



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2020 – 05:20 PM BST

PDB ID : 5FIF  
Title : Carboxyltransferase domain of a single-chain bacterial carboxylase  
Authors : Hagmann, A.; Hunkeler, M.; Stuttfeld, E.; Maier, T.  
Deposited on : 2015-12-23  
Resolution : 2.49 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
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) : 2.13.1

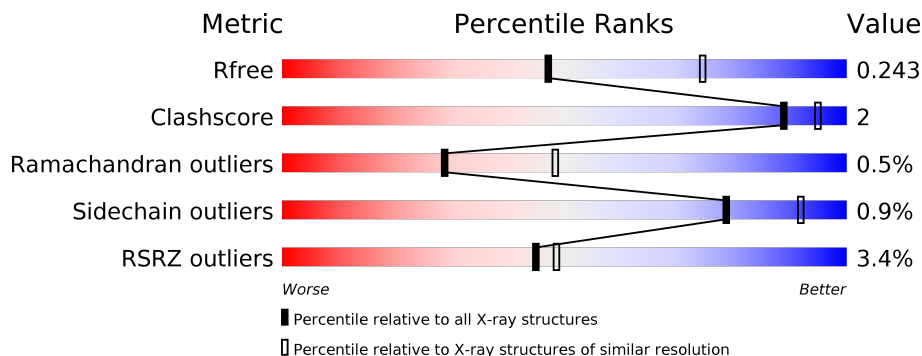
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.49 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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

Mol	Chain	Length	Quality of chain
1	A	566	3% 86% •• 10%
1	B	566	5% 86% 5% 8%
1	C	566	3% 84% 5% 10%
1	D	566	3% 88% 7% 5%
1	E	566	3% 84% • 11%
1	F	566	% 85% • 11%

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 45963 atoms, of which 22490 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 Carboxylase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	507	7466	2364	3723	676	693	10	0	2	0
1	B	519	7687	2429	3838	700	710	10	0	2	0
1	C	507	7487	2365	3742	681	689	10	0	0	0
1	D	536	7742	2505	3768	719	740	10	0	0	0
1	E	503	7348	2348	3637	671	682	10	0	1	0
1	F	506	7471	2363	3734	677	687	10	0	2	0

