



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 23, 2024 – 11:19 AM EDT

PDB ID : 1XA3  
Title : Crystal structure of CaiB, a type III CoA transferase in carnitine metabolism  
Authors : Stenmark, P.; Gurmu, D.; Nordlund, P.; Structural Proteomics in Europe (SPINE)  
Deposited on : 2004-08-25  
Resolution : 1.85 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.

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 : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 1.20.1  
EDS : 3.0  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.003 (Gargrove)  
Density-Fitness : 1.0.11  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

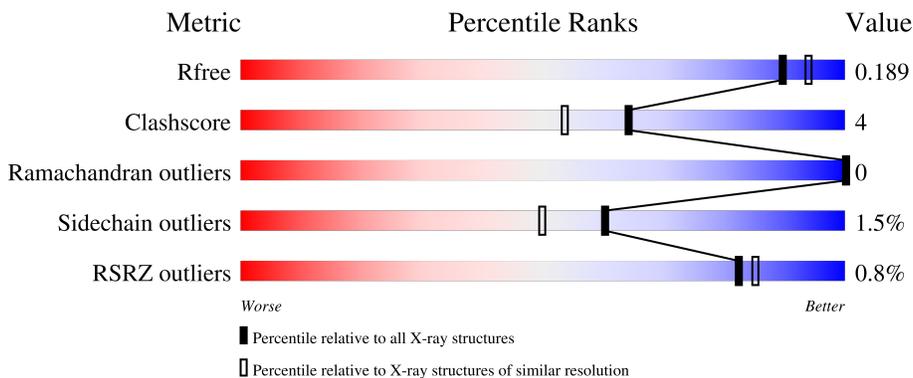
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.85 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))
$R_{free}$	164625	3097 (1.86-1.86)
Clashscore	180529	3359 (1.86-1.86)
Ramachandran outliers	177936	3335 (1.86-1.86)
Sidechain outliers	177891	3335 (1.86-1.86)
RSRZ outliers	164620	3097 (1.86-1.86)

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	437	
1	B	437	

## 2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 6932 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 Crotonobetainyl-CoA:carnitine CoA-transferase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	400	3127	2005	520	579	7	16	0	0	0
1	B	400	3127	2005	520	579	7	16	0	0	0

There are 98 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-23	MSE	-	expression tag	UNP P31572
A	-22	HIS	-	expression tag	UNP P31572
A	-21	HIS	-	expression tag	UNP P31572
A	-20	HIS	-	expression tag	UNP P31572
A	-19	HIS	-	expression tag	UNP P31572
A	-18	HIS	-	expression tag	UNP P31572
A	-17	HIS	-	expression tag	UNP P31572
A	-16	GLY	-	expression tag	UNP P31572
A	-15	SER	-	expression tag	UNP P31572
A	-14	THR	-	expression tag	UNP P31572
A	-13	SER	-	expression tag	UNP P31572
A	-12	LEU	-	expression tag	UNP P31572
A	-11	TYR	-	expression tag	UNP P31572
A	-10	LYS	-	expression tag	UNP P31572
A	-9	LYS	-	expression tag	UNP P31572
A	-8	ALA	-	expression tag	UNP P31572
A	-7	GLY	-	expression tag	UNP P31572
A	-6	SER	-	expression tag	UNP P31572
A	-5	GLU	-	expression tag	UNP P31572
A	-4	THR	-	expression tag	UNP P31572
A	-3	LEU	-	expression tag	UNP P31572
A	-2	TYR	-	expression tag	UNP P31572
A	-1	ILE	-	expression tag	UNP P31572
A	0	GLN	-	expression tag	UNP P31572
A	1	GLY	-	expression tag	UNP P31572

