



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 31, 2017 – 12:15 AM EDT

PDB ID : 3MFD  
Title : The Structure of the Beta-lactamase superfamily domain of D-alanyl-D-alanine carboxypeptidase from *Bacillus subtilis*  
Authors : Cuff, M.E.; Rakowski, E.; Buck, K.; Joachimiak, A.; Midwest Center for Structural Genomics (MCSG)  
Deposited on : unknown  
Resolution : 1.75 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

<http://wwpdb.org/validation/2016/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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030345  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030345

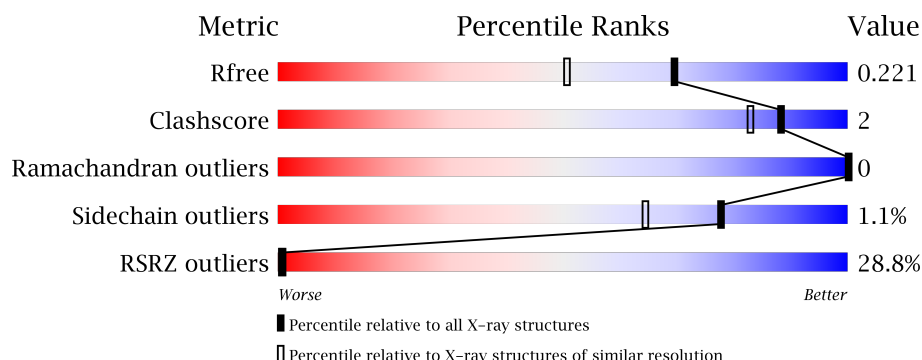
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.75 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))
$R_{free}$	100719	1762 (1.76-1.76)
Clashscore	112137	1889 (1.76-1.76)
Ramachandran outliers	110173	1868 (1.76-1.76)
Sidechain outliers	110143	1868 (1.76-1.76)
RSRZ outliers	101464	1770 (1.76-1.76)

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. 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	334	<div> <div>25%</div> <div>94%</div> </div>
1	B	334	<div> <div>27%</div> <div>84%</div> <div>7%</div> <div>8%</div> </div>

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	CIT	A	364	-	-	-	X
3	EDO	A	359	-	-	-	X
3	EDO	A	360	-	-	-	X
3	EDO	A	363	-	-	-	X

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6071 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.

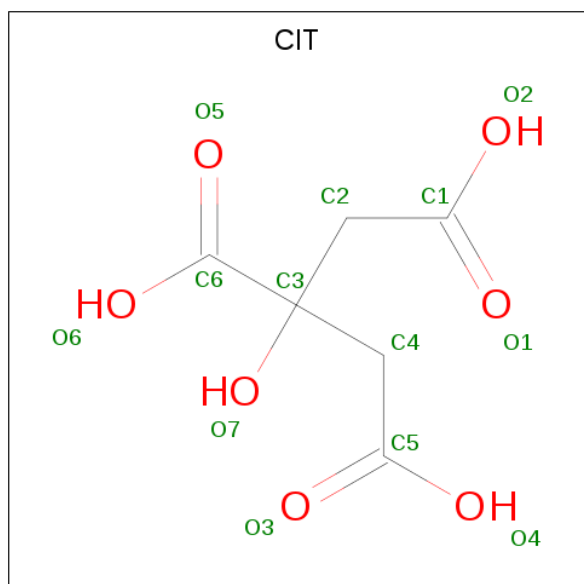
- Molecule 1 is a protein called D-alanyl-D-alanine carboxypeptidase dacB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	326	Total	C	N	O	Se	0	18	0
			2696	1718	450	514	14			
1	B	306	Total	C	N	O	Se	0	16	0
			2518	1599	421	484	14			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	25	SER	-	EXPRESSION TAG	UNP P35150
A	26	ASN	-	EXPRESSION TAG	UNP P35150
B	25	SER	-	EXPRESSION TAG	UNP P35150
B	26	ASN	-	EXPRESSION TAG	UNP P35150

- Molecule 2 is CITRIC ACID (three-letter code: CIT) (formula:  $C_6H_8O_7$ ).



