

# wwPDB X-ray Structure Validation Summary Report (i)

#### May 24, 2020 – 09:26 pm BST

PDB ID : 3GEM

Title : Crystal structure of short-chain dehydrogenase from Pseudomonas syringae Authors Osipiuk, J.; Xu, X.; Cui, H.; Nocek, B.; Savchenko, A.; Edwards, A.M.;

Joachimiak, A.; Midwest Center for Structural Genomics (MCSG)

Deposited on 2009-02-25

1.83 Å(reported) Resolution

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 A user guide is available at

https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity 4.02b-467

> 1.8.5 (274361), CSD as541be (2020) Mogul

Xtriage (Phenix) 1.13 EDS 2.11

20191225.v01 (using entries in the PDB archive December 25th 2019) Percentile statistics

> Refmac 5.8.0158

7.0.044 (Gargrove) CCP4 Engh & Huber (2001)

Ideal geometry (proteins) Ideal geometry (DNA, RNA) Parkinson et al. (1996)

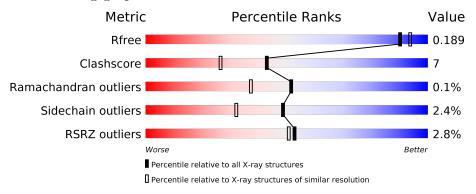
Validation Pipeline (wwPDB-VP) 2.11

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X-RAY DIFFRACTION

The reported resolution of this entry is 1.83 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	$\begin{array}{c} \text{Whole archive} \\ (\#\text{Entries}) \end{array}$	$\begin{array}{c} {\rm Similar \; resolution} \\ (\#{\rm Entries, \; resolution \; range(\AA)}) \end{array}$
$R_{free}$	130704	4003 (1.86-1.82)
Clashscore	141614	4233 (1.86-1.82)
Ramachandran outliers	138981	4185 (1.86-1.82)
Sidechain outliers	138945	4186 (1.86-1.82)
RSRZ outliers	127900	3957 (1.86-1.82)

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 >=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 <=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	260	71%	10% ••	17%
1	В	260	76%	9%	15%
1	С	260	78%	8%	14%
1	D	260	70%	12%	18%

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 crite-



ria:

$oxed{N}$	/Iol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
	2	ACT	В	239	_	-	X	-



# 2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 7638 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 Short chain dehydrogenase.

Mol	Chain	Residues		$\mathbf{Atoms}$					ZeroOcc	AltConf	Trace	
1	Λ	217	Total	С	N	О	S	Se	0	10	0	
1	A	211	1708	1088	300	312	4	4	U	10	U	
1	В	221	Total	С	N	О	S	Se	0	7	0	
1	Ъ	221	1721	1094	302	317	4	4		1	0	
1	C	224	Total	С	N	О	S	Se	0	13		
1		224	1781	1129	319	326	4	3	0	15	0	
1	1 D	D	214	Total	С	N	О	S	Se	0	11	0
1		D $\mid$ 214 $\mid$	1708	1086	299	315	4	4	U	11	U	

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-21	MSE	=	EXPRESSION TAG	UNP Q48MN0
A	-20	GLY	-	EXPRESSION TAG	UNP Q48MN0
A	-19	SER	-	EXPRESSION TAG	UNP Q48MN0
A	-18	SER	=	EXPRESSION TAG	UNP Q48MN0
A	-17	HIS	=	EXPRESSION TAG	UNP Q48MN0
A	-16	HIS	_	EXPRESSION TAG	UNP Q48MN0
A	-15	HIS	=	EXPRESSION TAG	UNP Q48MN0
A	-14	HIS	_	EXPRESSION TAG	UNP Q48MN0
A	-13	HIS	=	EXPRESSION TAG	UNP Q48MN0
A	-12	HIS	=	EXPRESSION TAG	UNP Q48MN0
A	-11	SER	=	EXPRESSION TAG	UNP Q48MN0
A	-10	SER	=	EXPRESSION TAG	UNP Q48MN0
A	-9	GLY	=	EXPRESSION TAG	UNP Q48MN0
A	-8	ARG	=	EXPRESSION TAG	UNP Q48MN0
A	-7	GLU	=	EXPRESSION TAG	UNP Q48MN0
A	-6	ASN	=	EXPRESSION TAG	UNP Q48MN0
A	-5	LEU	-	EXPRESSION TAG	UNP Q48MN0
A	-4	TYR	=	EXPRESSION TAG	UNP Q48MN0
A	-3	PHE	-	EXPRESSION TAG	UNP Q48MN0
A	-2	GLN	=	EXPRESSION TAG	UNP Q48MN0
Α	-1	GLY	-	EXPRESSION TAG	UNP Q48MN0



