



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 14, 2024 – 06:09 am GMT

PDB ID : 6YI4  
Title : Structure of IMP-13 metallo-beta-lactamase complexed with citrate anion  
Authors : Zak, K.M.; Zhou, R.X.; Softley, C.A.; Bostock, M.J.; Sattler, M.; Popowicz, G.M.  
Deposited on : 2020-03-31  
Resolution : 1.70 Å(reported)

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

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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 : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
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) : 2.36

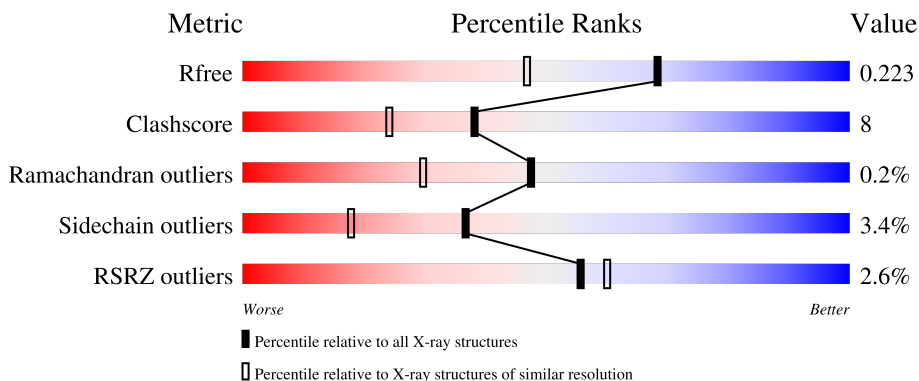
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.70 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	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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	AAA	226	 85% 10% .
1	BBB	226	 83% 12% . .
1	CCC	226	 86% 9% . .

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	ACT	BBB	401	-	-	X	-
5	ACT	BBB	402	-	-	X	-

## 2 Entry composition [i](#)

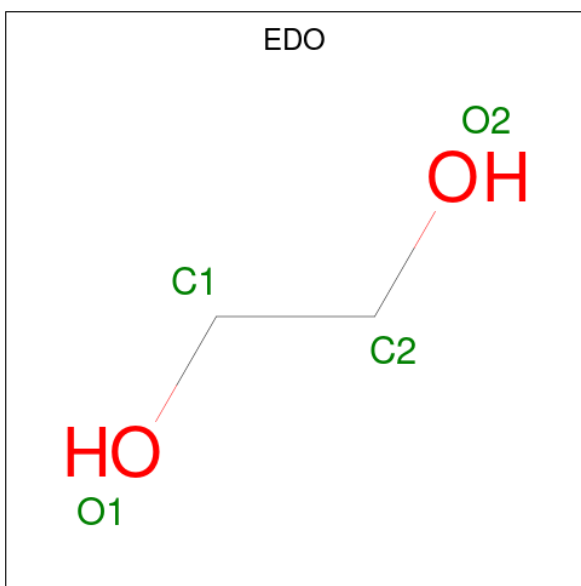
There are 7 unique types of molecules in this entry. The entry contains 10874 atoms, of which 5230 are hydrogens and 0 are deuteriums.

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 Beta-lactamase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
1	AAA	217	Total 3440	C 1116	H 1719	N 280	O 322	S 3	80	1	0
1	BBB	217	Total 3462	C 1124	H 1729	N 282	O 324	S 3	83	3	0
1	CCC	219	Total 3449	C 1110	H 1730	N 282	O 324	S 3	82	0	0

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



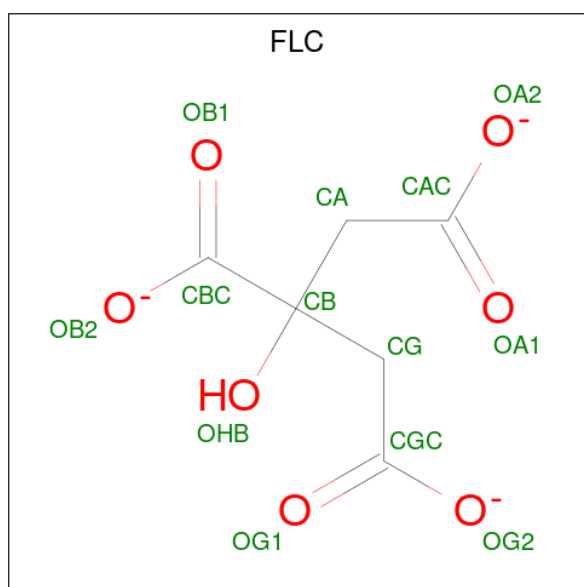
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
2	AAA	1	Total 10	C 2	H 6	O 2	1	0
2	AAA	1	Total 10	C 2	H 6	O 2	1	0
2	AAA	1	Total 10	C 2	H 6	O 2	1	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	AAA	1	Total	C	H	O	1	0
			10	2	6	2		
2	AAA	1	Total	C	H	O	1	0
			10	2	6	2		