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

- Molecule 3 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
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		

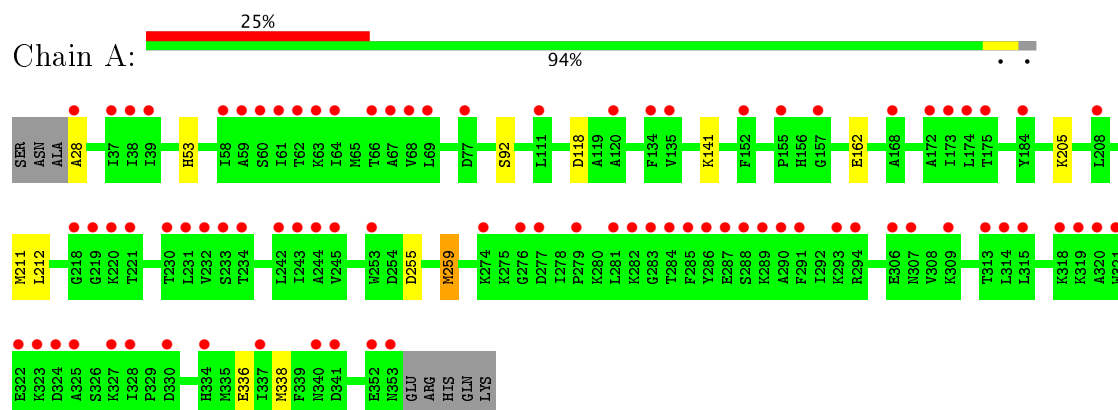
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	434	Total 434	O 434	0	0
4	B	339	Total 339	O 339	0	0

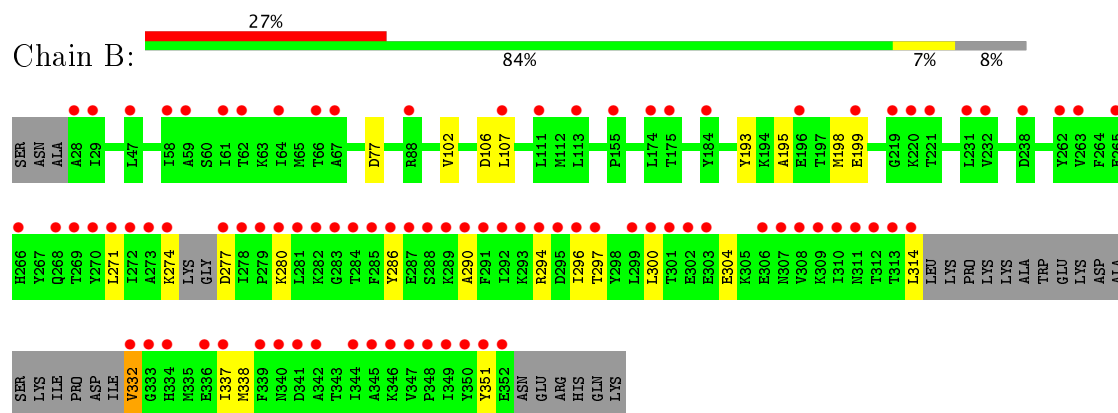
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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: D-alanyl-D-alanine carboxypeptidase dacB



- Molecule 1: D-alanyl-D-alanine carboxypeptidase dacB



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	100.44Å 100.44Å 171.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.78 – 1.75 34.78 – 1.75	Depositor EDS
% Data completeness (in resolution range)	98.5 (34.78-1.75) 98.5 (34.78-1.75)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.89 (at 1.75Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.165 , 0.190 0.202 , 0.221	Depositor DCC
$R_{free}$ test set	4385 reflections (5.00%)	DCC
Wilson B-factor (Å <sup>2</sup> )	23.3	Xtriage
Anisotropy	0.473	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 44.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	6071	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.54% 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, 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	0.68	0/2761	0.73	2/3691 (0.1%)
1	B	0.63	0/2560	0.67	1/3422 (0.0%)
All	All	0.66	0/5321	0.70	3/7113 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	259	MSE	CG-SE-CE	-11.53	73.54	98.90
1	B	106	ASP	CB-CG-OD1	5.74	123.47	118.30
1	A	118	ASP	CB-CG-OD1	5.52	123.27	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	2696	0	2745	11	0
1	B	2518	0	2521	12	0
2	A	39	0	15	3	0
2	B	13	0	5	1	0
3	A	16	0	24	1	0
3	B	16	0	24	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	434	0	0	2	2
4	B	339	0	0	0	2
All	All	6071	0	5334	24	2

