



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 17, 2023 – 09:36 PM EST

PDB ID : 2QEU  
Title : Crystal structure of putative carboxymuconolactone decarboxylase (YP\_555818.1) from Burkholderia xenovorans LB400 at 1.65 Å resolution  
Authors : Joint Center for Structural Genomics (JCSG)  
Deposited on : 2007-06-26  
Resolution : 1.65 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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 : 2.31.2  
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) : 2.31.2

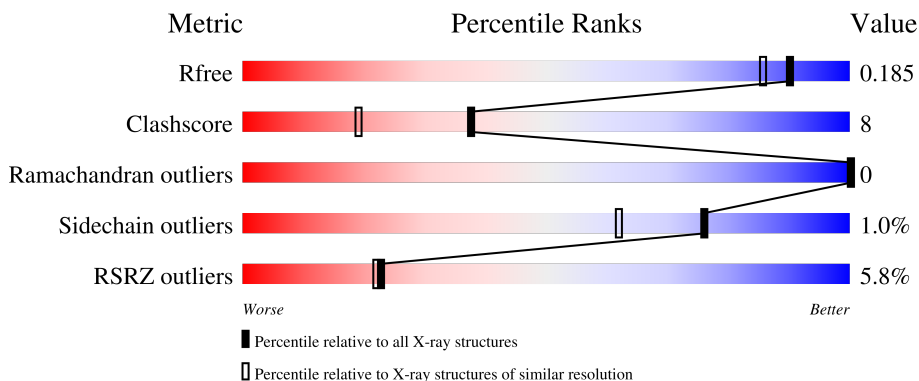
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.65 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	1827 (1.66-1.66)
Clashscore	141614	1931 (1.66-1.66)
Ramachandran outliers	138981	1891 (1.66-1.66)
Sidechain outliers	138945	1891 (1.66-1.66)
RSRZ outliers	127900	1791 (1.66-1.66)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	141	
1	B	141	
1	C	141	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ACT	A	142	-	-	X	-
2	ACT	A	143	-	-	X	-
2	ACT	A	144	-	-	X	-
3	CIT	A	146	-	X	-	-
3	CIT	B	142	-	X	-	-
3	CIT	C	142	-	X	-	-

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 3764 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 Putative carboxymuconolactone decarboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	Se			
1	A	132	1084	690	185	204	5	0	9	0
1	B	133	1084	691	188	200	5	0	8	0
1	C	132	1081	687	186	203	5	0	8	0

There are 21 discrepancies between the modelled and reference sequences:

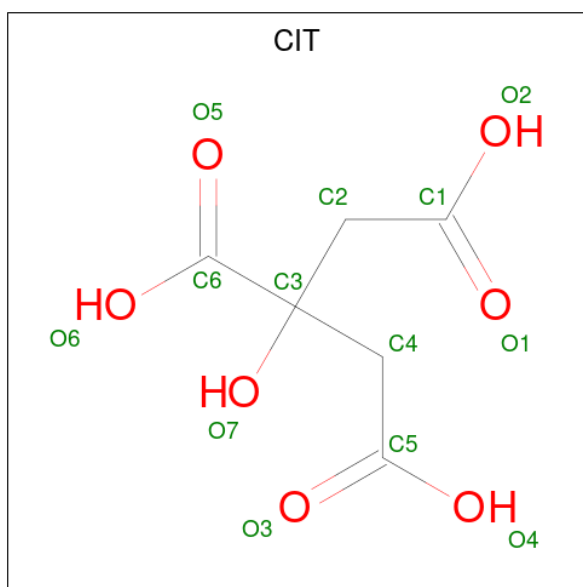
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP Q13HH1
A	1	MSE	MET	modified residue	UNP Q13HH1
A	24	MSE	MET	modified residue	UNP Q13HH1
A	48	MSE	MET	modified residue	UNP Q13HH1
A	52	MSE	MET	modified residue	UNP Q13HH1
A	92	MSE	MET	modified residue	UNP Q13HH1
A	114	MSE	MET	modified residue	UNP Q13HH1
B	0	GLY	-	expression tag	UNP Q13HH1
B	1	MSE	MET	modified residue	UNP Q13HH1
B	24	MSE	MET	modified residue	UNP Q13HH1
B	48	MSE	MET	modified residue	UNP Q13HH1
B	52	MSE	MET	modified residue	UNP Q13HH1
B	92	MSE	MET	modified residue	UNP Q13HH1
B	114	MSE	MET	modified residue	UNP Q13HH1
C	0	GLY	-	expression tag	UNP Q13HH1
C	1	MSE	MET	modified residue	UNP Q13HH1
C	24	MSE	MET	modified residue	UNP Q13HH1
C	48	MSE	MET	modified residue	UNP Q13HH1
C	52	MSE	MET	modified residue	UNP Q13HH1
C	92	MSE	MET	modified residue	UNP Q13HH1
C	114	MSE	MET	modified residue	UNP Q13HH1