There are 180 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-29	MET	-	initiating methionine	UNP Q9RYK2
A	-28	ALA	-	expression tag	UNP Q9RYK2
A	-27	HIS	-	expression tag	UNP Q9RYK2
A	-26	HIS	-	expression tag	UNP Q9RYK2
A	-25	HIS	-	expression tag	UNP Q9RYK2
A	-24	HIS	-	expression tag	UNP Q9RYK2
A	-23	HIS	-	expression tag	UNP Q9RYK2
A	-22	HIS	-	expression tag	UNP Q9RYK2
A	-21	HIS	-	expression tag	UNP Q9RYK2
A	-20	HIS	-	expression tag	UNP Q9RYK2
A	-19	HIS	-	expression tag	UNP Q9RYK2
A	-18	HIS	-	expression tag	UNP Q9RYK2
A	-17	LYS	-	expression tag	UNP Q9RYK2
A	-16	LEU	-	expression tag	UNP Q9RYK2
A	-15	THR	-	expression tag	UNP Q9RYK2
A	-14	SER	-	expression tag	UNP Q9RYK2
A	-13	LEU	-	expression tag	UNP Q9RYK2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-12	TYR	-	expression tag	UNP Q9RYK2
A	-11	LYS	-	expression tag	UNP Q9RYK2
A	-10	LYS	-	expression tag	UNP Q9RYK2
A	-9	ALA	-	expression tag	UNP Q9RYK2
A	-8	GLY	-	expression tag	UNP Q9RYK2
A	-7	LEU	-	expression tag	UNP Q9RYK2
A	-6	GLU	-	expression tag	UNP Q9RYK2
A	-5	ASN	-	expression tag	UNP Q9RYK2
A	-4	LEU	-	expression tag	UNP Q9RYK2
A	-3	TYR	-	expression tag	UNP Q9RYK2
A	-2	PHE	-	expression tag	UNP Q9RYK2
A	-1	GLN	-	expression tag	UNP Q9RYK2
A	0	GLY	-	expression tag	UNP Q9RYK2
B	-29	MET	-	initiating methionine	UNP Q9RYK2
B	-28	ALA	-	expression tag	UNP Q9RYK2
B	-27	HIS	-	expression tag	UNP Q9RYK2
B	-26	HIS	-	expression tag	UNP Q9RYK2
B	-25	HIS	-	expression tag	UNP Q9RYK2
B	-24	HIS	-	expression tag	UNP Q9RYK2
B	-23	HIS	-	expression tag	UNP Q9RYK2
B	-22	HIS	-	expression tag	UNP Q9RYK2
B	-21	HIS	-	expression tag	UNP Q9RYK2
B	-20	HIS	-	expression tag	UNP Q9RYK2
B	-19	HIS	-	expression tag	UNP Q9RYK2
B	-18	HIS	-	expression tag	UNP Q9RYK2
B	-17	LYS	-	expression tag	UNP Q9RYK2
B	-16	LEU	-	expression tag	UNP Q9RYK2
B	-15	THR	-	expression tag	UNP Q9RYK2
B	-14	SER	-	expression tag	UNP Q9RYK2
B	-13	LEU	-	expression tag	UNP Q9RYK2
B	-12	TYR	-	expression tag	UNP Q9RYK2
B	-11	LYS	-	expression tag	UNP Q9RYK2
B	-10	LYS	-	expression tag	UNP Q9RYK2
B	-9	ALA	-	expression tag	UNP Q9RYK2
B	-8	GLY	-	expression tag	UNP Q9RYK2
B	-7	LEU	-	expression tag	UNP Q9RYK2
B	-6	GLU	-	expression tag	UNP Q9RYK2
B	-5	ASN	-	expression tag	UNP Q9RYK2
B	-4	LEU	-	expression tag	UNP Q9RYK2
B	-3	TYR	-	expression tag	UNP Q9RYK2
B	-2	PHE	-	expression tag	UNP Q9RYK2
B	-1	GLN	-	expression tag	UNP Q9RYK2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	0	GLY	-	expression tag	UNP Q9RYK2
C	-29	MET	-	initiating methionine	UNP Q9RYK2
C	-28	ALA	-	expression tag	UNP Q9RYK2
C	-27	HIS	-	expression tag	UNP Q9RYK2
C	-26	HIS	-	expression tag	UNP Q9RYK2
C	-25	HIS	-	expression tag	UNP Q9RYK2
C	-24	HIS	-	expression tag	UNP Q9RYK2
C	-23	HIS	-	expression tag	UNP Q9RYK2
C	-22	HIS	-	expression tag	UNP Q9RYK2
C	-21	HIS	-	expression tag	UNP Q9RYK2
C	-20	HIS	-	expression tag	UNP Q9RYK2
C	-19	HIS	-	expression tag	UNP Q9RYK2
C	-18	HIS	-	expression tag	UNP Q9RYK2
C	-17	LYS	-	expression tag	UNP Q9RYK2
C	-16	LEU	-	expression tag	UNP Q9RYK2
C	-15	THR	-	expression tag	UNP Q9RYK2
C	-14	SER	-	expression tag	UNP Q9RYK2
C	-13	LEU	-	expression tag	UNP Q9RYK2
C	-12	TYR	-	expression tag	UNP Q9RYK2
C	-11	LYS	-	expression tag	UNP Q9RYK2
C	-10	LYS	-	expression tag	UNP Q9RYK2
C	-9	ALA	-	expression tag	UNP Q9RYK2
C	-8	GLY	-	expression tag	UNP Q9RYK2
C	-7	LEU	-	expression tag	UNP Q9RYK2
C	-6	GLU	-	expression tag	UNP Q9RYK2
C	-5	ASN	-	expression tag	UNP Q9RYK2
C	-4	LEU	-	expression tag	UNP Q9RYK2
C	-3	TYR	-	expression tag	UNP Q9RYK2
C	-2	PHE	-	expression tag	UNP Q9RYK2
C	-1	GLN	-	expression tag	UNP Q9RYK2
C	0	GLY	-	expression tag	UNP Q9RYK2
D	-29	MET	-	initiating methionine	UNP Q9RYK2
D	-28	ALA	-	expression tag	UNP Q9RYK2
D	-27	HIS	-	expression tag	UNP Q9RYK2
D	-26	HIS	-	expression tag	UNP Q9RYK2
D	-25	HIS	-	expression tag	UNP Q9RYK2
D	-24	HIS	-	expression tag	UNP Q9RYK2
D	-23	HIS	-	expression tag	UNP Q9RYK2
D	-22	HIS	-	expression tag	UNP Q9RYK2
D	-21	HIS	-	expression tag	UNP Q9RYK2
D	-20	HIS	-	expression tag	UNP Q9RYK2
D	-19	HIS	-	expression tag	UNP Q9RYK2

