1103	-	10,11,17	0.80	0	15,16,23	1.78	3 (20%)
4	BTN	D	1104	-	10,10,17	0.59	0	11,14,23	2.25	3 (27%)
7	GOL	D	1101	-	5,5,5	0.49	0	5,5,5	1.51	2 (40%)
3	3PY	B	1102	-	2,6,6	0.19	0	2,7,7	1.94	1 (50%)
3	3PY	C	1102	-	2,6,6	0.24	0	2,7,7	1.62	1 (50%)
3	3PY	A	1102	-	2,6,6	0.21	0	2,7,7	1.14	0
7	GOL	A	1106	-	5,5,5	0.28	0	5,5,5	1.02	0
4	BTN	B	1103	-	10,11,17	0.53	0	15,16,23	2.00	2 (13%)
4	BTN	A	1103	-	10,10,17	0.77	0	11,14,23	1.44	2 (18%)
3	3PY	D	1103	-	2,6,6	0.70	0	2,7,7	0.26	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
4	BTN	C	1103	-	-	-	0/2/2/2
4	BTN	D	1104	-	-	-	0/2/2/2
7	GOL	D	1101	-	-	2/4/4/4	-
3	3PY	B	1102	-	-	1/2/6/6	-
3	3PY	C	1102	-	-	0/2/6/6	-
3	3PY	A	1102	-	-	2/2/6/6	-
7	GOL	A	1106	-	-	2/4/4/4	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	BTN	B	1103	-	-	-	0/2/2/2
4	BTN	A	1103	-	-	-	0/2/2/2
3	3PY	D	1103	-	-	1/2/6/6	-

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1103	BTN	C2-C4-N2	6.42	118.78	113.11
4	C	1103	BTN	C2-C4-N2	5.37	117.86	113.11
4	D	1104	BTN	C4-C2-S1	-4.58	102.63	106.33
4	D	1104	BTN	C2-C4-C5	4.07	113.34	108.28
4	D	1104	BTN	C6-C5-N1	-3.74	108.28	113.03
4	A	1103	BTN	C6-C5-N1	-2.96	109.27	113.03
4	B	1103	BTN	C4-C2-S1	-2.50	102.85	105.19
3	B	1102	3PY	O4-C3-C2	-2.47	106.04	112.48
4	A	1103	BTN	C6-C5-C4	2.35	111.20	108.28
4	C	1103	BTN	C4-N2-C3	2.32	114.78	112.62
4	C	1103	BTN	C5-C4-N2	-2.12	100.39	102.67
7	D	1101	GOL	O2-C2-C1	2.08	118.30	109.12
3	C	1102	3PY	O3-C2-C3	2.06	123.69	120.50
7	D	1101	GOL	C3-C2-C1	-2.01	103.91	111.70

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	D	1101	GOL	C1-C2-C3-O3
7	D	1101	GOL	O2-C2-C3-O3
3	B	1102	3PY	O3-C2-C3-O4
3	A	1102	3PY	C1-C2-C3-O4
7	A	1106	GOL	O1-C1-C2-C3
3	D	1103	3PY	O3-C2-C3-O4
7	A	1106	GOL	O1-C1-C2-O2
3	A	1102	3PY	O3-C2-C3-O4

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	D	1101	GOL	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1102	3PY	1	0
7	A	1106	GOL	3	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, 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	596/632 (94%)	-0.24	3 (0%) 91 89	34, 56, 84, 138	13 (2%)
1	B	593/632 (93%)	0.37	62 (10%) 6 4	40, 86, 160, 212	5 (0%)
1	C	596/632 (94%)	-0.00	24 (4%) 38 32	45, 70, 120, 158	10 (1%)
1	D	593/632 (93%)	0.34	64 (10%) 5 3	45, 88, 146, 188	8 (1%)
All	All	2378/2528 (94%)	0.12	153 (6%) 19 15	34, 72, 140, 212	36 (1%)