- Molecule 3 is CITRATE ANION (three-letter code: FLC) (formula:  $C_6H_5O_7$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	AAA	1	Total	C	H	O	1	0
			18	6	5	7		
3	CCC	1	Total	C	H	O	1	0
			18	6	5	7		

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

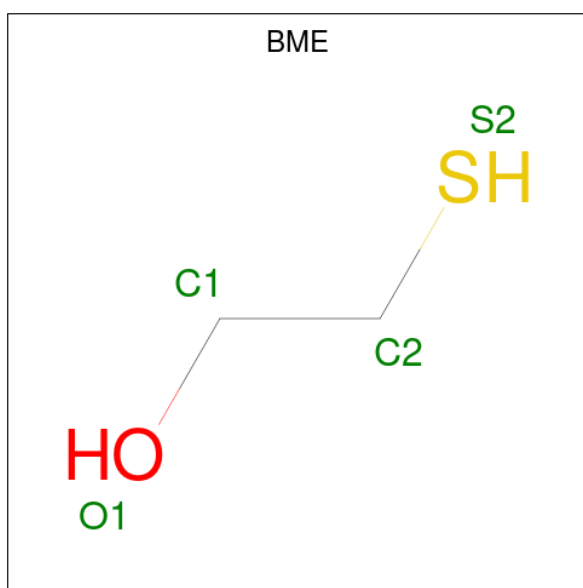
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	AAA	2	Total	Zn	0	0
			2	2		
4	BBB	2	Total	Zn	0	0
			2	2		
4	CCC	2	Total	Zn	0	0
			2	2		

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula:  $C_2H_3O_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	BBB	1	Total	C	H	O	0	0
			7	2	3	2		
5	BBB	1	Total	C	H	O	0	0
			7	2	3	2		

- Molecule 6 is BETA-MERCAPTOETHANOL (three-letter code: BME) (formula:  $C_2H_6OS$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	CCC	1	Total	C	H	O	S	1	0
			10	2	6	1	1		

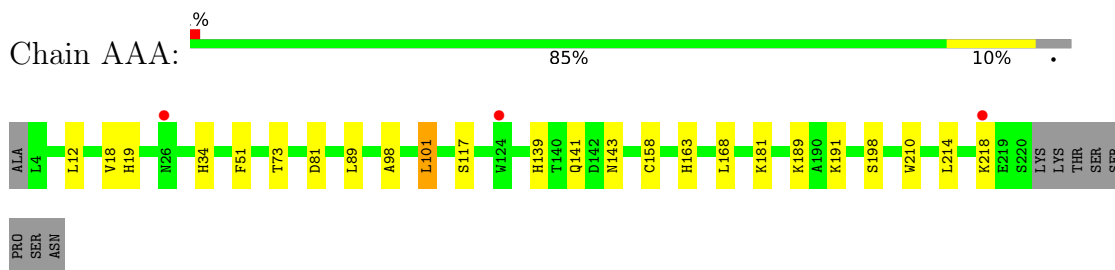
- Molecule 7 is water.

<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
7	AAA	162	Total 162	O 162	0	0
7	BBB	137	Total 137	O 137	0	0
7	CCC	108	Total 108	O 108	0	0

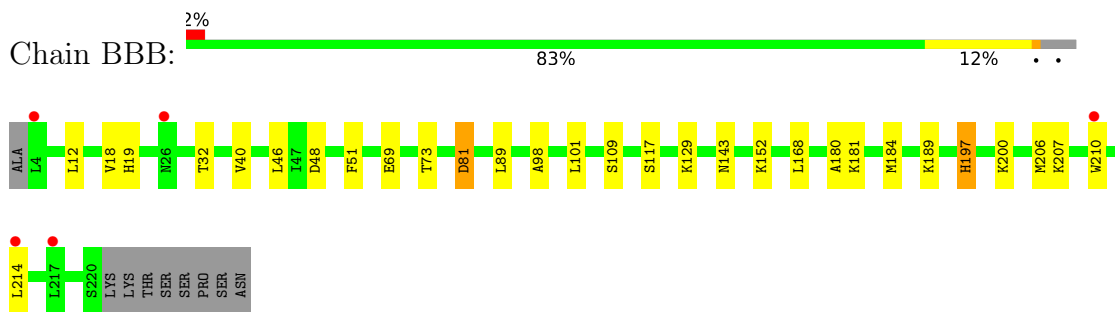
### 3 Residue-property plots [i](#)

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.