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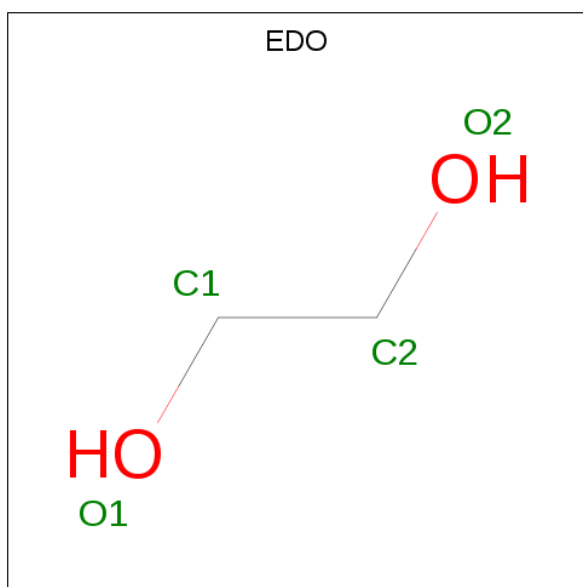
Chain	Residue	Modelled	Actual	Comment	Reference
D	-18	HIS	-	expression tag	UNP Q9RYK2
D	-17	LYS	-	expression tag	UNP Q9RYK2
D	-16	LEU	-	expression tag	UNP Q9RYK2
D	-15	THR	-	expression tag	UNP Q9RYK2
D	-14	SER	-	expression tag	UNP Q9RYK2
D	-13	LEU	-	expression tag	UNP Q9RYK2
D	-12	TYR	-	expression tag	UNP Q9RYK2
D	-11	LYS	-	expression tag	UNP Q9RYK2
D	-10	LYS	-	expression tag	UNP Q9RYK2
D	-9	ALA	-	expression tag	UNP Q9RYK2
D	-8	GLY	-	expression tag	UNP Q9RYK2
D	-7	LEU	-	expression tag	UNP Q9RYK2
D	-6	GLU	-	expression tag	UNP Q9RYK2
D	-5	ASN	-	expression tag	UNP Q9RYK2
D	-4	LEU	-	expression tag	UNP Q9RYK2
D	-3	TYR	-	expression tag	UNP Q9RYK2
D	-2	PHE	-	expression tag	UNP Q9RYK2
D	-1	GLN	-	expression tag	UNP Q9RYK2
D	0	GLY	-	expression tag	UNP Q9RYK2
E	-29	MET	-	initiating methionine	UNP Q9RYK2
E	-28	ALA	-	expression tag	UNP Q9RYK2
E	-27	HIS	-	expression tag	UNP Q9RYK2
E	-26	HIS	-	expression tag	UNP Q9RYK2
E	-25	HIS	-	expression tag	UNP Q9RYK2
E	-24	HIS	-	expression tag	UNP Q9RYK2
E	-23	HIS	-	expression tag	UNP Q9RYK2
E	-22	HIS	-	expression tag	UNP Q9RYK2
E	-21	HIS	-	expression tag	UNP Q9RYK2
E	-20	HIS	-	expression tag	UNP Q9RYK2
E	-19	HIS	-	expression tag	UNP Q9RYK2
E	-18	HIS	-	expression tag	UNP Q9RYK2
E	-17	LYS	-	expression tag	UNP Q9RYK2
E	-16	LEU	-	expression tag	UNP Q9RYK2
E	-15	THR	-	expression tag	UNP Q9RYK2
E	-14	SER	-	expression tag	UNP Q9RYK2
E	-13	LEU	-	expression tag	UNP Q9RYK2
E	-12	TYR	-	expression tag	UNP Q9RYK2
E	-11	LYS	-	expression tag	UNP Q9RYK2
E	-10	LYS	-	expression tag	UNP Q9RYK2
E	-9	ALA	-	expression tag	UNP Q9RYK2
E	-8	GLY	-	expression tag	UNP Q9RYK2
E	-7	LEU	-	expression tag	UNP Q9RYK2

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-6	GLU	-	expression tag	UNP Q9RYK2
E	-5	ASN	-	expression tag	UNP Q9RYK2
E	-4	LEU	-	expression tag	UNP Q9RYK2
E	-3	TYR	-	expression tag	UNP Q9RYK2
E	-2	PHE	-	expression tag	UNP Q9RYK2
E	-1	GLN	-	expression tag	UNP Q9RYK2
E	0	GLY	-	expression tag	UNP Q9RYK2
F	-29	MET	-	initiating methionine	UNP Q9RYK2
F	-28	ALA	-	expression tag	UNP Q9RYK2
F	-27	HIS	-	expression tag	UNP Q9RYK2
F	-26	HIS	-	expression tag	UNP Q9RYK2
F	-25	HIS	-	expression tag	UNP Q9RYK2
F	-24	HIS	-	expression tag	UNP Q9RYK2
F	-23	HIS	-	expression tag	UNP Q9RYK2
F	-22	HIS	-	expression tag	UNP Q9RYK2
F	-21	HIS	-	expression tag	UNP Q9RYK2
F	-20	HIS	-	expression tag	UNP Q9RYK2
F	-19	HIS	-	expression tag	UNP Q9RYK2
F	-18	HIS	-	expression tag	UNP Q9RYK2
F	-17	LYS	-	expression tag	UNP Q9RYK2
F	-16	LEU	-	expression tag	UNP Q9RYK2
F	-15	THR	-	expression tag	UNP Q9RYK2
F	-14	SER	-	expression tag	UNP Q9RYK2
F	-13	LEU	-	expression tag	UNP Q9RYK2
F	-12	TYR	-	expression tag	UNP Q9RYK2
F	-11	LYS	-	expression tag	UNP Q9RYK2
F	-10	LYS	-	expression tag	UNP Q9RYK2
F	-9	ALA	-	expression tag	UNP Q9RYK2
F	-8	GLY	-	expression tag	UNP Q9RYK2
F	-7	LEU	-	expression tag	UNP Q9RYK2
F	-6	GLU	-	expression tag	UNP Q9RYK2
F	-5	ASN	-	expression tag	UNP Q9RYK2
F	-4	LEU	-	expression tag	UNP Q9RYK2
F	-3	TYR	-	expression tag	UNP Q9RYK2
F	-2	PHE	-	expression tag	UNP Q9RYK2
F	-1	GLN	-	expression tag	UNP Q9RYK2
F	0	GLY	-	expression tag	UNP Q9RYK2

- Molecule 2 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	0	0
			10	2	6	2		
2	D	1	Total	C	H	O	0	0
			10	2	6	2		
2	D	1	Total	C	H	O	0	0
			10	2	6	2		
2	E	1	Total	C	H	O	0	0
			10	2	6	2		
2	E	1	Total	C	H	O	0	0
			10	2	6	2		
2	F	1	Total	C	H	O	0	0
			10	2	6	2		
2	F	1	Total	C	H	O	0	0
			10	2	6	2		
2	F	1	Total	C	H	O	0	0
			10	2	6	2		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	104	Total	O	0	0
			104	104		
3	B	89	Total	O	0	0
			89	89		
3	C	145	Total	O	0	0
			145	145		
3	D	91	Total	O	0	0
			91	91		