- Molecule 2 is ACETATE ION (three-letter code: ACT) (formula: C<sub>2</sub>H<sub>3</sub>O<sub>2</sub>).



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

- Molecule 3 is CITRIC ACID (three-letter code: CIT) (formula: C<sub>6</sub>H<sub>8</sub>O<sub>7</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			13	6	7		
3	B	1	Total	C	O	0	0
			13	6	7		
3	C	1	Total	C	O	0	0
			13	6	7		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	1
			12	6	6		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C O 6 3 3	0	0
4	C	1	Total C O 6 3 3	0	0
4	C	1	Total C O 12 6 6	0	1

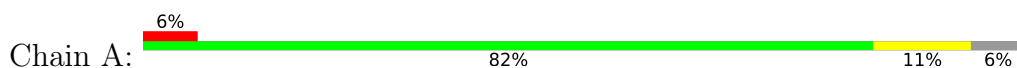
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	135	Total O 137 137	0	2
5	B	122	Total O 122 122	0	0
5	C	153	Total O 153 153	0	0

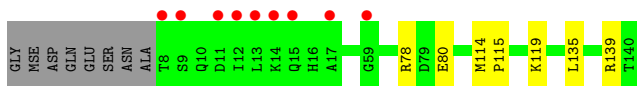
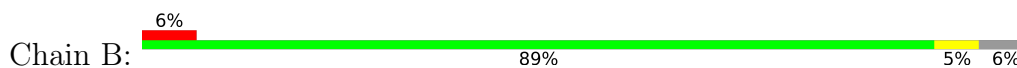
### 3 Residue-property plots [i](#)

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

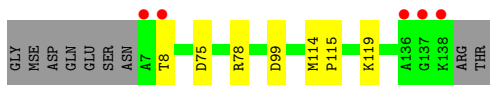
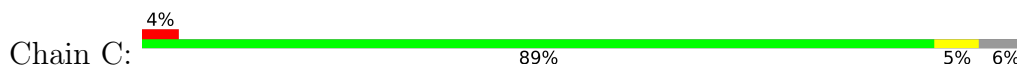
- Molecule 1: Putative carboxymuconolactone decarboxylase



- Molecule 1: Putative carboxymuconolactone decarboxylase



- Molecule 1: Putative carboxymuconolactone decarboxylase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	71.17Å 71.17Å 325.50Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.76 – 1.65 29.76 – 1.65	Depositor EDS
% Data completeness (in resolution range)	100.0 (29.76-1.65) 100.0 (29.76-1.65)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	0.15	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.17 (at 1.65Å)	Xtrriage
Refinement program	REFMAC 5.2.0019, PHENIX	Depositor
R, $R_{free}$	0.152 , 0.180 0.161 , 0.185	Depositor DCC
$R_{free}$ test set	3039 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	17.1	Xtrriage
Anisotropy	0.342	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 45.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	3764	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	12.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.31% 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: ACT, GOL, CIT

