



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 13, 2024 – 02:02 AM EDT

PDB ID : 3KKE  
Title : Crystal structure of a LacI family transcriptional regulator from *Mycobacterium smegmatis*  
Authors : Bonanno, J.B.; Rutter, M.; Bain, K.T.; Do, J.; Ozyurt, S.; Wasserman, S.; Sauder, J.M.; Burley, S.K.; Almo, S.C.; New York SGX Research Center for Structural Genomics (NYSGXRC)  
Deposited on : 2009-11-05  
Resolution : 2.20 Å(reported)

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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	:	2.36.2
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)	:	2.36.2

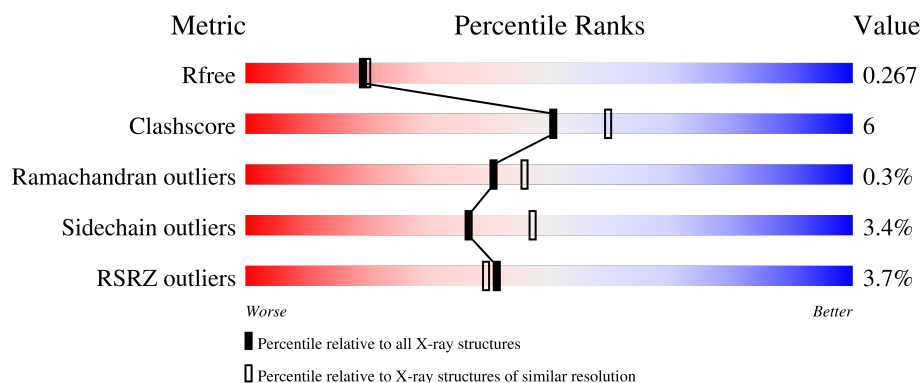
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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	303	<div> <div>79%</div> <div>12%</div> <div>8%</div> </div>
1	B	303	<div> <div>86%</div> <div>10%</div> <div>.</div> </div>
1	C	303	<div> <div>3%</div> <div>84%</div> <div>10%</div> <div>6%</div> </div>
1	D	303	<div> <div>10%</div> <div>74%</div> <div>16%</div> <div>9%</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	ACT	A	350	-	-	X	-
2	ACT	D	1	-	-	X	-

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8251 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 LacI family Transcriptional regulator.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	278	Total	C	N	O	S	0	0	0
			1992	1246	348	394	4			
1	B	291	Total	C	N	O	S	0	0	0
			2096	1307	372	413	4			
1	C	285	Total	C	N	O	S	0	0	0
			2046	1277	360	405	4			
1	D	277	Total	C	N	O	S	0	0	0
			1970	1238	345	383	4			

There are 44 discrepancies between the modelled and reference sequences:

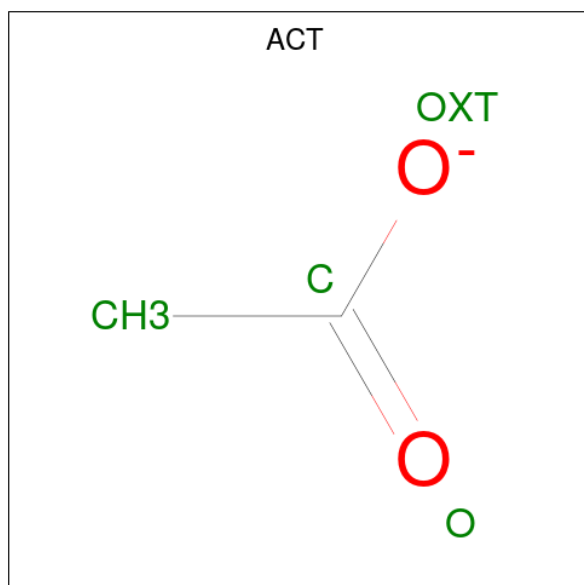
Chain	Residue	Modelled	Actual	Comment	Reference
A	47	MET	-	expression tag	UNP A0QPR6
A	48	SER	-	expression tag	UNP A0QPR6
A	49	LEU	-	expression tag	UNP A0QPR6
A	342	GLU	-	expression tag	UNP A0QPR6
A	343	GLY	-	expression tag	UNP A0QPR6
A	344	HIS	-	expression tag	UNP A0QPR6
A	345	HIS	-	expression tag	UNP A0QPR6
A	346	HIS	-	expression tag	UNP A0QPR6
A	347	HIS	-	expression tag	UNP A0QPR6
A	348	HIS	-	expression tag	UNP A0QPR6
A	349	HIS	-	expression tag	UNP A0QPR6
B	47	MET	-	expression tag	UNP A0QPR6
B	48	SER	-	expression tag	UNP A0QPR6
B	49	LEU	-	expression tag	UNP A0QPR6
B	342	GLU	-	expression tag	UNP A0QPR6
B	343	GLY	-	expression tag	UNP A0QPR6
B	344	HIS	-	expression tag	UNP A0QPR6
B	345	HIS	-	expression tag	UNP A0QPR6
B	346	HIS	-	expression tag	UNP A0QPR6
B	347	HIS	-	expression tag	UNP A0QPR6
B	348	HIS	-	expression tag	UNP A0QPR6