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Chain	Residue	Modelled	Actual	Comment	Reference
A	0	HIS	_	EXPRESSION TAG	UNP Q48MN0
A	237	GLY	-	EXPRESSION TAG	UNP Q48MN0
A	238	SER	-	EXPRESSION TAG	UNP Q48MN0
В	-21	MSE	-	EXPRESSION TAG	UNP Q48MN0
В	-20	GLY	-	EXPRESSION TAG	UNP Q48MN0
В	-19	SER	_	EXPRESSION TAG	UNP Q48MN0
В	-18	SER	_	EXPRESSION TAG	UNP Q48MN0
В	-17	HIS	-	EXPRESSION TAG	UNP Q48MN0
В	-16	HIS	_	EXPRESSION TAG	UNP Q48MN0
В	-15	HIS	_	EXPRESSION TAG	UNP Q48MN0
В	-14	HIS	_	EXPRESSION TAG	UNP Q48MN0
В	-13	HIS	_	EXPRESSION TAG	UNP Q48MN0
В	-12	HIS	_	EXPRESSION TAG	UNP Q48MN0
В	-11	SER	_	EXPRESSION TAG	UNP Q48MN0
В	-10	SER	_	EXPRESSION TAG	UNP Q48MN0
В	-9	GLY	_	EXPRESSION TAG	UNP Q48MN0
В	-8	ARG	-	EXPRESSION TAG	UNP Q48MN0
В	-7	GLU	_	EXPRESSION TAG	UNP Q48MN0
В	-6	ASN	_	EXPRESSION TAG	UNP Q48MN0
В	-5	LEU	-	EXPRESSION TAG	UNP Q48MN0
В	-4	TYR	-	EXPRESSION TAG	UNP Q48MN0
В	-3	PHE	-	EXPRESSION TAG	UNP Q48MN0
В	-2	GLN	-	EXPRESSION TAG	UNP Q48MN0
В	-1	GLY	-	EXPRESSION TAG	UNP Q48MN0
В	0	HIS	_	EXPRESSION TAG	UNP Q48MN0
В	237	GLY	-	EXPRESSION TAG	UNP Q48MN0
В	238	SER	_	EXPRESSION TAG	UNP Q48MN0
С	-21	MSE	_	EXPRESSION TAG	UNP Q48MN0
С	-20	GLY	_	EXPRESSION TAG	UNP Q48MN0
С	-19	SER	_	EXPRESSION TAG	UNP Q48MN0
С	-18	SER		EXPRESSION TAG	UNP Q48MN0
С	-17	HIS	-	EXPRESSION TAG	UNP Q48MN0
С	-16	HIS	-	EXPRESSION TAG	UNP Q48MN0
С	-15	HIS	-	EXPRESSION TAG	UNP Q48MN0
С	-14	HIS	-	EXPRESSION TAG	UNP Q48MN0
С	-13	HIS	-	EXPRESSION TAG	UNP Q48MN0
С	-12	HIS	-	EXPRESSION TAG	UNP Q48MN0
С	-11	SER	-	EXPRESSION TAG	UNP Q48MN0
С	-10	SER	-	EXPRESSION TAG	UNP Q48MN0
С	-9	GLY	-	EXPRESSION TAG	UNP Q48MN0
С	-8	ARG	-	EXPRESSION TAG	UNP Q48MN0
С	-7	GLU	-	EXPRESSION TAG	UNP Q48MN0

