



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 09:29 am GMT

PDB ID : 2CBV  
Title : BETA-GLUCOSIDASE FROM THERMOTOGA MARITIMA IN COMPLEX WITH CALYSTEGINE B2  
Authors : Gloster, T.M.; Madsen, R.; Davies, G.J.  
Deposited on : 2006-01-09  
Resolution : 1.95 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	:	trunk28620
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)	:	recalc28949

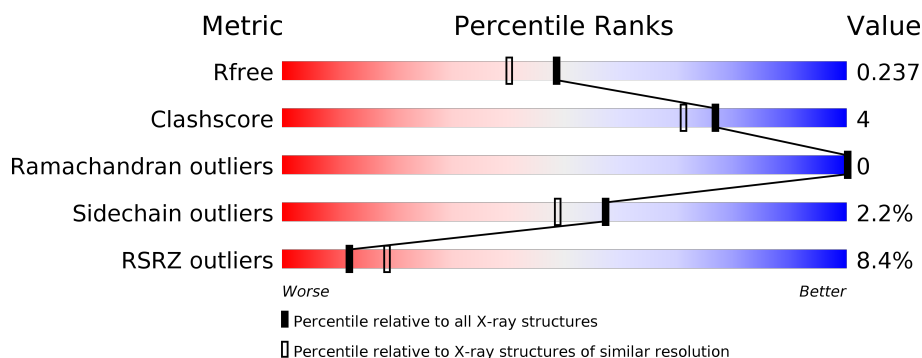
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.95 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	2004 (1.96-1.96)
Clashscore	112137	2136 (1.96-1.96)
Ramachandran outliers	110173	2117 (1.96-1.96)
Sidechain outliers	110143	2117 (1.96-1.96)
RSRZ outliers	101464	2018 (1.96-1.96)

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	468	<div> <div>6%</div> <div>87%</div> <div>7% • 5%</div> </div>
1	B	468	<div> <div>10%</div> <div>87%</div> <div>6% • 6%</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
3	ACT	A	1448	-	-	-	X

## 2 Entry composition [i](#)

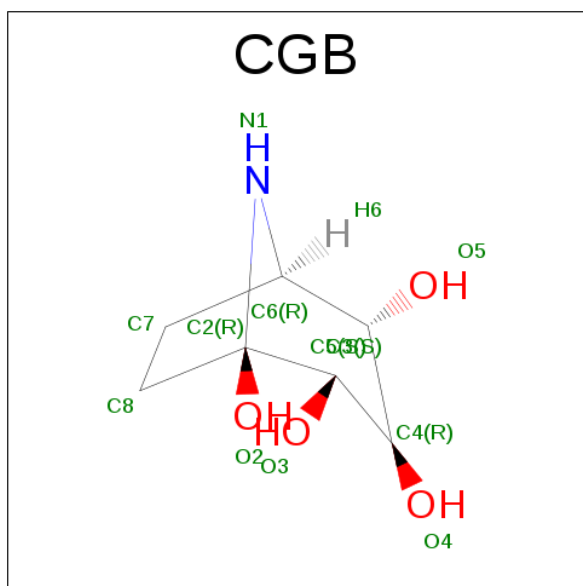
There are 4 unique types of molecules in this entry. The entry contains 8168 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 BETA-GLUCOSIDASE A.

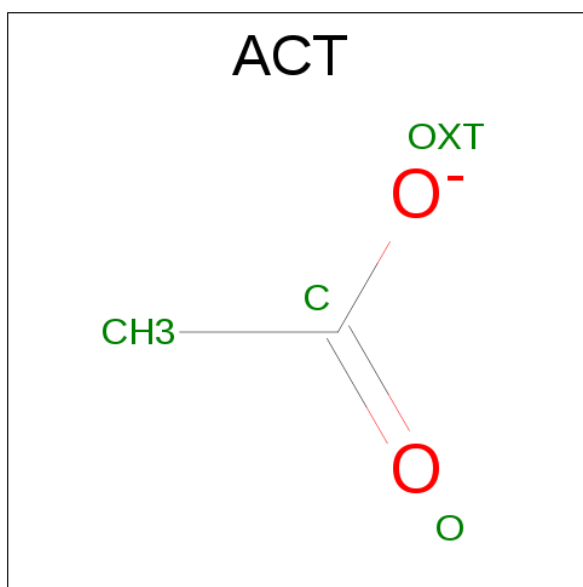
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	443	Total	C	N	O	S	0	20	0
			3759	2450	626	676	7			
1	B	442	Total	C	N	O	S	0	16	0
			3688	2402	617	662	7			

- Molecule 2 is CALYSTEGINE B2 (three-letter code: CGB) (formula:  $C_7H_{13}NO_4$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			12	7	1	4		
2	B	1	Total	C	N	O	0	0
			12	7	1	4		

- Molecule 3 is ACETATE ION (three-letter code: ACT) (formula:  $C_2H_3O_2$ ).