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Chain	Residue	Modelled	Actual	Comment	Reference
B	349	HIS	-	expression tag	UNP A0QPR6
C	47	MET	-	expression tag	UNP A0QPR6
C	48	SER	-	expression tag	UNP A0QPR6
C	49	LEU	-	expression tag	UNP A0QPR6
C	342	GLU	-	expression tag	UNP A0QPR6
C	343	GLY	-	expression tag	UNP A0QPR6
C	344	HIS	-	expression tag	UNP A0QPR6
C	345	HIS	-	expression tag	UNP A0QPR6
C	346	HIS	-	expression tag	UNP A0QPR6
C	347	HIS	-	expression tag	UNP A0QPR6
C	348	HIS	-	expression tag	UNP A0QPR6
C	349	HIS	-	expression tag	UNP A0QPR6
D	47	MET	-	expression tag	UNP A0QPR6
D	48	SER	-	expression tag	UNP A0QPR6
D	49	LEU	-	expression tag	UNP A0QPR6
D	342	GLU	-	expression tag	UNP A0QPR6
D	343	GLY	-	expression tag	UNP A0QPR6
D	344	HIS	-	expression tag	UNP A0QPR6
D	345	HIS	-	expression tag	UNP A0QPR6
D	346	HIS	-	expression tag	UNP A0QPR6
D	347	HIS	-	expression tag	UNP A0QPR6
D	348	HIS	-	expression tag	UNP A0QPR6
D	349	HIS	-	expression tag	UNP A0QPR6

- Molecule 2 is ACETATE ION (three-letter code: ACT) (formula:  $C_2H_3O_2$ ).



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

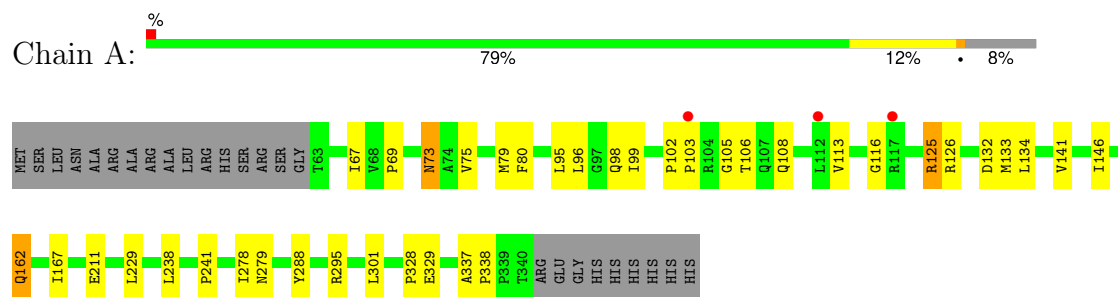
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	44	Total O 44 44	0	0
3	B	60	Total O 60 60	0	0
3	C	19	Total O 19 19	0	0
3	D	4	Total O 4 4	0	0

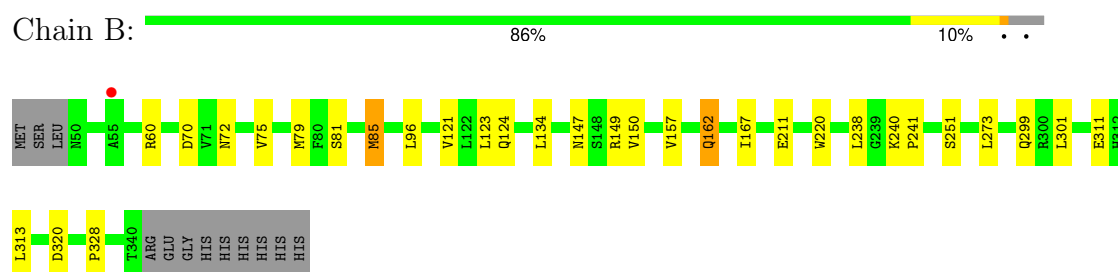
### 3 Residue-property plots [i](#)

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.