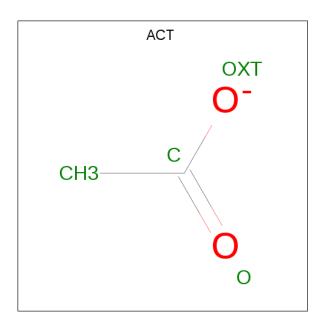


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	Residue	Modelled	Actual	Comment	Reference
С	-6	ASN	=	EXPRESSION TAG	UNP Q48MN0
С	-5	LEU	-	EXPRESSION TAG	UNP Q48MN0
С	-4	TYR	-	EXPRESSION TAG	UNP Q48MN0
С	-3	PHE	_	EXPRESSION TAG	UNP Q48MN0
С	-2	GLN	=	EXPRESSION TAG	UNP Q48MN0
С	-1	GLY	=	EXPRESSION TAG	UNP Q48MN0
С	0	HIS	-	EXPRESSION TAG	UNP Q48MN0
С	237	GLY	-	EXPRESSION TAG	UNP Q48MN0
С	238	SER	-	EXPRESSION TAG	UNP Q48MN0
D	-21	MSE	-	EXPRESSION TAG	UNP Q48MN0
D	-20	GLY	-	EXPRESSION TAG	UNP Q48MN0
D	-19	SER	=	EXPRESSION TAG	UNP Q48MN0
D	-18	SER	-	EXPRESSION TAG	UNP Q48MN0
D	-17	HIS	-	EXPRESSION TAG	UNP Q48MN0
D	-16	HIS	-	EXPRESSION TAG	UNP Q48MN0
D	-15	HIS	_	EXPRESSION TAG	UNP Q48MN0
D	-14	HIS	1	EXPRESSION TAG	UNP Q48MN0
D	-13	HIS	-	EXPRESSION TAG	UNP Q48MN0
D	-12	HIS	-	EXPRESSION TAG	UNP Q48MN0
D	-11	SER	-	EXPRESSION TAG	UNP Q48MN0
D	-10	SER	-	EXPRESSION TAG	UNP Q48MN0
D	-9	GLY	=	EXPRESSION TAG	UNP Q48MN0
D	-8	ARG	-	EXPRESSION TAG	UNP Q48MN0
D	-7	GLU	=	EXPRESSION TAG	UNP Q48MN0
D	-6	ASN	-	EXPRESSION TAG	UNP Q48MN0
D	-5	LEU	-	EXPRESSION TAG	UNP Q48MN0
D	-4	TYR	-	EXPRESSION TAG	UNP Q48MN0
D	-3	PHE	ı	EXPRESSION TAG	UNP Q48MN0
D	-2	GLN	=	EXPRESSION TAG	UNP Q48MN0
D	-1	GLY	=	EXPRESSION TAG	UNP Q48MN0
D	0	HIS	·	EXPRESSION TAG	UNP Q48MN0
D	237	GLY	=	EXPRESSION TAG	UNP Q48MN0
D	238	SER	-	EXPRESSION TAG	UNP Q48MN0

 $\bullet$  Molecule 2 is ACETATE ION (three-letter code: ACT) (formula:  $\mathrm{C_2H_3O_2}).$ 