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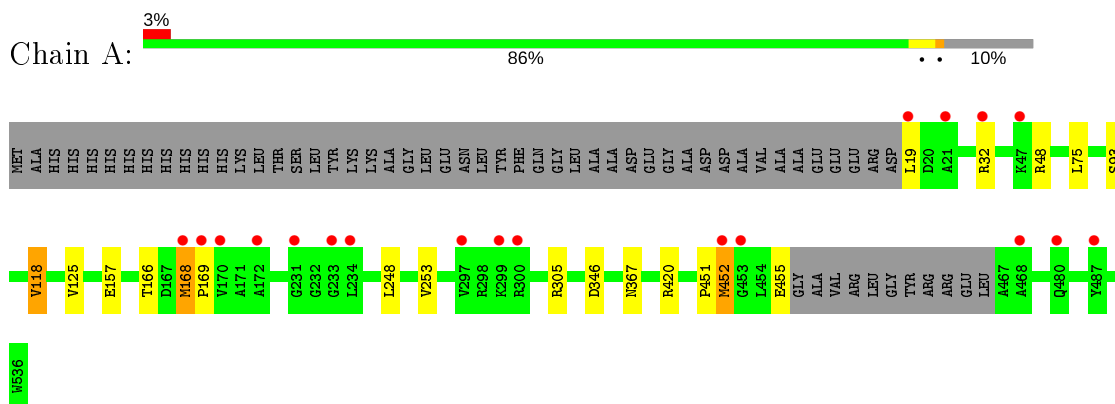
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
3	E	117	Total 117	O 117	0	0
3	F	136	Total 136	O 136	0	0

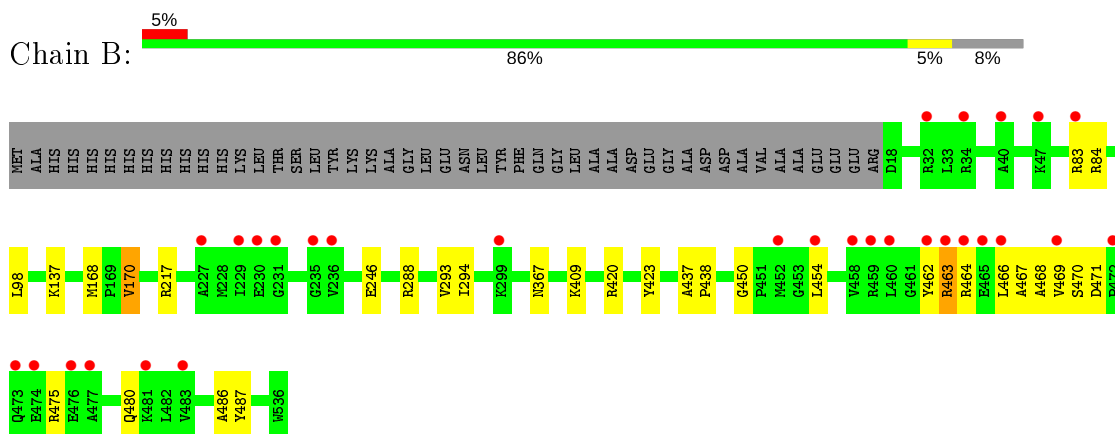
### 3 Residue-property plots [i](#)

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.