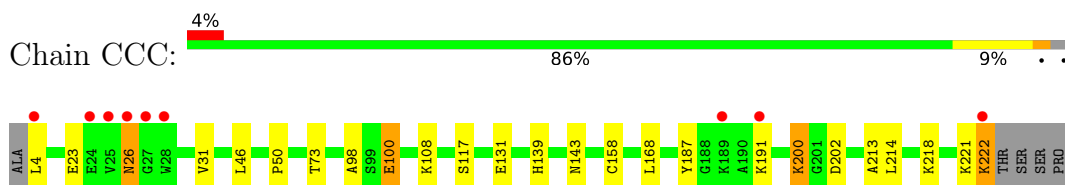
- Molecule 1: Beta-lactamase



- Molecule 1: Beta-lactamase



- Molecule 1: Beta-lactamase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	47.67Å 90.47Å 88.52Å 90.00° 100.85° 90.00°	Depositor
Resolution (Å)	46.87 – 1.70 46.82 – 1.70	Depositor EDS
% Data completeness (in resolution range)	99.7 (46.87-1.70) 99.8 (46.82-1.70)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.43 (at 1.70Å)	Xtrriage
Refinement program	REFMAC 5.8.0257	Depositor
R, $R_{free}$	0.180 , 0.213 0.189 , 0.223	Depositor DCC
$R_{free}$ test set	3820 reflections (4.73%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	25.1	Xtrriage
Anisotropy	0.404	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.42 , 49.9	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	10874	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.64% 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, ACT, ZN, BME, FLC

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	AAA	0.77	0/1770	0.85	0/2399
1	BBB	0.81	2/1789 (0.1%)	0.89	8/2425 (0.3%)
1	CCC	0.73	1/1761 (0.1%)	0.81	0/2382
All	All	0.77	3/5320 (0.1%)	0.85	8/7206 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	BBB	197[A]	HIS	CE1-NE2	6.91	1.48	1.32
1	BBB	197[B]	HIS	CE1-NE2	6.91	1.48	1.32
1	CCC	100	GLU	CD-OE1	-5.57	1.19	1.25

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	BBB	81[A]	ASP	CA-CB-CG	6.91	128.60	113.40
1	BBB	81[B]	ASP	CA-CB-CG	6.91	128.60	113.40
1	BBB	197[A]	HIS	CB-CA-C	6.61	123.62	110.40
1	BBB	197[B]	HIS	CB-CA-C	6.61	123.62	110.40
1	BBB	197[A]	HIS	CA-CB-CG	5.95	123.72	113.60

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	AAA	1721	1719	1711	16	0
1	BBB	1733	1729	1722	40	0
1	CCC	1719	1730	1719	14	0
2	AAA	20	30	30	0	0
3	AAA	13	5	4	0	0
3	CCC	13	5	4	0	0
4	AAA	2	0	0	0	0
4	BBB	2	0	0	0	0
4	CCC	2	0	0	0	0
5	BBB	8	6	6	9	0
6	CCC	4	6	6	1	0
7	AAA	162	0	0	7	1
7	BBB	137	0	0	12	1
7	CCC	108	0	0	5	0
All	All	5644	5230	5202	79	1

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.

The worst 5 of 79 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:BBB:184:MET:HE1	1:BBB:210[B]:TRP:NE1	1.15	1.44
1:BBB:184:MET:HE1	1:BBB:210[B]:TRP:CD1	1.74	1.23
1:BBB:101:LEU:HD12	7:BBB:545:HOH:O	1.46	1.14
1:BBB:184:MET:CE	1:BBB:210[B]:TRP:NE1	2.11	1.14
5:BBB:402:ACT:H3	7:BBB:503:HOH:O	0.85	1.00

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:AAA:474:HOH:O	7:BBB:603:HOH:O[2_646]	2.01	0.19

## 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	AAA	216/226 (96%)	210 (97%)	6 (3%)	0	100	100
1	BBB	218/226 (96%)	213 (98%)	4 (2%)	1 (0%)	29	13
1	CCC	217/226 (96%)	210 (97%)	7 (3%)	0	100	100
All	All	651/678 (96%)	633 (97%)	17 (3%)	1 (0%)	47	30

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	BBB	48	ASP

### 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	AAA	189/196 (96%)	183 (97%)	6 (3%)	39	20
1	BBB	191/196 (97%)	186 (97%)	5 (3%)	46	28
1	CCC	189/196 (96%)	181 (96%)	8 (4%)	30	12
All	All	569/588 (97%)	550 (97%)	19 (3%)	37	19

5 of 19 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	CCC	168	LEU
1	CCC	218	LYS