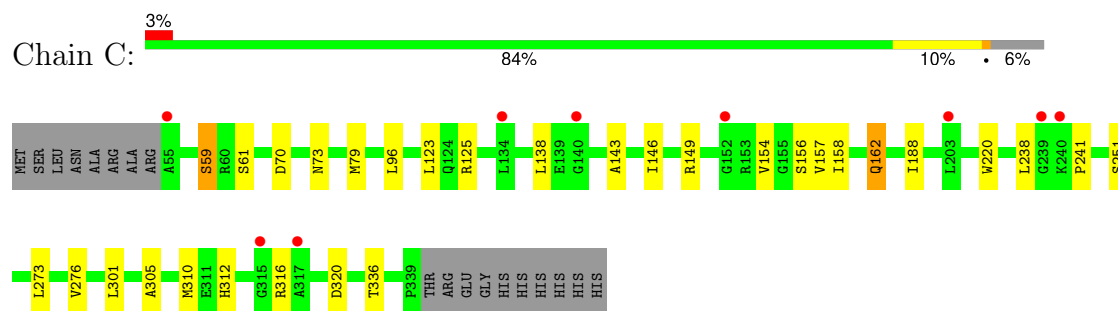
- Molecule 1: LacI family Transcriptional regulator



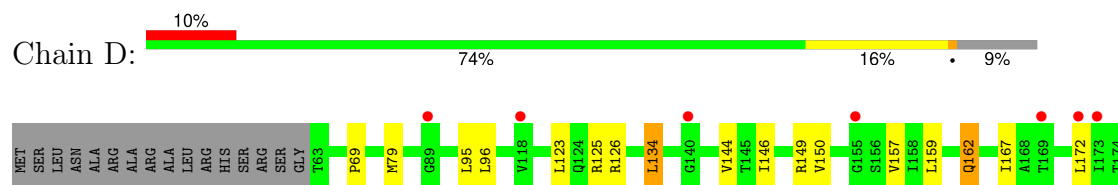
- Molecule 1: LacI family Transcriptional regulator

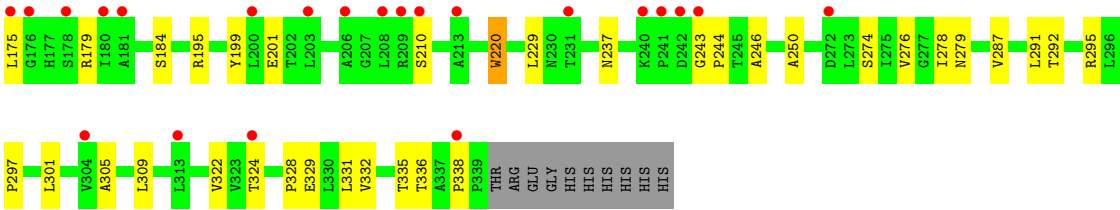


- Molecule 1: LacI family Transcriptional regulator



- Molecule 1: LacI family Transcriptional regulator







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	64.60Å 65.47Å 116.03Å 90.00° 90.72° 90.00°	Depositor
Resolution (Å)	20.00 – 2.20 33.37 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.2 (20.00-2.20) 99.2 (33.37-2.20)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.45 (at 2.20Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.194 , 0.247 0.214 , 0.267	Depositor DCC
$R_{free}$ test set	2460 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	34.7	Xtriage
Anisotropy	0.464	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 44.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.011 for -k,-h,-l 0.009 for k,h,-l 0.032 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	8251	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.65% 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: 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	0.73	0/2022	0.78	0/2772
1	B	0.80	0/2127	0.84	5/2911 (0.2%)
1	C	0.64	0/2077	0.72	0/2844
1	D	0.54	0/2000	0.63	0/2743
All	All	0.69	0/8226	0.75	5/11270 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	149	ARG	NE-CZ-NH1	6.66	123.63	120.30
1	B	79	MET	CG-SD-CE	-5.99	90.62	100.20
1	B	149	ARG	NE-CZ-NH2	-5.90	117.35	120.30
1	B	320	ASP	CB-CG-OD1	5.78	123.50	118.30
1	B	85	MET	CA-CB-CG	5.05	121.88	113.30