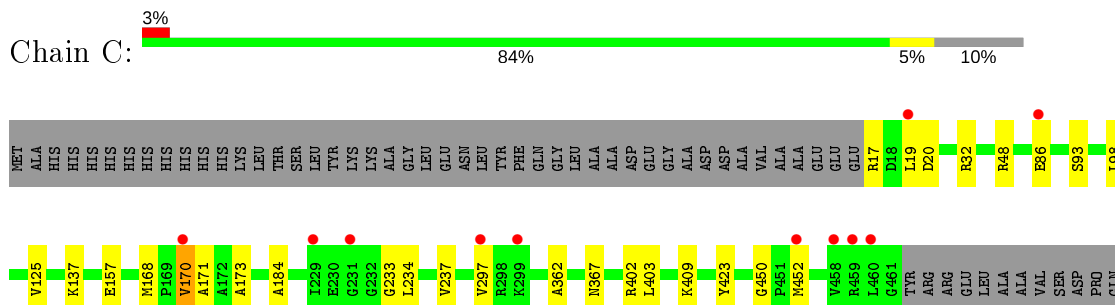
- Molecule 1: Carboxylase

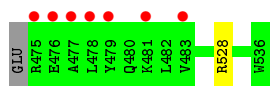


- Molecule 1: Carboxylase

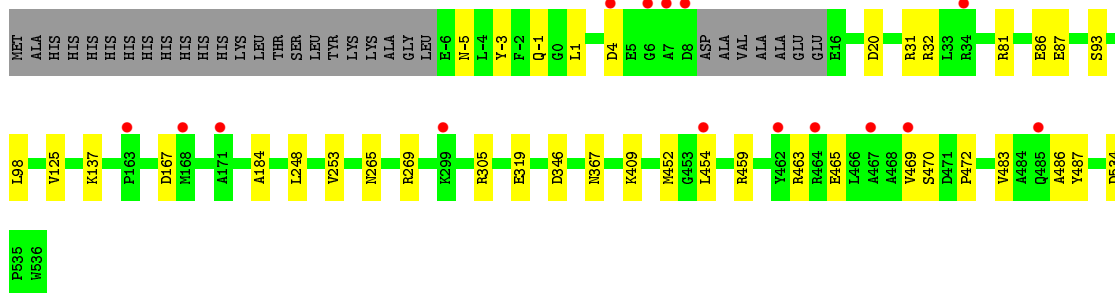
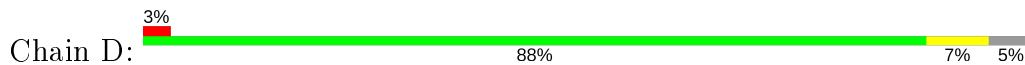


- Molecule 1: Carboxylase

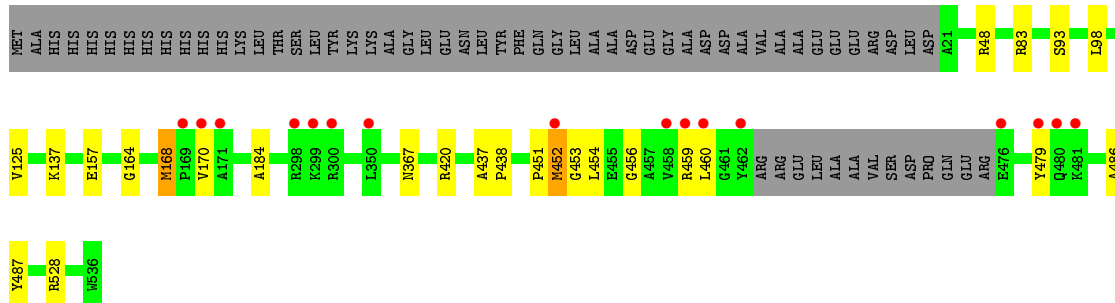
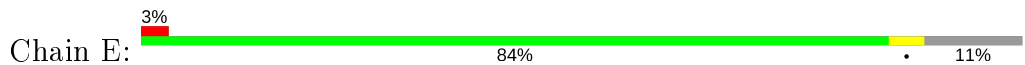




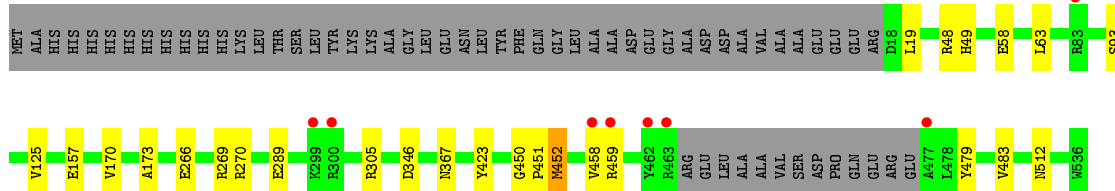
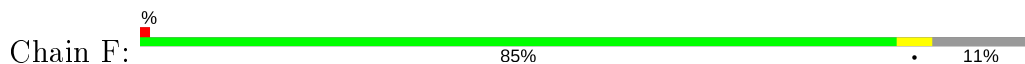
• Molecule 1: Carboxylase



• Molecule 1: Carboxylase



• Molecule 1: Carboxylase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	111.47Å 149.57Å 189.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	69.55 – 2.49 69.55 – 2.49	Depositor EDS
% Data completeness (in resolution range)	99.6 (69.55-2.49) 99.6 (69.55-2.49)	Depositor EDS
$R_{merge}$	0.21	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.04 (at 2.48Å)	Xtrriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, $R_{free}$	0.202 , 0.242 0.204 , 0.243	Depositor DCC
$R_{free}$ test set	2204 reflections (2.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	40.8	Xtrriage
Anisotropy	0.245	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 28.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	45963	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	49.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.33% 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: EDO

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	0.27	0/3831	0.48	1/5218 (0.0%)
1	B	0.26	0/3934	0.47	1/5357 (0.0%)
1	C	0.27	0/3819	0.47	2/5199 (0.0%)
1	D	0.26	0/4052	0.44	0/5515
1	E	0.27	0/3790	0.44	0/5161
1	F	0.27	0/3821	0.44	0/5203
All	All	0.27	0/23247	0.46	4/31653 (0.0%)

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	A	0	1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	B	170	VAL	CG1-CB-CG2	11.45	129.22	110.90
1	A	118	VAL	CG1-CB-CG2	8.47	124.45	110.90
1	C	297	VAL	CG1-CB-CG2	7.90	123.55	110.90
1	C	297	VAL	CA-CB-CG2	5.40	118.99	110.90

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	452	MET	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	3743	3723	3720	9	0
1	B	3849	3838	3838	17	0
1	C	3745	3742	3741	16	0
1	D	3974	3768	3946	21	0
1	E	3711	3637	3702	15	0
1	F	3737	3734	3723	15	0
2	A	4	6	6	0	0
2	D	8	12	12	0	0
2	E	8	12	12	0	0
2	F	12	18	18	0	0
3	A	104	0	0	0	0
3	B	89	0	0	0	0
3	C	145	0	0	0	0
3	D	91	0	0	0	0
3	E	117	0	0	0	0
3	F	136	0	0	1	0
All	All	23473	22490	22718	87	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 2.

