



# Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 08:02 pm BST

PDB ID : 3HA1  
Title : Alanine racemase from Bacillus Anthracis (Ames)  
Authors : Counago, R.M.; Davlieva, M.; Strych, U.; Hill, R.E.; Krause, K.L.  
Deposited on : 2009-04-30  
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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
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) : 2.11

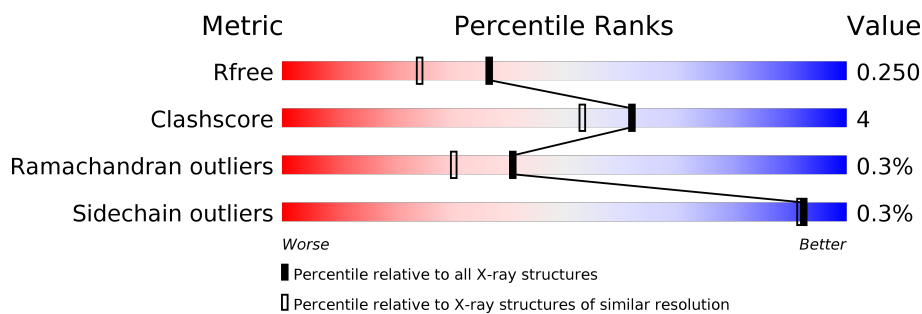
# 1 Overall quality at a glance

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))
$R_{free}$	130704	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (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 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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	397	
1	B	397	

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	398	-	-	X	-

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6434 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 Alanine racemase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	386	Total	C	N	O	P	S	0	0	0
			3040	1969	505	559	1	6			
1	B	386	Total	C	N	O	P	S	0	0	0
			3026	1960	504	555	1	6			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	390	LEU	-	EXPRESSION TAG	UNP Q81VF6
A	391	GLU	-	EXPRESSION TAG	UNP Q81VF6
A	392	GLU	-	EXPRESSION TAG	UNP Q81VF6
A	393	ASN	-	EXPRESSION TAG	UNP Q81VF6
A	394	LEU	-	EXPRESSION TAG	UNP Q81VF6
A	395	TYR	-	EXPRESSION TAG	UNP Q81VF6
A	396	PHE	-	EXPRESSION TAG	UNP Q81VF6
A	397	GLN	-	EXPRESSION TAG	UNP Q81VF6
B	390	LEU	-	EXPRESSION TAG	UNP Q81VF6
B	391	GLU	-	EXPRESSION TAG	UNP Q81VF6
B	392	GLU	-	EXPRESSION TAG	UNP Q81VF6
B	393	ASN	-	EXPRESSION TAG	UNP Q81VF6
B	394	LEU	-	EXPRESSION TAG	UNP Q81VF6
B	395	TYR	-	EXPRESSION TAG	UNP Q81VF6
B	396	PHE	-	EXPRESSION TAG	UNP Q81VF6
B	397	GLN	-	EXPRESSION TAG	UNP Q81VF6

- Molecule 2 is ACETATE ION (three-letter code: ACT) (formula: C<sub>2</sub>H<sub>3</sub>O<sub>2</sub>).



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

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Cl	0	0
			1	1		
3	A	1	Total	Cl	0	0
			1	1		

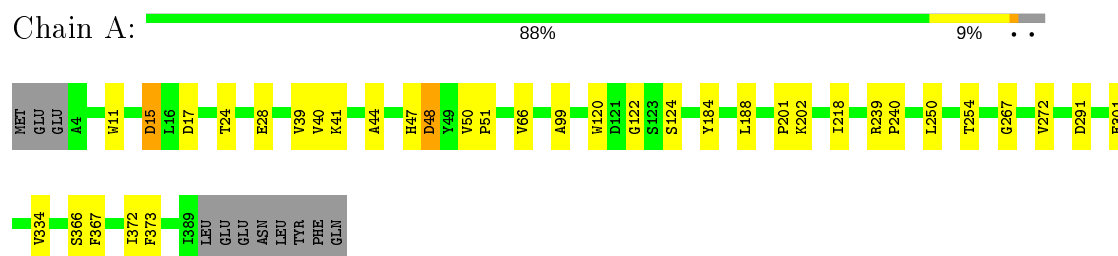
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	185	Total	O	0	0
			185	185		
4	B	173	Total	O	0	0
			173	173		

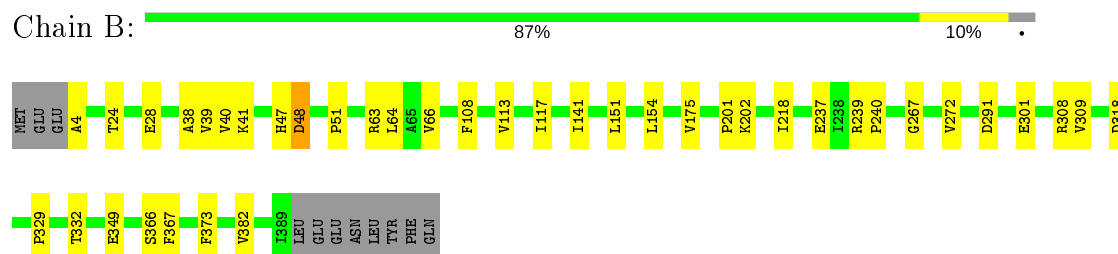
### 3 Residue-property plots [i](#)

