



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 26, 2020 – 05:19 am BST

PDB ID : 4LOC  
Title : Structure of the carboxyl transferase domain from *Rhizobium etli* pyruvate carboxylase with oxamate and biotin  
Authors : Lietzan, A.D.; St.Maurice, M.  
Deposited on : 2013-07-12  
Resolution : 2.26 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](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

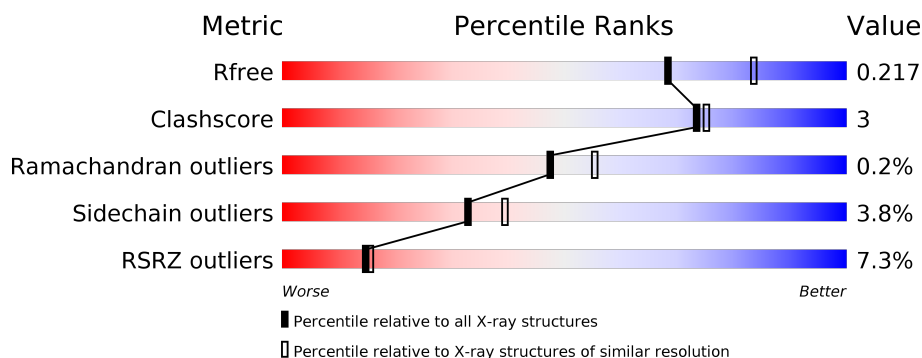
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.26 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	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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	632	<div> <div>2%</div> <div>84%</div> <div>10%</div> <div>6%</div> </div>
1	B	632	<div> <div>12%</div> <div>83%</div> <div>10%</div> <div>6%</div> </div>
1	C	632	<div> <div>10%</div> <div>86%</div> <div>7%</div> <div>6%</div> </div>
1	D	632	<div> <div>4%</div> <div>84%</div> <div>10%</div> <div>6%</div> </div>

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 18570 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	595	Total	C	N	O	S	0	3	0
			4572	2908	771	870	23			
1	B	593	Total	C	N	O	S	0	1	0
			4389	2784	743	839	23			
1	C	595	Total	C	N	O	S	0	1	0
			4456	2841	746	846	23			
1	D	596	Total	C	N	O	S	0	1	0
			4507	2868	761	855	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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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 MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

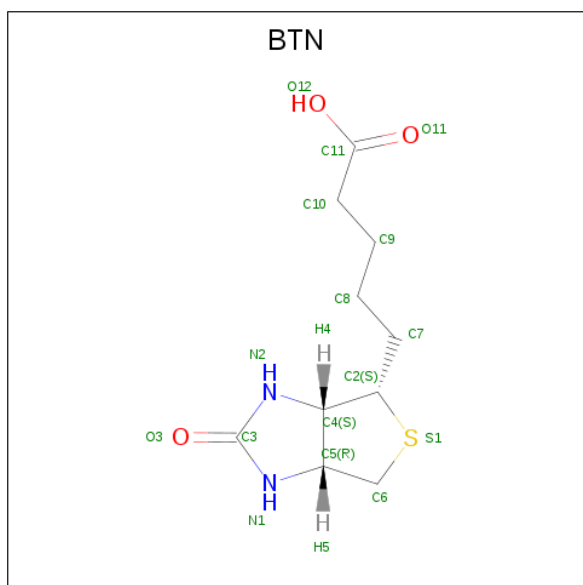
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Cl 1 1	0	0

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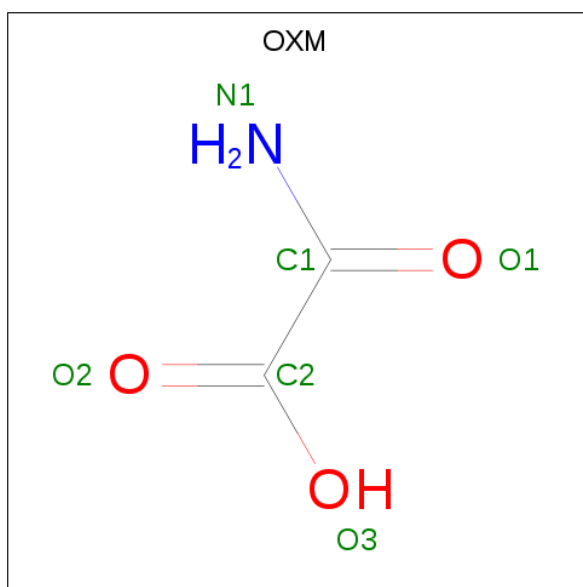
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	1	Total	Cl	0	0
			1	1		
4	C	1	Total	Cl	0	0
			1	1		

- Molecule 5 is BIOTIN (three-letter code: BTN) (formula:  $C_{10}H_{16}N_2O_3S$ ).