All (87) 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:E:451:PRO:O	1:E:453:GLY:N	2.17	0.77
1:E:459:ARG:HG3	1:E:479:TYR:CE1	2.29	0.67
1:D:465:GLU:O	1:D:469:VAL:HG23	1.98	0.64
1:C:32:ARG:NH2	1:C:86:GLU:OE2	2.31	0.64
1:D:31:ARG:NH1	1:D:87:GLU:OE2	2.31	0.63
1:F:512:ASN:OD1	3:F:701:HOH:O	2.15	0.63
1:D:-3:TYR:CE2	1:D:1:LEU:HD11	2.34	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:467:ALA:O	1:B:469:VAL:N	2.33	0.60
1:D:-5:ASN:O	1:D:-1:GLN:HG3	2.02	0.60
1:A:32:ARG:NH2	1:A:75:LEU:O	2.36	0.58
1:B:217:ARG:NH1	1:B:246:GLU:OE2	2.39	0.56
1:B:469:VAL:O	1:B:470:SER:OG	2.21	0.56
1:D:265:ASN:OD1	1:D:269:ARG:NH1	2.40	0.55
1:E:48:ARG:NH2	1:E:157:GLU:OE1	2.38	0.54
1:C:402:ARG:NE	1:D:534:ASP:OD1	2.40	0.54
1:C:48:ARG:NH2	1:C:157:GLU:OE1	2.39	0.54
1:B:454:LEU:HD11	1:B:486:ALA:HB1	1.91	0.53
1:F:459:ARG:HG3	1:F:479:TYR:CE1	2.44	0.52
1:E:459:ARG:HG3	1:E:479:TYR:HE1	1.72	0.52
1:A:168:MET:HB2	1:A:169:PRO:HA	1.92	0.51
1:C:17:ARG:NH2	1:F:289:GLU:OE1	2.44	0.51
1:E:456:GLY:O	1:E:460:LEU:HG	2.11	0.51
1:C:184:ALA:O	1:D:409:LYS:NZ	2.44	0.50
1:E:83:ARG:NH1	1:E:164:GLY:O	2.44	0.50
1:F:48:ARG:NH2	1:F:157:GLU:OE1	2.42	0.50
1:A:48:ARG:NH2	1:A:157:GLU:OE1	2.43	0.49
1:A:93:SER:HA	1:A:125:VAL:HG13	1.95	0.49
1:E:454:LEU:HD22	1:E:486:ALA:HB1	1.93	0.49
1:F:305:ARG:NH2	1:F:346:ASP:OD2	2.46	0.48
1:B:288:ARG:NH1	1:D:20:ASP:OD1	2.46	0.48
1:B:454:LEU:HD23	1:B:487:TYR:CE2	2.49	0.48
1:D:305:ARG:NH1	1:D:319:GLU:OE2	2.47	0.48
1:D:98:LEU:O	1:D:137:LYS:NZ	2.35	0.47
1:B:467:ALA:O	1:B:475:ARG:HD3	2.14	0.47
1:B:83:ARG:HG3	1:B:84:ARG:HG3	1.96	0.47
1:D:454:LEU:HD21	1:D:486:ALA:HB3	1.96	0.47
1:D:32:ARG:NH2	1:D:86:GLU:OE2	2.48	0.47
1:B:462:TYR:CD1	1:B:466:LEU:HD13	2.50	0.47
1:B:423:TYR:HA	1:B:450:GLY:O	2.14	0.47
1:C:170:VAL:HG21	1:C:173:ALA:HB2	1.97	0.47
1:F:458:VAL:HG11	1:F:483:VAL:HG22	1.97	0.46
1:E:454:LEU:HD12	1:E:487:TYR:CD1	2.50	0.46
1:B:467:ALA:O	1:B:469:VAL:HG23	2.16	0.46
1:B:409:LYS:NZ	1:E:184:ALA:O	2.48	0.46
1:F:266:GLU:O	1:F:270:ARG:HG2	2.16	0.45
1:A:305:ARG:NH2	1:A:346:ASP:OD1	2.49	0.45
1:C:409:LYS:NZ	1:D:184:ALA:O	2.50	0.45
1:D:454:LEU:HD11	1:D:487:TYR:N	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:459:ARG:CG	1:F:479:TYR:CE1	2.99	0.45
1:B:454:LEU:HD23	1:B:487:TYR:CD2	2.52	0.45
1:A:32:ARG:HH12	1:A:75:LEU:HB3	1.82	0.45
1:C:170:VAL:HG23	1:C:171:ALA:N	2.31	0.44
1:C:93:SER:HA	1:C:125:VAL:HG13	1.99	0.44
1:E:93:SER:HA	1:E:125:VAL:HG13	1.99	0.44
1:F:451:PRO:O	1:F:452:MET:O	2.34	0.44
1:C:17:ARG:NH2	1:C:19:LEU:HD11	2.33	0.44
1:C:423:TYR:HA	1:C:450:GLY:O	2.18	0.44
1:D:93:SER:HA	1:D:125:VAL:HG13	2.01	0.43
1:E:459:ARG:CG	1:E:479:TYR:CE1	3.01	0.43
1:D:305:ARG:NH2	1:D:346:ASP:OD2	2.52	0.43
1:A:168:MET:CB	1:A:169:PRO:CA	2.97	0.43
1:D:248:LEU:HB3	1:D:253:VAL:HB	2.00	0.43
1:C:233:GLY:O	1:C:234:LEU:HB2	2.19	0.42
1:D:454:LEU:HD22	1:D:483:VAL:HG13	2.01	0.42
1:E:452:MET:HG3	1:E:453:GLY:N	2.34	0.42
1:E:437:ALA:N	1:E:438:PRO:CD	2.82	0.42
1:F:63:LEU:HD12	1:F:269:ARG:HG2	2.01	0.42
1:B:98:LEU:O	1:B:137:LYS:NZ	2.49	0.42
1:A:248:LEU:HB3	1:A:253:VAL:HB	2.02	0.42
1:B:293:VAL:HG13	1:B:294:ILE:HG13	2.02	0.42
1:C:234:LEU:O	1:C:237:VAL:HG22	2.20	0.42
1:D:470:SER:O	1:D:472:PRO:HD3	2.19	0.42
1:E:98:LEU:O	1:E:137:LYS:NZ	2.50	0.41
1:F:49:HIS:HE2	1:F:58:GLU:CD	2.23	0.41
1:B:463:ARG:HG2	1:B:464:ARG:N	2.36	0.41
1:E:168:MET:HE3	1:E:170:VAL:HG12	2.02	0.41
1:F:170:VAL:HG21	1:F:173:ALA:HB2	2.01	0.41
1:B:437:ALA:N	1:B:438:PRO:CD	2.84	0.41
1:C:19:LEU:N	1:C:19:LEU:HD12	2.35	0.41
1:C:362:ALA:HB3	1:C:403:LEU:HD21	2.03	0.41
1:C:98:LEU:O	1:C:137:LYS:NZ	2.54	0.41
1:F:423:TYR:HA	1:F:450:GLY:O	2.21	0.41
1:F:458:VAL:HG13	1:F:479:TYR:HE1	1.86	0.41
1:D:459:ARG:O	1:D:463:ARG:HB2	2.21	0.41
1:D:81:ARG:N	1:D:167:ASP:OD2	2.48	0.40
1:F:93:SER:HA	1:F:125:VAL:HG13	2.02	0.40
1:A:455:GLU:N	1:A:455:GLU:OE1	2.54	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	505/566 (89%)	485 (96%)	16 (3%)	4 (1%)	19	35
1	B	519/566 (92%)	493 (95%)	22 (4%)	4 (1%)	19	35
1	C	503/566 (89%)	488 (97%)	14 (3%)	1 (0%)	47	68
1	D	532/566 (94%)	512 (96%)	19 (4%)	1 (0%)	47	68
1	E	500/566 (88%)	484 (97%)	14 (3%)	2 (0%)	34	54
1	F	504/566 (89%)	488 (97%)	14 (3%)	2 (0%)	34	54
All	All	3063/3396 (90%)	2950 (96%)	99 (3%)	14 (0%)	29	48