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. 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. 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: Alanine racemase



#### • Molecule 1: Alanine racemase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	49.62Å 141.27Å 60.12Å 90.00° 103.11° 90.00°	Depositor
Resolution (Å)	32.79 – 1.95 32.79 – 1.95	Depositor EDS
% Data completeness (in resolution range)	91.1 (32.79-1.95) 91.2 (32.79-1.95)	Depositor EDS
$R_{merge}$	0.03	Depositor
$R_{sym}$	0.03	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.06 (at 1.95Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.160 , 0.201 0.222 , 0.250	Depositor DCC
$R_{free}$ test set	1627 reflections (3.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	29.7	Xtriage
Anisotropy	0.216	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 33.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	6434	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.83% 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: CL, LLP, 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	0.81	0/3088	0.74	1/4209 (0.0%)
1	B	0.80	0/3074	0.71	0/4192
All	All	0.80	0/6162	0.72	1/8401 (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	A	15	ASP	CB-CG-OD1	5.14	122.92	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	3040	0	2992	27	0
1	B	3026	0	2957	27	0
2	A	4	0	3	2	0
2	B	4	0	3	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	185	0	0	1	0
4	B	173	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	6434	0	5955	53	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 (53) 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:184:TYR:CE2	1:A:188:LEU:HD11	2.06	0.90
2:A:398:ACT:H1	1:B:41:LLP:H4'1	1.60	0.83
1:A:40:VAL:HG23	1:A:66:VAL:HG12	1.70	0.73
1:A:184:TYR:HE2	1:A:188:LEU:HD11	1.52	0.71
1:A:11:TRP:CD1	1:A:372:ILE:HD12	2.32	0.65
1:A:41:LLP:H4'1	2:B:398:ACT:H1	1.82	0.62
1:B:201:PRO:O	1:B:202:LYS:HB2	2.00	0.62
1:B:39:VAL:HG11	1:B:41:LLP:HE3	1.81	0.62
1:B:301:GLU:HA	1:B:309:VAL:O	2.01	0.61
1:B:267:GLY:HA3	1:B:272:VAL:HG13	1.86	0.58
1:B:175:VAL:HG23	1:B:237:GLU:HG2	1.84	0.58
1:A:254:THR:CG2	1:A:334:VAL:HB	2.33	0.57
1:A:239:ARG:HB3	1:A:240:PRO:HD3	1.88	0.56
1:B:308:ARG:NH2	1:B:349:GLU:OE1	2.39	0.54
1:A:291:ASP:HA	1:A:366:SER:HB3	1.91	0.52
1:A:267:GLY:HA3	1:A:272:VAL:HG13	1.91	0.52
1:B:201:PRO:O	1:B:202:LYS:CB	2.58	0.51
1:B:40:VAL:HG23	1:B:66:VAL:HG12	1.92	0.51
1:B:63:ARG:HD3	4:B:528:HOH:O	2.11	0.51
1:B:24:THR:O	1:B:28:GLU:HG3	2.10	0.51
1:B:39:VAL:CG1	1:B:41:LLP:HE3	2.41	0.51
1:B:47:HIS:O	1:B:48:ASP:HB2	2.11	0.50
1:A:254:THR:HG22	1:A:334:VAL:HB	1.92	0.49
1:B:51:PRO:HG2	1:B:373:PHE:CZ	2.48	0.49
1:A:301:GLU:HB2	4:A:451:HOH:O	2.13	0.48
1:B:291:ASP:HA	1:B:366:SER:HB3	1.95	0.48
1:B:113:VAL:O	1:B:117:ILE:HG12	2.13	0.48
1:A:51:PRO:HG2	1:A:373:PHE:CZ	2.49	0.47
1:B:38:ALA:HB3	1:B:64:LEU:HD23	1.96	0.47
1:A:47:HIS:O	1:A:48:ASP:HB2	2.13	0.47
1:A:40:VAL:O	1:A:41:LLP:C	2.63	0.46
1:A:254:THR:HG23	1:A:334:VAL:HB	1.97	0.46
1:A:201:PRO:O	1:A:202:LYS:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:THR:O	1:A:28:GLU:HG3	2.16	0.45
1:A:99:ALA:HB1	1:A:124:SER:HB2	1.97	0.45
1:B:4:ALA:HB3	1:B:382:VAL:HB	1.99	0.45
1:B:218:ILE:HA	1:B:218:ILE:HD12	1.67	0.45
1:A:40:VAL:O	1:A:44:ALA:N	2.48	0.44
1:B:237:GLU:HB2	4:B:403:HOH:O	2.17	0.44
1:A:47:HIS:NE2	1:A:250:LEU:HB2	2.33	0.44
2:A:398:ACT:H1	1:B:41:LLP:C4'	2.41	0.43
1:A:218:ILE:HD12	1:A:218:ILE:HA	1.65	0.42
1:A:41:LLP:HD3	1:B:318:ASP:OD2	2.20	0.41
1:B:151:LEU:HA	1:B:154:LEU:HD12	2.02	0.41
1:A:39:VAL:HG11	1:A:41:LLP:HE3	2.02	0.41
1:B:108:PHE:HB2	1:B:141:ILE:HG13	2.03	0.41
1:B:239:ARG:N	1:B:240:PRO:CD	2.83	0.41
1:A:40:VAL:O	1:A:44:ALA:HA	2.21	0.41
1:A:15:ASP:OD1	1:A:17:ASP:HB2	2.21	0.41
1:B:41:LLP:NZ	1:B:41:LLP:O3	2.51	0.40
1:A:120:TRP:CH2	1:A:122:GLY:HA2	2.56	0.40
1:A:50:VAL:HB	1:A:51:PRO:HD3	2.04	0.40
1:B:329:PRO:HD2	1:B:332:THR:OG1	2.22	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	383/397 (96%)	368 (96%)	14 (4%)	1 (0%)	41	30
1	B	383/397 (96%)	366 (96%)	16 (4%)	1 (0%)	41	30
All	All	766/794 (96%)	734 (96%)	30 (4%)	2 (0%)	41	30