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

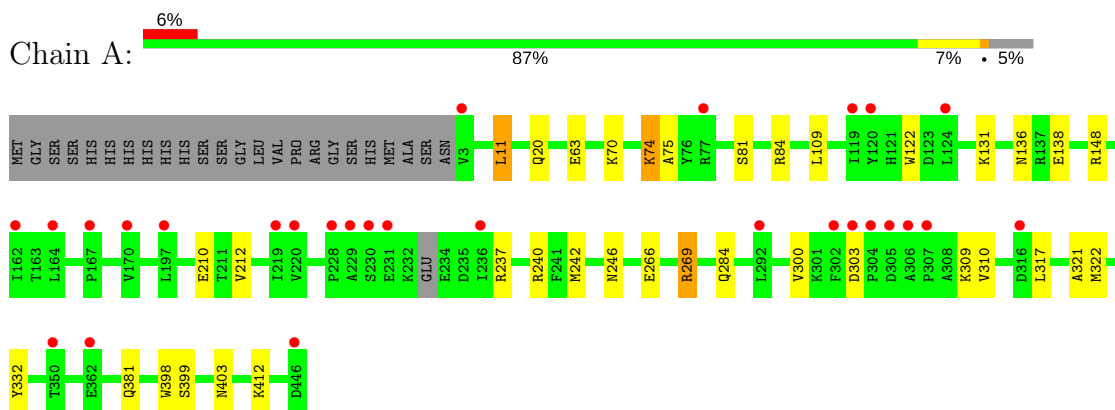
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	419	Total	O	0	57
			419	419		
4	B	270	Total	O	0	37
			270	270		

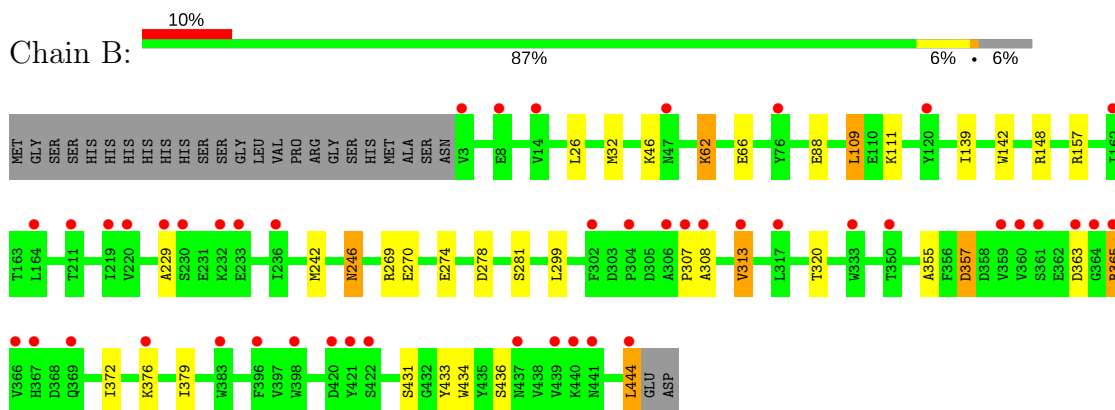
### 3 Residue-property plots [i](#)

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: BETA-GLUCOSIDASE A



#### • Molecule 1: BETA-GLUCOSIDASE A



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	94.26Å 94.31Å 113.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	72.55 – 1.95 39.53 – 1.95	Depositor EDS
% Data completeness (in resolution range)	99.1 (72.55-1.95) 99.1 (39.53-1.95)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.15 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.183 , 0.238 0.182 , 0.237	Depositor DCC
$R_{free}$ test set	3701 reflections (5.31%)	DCC
Wilson B-factor (Å <sup>2</sup> )	28.7	Xtriage
Anisotropy	0.005	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 60.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.012 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	8168	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.30% 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: CGB, ACT

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	0.71	0/3940	0.69	0/5341
1	B	0.66	0/3846	0.64	1/5222 (0.0%)
All	All	0.69	0/7786	0.67	1/10563 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	444	LEU	CA-CB-CG	5.13	127.10	115.30

