



# wwPDB X-ray Structure Validation Summary Report

Jun 12, 2024 – 08:31 AM EDT

PDB ID : 6NVT  
Title : Crystal structure of TLA-1 extended spectrum Beta-lactamase  
Authors : Rudino-Pinera, E.; Cifuentes-Castro, V.H.; Rodriguez-Almazan, C.  
Deposited on : 2019-02-05  
Resolution : 2.20 Å(reported)

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](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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

---

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 : 2.36.2  
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

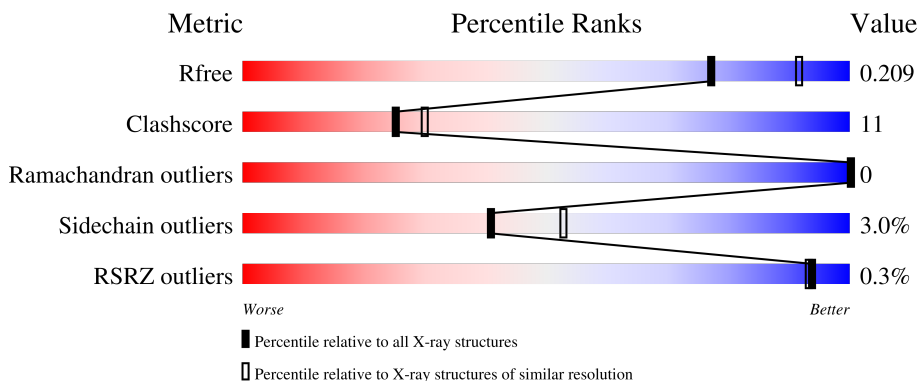
# 1 Overall quality at a glance

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	276	 89% 9% .
1	B	276	 88% 12% .
1	C	276	 85% 14% .
1	D	276	 85% 13% .

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
4	ACT	A	309	-	-	X	-
4	ACT	A	310	-	-	X	-
4	ACT	A	312	-	-	X	-
4	ACT	A	313	-	-	X	-
4	ACT	A	314	-	-	X	-
4	ACT	A	317	-	-	X	-
4	ACT	A	318	-	-	X	-
4	ACT	A	320	-	-	X	-
4	ACT	B	309	-	-	X	-
4	ACT	C	315	-	-	X	-
4	ACT	C	317	-	-	X	-
4	ACT	C	319	-	-	X	-
4	ACT	C	320	-	-	X	-
4	ACT	D	309	-	-	X	-
4	ACT	D	310	-	-	X	-
4	ACT	D	311	-	-	X	-
4	ACT	D	312	-	-	X	-
4	ACT	D	314	-	-	X	-
4	ACT	D	315	-	-	X	-
4	ACT	D	316	-	-	X	-
4	ACT	D	318	-	-	X	-
4	ACT	D	319	-	-	X	-

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 10170 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-lactamase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	276	Total 2201	C 1402	N 371	O 423	S 5	7	3	0
1	B	276	Total 2201	C 1405	N 368	O 423	S 5	9	3	0
1	C	276	Total 2213	C 1412	N 371	O 425	S 5	16	5	0
1	D	276	Total 2213	C 1410	N 369	O 429	S 5	9	4	0

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
2	A	1	Total 5	O 4	S 1	0	0
2	A	1	Total 5	O 4	S 1	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0

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

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

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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*



*Continued from previous page...*

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


- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	254	Total	O	0	0
			254	254		
5	B	263	Total	O	0	0
			263	263		
5	C	256	Total	O	0	0
			256	256		
5	D	263	Total	O	0	0
			263	263		

### 3 Residue-property plots


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.