Mol	Chain	Residues	${f Atoms}$			ZeroOcc	AltConf
2	В	1	Total 4	C 2	O 2	0	0

### • Molecule 3 is water.

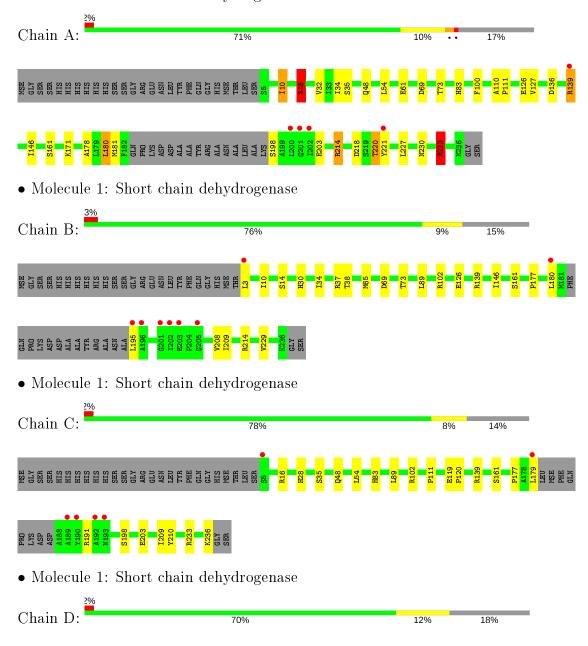
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	195	Total O 195 195	0	0
3	В	182	Total O 182 182	0	0
3	С	186	Total O 186 186	0	2
3	D	153	Total O 153 153	0	0



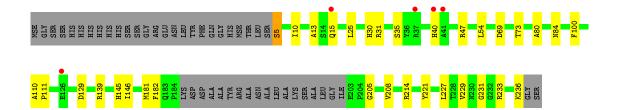
# 3 Residue-property plots (i)

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: Short chain dehydrogenase









# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	74.20Å 73.77Å 162.17Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $90.00^{\circ}$	Depositor
Resolution (Å)	49.80 - 1.83	Depositor
Resolution (A)	49.79 - 1.83	EDS
% Data completeness	99.6 (49.80-1.83)	Depositor
(in resolution range)	99.6 (49.79-1.83)	EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	3.13 (at 1.83Å)	Xtriage
Refinement program	REFMAC 5.5.0054	Depositor
D D.	0.149 , 0.182	Depositor
$R, R_{free}$	0.159 , $0.189$	DCC
$R_{free}$ test set	3951  reflections  (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	20.3	Xtriage
Anisotropy	0.074	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.34 , 42.5	EDS
L-test for twinning <sup>2</sup>	$< L >=0.49, < L^2>=0.32$	Xtriage
Estimated twinning fraction	0.017 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	7638	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.87% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>Theoretical values of <|L|>,  $< L^2>$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

# 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		
10101		RMSZ	# Z >5	RMSZ	# Z  > 5	
1	A	0.88	0/1765	0.91	8/2387~(0.3%)	
1	В	0.87	0/1764	0.83	0/2385	
1	С	0.86	0/1846	0.88	2/2499~(0.1%)	
1	D	0.86	0/1757	0.86	2/2378~(0.1%)	
All	All	0.87	0/7132	0.87	12/9649~(0.1%)	

There are no bond length outliers.

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^o)$
1	С	233[A]	ARG	NE-CZ-NH2	-7.84	116.38	120.30
1	С	233[B]	ARG	NE-CZ-NH2	-7.84	116.38	120.30
1	A	16[A]	ARG	NE-CZ-NH1	6.29	123.45	120.30
1	A	16[B]	ARG	NE-CZ-NH1	6.29	123.45	120.30
1	A	214[A]	ARG	NE-CZ-NH2	-5.51	117.55	120.30

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	1708	0	1761	36	0
1	В	1721	0	1769	21	0



$\alpha \cdots$	· ·	•	
Continued	trom	mromanne	maaa
-	110116	DICUIUU	$Du_iu_{C}$

Mol	Chain	Non-H	H(model)	$\mathbf{H}(\mathbf{added})$	Clashes	Symm-Clashes
1	С	1781	0	1832	13	0
1	D	1708	0	1741	32	0
2	В	4	0	3	10	0
3	A	195	0	0	7	0
3	В	182	0	0	3	0
3	С	186	0	0	3	0
3	D	153	0	0	5	0
All	All	7638	0	7106	95	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 7.