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	3759	0	3679	23	0
1	B	3688	0	3560	28	0
2	A	12	0	13	1	0
2	B	12	0	13	0	0
3	A	4	0	3	1	0
3	B	4	0	3	1	0
4	A	419	0	0	9	0
4	B	270	0	0	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	8168	0	7271	52	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (52) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63[A]:GLU:HG3	4:A:2098:HOH:O	1.30	1.24
1:B:365:ARG:HG2	1:B:365:ARG:HH11	1.17	1.06
1:A:212:VAL:HG11	4:A:2215:HOH:O	1.69	0.91
1:A:266[A]:GLU:OE2	4:A:2280:HOH:O	1.93	0.86
1:B:148[A]:ARG:NH1	4:B:2116[A]:HOH:O	2.11	0.83
1:A:70[A]:LYS:HD2	4:A:2111:HOH:O	1.86	0.76
1:B:372:ILE:CD1	1:B:431:SER:HA	2.18	0.72
1:B:357[A]:ASP:OD2	4:B:2247:HOH:O	2.10	0.69
3:A:1448:ACT:H3	4:A:2013:HOH:O	1.95	0.67
1:B:270[A]:GLU:HG2	4:B:2189:HOH:O	1.94	0.67
1:A:74[A]:LYS:HE3	4:B:2200[A]:HOH:O	1.94	0.66
1:B:278:ASP:O	3:B:1446:ACT:C	2.45	0.65
1:B:365:ARG:HH11	1:B:365:ARG:CG	2.00	0.64
1:B:365:ARG:HG2	1:B:365:ARG:NH1	1.96	0.63
1:B:376:LYS:HB3	1:B:434:TRP:CZ2	2.35	0.62
1:B:372:ILE:HD11	1:B:431:SER:HA	1.80	0.61
1:A:136:ASN:OD1	1:A:138[B]:GLU:HG3	2.01	0.60
1:A:148[B]:ARG:NH2	1:A:210:GLU:OE2	2.34	0.60
1:A:70[A]:LYS:HG3	4:A:2106:HOH:O	2.02	0.59
1:B:372:ILE:HD13	1:B:431:SER:HA	1.84	0.58
1:A:237:ARG:HH22	1:A:240[A]:ARG:HH22	1.51	0.57
1:B:299:LEU:HD23	1:B:313:VAL:HG22	1.87	0.55
1:B:26:LEU:HD21	1:B:32:MET:HG2	1.90	0.54
1:A:242:MET:O	1:A:246[B]:ASN:HB2	2.09	0.53
1:A:269[B]:ARG:HG3	4:A:2133:HOH:O	2.09	0.52
1:B:365:ARG:NH1	1:B:365:ARG:CG	2.65	0.51
1:B:274[A]:GLU:HB3	4:B:2192:HOH:O	2.09	0.51
1:A:300:VAL:HG13	1:A:310:VAL:HG13	1.93	0.50
1:B:66:GLU:HG2	1:B:111:LYS:NZ	2.27	0.49
1:B:307:PRO:O	1:B:308:ALA:HB3	2.14	0.48
1:A:20:GLN:O	1:A:403:ASN:HB2	2.14	0.48
1:A:11:LEU:HG	1:A:75:ALA:HB2	1.98	0.46
1:B:62:LYS:HB2	4:B:2053:HOH:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:242:MET:O	1:B:246[B]:ASN:HB2	2.17	0.45
1:B:320:THR:HB	1:B:355:ALA:O	2.17	0.45
1:A:131[B]:LYS:NZ	4:A:2183:HOH:O	2.43	0.44
1:A:303:ASP:O	1:A:309:LYS:HA	2.17	0.44
1:B:229:ALA:HA	1:B:299:LEU:HD11	2.00	0.44
1:A:321:ALA:O	1:A:412:LYS:HE3	2.19	0.43
1:A:122:TRP:CH2	2:A:1447:CGB:H8C2	2.53	0.43
1:A:322:MET:SD	1:A:412:LYS:HG3	2.59	0.43
1:B:109:LEU:HD21	1:B:157:ARG:HB3	2.01	0.42
1:B:379:ILE:HG22	1:B:444:LEU:HD21	2.03	0.41
1:B:433:TYR:O	1:B:436:SER:HB3	2.21	0.41
1:B:139:ILE:HA	1:B:142:TRP:CE3	2.55	0.41
1:A:398:TRP:HA	1:A:399:SER:HA	1.85	0.40
1:A:81:SER:HB3	1:A:84:ARG:HG3	2.02	0.40
1:B:376:LYS:HB3	1:B:434:TRP:HZ2	1.82	0.40
1:A:284:GLN:NE2	4:A:2295:HOH:O	2.51	0.40
1:A:332:TYR:HB3	1:A:381:GLN:HE21	1.86	0.40
1:B:270[B]:GLU:OE1	4:B:2184[B]:HOH:O	2.21	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	462/468 (99%)	452 (98%)	10 (2%)	0	100	100
1	B	457/468 (98%)	447 (98%)	10 (2%)	0	100	100
All	All	919/936 (98%)	899 (98%)	20 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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	398/399 (100%)	391 (98%)	7 (2%)	64	57
1	B	383/399 (96%)	368 (96%)	15 (4%)	37	22
All	All	781/798 (98%)	759 (97%)	22 (3%)	57	37