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	0.86	0/1096	0.80	2/1470 (0.1%)
1	B	0.74	0/1097	0.72	0/1472
1	C	0.87	0/1093	0.78	1/1466 (0.1%)
All	All	0.83	0/3286	0.77	3/4408 (0.1%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	49	ARG	NE-CZ-NH2	-5.86	117.37	120.30
1	C	75	ASP	CB-CG-OD2	-5.18	113.64	118.30
1	A	89	ARG	NE-CZ-NH1	5.15	122.88	120.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1084	0	1090	28	0
1	B	1084	0	1093	20	0
1	C	1081	0	1091	14	0
2	A	20	0	15	15	0
2	B	4	0	3	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	4	0	3	1	0
3	A	13	0	5	3	0
3	B	13	0	5	0	0
3	C	13	0	5	1	0
4	A	12	0	16	3	0
4	B	6	0	8	0	0
4	C	18	0	24	4	0
5	A	137	0	0	3	0
5	B	122	0	0	0	0
5	C	153	0	0	4	0
All	All	3764	0	3358	52	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 8.

All (52) 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:82:ILE:H	2:A:142:ACT:H1	1.21	1.03
1:A:119[B]:LYS:NZ	1:B:78[B]:ARG:NH1	2.24	0.86
1:A:119[B]:LYS:NZ	1:B:78[B]:ARG:HH12	1.74	0.82
1:A:81:PRO:HD2	2:A:142:ACT:H3	1.67	0.76
1:B:119[A]:LYS:NZ	1:C:78[A]:ARG:NH1	2.34	0.75
4:A:147[B]:GOL:H11	4:C:144[B]:GOL:O3	1.87	0.74
1:A:119[B]:LYS:HZ3	1:B:78[B]:ARG:HH12	1.35	0.74
1:A:119[B]:LYS:HZ2	1:B:78[B]:ARG:NH1	1.87	0.72
1:A:78[B]:ARG:NH1	5:A:276:HOH:O	2.24	0.71
1:B:135[A]:LEU:HD11	1:B:139:ARG:CZ	2.22	0.69
1:C:78[A]:ARG:HD2	5:C:145:HOH:O	1.94	0.68
1:A:80:GLU:OE1	3:A:146:CIT:H21	1.94	0.68
1:B:119[A]:LYS:NZ	1:C:78[A]:ARG:HH12	1.91	0.67
1:A:82:ILE:N	2:A:142:ACT:H1	2.04	0.66
1:B:119[A]:LYS:HZ3	1:C:78[A]:ARG:HH12	1.43	0.65
1:A:11[B]:ASP:O	1:A:15[B]:GLN:HG3	1.98	0.63
1:C:119[A]:LYS:NZ	5:C:253:HOH:O	2.33	0.62
1:B:119[A]:LYS:HZ2	1:C:78[A]:ARG:NH1	1.99	0.59
1:A:119[B]:LYS:HD3	1:B:78[B]:ARG:NH1	2.20	0.56
3:A:146:CIT:O2	3:A:146:CIT:O6	2.22	0.56
1:A:79:ASP:O	1:C:119[A]:LYS:NZ	2.39	0.56
1:A:119[B]:LYS:CD	1:B:78[B]:ARG:NH1	2.70	0.55
4:A:147[A]:GOL:O1	4:C:144[A]:GOL:H32	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:119[A]:LYS:HD3	1:C:78[A]:ARG:NH1	2.23	0.54
1:A:60:ALA:CB	2:A:144:ACT:H1	2.39	0.53
1:B:119[A]:LYS:HZ3	1:C:78[A]:ARG:NH1	2.04	0.53
2:A:142:ACT:H2	5:A:256:HOH:O	2.10	0.52
3:A:146:CIT:O2	3:A:146:CIT:C6	2.58	0.52
1:A:67:LYS:NZ	2:A:144:ACT:OXT	2.41	0.51
1:A:60:ALA:CB	2:A:144:ACT:CH3	2.89	0.50
1:A:119[B]:LYS:HZ2	1:B:78[B]:ARG:HH11	1.56	0.50
3:C:142:CIT:C1	5:C:266:HOH:O	2.60	0.48
1:A:78[A]:ARG:HA	2:A:143:ACT:H3	1.95	0.48
1:C:119[B]:LYS:NZ	5:C:278:HOH:O	2.45	0.48
1:A:86:ASN:ND2	2:A:145:ACT:H2	2.28	0.48
1:B:119[A]:LYS:HZ2	1:C:78[A]:ARG:HH11	1.63	0.47
2:A:143:ACT:H2	4:C:144[A]:GOL:O2	2.15	0.47
1:A:119[B]:LYS:CE	1:B:78[B]:ARG:HH12	2.28	0.46
1:B:119[A]:LYS:CD	1:C:78[A]:ARG:NH1	2.78	0.46
4:A:147[A]:GOL:HO1	4:C:144[A]:GOL:C3	2.29	0.46
1:C:99:ASP:OD1	2:C:141:ACT:H2	2.16	0.45
1:A:43:ASP:O	1:A:47[B]:ARG:HG3	2.17	0.45
1:A:119[B]:LYS:HZ3	1:B:78[B]:ARG:NH1	1.99	0.44
1:C:114:MSE:N	1:C:115:PRO:CD	2.80	0.44
2:A:142:ACT:CH3	5:A:256:HOH:O	2.63	0.44
1:A:119[B]:LYS:HD3	1:B:78[B]:ARG:CZ	2.48	0.44
1:A:60:ALA:HB2	2:A:144:ACT:CH3	2.47	0.44
1:A:60:ALA:HB1	2:A:144:ACT:H1	2.01	0.42
1:A:11[B]:ASP:OD1	1:A:15[B]:GLN:OE1	2.38	0.42
1:A:67:LYS:NZ	2:A:144:ACT:H1	2.33	0.42
1:A:60:ALA:HB2	2:A:144:ACT:H3	2.01	0.42
1:B:114:MSE:N	1:B:115:PRO:CD	2.85	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	139/141 (99%)	137 (99%)	2 (1%)	0	100	100
1	B	139/141 (99%)	139 (100%)	0	0	100	100
1	C	138/141 (98%)	136 (99%)	2 (1%)	0	100	100
All	All	416/423 (98%)	412 (99%)	4 (1%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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	111/106 (105%)	109 (98%)	2 (2%)	59	36
1	B	109/106 (103%)	107 (98%)	2 (2%)	59	36
1	C	111/106 (105%)	110 (99%)	1 (1%)	78	66
All	All	331/318 (104%)	326 (98%)	5 (2%)	76	44