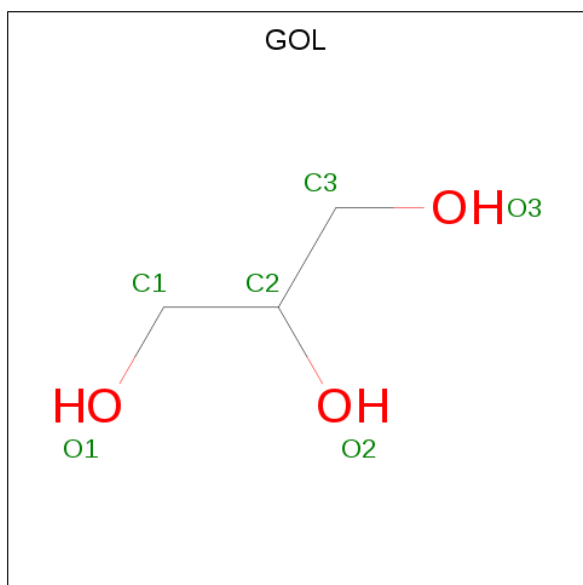
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	S	0	0
			16	10	2	3	1		
5	B	1	Total	C	N	O	S	0	0
			16	10	2	3	1		
5	C	1	Total	C	N	O	S	0	0
			16	10	2	3	1		
5	D	1	Total	C	N	O	S	0	0
			16	10	2	3	1		

- Molecule 6 is OXAMIC ACID (three-letter code: OXM) (formula:  $C_2H_3NO_3$ ).



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

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



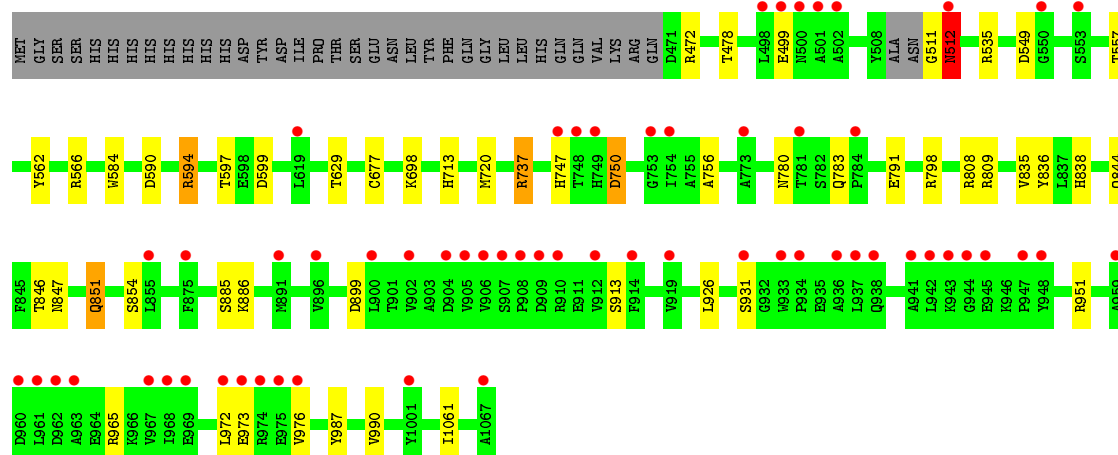
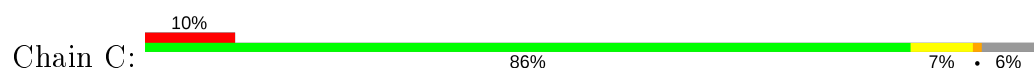


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			6	3	3		
7	C	1	Total	C	O	0	0
			6	3	3		