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Mol	Chain	Res	Type
1	CCC	222	LYS
1	CCC	200	LYS
1	BBB	143	ASN

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](#)

Of 16 ligands modelled in this entry, 6 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	$\# Z  > 2$
2	EDO	AAA	304	-	3,3,3	0.26	0	2,2,2	0.32	0
5	ACT	BBB	401	-	3,3,3	0.83	0	3,3,3	0.85	0
3	FLC	CCC	402	4	12,12,12	0.89	0	17,17,17	2.87	7 (41%)
2	EDO	AAA	305	-	3,3,3	0.07	0	2,2,2	0.19	0
6	BME	CCC	401	-	3,3,3	0.29	0	1,2,2	0.71	0
3	FLC	AAA	306	4	12,12,12	1.23	2 (16%)	17,17,17	1.77	2 (11%)
2	EDO	AAA	301	-	3,3,3	0.05	0	2,2,2	0.14	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	EDO	AAA	302	-	3,3,3	0.26	0	2,2,2	0.30	0
2	EDO	AAA	303	-	3,3,3	0.08	0	2,2,2	0.06	0
5	ACT	BBB	402	4	3,3,3	1.27	0	3,3,3	1.14	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	AAA	304	-	-	0/1/1/1	-
3	FLC	CCC	402	4	-	2/16/16/16	-
2	EDO	AAA	305	-	-	1/1/1/1	-
6	BME	CCC	401	-	-	0/1/1/1	-
3	FLC	AAA	306	4	-	4/16/16/16	-
2	EDO	AAA	301	-	-	0/1/1/1	-
2	EDO	AAA	302	-	-	1/1/1/1	-
2	EDO	AAA	303	-	-	1/1/1/1	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	AAA	306	FLC	OAI-CAC	2.18	1.29	1.22
3	AAA	306	FLC	OB1-CBC	2.15	1.29	1.22

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	CCC	402	FLC	OHB-CB-CBC	-7.02	99.00	108.86
3	CCC	402	FLC	OHB-CB-CA	6.02	123.49	109.40
3	AAA	306	FLC	OB1-CBC-CB	-5.12	115.00	122.25
3	CCC	402	FLC	OB2-CBC-CB	-3.96	106.17	113.05
3	AAA	306	FLC	OB2-CBC-CB	3.59	119.29	113.05

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	AAA	305	EDO	O1-C1-C2-O2
2	AAA	302	EDO	O1-C1-C2-O2
2	AAA	303	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
3	CCC	402	FLC	CB-CG-CGC-OG1
3	AAA	306	FLC	CA-CB-CBC-OB2

There are no ring outliers.

3 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	BBB	401	ACT	4	0
6	CCC	401	BME	1	0
5	BBB	402	ACT	7	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	AAA	217/226 (96%)	-0.11	3 (1%) 75 79	17, 25, 44, 67	0
1	BBB	217/226 (96%)	0.10	5 (2%) 60 65	18, 29, 52, 72	0
1	CCC	219/226 (96%)	0.22	9 (4%) 37 41	20, 33, 58, 88	0
All	All	653/678 (96%)	0.07	17 (2%) 56 60	17, 29, 52, 88	0

The worst 5 of 17 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	CCC	26	ASN	5.1
1	CCC	4	LEU	4.7
1	CCC	28	TRP	4.6
1	BBB	210[A]	TRP	4.2
1	BBB	214	LEU	3.1

### 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	EDO	AAA	305	4/4	0.50	0.22	71,72,74,74	1
2	EDO	AAA	303	4/4	0.70	0.18	62,68,70,70	1
2	EDO	AAA	304	4/4	0.74	0.26	50,54,57,57	1
2	EDO	AAA	301	4/4	0.77	0.14	53,55,65,65	1
6	BME	CCC	401	4/4	0.84	0.21	42,58,80,80	1
5	ACT	BBB	402	4/4	0.88	0.10	26,26,36,43	0
5	ACT	BBB	401	4/4	0.90	0.19	33,33,49,49	0
3	FLC	CCC	402	13/13	0.92	0.09	24,30,34,34	1
2	EDO	AAA	302	4/4	0.92	0.14	52,54,67,67	1
4	ZN	BBB	403	1/1	0.93	0.20	26,26,26,26	0
3	FLC	AAA	306	13/13	0.95	0.09	22,27,34,35	1
4	ZN	BBB	404	1/1	0.96	0.18	29,29,29,29	0
4	ZN	CCC	403	1/1	0.98	0.17	21,21,21,21	0
4	ZN	CCC	404	1/1	0.99	0.10	25,25,25,25	0
4	ZN	AAA	308	1/1	1.00	0.12	20,20,20,20	0
4	ZN	AAA	307	1/1	1.00	0.20	15,15,15,15	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.