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29[A]	GLU
1	A	29[B]	GLU
1	B	80[A]	GLU
1	B	80[B]	GLU
1	C	8	THR

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

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

16 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	GOL	C	144[B]	-	5,5,5	0.48	0	5,5,5	0.46	0
3	CIT	B	142	-	12,12,12	1.38	1 (8%)	17,17,17	2.39	6 (35%)
4	GOL	A	147[B]	-	5,5,5	0.47	0	5,5,5	0.74	0
4	GOL	C	143	-	5,5,5	0.55	0	5,5,5	0.91	0
2	ACT	A	143	-	3,3,3	1.22	0	3,3,3	1.33	0
2	ACT	C	141	-	3,3,3	1.01	0	3,3,3	1.11	0
3	CIT	C	142	-	12,12,12	1.66	2 (16%)	17,17,17	5.59	13 (76%)
4	GOL	A	147[A]	-	5,5,5	0.42	0	5,5,5	0.36	0
4	GOL	B	143	-	5,5,5	0.47	0	5,5,5	0.82	0
2	ACT	A	141	-	3,3,3	0.60	0	3,3,3	1.77	2 (66%)
2	ACT	B	141	-	3,3,3	0.74	0	3,3,3	1.45	0
2	ACT	A	145	-	3,3,3	1.05	0	3,3,3	0.61	0
3	CIT	A	146	-	12,12,12	1.71	2 (16%)	17,17,17	4.56	12 (70%)
2	ACT	A	144	-	3,3,3	1.30	0	3,3,3	0.81	0
2	ACT	A	142	-	3,3,3	1.01	0	3,3,3	1.88	1 (33%)
4	GOL	C	144[A]	-	5,5,5	0.47	0	5,5,5	0.55	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	GOL	C	144[B]	-	-	0/4/4/4	-
3	CIT	B	142	-	-	11/16/16/16	-
4	GOL	A	147[B]	-	-	2/4/4/4	-
4	GOL	C	143	-	-	2/4/4/4	-
4	GOL	A	147[A]	-	-	0/4/4/4	-
3	CIT	C	142	-	-	5/16/16/16	-
4	GOL	B	143	-	-	4/4/4/4	-
3	CIT	A	146	-	-	5/16/16/16	-
4	GOL	C	144[A]	-	-	2/4/4/4	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	146	CIT	C4-C3	4.01	1.58	1.53
3	C	142	CIT	O3-C5	2.84	1.31	1.22
3	A	146	CIT	O7-C3	2.70	1.48	1.43
3	C	142	CIT	C4-C3	2.68	1.57	1.53
3	B	142	CIT	O2-C1	-2.11	1.23	1.30