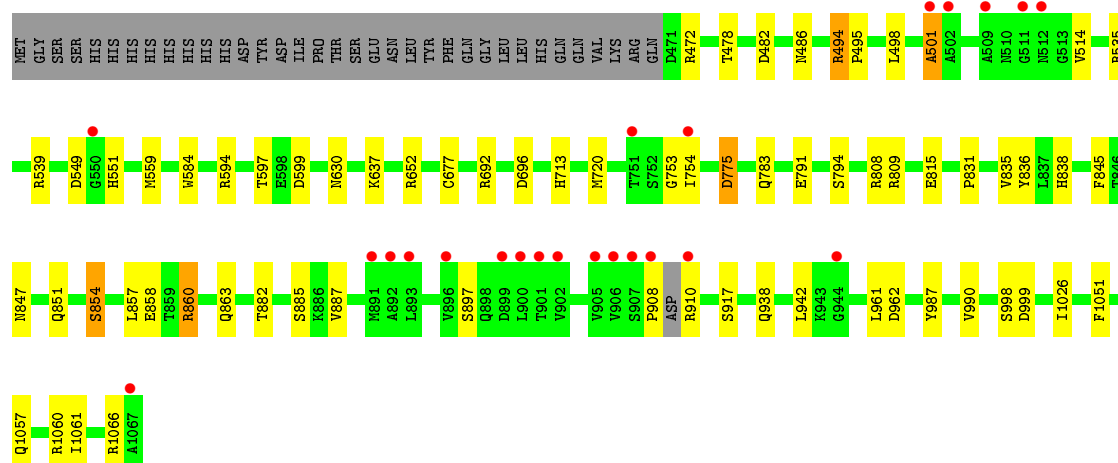
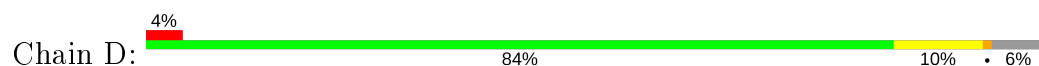
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	213	Total	O	0	0
			213	213		
8	B	97	Total	O	0	0
			97	97		
8	C	79	Total	O	0	0
			79	79		
8	D	146	Total	O	0	0
			146	146		





• Molecule 1: Pyruvate carboxylase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	83.87Å 157.12Å 244.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.75 – 2.26 43.71 – 2.26	Depositor EDS
% Data completeness (in resolution range)	98.0 (43.75-2.26) 98.1 (43.71-2.26)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.74 (at 2.27Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, $R_{free}$	0.176 , 0.216 0.184 , 0.217	Depositor DCC
$R_{free}$ test set	7444 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	39.4	Xtriage
Anisotropy	0.113	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 38.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	18570	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.49% 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, MG, CL, ZN, OXM, 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	1.01	2/4665 (0.0%)	1.03	18/6338 (0.3%)
1	B	0.80	2/4474 (0.0%)	0.89	9/6103 (0.1%)
1	C	0.74	0/4542	0.86	9/6189 (0.1%)
1	D	0.89	3/4593 (0.1%)	0.93	11/6251 (0.2%)
All	All	0.87	7/18274 (0.0%)	0.93	47/24881 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1040	SER	CB-OG	9.52	1.54	1.42
1	D	815	GLU	CD-OE2	-5.78	1.19	1.25
1	B	791	GLU	CD-OE1	-5.76	1.19	1.25
1	A	815	GLU	CD-OE1	-5.72	1.19	1.25
1	D	815	GLU	CD-OE1	-5.44	1.19	1.25

The worst 5 of 47 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	594[A]	ARG	NE-CZ-NH1	-10.88	114.86	120.30
1	A	594[B]	ARG	NE-CZ-NH1	-10.88	114.86	120.30
1	D	535	ARG	NE-CZ-NH2	-9.95	115.32	120.30
1	D	594	ARG	NE-CZ-NH2	9.41	125.00	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	594	ARG	NE-CZ-NH1	-9.40	115.60	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	512	ASN	Peptide

## 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	4572	0	4488	33	0
1	B	4389	0	4132	31	0
1	C	4456	0	4273	24	0
1	D	4507	0	4379	35	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	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	16	0	15	0	0
5	B	16	0	15	1	0
5	C	16	0	15	0	0
5	D	16	0	15	1	0
6	A	6	0	2	0	0
6	B	6	0	2	0	0
6	C	6	0	2	0	0
6	D	6	0	2	0	0
7	B	6	0	8	1	0
7	C	6	0	8	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	A	213	0	0	10	0
8	B	97	0	0	3	0
8	C	79	0	0	1	0
8	D	146	0	0	7	0
All	All	18570	0	17356	118	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.