All (153) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	912	VAL	7.3
1	D	944	GLY	6.8
1	D	907	SER	6.0
1	D	941	ALA	5.7
1	D	908	PRO	5.4
1	B	911	GLU	5.3
1	B	1048	VAL	5.3
1	D	942	LEU	5.3
1	D	947	PRO	5.1
1	B	909	ASP	4.9
1	B	1047	MET	4.8
1	D	909	ASP	4.8
1	D	961	LEU	4.8
1	B	905	VAL	4.8
1	B	902	VAL	4.7
1	D	1046	GLY	4.6
1	B	1051	PHE	4.6
1	C	944	GLY	4.6
1	B	907	SER	4.6
1	B	906	VAL	4.5
1	C	902	VAL	4.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	910	ARG	4.4
1	C	509	ALA	4.4
1	C	900	LEU	4.3
1	C	905	VAL	4.1
1	D	906	VAL	4.0
1	D	950	VAL	4.0
1	B	914	PHE	4.0
1	B	939	LYS	4.0
1	B	942	LEU	3.9
1	B	908	PRO	3.9
1	B	922	LEU	3.9
1	B	950	VAL	3.8
1	B	924	GLY	3.7
1	D	914	PHE	3.7
1	B	913	SER	3.7
1	B	944	GLY	3.7
1	D	1051	PHE	3.7
1	D	910	ARG	3.7
1	B	1046	GLY	3.7
1	D	1044	SER	3.7
1	D	875	PHE	3.6
1	D	921	MET	3.6
1	D	705	VAL	3.5
1	C	906	VAL	3.5
1	B	947	PRO	3.5
1	D	676	LEU	3.4
1	C	909	ASP	3.4
1	D	891[A]	MET	3.3
1	C	912	VAL	3.3
1	D	905	VAL	3.3
1	B	968	ILE	3.2
1	D	638	TYR	3.2
1	D	976	VAL	3.1
1	B	948	TYR	3.1
1	D	933	TRP	3.0
1	D	959	ALA	3.0
1	C	485	VAL	3.0
1	D	675	LYS	3.0
1	C	907	SER	3.0
1	B	903	ALA	3.0
1	B	981	PHE	2.9
1	C	908	PRO	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	976	VAL	2.9
1	D	923	LYS	2.9
1	D	1047	MET	2.8
1	B	639	PHE	2.8
1	B	894	MET	2.8
1	B	933	TRP	2.8
1	C	963	ALA	2.8
1	B	972	LEU	2.8
1	B	941	ALA	2.8
1	B	943	LYS	2.8
1	B	974	ARG	2.8
1	B	1019	GLY	2.8
1	D	911	GLU	2.7
1	D	912	VAL	2.7
1	D	898	GLN	2.7
1	C	501	ALA	2.7
1	C	1067	ALA	2.7
1	B	1018	ASP	2.7
1	B	1042	THR	2.7
1	D	1043	ASP	2.6
1	B	952	PRO	2.6
1	B	904	ASP	2.6
1	C	510	ASN	2.6
1	B	1049	THR	2.5
1	D	968	ILE	2.5
1	D	525	LEU	2.5
1	D	904	ASP	2.5
1	D	928	GLN	2.5
1	B	1023	PHE	2.5
1	B	1067	ALA	2.4
1	D	948	TYR	2.4
1	D	1067	ALA	2.4
1	C	901	THR	2.4
1	D	922	LEU	2.4
1	D	939	LYS	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	D	902	VAL	2.4
1	D	1048	VAL	2.3
1	A	968	ILE	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	975	GLU	2.3
1	B	485	VAL	2.3
1	C	974	ARG	2.3
1	D	632	PRO	2.3
1	D	900	LEU	2.3
1	D	951	ARG	2.3
1	D	1041	ALA	2.3
1	D	530	PHE	2.3
1	C	904	ASP	2.3
1	C	910	ARG	2.3
1	C	903	ALA	2.3
1	B	891[A]	MET	2.2
1	B	1001	TYR	2.2
1	D	677	CYS	2.2
1	C	961	LEU	2.2
1	D	946	LYS	2.2
1	B	472	ARG	2.2
1	D	949	THR	2.2
1	B	923	LYS	2.2
1	D	897	SER	2.2
1	C	891[A]	MET	2.2
1	D	1042	THR	2.2
1	A	780	ASN	2.2
1	B	934	PRO	2.2
1	D	903	ALA	2.2
1	B	937	LEU	2.2
1	D	940	LYS	2.1
1	B	483	VAL	2.1
1	B	1057	GLN	2.1
1	B	970	LYS	2.1
1	B	897	SER	2.1
1	D	511	GLY	2.1
1	D	958	GLU	2.1
1	B	1040	SER	2.1
1	B	1039	VAL	2.1
1	B	900	LEU	2.1
1	B	1043	ASP	2.1
1	D	972	LEU	2.1
1	D	896	VAL	2.1
1	D	937	LEU	2.0
1	B	1016	LEU	2.0
1	D	1039	VAL	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	945	GLU	2.0
1	B	487	GLY	2.0
1	D	945	GLU	2.0
1	B	946	LYS	2.0
1	C	948	TYR	2.0
1	A	779	GLY	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. 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
1	KCX	D	718	12/13	0.96	0.19	68,72,87,90	0
1	KCX	B	718	12/13	0.96	0.17	59,60,65,68	0
1	KCX	C	718	12/13	0.97	0.22	48,51,61,62	0
1	KCX	A	718	12/13	0.99	0.18	40,42,44,46	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. 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
5	MG	D	1105	1/1	0.78	0.21	66,66,66,66	0
5	MG	C	1104	1/1	0.84	0.07	61,61,61,61	0
6	CL	C	1105	1/1	0.87	0.18	80,80,80,80	0
4	BTN	B	1103	10/16	0.89	0.29	82,94,104,106	0
4	BTN	D	1104	9/16	0.91	0.22	76,81,86,89	0
7	GOL	D	1101	6/6	0.92	0.28	53,62,68,68	0
5	MG	B	1104	1/1	0.92	0.18	60,60,60,60	0
5	MG	A	1104	1/1	0.93	0.05	58,58,58,58	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	3PY	B	1102	7/7	0.94	0.14	64,70,72,78	0
6	CL	B	1105	1/1	0.94	0.06	89,89,89,89	0
7	GOL	A	1106	6/6	0.95	0.31	58,63,67,72	0
4	BTN	C	1103	10/16	0.96	0.15	67,77,81,87	0
2	ZN	D	1102	1/1	0.96	0.17	69,69,69,69	0
4	BTN	A	1103	9/16	0.96	0.16	58,70,73,77	0
6	CL	A	1105	1/1	0.97	0.16	61,61,61,61	0
3	3PY	C	1102	7/7	0.97	0.20	53,59,60,68	0
3	3PY	A	1102	7/7	0.97	0.21	44,48,52,62	0
3	3PY	D	1103	7/7	0.97	0.17	74,82,88,92	0
2	ZN	A	1101	1/1	0.99	0.17	44,44,44,44	0
2	ZN	C	1101	1/1	1.00	0.17	54,54,54,54	0
2	ZN	B	1101	1/1	1.00	0.13	61,61,61,61	0

6.5 Other polymers [i](#)

There are no such residues in this entry.