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	142	CIT	C2-C3-C6	10.15	131.92	110.11
3	C	142	CIT	O7-C3-C4	9.84	132.41	109.40
3	A	146	CIT	O7-C3-C4	8.82	130.03	109.40
3	C	142	CIT	O7-C3-C6	-8.18	97.38	108.86
3	C	142	CIT	C4-C3-C6	-7.13	94.78	110.11
3	C	142	CIT	O7-C3-C2	-7.02	92.98	109.40
3	C	142	CIT	O6-C6-C3	6.45	124.25	113.05
3	A	146	CIT	O7-C3-C2	-6.41	94.41	109.40
3	C	142	CIT	O5-C6-C3	-6.40	113.19	122.25
3	A	146	CIT	C4-C3-C6	-6.22	96.74	110.11
3	A	146	CIT	C2-C3-C6	6.01	123.03	110.11
3	A	146	CIT	O6-C6-C3	5.90	123.30	113.05
3	C	142	CIT	C3-C2-C1	-5.33	100.90	113.81
3	A	146	CIT	O5-C6-C3	-5.27	114.79	122.25
3	A	146	CIT	C3-C2-C1	-5.22	101.18	113.81
3	B	142	CIT	O7-C3-C4	4.82	120.67	109.40
3	C	142	CIT	C3-C4-C5	4.64	125.04	113.81
3	B	142	CIT	C2-C3-C6	4.32	119.38	110.11
3	A	146	CIT	C3-C4-C5	4.24	124.09	113.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	142	CIT	O7-C3-C2	-4.05	99.93	109.40
3	A	146	CIT	O7-C3-C6	-3.87	103.42	108.86
3	A	146	CIT	O2-C1-O1	-3.83	113.76	123.30
3	B	142	CIT	C4-C3-C6	-3.64	102.30	110.11
3	A	146	CIT	O2-C1-C2	3.39	125.24	114.35
3	B	142	CIT	O7-C3-C6	-3.16	104.43	108.86
3	C	142	CIT	O4-C5-O3	-3.11	115.54	123.30
3	C	142	CIT	O2-C1-C2	2.74	123.16	114.35
2	A	142	ACT	OXT-C-O	-2.65	112.30	122.05
3	A	146	CIT	O4-C5-O3	-2.60	116.82	123.30
3	C	142	CIT	O4-C5-C4	2.50	122.37	114.35
3	B	142	CIT	O6-C6-C3	2.44	117.28	113.05
2	A	141	ACT	OXT-C-CH3	2.26	124.51	115.18
3	C	142	CIT	O2-C1-O1	-2.08	118.12	123.30
2	A	141	ACT	OXT-C-O	-2.04	114.52	122.05