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	1992	0	1968	25	0
1	B	2096	0	2089	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2046	0	2021	18	0
1	D	1970	0	1949	35	0
2	A	8	0	6	3	0
2	B	4	0	3	0	0
2	C	4	0	3	0	0
2	D	4	0	3	2	0
3	A	44	0	0	0	0
3	B	60	0	0	0	0
3	C	19	0	0	0	0
3	D	4	0	0	0	0
All	All	8251	0	8042	92	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 6.

The worst 5 of 92 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:D:162:GLN:HE21	1:D:162:GLN:H	1.07	0.98
1:C:162:GLN:H	1:C:162:GLN:HE21	1.18	0.90
1:B:134:LEU:HD23	1:B:150:VAL:HG22	1.52	0.89
2:A:350:ACT:H1	1:D:287:VAL:HB	1.57	0.87
1:B:162:GLN:HE21	1:B:162:GLN:H	1.22	0.87

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	276/303 (91%)	266 (96%)	8 (3%)	2 (1%)	22	22
1	B	289/303 (95%)	283 (98%)	6 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	283/303 (93%)	271 (96%)	11 (4%)	1 (0%)	34	37
1	D	275/303 (91%)	263 (96%)	12 (4%)	0	100	100
All	All	1123/1212 (93%)	1083 (96%)	37 (3%)	3 (0%)	41	46

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	116	GLY
1	A	241	PRO
1	C	241	PRO

### 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	205/237 (86%)	196 (96%)	9 (4%)	28	35
1	B	217/237 (92%)	212 (98%)	5 (2%)	50	63
1	C	211/237 (89%)	207 (98%)	4 (2%)	57	71
1	D	199/237 (84%)	189 (95%)	10 (5%)	24	30
All	All	832/948 (88%)	804 (97%)	28 (3%)	37	47

5 of 28 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	59	SER
1	D	274	SER
1	C	188	ILE
1	D	210	SER
1	C	162	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	162	GLN
1	B	299	GLN
1	D	162	GLN
1	C	162	GLN
1	B	124	GLN

### 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](#)

5 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	ACT	A	1	-	3,3,3	0.76	0	3,3,3	1.58	0
2	ACT	D	1	-	3,3,3	0.83	0	3,3,3	1.17	0
2	ACT	A	350	-	3,3,3	0.51	0	3,3,3	1.49	1 (33%)
2	ACT	C	1	-	3,3,3	0.78	0	3,3,3	1.57	1 (33%)
2	ACT	B	1	-	3,3,3	0.79	0	3,3,3	1.33	0

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	350	ACT	OXT-C-CH3	2.08	123.78	115.05
2	C	1	ACT	OXT-C-CH3	2.01	123.50	115.05

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1	ACT	2	0
2	A	350	ACT	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	278/303 (91%)	-0.02	3 (1%) 80 79	24, 34, 50, 58	0
1	B	291/303 (96%)	-0.26	1 (0%) 94 93	21, 30, 43, 52	0
1	C	285/303 (94%)	0.14	9 (3%) 47 45	26, 42, 54, 61	0
1	D	277/303 (91%)	0.71	29 (10%) 6 5	35, 49, 61, 66	0
All	All	1131/1212 (93%)	0.14	42 (3%) 41 39	21, 39, 56, 66	0

The worst 5 of 42 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	208	LEU	4.7
1	D	89	GLY	4.6
1	D	140	GLY	4.1
1	D	206	ALA	4.0
1	D	178	SER	3.8

### 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	ACT	A	350	4/4	0.91	0.14	58,58,59,59	0
2	ACT	C	1	4/4	0.91	0.23	43,43,44,44	0
2	ACT	B	1	4/4	0.95	0.18	39,39,40,40	0
2	ACT	A	1	4/4	0.97	0.19	39,39,40,40	0
2	ACT	D	1	4/4	0.97	0.16	52,52,52,53	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.