The worst 5 of 118 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:885:SER:N	8:A:1355:HOH:O	1.76	1.18
1:D:630:ASN:HB2	8:D:1268:HOH:O	1.64	0.97
1:A:677:CYS:H	1:A:713:HIS:HD2	1.19	0.90
1:C:780:ASN:H	7:C:1103:GOL:H12	1.36	0.90
1:C:677:CYS:H	1:C:713:HIS:HD2	1.22	0.88

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	593/632 (94%)	577 (97%)	15 (2%)	1 (0%)	47	55
1	B	587/632 (93%)	567 (97%)	18 (3%)	2 (0%)	41	46
1	C	591/632 (94%)	563 (95%)	27 (5%)	1 (0%)	47	55
1	D	592/632 (94%)	573 (97%)	18 (3%)	1 (0%)	47	55
All	All	2363/2528 (94%)	2280 (96%)	78 (3%)	5 (0%)	47	55

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	501	ALA
1	C	512	ASN
1	D	501	ALA
1	B	930	PRO
1	B	843	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	472/519 (91%)	455 (96%)	17 (4%)	35	42
1	B	427/519 (82%)	408 (96%)	19 (4%)	28	32
1	C	439/519 (85%)	421 (96%)	18 (4%)	30	36
1	D	455/519 (88%)	441 (97%)	14 (3%)	40	49
All	All	1793/2076 (86%)	1725 (96%)	68 (4%)	33	39

5 of 68 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	913	SER
1	C	557	THR
1	D	860	ARG
1	B	926	LEU
1	B	999	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 29 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	783	GLN
1	C	486	ASN
1	D	713	HIS
1	B	862	HIS
1	C	577	ASN



### 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	C	718	1,2	7,11,12	0.87	0	4,12,14	2.79	2 (50%)
1	KCX	B	718	1,2	7,11,12	0.79	0	4,12,14	3.16	2 (50%)
1	KCX	D	718	1,2	7,11,12	0.78	0	4,12,14	1.76	2 (50%)
1	KCX	A	718	1,2	7,11,12	1.25	1 (14%)	4,12,14	2.73	2 (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	KCX	C	718	1,2	-	1/7/10/12	-
1	KCX	B	718	1,2	-	1/7/10/12	-
1	KCX	D	718	1,2	-	1/7/10/12	-
1	KCX	A	718	1,2	-	1/7/10/12	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	718	KCX	CE-NZ	2.01	1.50	1.45

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	718	KCX	CE-NZ-CX	5.36	132.02	122.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	718	KCX	CE-NZ-CX	4.40	130.39	122.95
1	A	718	KCX	CE-NZ-CX	4.15	129.98	122.95
1	C	718	KCX	CD-CE-NZ	3.41	120.66	111.49
1	A	718	KCX	CD-CE-NZ	3.29	120.33	111.49

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	C	718	KCX	O-C-CA-CB
1	B	718	KCX	O-C-CA-CB
1	D	718	KCX	O-C-CA-CB
1	A	718	KCX	O-C-CA-CB

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	$\# Z  > 2$
5	BTN	B	1104	-	14,17,17	0.90	0	19,23,23	2.33	8 (42%)
5	BTN	A	1104	-	14,17,17	1.27	1 (7%)	19,23,23	1.87	6 (31%)
6	OXM	B	1105	-	2,5,5	0.88	0	2,6,6	1.85	1 (50%)
6	OXM	D	1105	-	2,5,5	0.32	0	2,6,6	2.03	1 (50%)
6	OXM	C	1106	-	2,5,5	0.67	0	2,6,6	0.82	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	OXM	A	1105	-	2,5,5	2.05	1 (50%)	2,6,6	1.08	0
7	GOL	C	1103	-	5,5,5	0.66	0	5,5,5	1.56	1 (20%)
5	BTN	D	1104	-	14,17,17	0.89	0	19,23,23	1.72	6 (31%)
5	BTN	C	1105	-	14,17,17	0.86	0	19,23,23	1.52	3 (15%)
7	GOL	B	1101	-	5,5,5	0.50	0	5,5,5	1.95	2 (40%)