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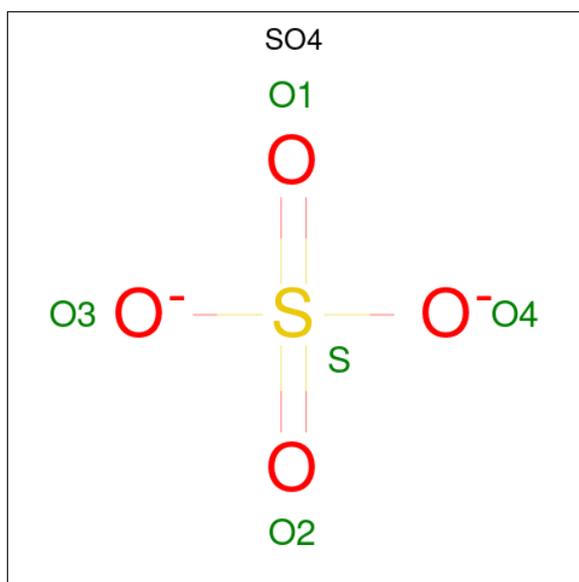
Chain	Residue	Modelled	Actual	Comment	Reference
A	6	MSE	MET	modified residue	UNP P31572
A	32	MSE	MET	modified residue	UNP P31572
A	86	MSE	MET	modified residue	UNP P31572
A	161	MSE	MET	modified residue	UNP P31572
A	200	MSE	MET	modified residue	UNP P31572
A	204	MSE	MET	modified residue	UNP P31572
A	207	MSE	MET	modified residue	UNP P31572
A	212	MSE	MET	modified residue	UNP P31572
A	213	MSE	MET	modified residue	UNP P31572
A	221	MSE	MET	modified residue	UNP P31572
A	225	MSE	MET	modified residue	UNP P31572
A	248	MSE	MET	modified residue	UNP P31572
A	346	MSE	MET	modified residue	UNP P31572
A	357	MSE	MET	modified residue	UNP P31572
A	371	MSE	MET	modified residue	UNP P31572
A	376	MSE	MET	modified residue	UNP P31572
A	406	SER	-	expression tag	UNP P31572
A	407	THR	-	expression tag	UNP P31572
A	408	HIS	-	expression tag	UNP P31572
A	409	HIS	-	expression tag	UNP P31572
A	410	HIS	-	expression tag	UNP P31572
A	411	HIS	-	expression tag	UNP P31572
A	412	HIS	-	expression tag	UNP P31572
A	413	HIS	-	expression tag	UNP P31572
B	-23	MSE	-	expression tag	UNP P31572
B	-22	HIS	-	expression tag	UNP P31572
B	-21	HIS	-	expression tag	UNP P31572
B	-20	HIS	-	expression tag	UNP P31572
B	-19	HIS	-	expression tag	UNP P31572
B	-18	HIS	-	expression tag	UNP P31572
B	-17	HIS	-	expression tag	UNP P31572
B	-16	GLY	-	expression tag	UNP P31572
B	-15	SER	-	expression tag	UNP P31572
B	-14	THR	-	expression tag	UNP P31572
B	-13	SER	-	expression tag	UNP P31572
B	-12	LEU	-	expression tag	UNP P31572
B	-11	TYR	-	expression tag	UNP P31572
B	-10	LYS	-	expression tag	UNP P31572
B	-9	LYS	-	expression tag	UNP P31572
B	-8	ALA	-	expression tag	UNP P31572
B	-7	GLY	-	expression tag	UNP P31572
B	-6	SER	-	expression tag	UNP P31572