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	48	ASP
1	B	48	ASP

### 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	315/336 (94%)	314 (100%)	1 (0%)	92	92
1	B	309/336 (92%)	308 (100%)	1 (0%)	92	92
All	All	624/672 (93%)	622 (100%)	2 (0%)	92	92

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	367	PHE
1	B	367	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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
1	LLP	B	41	1	23,24,25	1.72	4 (17%)	25,32,34	1.73	5 (20%)
1	LLP	A	41	1	23,24,25	1.99	7 (30%)	25,32,34	1.73	5 (20%)

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
1	LLP	B	41	1	-	5/16/17/19	0/1/1/1
1	LLP	A	41	1	-	4/16/17/19	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	41	LLP	O3-C3	-5.83	1.23	1.37
1	A	41	LLP	O3-C3	-5.44	1.24	1.37
1	A	41	LLP	C2-N1	3.20	1.39	1.33
1	A	41	LLP	C4-C4'	2.97	1.52	1.46
1	A	41	LLP	OP4-C5'	2.88	1.55	1.45
1	A	41	LLP	C4'-NZ	2.79	1.36	1.27
1	A	41	LLP	C6-N1	2.47	1.39	1.34
1	B	41	LLP	C2-N1	2.47	1.38	1.33
1	A	41	LLP	CE-NZ	2.22	1.51	1.46
1	B	41	LLP	C4-C5	-2.11	1.39	1.42
1	B	41	LLP	C4-C4'	2.02	1.50	1.46

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	41	LLP	OP4-C5'-C5	5.58	119.99	109.35
1	A	41	LLP	CD-CE-NZ	3.86	120.38	110.93
1	B	41	LLP	C4-C4'-NZ	-3.22	109.52	124.31
1	A	41	LLP	C3-C4-C5	3.12	120.66	118.26
1	B	41	LLP	CE-NZ-C4'	-3.05	109.54	118.90
1	A	41	LLP	OP4-C5'-C5	2.79	114.67	109.35
1	A	41	LLP	C4-C4'-NZ	-2.69	111.97	124.31
1	A	41	LLP	OP4-P-OP1	2.45	113.36	106.47
1	B	41	LLP	C5-C6-N1	-2.23	120.10	123.82
1	B	41	LLP	C3-C4-C5	2.01	119.80	118.26

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	41	LLP	C4-C4'-NZ-CE
1	A	41	LLP	C4-C4'-NZ-CE
1	B	41	LLP	CG-CD-CE-NZ
1	A	41	LLP	CG-CD-CE-NZ
1	B	41	LLP	CE-CD-CG-CB
1	B	41	LLP	CD-CE-NZ-C4'
1	A	41	LLP	CD-CE-NZ-C4'
1	A	41	LLP	C3-C4-C4'-NZ
1	B	41	LLP	C3-C4-C4'-NZ

There are no ring outliers.

2 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	41	LLP	5	0
1	A	41	LLP	4	0

## 5.5 Carbohydrates

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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	B	398	-	1,3,3	2.67	1 (100%)	0,3,3	0.00	-
2	ACT	A	398	-	1,3,3	3.24	1 (100%)	0,3,3	0.00	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	398	ACT	CH3-C	3.24	1.52	1.48
2	B	398	ACT	CH3-C	2.67	1.52	1.48

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	398	ACT	1	0
2	A	398	ACT	2	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 ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.3 Carbohydrates ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.4 Ligands ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.5 Other polymers ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.