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	147[B]	GOL	O1-C1-C2-C3
4	B	143	GOL	C1-C2-C3-O3
4	C	144[A]	GOL	C1-C2-C3-O3
4	B	143	GOL	O1-C1-C2-C3
4	C	143	GOL	C1-C2-C3-O3
4	A	147[B]	GOL	O1-C1-C2-O2
4	B	143	GOL	O2-C2-C3-O3
3	A	146	CIT	C1-C2-C3-O7
3	B	142	CIT	C2-C3-C4-C5
3	C	142	CIT	C1-C2-C3-O7
4	C	143	GOL	O2-C2-C3-O3
3	B	142	CIT	O7-C3-C4-C5
3	B	142	CIT	C4-C3-C6-O6
3	B	142	CIT	C6-C3-C4-C5
4	B	143	GOL	O1-C1-C2-O2
3	B	142	CIT	C4-C3-C6-O5
3	A	146	CIT	C3-C4-C5-O3
3	C	142	CIT	C3-C4-C5-O3
3	B	142	CIT	C1-C2-C3-O7
3	B	142	CIT	C1-C2-C3-C4
3	A	146	CIT	C3-C4-C5-O4
3	B	142	CIT	O7-C3-C6-O5

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Mol	Chain	Res	Type	Atoms
3	B	142	CIT	O7-C3-C6-O6
3	C	142	CIT	C3-C4-C5-O4
3	C	142	CIT	O1-C1-C2-C3
4	C	144[A]	GOL	O2-C2-C3-O3
3	A	146	CIT	O1-C1-C2-C3
3	C	142	CIT	O2-C1-C2-C3
3	A	146	CIT	O2-C1-C2-C3
3	B	142	CIT	C3-C4-C5-O3
3	B	142	CIT	C3-C4-C5-O4

There are no ring outliers.

11 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	144[B]	GOL	1	0
4	A	147[B]	GOL	1	0
2	A	143	ACT	2	0
2	C	141	ACT	1	0
3	C	142	CIT	1	0
4	A	147[A]	GOL	2	0
2	A	145	ACT	1	0
3	A	146	CIT	3	0
2	A	144	ACT	7	0
2	A	142	ACT	5	0
4	C	144[A]	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, 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	127/141 (90%)	-0.11	8 (6%) 20 19	3, 8, 22, 49	0
1	B	128/141 (90%)	0.23	9 (7%) 16 15	3, 11, 21, 42	0
1	C	127/141 (90%)	-0.27	5 (3%) 39 39	3, 6, 19, 54	0
All	All	382/423 (90%)	-0.05	22 (5%) 23 22	3, 8, 22, 54	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	7	ALA	9.4
1	C	136	ALA	6.7
1	B	12	ILE	6.6
1	A	137	GLY	5.7
1	C	137	GLY	5.6
1	C	138	LYS	5.2
1	A	8	THR	5.0
1	C	7	ALA	4.5
1	A	138	LYS	4.4
1	B	8	THR	4.3
1	A	136	ALA	4.2
1	B	9	SER	3.9
1	B	14	LYS	3.4
1	B	11	ASP	3.3
1	B	13	LEU	3.3
1	B	15	GLN	3.3
1	B	17	ALA	2.9
1	A	9	SER	2.8
1	A	135	LEU	2.5
1	A	10	GLN	2.4
1	B	59	GLY	2.3
1	C	8	THR	2.3

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	ACT	C	141	4/4	0.31	0.23	25,37,38,39	0
2	ACT	A	142	4/4	0.70	0.26	22,35,39,40	0
2	ACT	A	141	4/4	0.77	0.13	49,51,52,53	0
2	ACT	A	143	4/4	0.79	0.26	38,40,42,46	0
2	ACT	B	141	4/4	0.80	0.19	50,55,56,58	0
2	ACT	A	144	4/4	0.84	0.51	25,27,29,37	0
3	CIT	B	142	13/13	0.84	0.16	19,47,69,76	0
4	GOL	B	143	6/6	0.85	0.18	30,35,39,40	0
4	GOL	A	147[B]	6/6	0.87	0.29	18,33,37,42	6
4	GOL	A	147[A]	6/6	0.87	0.29	13,29,36,38	6
2	ACT	A	145	4/4	0.88	0.24	26,28,34,37	0
3	CIT	C	142	13/13	0.89	0.14	6,19,38,52	0
3	CIT	A	146	13/13	0.90	0.12	4,20,46,47	0
4	GOL	C	144[A]	6/6	0.91	0.27	19,33,36,41	6
4	GOL	C	144[B]	6/6	0.91	0.27	8,19,29,29	6
4	GOL	C	143	6/6	0.92	0.24	13,28,35,40	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.