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	168	MET
1	B	463	ARG
1	B	468	ALA
1	D	452	MET
1	E	452	MET
1	F	452	MET
1	C	452	MET
1	A	452	MET
1	A	451	PRO
1	B	471	ASP
1	F	19	LEU
1	E	420	ARG
1	A	420	ARG
1	B	420	ARG

### 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	361/405 (89%)	357 (99%)	4 (1%)	73	89
1	B	370/405 (91%)	366 (99%)	4 (1%)	73	89
1	C	359/405 (89%)	354 (99%)	5 (1%)	67	86
1	D	381/405 (94%)	379 (100%)	2 (0%)	88	96
1	E	355/405 (88%)	352 (99%)	3 (1%)	81	93
1	F	358/405 (88%)	357 (100%)	1 (0%)	92	97
All	All	2184/2430 (90%)	2165 (99%)	19 (1%)	78	92

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	LEU
1	A	118	VAL
1	A	166	THR
1	A	367	ASN
1	B	168	MET
1	B	170	VAL
1	B	367	ASN
1	B	480	GLN
1	C	20	ASP
1	C	168	MET
1	C	170	VAL
1	C	367	ASN
1	C	528	ARG
1	D	4	ASP
1	D	367	ASN
1	E	168	MET
1	E	367	ASN
1	E	528	ARG
1	F	367	ASN

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

### 5.3.3 RNA

There are no RNA molecules in this entry.

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

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	EDO	F	603	-	3,3,3	0.47	0	2,2,2	0.33	0
2	EDO	E	601	-	3,3,3	0.40	0	2,2,2	0.45	0
2	EDO	D	602	-	3,3,3	0.45	0	2,2,2	0.47	0
2	EDO	A	601	-	3,3,3	0.46	0	2,2,2	0.34	0
2	EDO	E	602	-	3,3,3	0.48	0	2,2,2	0.38	0
2	EDO	F	602	-	3,3,3	0.45	0	2,2,2	0.37	0
2	EDO	D	601	-	3,3,3	0.46	0	2,2,2	0.31	0
2	EDO	F	601	-	3,3,3	0.49	0	2,2,2	0.34	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	F	603	-	-	0/1/1/1	-
2	EDO	E	601	-	-	1/1/1/1	-
2	EDO	D	602	-	-	1/1/1/1	-
2	EDO	A	601	-	-	0/1/1/1	-
2	EDO	E	602	-	-	1/1/1/1	-
2	EDO	F	602	-	-	1/1/1/1	-
2	EDO	D	601	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	F	601	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	601	EDO	O1-C1-C2-O2
2	F	602	EDO	O1-C1-C2-O2
2	D	602	EDO	O1-C1-C2-O2
2	E	602	EDO	O1-C1-C2-O2