The worst 5 of 95 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$egin{array}{c}  ext{Interatomic} \  ext{distance} \ ( ext{Å}) \end{array}$	$egin{array}{c}  ext{Clash} \  ext{overlap } ( ext{Å}) \end{array}$
1:C:179:LEU:HD21	3:C:412:HOH:O	1.53	1.09
1:A:180:LEU:HB3	1:A:181:MSE:HE2	1.46	0.98
1:D:139[B]:ARG:HD2	1:D:139[B]:ARG:N	1.77	0.97
1:B:37[B]:ARG:H	2:B:239:ACT:H3	1.34	0.92
1:B:37[A]:ARG:H	2:B:239:ACT:H3	1.35	0.91

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	Perce	entiles
1	A	$223/260\ (86\%)$	217 (97%)	6 (3%)	0	100	100
1	В	224/260 (86%)	218 (97%)	5 (2%)	1 (0%)	34	20
1	С	$233/260 \ (90\%)$	228 (98%)	5 (2%)	0	100	100
1	D	$221/260 \; (85\%)$	214 (97%)	7 (3%)	0	100	100



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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	$\mathbf{ntiles}$
All	All	901/1040 (87%)	877 (97%)	23 (3%)	1 (0%)	51	37

#### All (1) Ramachandran outliers are listed below:

Mol	Chain	${f Res}$	Type	
1	В	180	LEU	

#### 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	187/205~(91%)	174 (93%)	13 (7%)	15 3
1	В	187/205 (91%)	185 (99%)	2 (1%)	73 64
1	С	192/205 (94%)	189 (98%)	3 (2%)	62 49
1	D	187/205 (91%)	183 (98%)	4 (2%)	53 38
All	All	753/820 (92%)	731 (97%)	22 (3%)	49 25

5 of 22 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	203	GLU
1	A	233[B]	ARG
1	D	100	PHE
1	A	220	THR
1	A	233[A]	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	$\operatorname{Res}$	Type
1	В	30	HIS
1	С	48	GLN
1	D	28	HIS
1	D	30	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 carbohydrates in this entry.

### 5.6 Ligand geometry (i)

1 ligand is 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	Tuno	Chain	hain Res	es Link	Bond lengths			Bond angles		
	Type			LIIIK	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	ACT	В	239	_	1,3,3	2.38	1 (100%)	0,3,3	0.00	-

#### All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	${ m Observed}({ m \AA})$	$\operatorname{Ideal}( ext{\AA})$
2	В	239	ACT	СН3-С	2.38	1.51	1.48

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	В	239	ACT	10	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,  $95^{th}$  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 $>$	$\#\mathrm{RSRZ}{>}2$	$OWAB(Å^2)$	Q < 0.9
1	A	213/260~(81%)	-0.01	5 (2%) 60 58	8, 13, 27, 36	0
1	В	217/260~(83%)	-0.19	8 (3%) 41 38	7, 14, 28, 37	0
1	С	221/260 (85%)	-0.32	6 (2%) 54 52	9, 15, 27, 33	0
1	D	210/260 (80%)	-0.22	5 (2%) 59 57	7, 15, 28, 37	0
All	All	861/1040 (82%)	-0.19	24 (2%) 53 51	7, 14, 28, 37	0

The worst 5 of 24 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	В	202	ILE	5.5
1	В	3	LEU	5.1
1	В	195	LEU	4.8
1	В	201	GLY	4.2
1	В	203	GLU	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 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. The B-factors column lists the minimum, median,  $95^{th}$  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	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q < 0.9
2	ACT	В	239	4/4	0.91	0.26	27,28,29,32	4

# 6.5 Other polymers (i)

There are no such residues in this entry.