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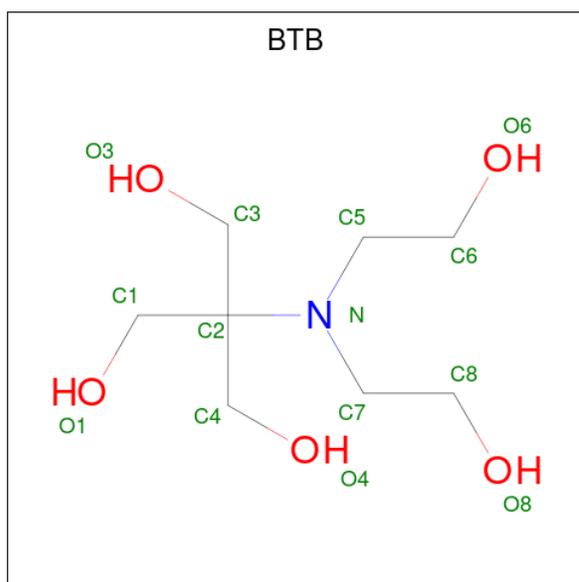
Chain	Residue	Modelled	Actual	Comment	Reference
B	-5	GLU	-	expression tag	UNP P31572
B	-4	THR	-	expression tag	UNP P31572
B	-3	LEU	-	expression tag	UNP P31572
B	-2	TYR	-	expression tag	UNP P31572
B	-1	ILE	-	expression tag	UNP P31572
B	0	GLN	-	expression tag	UNP P31572
B	1	GLY	-	expression tag	UNP P31572
B	6	MSE	MET	modified residue	UNP P31572
B	32	MSE	MET	modified residue	UNP P31572
B	86	MSE	MET	modified residue	UNP P31572
B	161	MSE	MET	modified residue	UNP P31572
B	200	MSE	MET	modified residue	UNP P31572
B	204	MSE	MET	modified residue	UNP P31572
B	207	MSE	MET	modified residue	UNP P31572
B	212	MSE	MET	modified residue	UNP P31572
B	213	MSE	MET	modified residue	UNP P31572
B	221	MSE	MET	modified residue	UNP P31572
B	225	MSE	MET	modified residue	UNP P31572
B	248	MSE	MET	modified residue	UNP P31572
B	346	MSE	MET	modified residue	UNP P31572
B	357	MSE	MET	modified residue	UNP P31572
B	371	MSE	MET	modified residue	UNP P31572
B	376	MSE	MET	modified residue	UNP P31572
B	406	SER	-	expression tag	UNP P31572
B	407	THR	-	expression tag	UNP P31572
B	408	HIS	-	expression tag	UNP P31572
B	409	HIS	-	expression tag	UNP P31572
B	410	HIS	-	expression tag	UNP P31572
B	411	HIS	-	expression tag	UNP P31572
B	412	HIS	-	expression tag	UNP P31572
B	413	HIS	-	expression tag	UNP P31572

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0

- Molecule 3 is 2-[BIS-(2-HYDROXY-ETHYL)-AMINO]-2-HYDROXYMETHYL-PROPAN E-1,3-DIOL (three-letter code: BTB) (formula: C<sub>8</sub>H<sub>19</sub>NO<sub>5</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 14 8 1 5	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	B	1	14	8	1	5	0	0

- Molecule 4 is water.

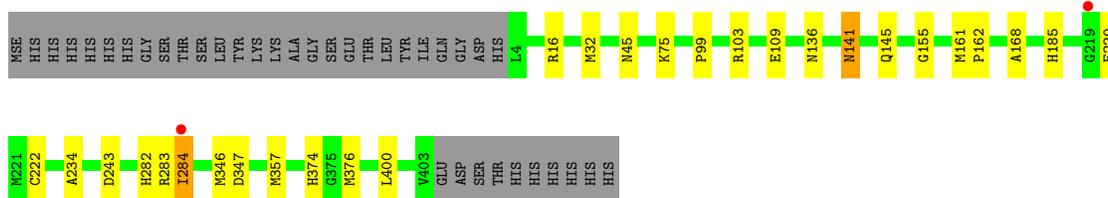
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	313	Total	O	0	0
			313	313		
4	B	327	Total	O	0	0
			327	327		

### 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.

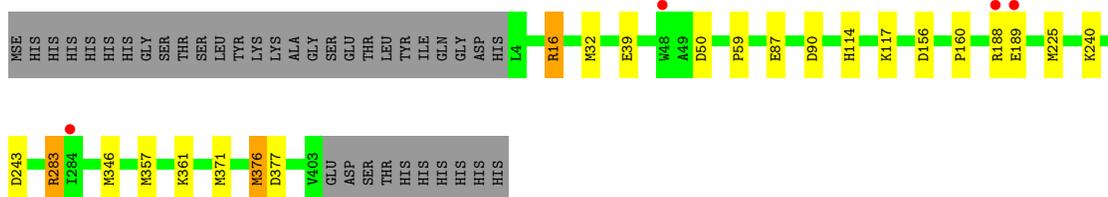
- Molecule 1: Crotonobetainyl-CoA:carnitine CoA-transferase

Chain A: 



- Molecule 1: Crotonobetainyl-CoA:carnitine CoA-transferase

Chain B: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	55.58Å 129.80Å 69.79Å 90.00° 109.48° 90.00°	Depositor
Resolution (Å)	30.00 – 1.85 30.00 – 1.85	Depositor EDS
% Data completeness (in resolution range)	96.7 (30.00-1.85) 96.7 (30.00-1.85)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.25 (at 1.85Å)	Xtrriage
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.143 , 0.178 0.158 , 0.189	Depositor DCC
$R_{free}$ test set	3866 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	17.0	Xtrriage
Anisotropy	0.293	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 41.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	6932	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	20.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.11% 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: BTB, SO4