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 (24) 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:162[B]:GLU:HA	1:A:162[B]:GLU:OE1	1.80	0.81
1:B:199[A]:GLU:O	1:B:199[A]:GLU:HG3	1.84	0.77
1:A:205:LYS:HD3	2:A:1:CIT:O6	1.89	0.71
1:A:28:ALA:N	4:A:759:HOH:O	2.27	0.67
1:B:314:LEU:HD23	1:B:332:VAL:CG1	2.26	0.65
1:A:92:SER:OG	2:A:1:CIT:O7	2.13	0.65
1:B:271:LEU:HA	1:B:297:THR:HG22	1.86	0.57
1:B:102[A]:VAL:HG11	1:B:107:LEU:HD21	1.88	0.55
1:B:286:TYR:HB3	1:B:290:ALA:HB2	1.90	0.54
2:B:1:CIT:O4	2:B:1:CIT:C6	2.56	0.53
1:B:271:LEU:HD21	1:B:274:LYS:HG2	1.90	0.53
1:A:162[B]:GLU:CA	1:A:162[B]:GLU:OE1	2.50	0.51
1:A:255:ASP:O	1:A:259:MSE:HG3	2.10	0.51
1:A:53:HIS:CG	3:A:361:EDO:H21	2.45	0.50
1:A:205:LYS:CD	2:A:1:CIT:O6	2.61	0.49
1:B:193:TYR:CE2	1:B:195:ALA:HA	2.49	0.48
1:A:336:GLU:HG2	1:A:338:MSE:SE	2.64	0.47
1:B:300:LEU:HD22	1:B:304:GLU:HB3	1.96	0.47
1:B:296:ILE:HG21	1:B:337:ILE:HD12	1.97	0.46
1:B:314:LEU:HD23	1:B:332:VAL:HG11	1.96	0.45
1:A:141:LYS:NZ	4:A:728:HOH:O	2.50	0.44
1:A:211:MSE:HG3	1:A:212:LEU:HG	2.00	0.44
1:B:195:ALA:HB3	1:B:198:MSE:O	2.20	0.41
1:B:332:VAL:HG23	1:B:351:TYR:HB2	2.01	0.41

All (2) 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)
4:A:727:HOH:O	4:B:646:HOH:O[8_565]	2.06	0.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:534:HOH:O	4:B:410:HOH:O[8_565]	2.12	0.08

## 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	342/334 (102%)	334 (98%)	8 (2%)	0	100	100
1	B	316/334 (95%)	306 (97%)	10 (3%)	0	100	100
All	All	658/668 (98%)	640 (97%)	18 (3%)	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	293/270 (108%)	293 (100%)	0	100	100
1	B	269/270 (100%)	261 (97%)	8 (3%)	46	21
All	All	562/540 (104%)	554 (99%)	8 (1%)	78	56

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	77[A]	ASP
1	B	77[B]	ASP

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Mol	Chain	Res	Type
1	B	277	ASP
1	B	280	LYS
1	B	294[A]	ARG
1	B	294[B]	ARG
1	B	332	VAL
1	B	338	MSE

Some 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

12 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	CIT	A	1	-	3,12,12	0.72	0	3,17,17	1.19	0
3	EDO	A	359	-	3,3,3	0.58	0	2,2,2	0.32	0
3	EDO	A	360	-	3,3,3	0.41	0	2,2,2	0.51	0
3	EDO	A	361	-	3,3,3	0.45	0	2,2,2	0.38	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	CIT	A	362	-	3,12,12	1.25	1 (33%)	3,17,17	1.87	1 (33%)
3	EDO	A	363	-	3,3,3	0.46	0	2,2,2	0.22	0
2	CIT	A	364	-	3,12,12	0.98	0	3,17,17	1.43	1 (33%)
2	CIT	B	1	-	3,12,12	1.46	1 (33%)	3,17,17	2.56	1 (33%)
3	EDO	B	359	-	3,3,3	0.38	0	2,2,2	0.37	0
3	EDO	B	360	-	3,3,3	0.49	0	2,2,2	0.38	0
3	EDO	B	361	-	3,3,3	0.52	0	2,2,2	0.36	0
3	EDO	B	362	-	3,3,3	0.51	0	2,2,2	0.11	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	CIT	A	1	-	-	0/6/16/16	0/0/0/0
3	EDO	A	359	-	-	0/1/1/1	0/0/0/0
3	EDO	A	360	-	-	0/1/1/1	0/0/0/0
3	EDO	A	361	-	-	0/1/1/1	0/0/0/0
2	CIT	A	362	-	-	0/6/16/16	0/0/0/0
3	EDO	A	363	-	-	0/1/1/1	0/0/0/0
2	CIT	A	364	-	-	0/6/16/16	0/0/0/0
2	CIT	B	1	-	-	0/6/16/16	0/0/0/0
3	EDO	B	359	-	-	0/1/1/1	0/0/0/0
3	EDO	B	360	-	-	0/1/1/1	0/0/0/0
3	EDO	B	361	-	-	0/1/1/1	0/0/0/0
3	EDO	B	362	-	-	0/1/1/1	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	CIT	C2-C3	-2.39	1.51	1.54
2	A	362	CIT	O7-C3	2.15	1.46	1.43