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
5	BTN	B	1104	-	-	5/5/28/28	0/2/2/2
5	BTN	A	1104	-	-	5/5/28/28	0/2/2/2
6	OXM	B	1105	-	-	0/0/4/4	-
6	OXM	D	1105	-	-	0/0/4/4	-
6	OXM	C	1106	-	-	0/0/4/4	-
6	OXM	A	1105	-	-	0/0/4/4	-
7	GOL	C	1103	-	-	1/4/4/4	-
5	BTN	D	1104	-	-	4/5/28/28	0/2/2/2
5	BTN	C	1105	-	-	4/5/28/28	0/2/2/2
7	GOL	B	1101	-	-	0/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1105	OXM	O1-C1	-2.83	1.18	1.24
5	A	1104	BTN	C7-C2	2.37	1.58	1.52

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1104	BTN	C8-C7-C2	5.91	125.86	113.86
5	D	1104	BTN	C6-C5-C4	3.99	112.12	108.66
5	C	1105	BTN	C6-C5-N1	-3.98	107.98	113.03
5	B	1104	BTN	C5-C4-N2	-3.45	98.96	102.67
5	A	1104	BTN	C2-C4-N2	3.44	116.21	113.13

There are no chirality outliers.

5 of 19 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1104	BTN	S1-C2-C7-C8
5	A	1104	BTN	C4-C2-C7-C8
5	C	1105	BTN	C11-C10-C9-C8
5	C	1105	BTN	S1-C2-C7-C8
5	C	1105	BTN	C4-C2-C7-C8

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1104	BTN	1	0
7	C	1103	GOL	3	0
5	D	1104	BTN	1	0
7	B	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	594/632 (93%)	-0.21	12 (2%) 65 68	23, 34, 57, 82	12 (2%)
1	B	592/632 (93%)	0.54	77 (13%) 3 3	26, 61, 122, 160	7 (1%)
1	C	594/632 (93%)	0.39	61 (10%) 6 6	33, 59, 96, 129	6 (1%)
1	D	595/632 (94%)	0.02	23 (3%) 39 42	29, 44, 80, 106	3 (0%)
All	All	2375/2528 (93%)	0.18	173 (7%) 15 15	23, 47, 101, 160	28 (1%)

The worst 5 of 173 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	512	ASN	6.5
1	B	908	PRO	5.9
1	C	944	GLY	5.7
1	C	906	VAL	5.6
1	C	959	ALA	5.6

### 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(Å <sup>2</sup> )	Q<0.9
1	KCX	C	718	12/13	0.96	0.29	40,41,43,46	0
1	KCX	B	718	12/13	0.96	0.20	38,41,48,48	0
1	KCX	D	718	12/13	0.99	0.21	31,32,34,35	0
1	KCX	A	718	12/13	0.99	0.18	21,23,25,26	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, 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
5	BTN	B	1104	16/16	0.73	0.28	55,71,80,82	0
3	MG	B	1103	1/1	0.87	0.17	32,32,32,32	0
7	GOL	B	1101	6/6	0.89	0.26	42,45,49,51	0
5	BTN	A	1104	16/16	0.90	0.15	44,55,73,74	0
7	GOL	C	1103	6/6	0.90	0.24	42,50,54,55	0
5	BTN	C	1105	16/16	0.90	0.16	53,62,72,78	0
5	BTN	D	1104	16/16	0.91	0.14	51,57,81,87	0
3	MG	C	1102	1/1	0.92	0.12	41,41,41,41	0
4	CL	D	1103	1/1	0.94	0.10	49,49,49,49	0
4	CL	C	1104	1/1	0.95	0.14	58,58,58,58	0
3	MG	D	1102	1/1	0.95	0.07	33,33,33,33	0
2	ZN	B	1102	1/1	0.95	0.12	41,41,41,41	0
6	OXM	D	1105	6/6	0.95	0.20	33,38,41,41	0
6	OXM	C	1106	6/6	0.96	0.19	42,44,48,49	0
6	OXM	B	1105	6/6	0.96	0.17	40,43,45,45	0
3	MG	A	1102	1/1	0.97	0.05	34,34,34,34	0
6	OXM	A	1105	6/6	0.98	0.18	30,36,37,42	0
2	ZN	A	1101	1/1	0.99	0.12	30,30,30,30	0
2	ZN	C	1101	1/1	0.99	0.11	41,41,41,41	0
2	ZN	D	1101	1/1	1.00	0.11	34,34,34,34	0
4	CL	A	1103	1/1	1.00	0.07	45,45,45,45	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.