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	0.78	1/3190 (0.0%)	0.78	2/4301 (0.0%)
1	B	0.76	2/3190 (0.1%)	0.80	6/4301 (0.1%)
All	All	0.77	3/6380 (0.0%)	0.79	8/8602 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	376	MSE	SE-CE	-6.20	1.58	1.95
1	A	222	CYS	CB-SG	-6.06	1.72	1.82
1	B	117	LYS	CD-CE	5.04	1.63	1.51

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	347	ASP	CB-CG-OD2	8.51	125.96	118.30
1	B	243	ASP	CB-CG-OD2	5.56	123.30	118.30
1	B	377	ASP	CB-CG-OD2	5.35	123.11	118.30
1	B	90	ASP	CB-CG-OD2	5.31	123.08	118.30
1	A	243	ASP	CB-CG-OD2	5.23	123.01	118.30

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	3127	0	3077	28	0
1	B	3127	0	3077	15	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
3	A	14	0	19	3	0
3	B	14	0	19	3	0
4	A	313	0	0	15	0
4	B	327	0	0	8	0
All	All	6932	0	6192	48	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 4.

The worst 5 of 48 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:32:MSE:HG2	4:A:1892:HOH:O	1.24	1.26
1:B:32:MSE:HG2	4:B:1875:HOH:O	1.17	1.25
1:A:16:ARG:HG3	4:A:1688:HOH:O	1.52	1.10
1:B:361:LYS:HE2	4:B:1890:HOH:O	1.71	0.90
3:B:1602:BTB:H62	3:B:1602:BTB:H81	1.63	0.81

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	398/437 (91%)	390 (98%)	8 (2%)	0	100	100
1	B	398/437 (91%)	392 (98%)	6 (2%)	0	100	100
All	All	796/874 (91%)	782 (98%)	14 (2%)	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	327/343 (95%)	323 (99%)	4 (1%)	67	59
1	B	327/343 (95%)	321 (98%)	6 (2%)	54	41
All	All	654/686 (95%)	644 (98%)	10 (2%)	60	50

5 of 10 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	240	LYS
1	B	283	ARG
1	B	357	MSE
1	A	357	MSE
1	B	160	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	390	ASN
1	B	153	GLN
1	A	267	HIS
1	A	279	GLN
1	A	282	HIS

### 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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

4 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
3	BTB	A	1601	-	13,13,13	0.93	1 (7%)	7,16,16	0.65	0
2	SO4	A	1501	-	4,4,4	0.61	0	6,6,6	0.50	0
2	SO4	B	1502	-	4,4,4	0.29	0	6,6,6	0.32	0
3	BTB	B	1602	-	13,13,13	0.64	0	7,16,16	1.01	1 (14%)

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
3	BTB	A	1601	-	-	3/21/21/21	-
3	BTB	B	1602	-	-	1/21/21/21	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1601	BTB	C4-C2	-2.34	1.50	1.53

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1602	BTB	O3-C3-C2	-2.38	105.80	111.40

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1601	BTB	N-C2-C3-O3
3	A	1601	BTB	C1-C2-C3-O3
3	A	1601	BTB	C3-C2-C4-O4
3	B	1602	BTB	C3-C2-C4-O4

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1601	BTB	3	0
3	B	1602	BTB	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 [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	384/437 (87%)	-0.41	2 (0%) 87 89	9, 17, 33, 43	0
1	B	384/437 (87%)	-0.35	4 (1%) 79 82	8, 18, 32, 45	0
All	All	768/874 (87%)	-0.38	6 (0%) 82 85	8, 18, 33, 45	0

The worst 5 of 6 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	284	ILE	4.9
1	A	219	GLY	2.5
1	B	48	TRP	2.3
1	B	284	ILE	2.2
1	B	189	GLU	2.1

### 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	SO4	B	1502	5/5	0.74	0.15	73,74,75,75	0
3	BTB	B	1602	14/14	0.90	0.10	23,27,30,34	0
3	BTB	A	1601	14/14	0.95	0.07	16,20,22,26	0
2	SO4	A	1501	5/5	0.98	0.13	21,25,27,28	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.