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data [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	507/566 (89%)	0.20	19 (3%) 41 45	34, 43, 65, 82	0
1	B	519/566 (91%)	0.26	30 (5%) 23 24	35, 45, 78, 115	0
1	C	507/566 (89%)	0.19	18 (3%) 42 46	30, 38, 69, 127	0
1	D	536/566 (94%)	0.18	15 (2%) 53 56	33, 44, 67, 118	0
1	E	503/566 (88%)	0.07	16 (3%) 47 51	31, 39, 61, 110	0
1	F	506/566 (89%)	0.08	8 (1%) 72 74	30, 37, 68, 123	0
All	All	3078/3396 (90%)	0.16	106 (3%) 45 48	30, 41, 68, 127	0

All (106) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	464	ARG	9.0
1	C	477	ALA	8.3
1	E	460	LEU	6.7
1	E	462	TYR	5.7
1	C	458	VAL	5.7
1	C	86	GLU	5.6
1	C	475	ARG	5.3
1	B	458	VAL	5.0
1	B	231	GLY	4.6
1	B	466	LEU	4.6
1	C	476	GLU	4.6
1	A	300	ARG	4.6
1	B	236	VAL	4.4
1	F	299	LYS	4.4
1	B	235	GLY	4.3
1	B	462	TYR	4.3
1	E	476	GLU	4.2
1	F	463	ARG	4.2
1	E	299	LYS	4.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	47	LYS	4.1
1	A	452	MET	4.0
1	A	233	GLY	4.0
1	D	454	LEU	3.9
1	A	231	GLY	3.9
1	A	234	LEU	3.9
1	E	169	PRO	3.8
1	C	479	TYR	3.8
1	E	452	MET	3.8
1	D	8	ASP	3.6
1	F	459	ARG	3.6
1	A	297	VAL	3.6
1	F	462	TYR	3.6
1	A	169	PRO	3.6
1	C	459	ARG	3.5
1	B	83	ARG	3.5
1	A	19	LEU	3.5
1	C	481	LYS	3.5
1	B	230	GLU	3.4
1	B	454	LEU	3.4
1	C	478	LEU	3.4
1	A	299	LYS	3.3
1	E	458	VAL	3.3
1	C	299	LYS	3.3
1	A	168	MET	3.2
1	C	483	VAL	3.2
1	A	21	ALA	3.2
1	C	297	VAL	3.1
1	D	299	LYS	3.0
1	C	460	LEU	3.0
1	B	477	ALA	3.0
1	A	170	VAL	2.9
1	D	469	VAL	2.9
1	B	472	PRO	2.9
1	D	467	ALA	2.9
1	F	300	ARG	2.9
1	D	464	ARG	2.9
1	D	462	TYR	2.8
1	D	6	GLY	2.8
1	C	229	ILE	2.8
1	B	229	ILE	2.7
1	E	479	TYR	2.7

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	481	LYS	2.7
1	C	231	GLY	2.7
1	D	4	ASP	2.7
1	D	163	PRO	2.6
1	B	459	ARG	2.5
1	B	40	ALA	2.5
1	B	465	GLU	2.5
1	A	468	ALA	2.5
1	B	476	GLU	2.5
1	C	170	VAL	2.4
1	B	463	ARG	2.4
1	E	459	ARG	2.4
1	B	469	VAL	2.4
1	B	483	VAL	2.4
1	B	299	LYS	2.4
1	E	300	ARG	2.4
1	B	474	GLU	2.4
1	F	83	ARG	2.3
1	D	485	GLN	2.3
1	E	171	ALA	2.3
1	F	477	ALA	2.3
1	A	172	ALA	2.3
1	C	452	MET	2.3
1	E	350	LEU	2.3
1	E	170	VAL	2.3
1	A	480	GLN	2.3
1	B	34	ARG	2.2
1	E	480	GLN	2.2
1	A	32	ARG	2.2
1	B	452	MET	2.2
1	B	32[A]	ARG	2.2
1	D	7	ALA	2.2
1	E	481	LYS	2.2
1	F	458	VAL	2.2
1	D	34	ARG	2.2
1	A	453	GLY	2.1
1	C	19	LEU	2.1
1	B	227	ALA	2.1
1	A	47	LYS	2.1
1	D	171	ALA	2.1
1	B	460	LEU	2.1
1	E	298	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	487	TYR	2.1
1	B	473	GLN	2.0
1	D	168	MET	2.0

## 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(Å <sup>2</sup> )	Q<0.9
2	EDO	E	602	4/4	0.80	0.24	37,44,47,49	0
2	EDO	A	601	4/4	0.87	0.35	44,53,56,63	0
2	EDO	D	602	4/4	0.90	0.18	47,57,61,66	0
2	EDO	E	601	4/4	0.91	0.25	35,42,44,48	0
2	EDO	F	602	4/4	0.93	0.14	37,44,45,47	0
2	EDO	F	601	4/4	0.93	0.24	37,45,47,47	0
2	EDO	F	603	4/4	0.94	0.21	36,43,46,51	0
2	EDO	D	601	4/4	0.98	0.19	43,51,51,52	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.