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	LEU
1	A	74[A]	LYS
1	A	74[B]	LYS
1	A	109	LEU
1	A	269[A]	ARG
1	A	269[B]	ARG
1	A	317	LEU
1	B	46	LYS
1	B	62	LYS
1	B	88	GLU
1	B	109	LEU
1	B	246[A]	ASN
1	B	246[B]	ASN
1	B	269[A]	ARG
1	B	269[B]	ARG
1	B	269[C]	ARG
1	B	281	SER
1	B	313	VAL
1	B	357[A]	ASP
1	B	357[B]	ASP
1	B	363	ASP
1	B	365	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	381	GLN
1	B	441	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

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	$\# Z  > 2$
2	CGB	A	1447	-	10,13,13	1.49	1 (10%)	11,21,21	0.76	0
3	ACT	A	1448	-	1,3,3	0.15	0	0,3,3	0.00	-
2	CGB	B	1445	-	10,13,13	1.25	1 (10%)	11,21,21	0.81	0
3	ACT	B	1446	-	1,3,3	4.48	1 (100%)	0,3,3	0.00	-

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	CGB	A	1447	-	-	0/0/29/29	0/0/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ACT	A	1448	-	-	0/0/0/0	0/0/0/0
2	CGB	B	1445	-	-	0/0/29/29	0/0/2/2
3	ACT	B	1446	-	-	0/0/0/0	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1447	CGB	C6-N1	-4.19	1.44	1.47
2	B	1445	CGB	C6-N1	-3.24	1.44	1.47
3	B	1446	ACT	CH3-C	4.48	1.54	1.48

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1447	CGB	1	0
3	A	1448	ACT	1	0
3	B	1446	ACT	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	443/468 (94%)	0.34	28 (6%)	21 30	15, 25, 47, 57	0
1	B	442/468 (94%)	0.65	46 (10%)	7 11	16, 32, 49, 56	0
All	All	885/936 (94%)	0.49	74 (8%)	12 18	15, 28, 49, 57	0

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	306	ALA	6.0
1	B	361[A]	SER	5.7
1	B	308	ALA	5.6
1	B	359	VAL	5.6
1	B	360	VAL	5.3
1	B	364	GLY	4.8
1	B	307	PRO	4.7
1	A	3	VAL	4.0
1	A	302	PHE	3.9
1	B	306	ALA	3.8
1	B	441	ASN	3.7
1	B	363	ASP	3.7
1	A	231	GLU	3.7
1	B	229	ALA	3.7
1	A	305	ASP	3.7
1	B	302	PHE	3.6
1	A	303	ASP	3.6
1	B	369	GLN	3.6
1	A	197	LEU	3.6
1	B	366	VAL	3.5
1	B	164	LEU	3.4
1	A	307	PRO	3.4
1	B	3	VAL	3.4
1	A	446	ASP	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	220	VAL	3.1
1	B	365	ARG	3.1
1	A	170	VAL	3.1
1	B	162	ILE	3.1
1	B	350	THR	3.0
1	B	233	GLU	2.8
1	B	304	PRO	2.8
1	B	422	SER	2.8
1	B	439	VAL	2.8
1	B	317	LEU	2.8
1	A	219	ILE	2.8
1	B	396	PHE	2.8
1	A	120	TYR	2.8
1	A	236	ILE	2.8
1	A	164	LEU	2.7
1	A	167	PRO	2.7
1	B	383	TRP	2.7
1	A	229	ALA	2.7
1	B	367	HIS	2.7
1	A	230	SER	2.7
1	B	444	LEU	2.7
1	B	437	ASN	2.6
1	A	162	ILE	2.6
1	A	316	ASP	2.5
1	A	228	PRO	2.5
1	B	420	ASP	2.5
1	B	219	ILE	2.5
1	B	220	VAL	2.4
1	B	376	LYS	2.4
1	A	124	LEU	2.4
1	B	76	TYR	2.4
1	B	230	SER	2.3
1	B	421	TYR	2.3
1	A	304	PRO	2.3
1	A	350	THR	2.3
1	A	362	GLU	2.3
1	B	211	THR	2.2
1	B	232	LYS	2.2
1	B	333	TRP	2.2
1	B	398	TRP	2.2
1	A	292	LEU	2.2
1	B	440	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	47	ASN	2.1
1	B	236	ILE	2.1
1	A	119	ILE	2.1
1	A	77	ARG	2.1
1	B	313	VAL	2.1
1	B	8	GLU	2.1
1	B	120	TYR	2.0
1	B	14	VAL	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	ACT	A	1448	4/4	0.90	0.17	3.73	34,35,35,36	0
3	ACT	B	1446	4/4	0.86	0.16	0.77	25,29,29,29	0
2	CGB	B	1445	12/12	0.96	0.17	0.72	25,27,29,29	0
2	CGB	A	1447	12/12	0.93	0.15	0.01	23,28,30,30	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.