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	CIT	C3-C4-C5	-4.16	108.45	114.95
2	A	362	CIT	C3-C4-C5	-3.10	110.11	114.95
2	A	364	CIT	C3-C2-C1	-2.15	111.59	114.95

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1	CIT	3	0
3	A	361	EDO	1	0
2	B	1	CIT	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.







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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 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	312/334 (93%)	1.46	84 (26%)  	9, 15, 39, 65	0
1	B	292/334 (87%)	1.75	90 (30%)  	10, 15, 73, 93	0
All	All	604/668 (90%)	1.60	174 (28%)  	9, 15, 43, 93	0

All (174) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	351	TYR	16.2
1	B	291	PHE	12.3
1	B	285	PHE	10.6
1	B	350	TYR	9.8
1	B	314	LEU	9.8
1	B	286	TYR	9.1
1	B	290	ALA	9.1
1	B	292	ILE	9.1
1	B	271	LEU	8.6
1	A	321	TRP	8.3
1	B	313	THR	8.1
1	B	294[A]	ARG	7.7
1	B	277	ASP	7.5
1	B	278	ILE	7.3
1	A	285	PHE	7.3
1	B	348	PRO	7.2
1	B	349	ILE	7.2
1	A	325	ALA	7.0
1	B	28	ALA	6.9
1	B	283	GLY	6.7
1	B	296	ILE	6.5
1	B	281	LEU	6.5
1	A	61	ILE	6.3
1	B	312	THR	6.2

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Mol	Chain	Res	Type	RSRZ
1	B	288	SER	6.1
1	A	28	ALA	6.1
1	B	273	ALA	6.1
1	A	322	GLU	5.9
1	B	332	VAL	5.7
1	A	64	ILE	5.6
1	B	64	ILE	5.5
1	A	232	VAL	5.2
1	B	352	GLU	5.2
1	A	324	ASP	5.2
1	B	333	GLY	5.0
1	A	231	LEU	5.0
1	B	282	LYS	5.0
1	A	319	LYS	4.9
1	A	283	GLY	4.8
1	B	340	ASN	4.8
1	A	290	ALA	4.8
1	A	328	ILE	4.7
1	A	315	LEU	4.7
1	A	289	LYS	4.7
1	A	174	LEU	4.7
1	B	339	PHE	4.6
1	B	308	VAL	4.6
1	A	288	SER	4.5
1	A	353	ASN	4.5
1	B	284	THR	4.4
1	B	270	TYR	4.4
1	B	347	VAL	4.4
1	B	279	PRO	4.3
1	A	320	ALA	4.3
1	B	311	ASN	4.2
1	B	61	ILE	4.2
1	B	289	LYS	4.2
1	A	282	LYS	4.2
1	A	219	GLY	4.1
1	B	303	GLU	3.9
1	B	272	ILE	3.9
1	B	336	GLU	3.9
1	B	232	VAL	3.9
1	A	341	ASP	3.8
1	B	287	GLU	3.8
1	B	341	ASP	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	297	THR	3.7
1	B	344	ILE	3.7
1	A	340	ASN	3.6
1	B	88[A]	ARG	3.6
1	A	245	VAL	3.6
1	B	342	ALA	3.6
1	A	111	LEU	3.6
1	A	175	THR	3.5
1	A	59	ALA	3.5
1	A	62	THR	3.5
1	B	231	LEU	3.5
1	B	345	ALA	3.5
1	B	274	LYS	3.5
1	A	243	ILE	3.4
1	B	269	THR	3.4
1	A	352	GLU	3.4
1	B	265[A]	GLU	3.4
1	A	291	PHE	3.4
1	A	286	TYR	3.4
1	B	262	TYR	3.4
1	B	310	ILE	3.4
1	A	327	LYS	3.4
1	A	314	LEU	3.3
1	B	295	ASP	3.3
1	B	196[A]	GLU	3.3
1	A	281	LEU	3.2
1	B	111	LEU	3.2
1	A	244	ALA	3.2
1	A	39	ILE	3.2
1	A	172	ALA	3.2
1	B	302	GLU	3.2
1	B	266	HIS	3.2
1	A	279	PRO	3.2
1	A	306[A]	GLU	3.2
1	A	337	ILE	3.2
1	A	323	LYS	3.1
1	A	58	ILE	3.1
1	A	284	THR	3.1
1	A	318	LYS	3.1
1	B	300	LEU	3.1
1	A	184	TYR	3.1
1	B	299	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	280	LYS	3.0
1	A	173	ILE	3.0
1	A	233	SER	3.0
1	A	287	GLU	2.9
1	B	199[A]	GLU	2.9
1	B	306	GLU	2.9
1	B	62	THR	2.9
1	A	60	SER	2.9
1	A	67	ALA	2.9
1	B	66	THR	2.9
1	A	66	THR	2.9
1	B	219	GLY	2.8
1	A	313	THR	2.8
1	B	238	ASP	2.8
1	A	221	THR	2.7
1	B	47	LEU	2.7
1	B	174	LEU	2.7
1	A	234	THR	2.7
1	B	309	LYS	2.7
1	A	277	ASP	2.7
1	B	221	THR	2.7
1	A	68	VAL	2.6
1	A	220	LYS	2.6
1	A	253	TRP	2.6
1	B	346	LYS	2.5
1	B	301	THR	2.5
1	B	268	GLN	2.5
1	A	63	LYS	2.5
1	B	67	ALA	2.5
1	A	155	PRO	2.5
1	B	29	ILE	2.5
1	A	274	LYS	2.5
1	A	294	ARG	2.5
1	A	334[A]	HIS	2.5
1	B	337	ILE	2.5
1	A	307	ASN	2.5
1	A	230	THR	2.4
1	B	155	PRO	2.4
1	A	330[A]	ASP	2.4
1	A	152	PHE	2.4
1	B	175	THR	2.4
1	A	37	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	293	LYS	2.3
1	A	120	ALA	2.3
1	A	38	ILE	2.3
1	B	58	ILE	2.3
1	A	157	GLY	2.3
1	A	69	LEU	2.3
1	A	208	LEU	2.3
1	A	218	GLY	2.3
1	A	242	LEU	2.3
1	A	276	GLY	2.3
1	B	263	VAL	2.2
1	B	113	LEU	2.2
1	B	307	ASN	2.2
1	B	184	TYR	2.2
1	B	220	LYS	2.2
1	A	134	PHE	2.2
1	A	293	LYS	2.2
1	B	107	LEU	2.1
1	A	135	VAL	2.1
1	A	77[A]	ASP	2.1
1	A	309	LYS	2.0
1	A	168	ALA	2.0
1	B	59	ALA	2.0
1	B	334	HIS	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 carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	EDO	A	360	4/4	0.87	0.25	6.89	44,47,49,50	0
2	CIT	A	364	13/13	0.74	0.28	5.08	67,70,72,74	0
3	EDO	A	359	4/4	0.64	0.26	3.40	54,56,56,56	0
3	EDO	A	363	4/4	0.78	0.19	2.46	50,50,51,51	0
2	CIT	A	1	13/13	0.83	0.31	1.84	17,37,44,45	13
2	CIT	B	1	13/13	0.86	0.18	0.25	25,30,37,37	0
3	EDO	A	361	4/4	0.71	0.38	-	76,76,77,77	0
3	EDO	B	361	4/4	0.80	0.17	-	46,48,48,49	0
2	CIT	A	362	13/13	0.43	0.34	-	77,79,81,82	0
3	EDO	B	360	4/4	0.43	0.28	-	81,82,82,82	0
3	EDO	B	362	4/4	0.70	0.39	-	77,78,78,78	0
3	EDO	B	359	4/4	0.79	0.36	-	68,68,68,69	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.