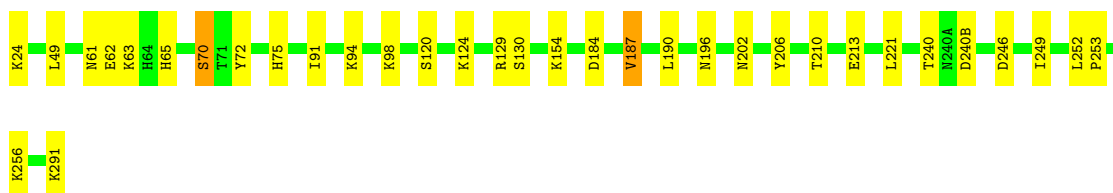
- Molecule 1: Beta-lactamase

Chain A:  89% 9%




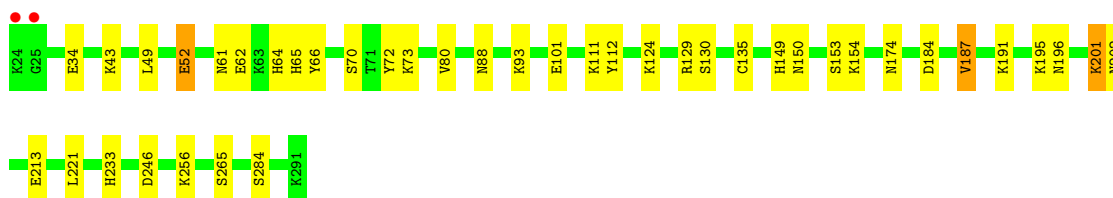
- Molecule 1: Beta-lactamase

Chain B:  88% 12%




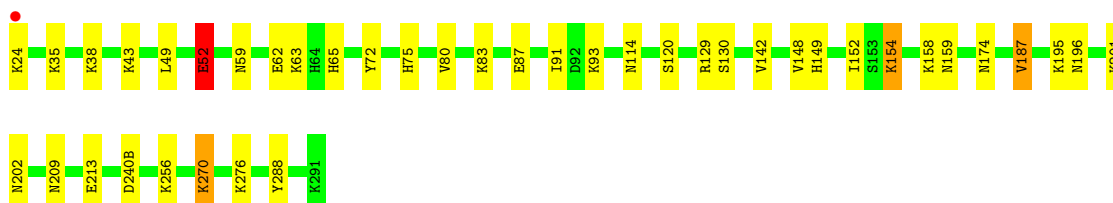
- Molecule 1: Beta-lactamase

Chain C:  % 85% 14%



- Molecule 1: Beta-lactamase

Chain D:  85% 13%



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	99.06Å 99.01Å 99.70Å 90.00° 90.04° 90.00°	Depositor
Resolution (Å)	35.15 – 2.20 35.15 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.9 (35.15-2.20) 99.7 (35.15-2.20)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.59 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, $R_{free}$	0.181 , 0.208 0.182 , 0.209	Depositor DCC
$R_{free}$ test set	4863 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	35.4	Xtriage
Anisotropy	0.053	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 43.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.007 for l,k,-h 0.009 for -h,-l,-k 0.007 for -h,l,k 0.469 for k,h,-l 0.469 for -k,-h,-l 0.008 for l,h,k 0.007 for k,l,h 0.007 for -l,-h,k 0.007 for -k,-l,h 0.477 for h,-k,-l 0.008 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	10170	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 7.20% 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: SO4, ACT, CL

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	1.39	2/2244 (0.1%)	0.89	5/3030 (0.2%)
1	B	1.37	1/2248 (0.0%)	0.87	4/3035 (0.1%)
1	C	1.37	1/2263 (0.0%)	0.85	0/3056
1	D	1.38	2/2257 (0.1%)	0.83	0/3048
All	All	1.38	6/9012 (0.1%)	0.86	9/12169 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	2
1	D	0	2
All	All	0	5

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	240	THR	C-N	9.53	1.55	1.34
1	B	240	THR	C-N	8.06	1.52	1.34
1	D	52[A]	GLU	CD-OE2	-5.57	1.19	1.25
1	D	52[B]	GLU	CD-OE2	-5.57	1.19	1.25
1	A	52	GLU	CD-OE2	-5.33	1.19	1.25

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	240	THR	O-C-N	10.54	139.56	122.70

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	240	THR	O-C-N	10.00	138.69	122.70
1	A	240	THR	CA-C-N	-9.44	96.43	117.20
1	B	240	THR	CA-C-N	-7.36	101.00	117.20
1	B	24	LYS	O-C-N	-5.22	114.32	123.20

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	52	GLU	Mainchain
1	C	284[A]	SER	Mainchain
1	C	284[B]	SER	Mainchain
1	D	52[A]	GLU	Mainchain
1	D	52[B]	GLU	Mainchain

## 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	2201	0	2248	29	1
1	B	2201	0	2249	29	0
1	C	2213	0	2262	45	0
1	D	2213	0	2246	61	1
2	A	35	0	0	2	0
2	B	35	0	0	1	0
2	C	50	0	0	3	0
2	D	30	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	1	0
3	C	4	0	0	3	0
3	D	2	0	0	1	0
4	A	48	0	36	24	1
4	B	24	0	18	8	0
4	C	28	0	21	8	0
4	D	48	0	36	30	0
5	A	254	0	0	21	0
5	B	263	0	0	11	0

*Continued on next page...*

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	256	0	0	16	0
5	D	263	0	0	19	1
All	All	10170	0	9116	194	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 11.

The worst 5 of 194 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:62:GLU:OE2	4:D:314:ACT:H1	1.36	1.24
1:D:174[A]:ASN:ND2	5:D:401:HOH:O	1.60	1.23
1:D:52[B]:GLU:CG	1:D:256:LYS:HD2	1.71	1.19
1:D:52[A]:GLU:HG3	1:D:256:LYS:HD2	1.16	1.16
1:D:52[B]:GLU:HG3	1:D:256:LYS:HD2	1.16	1.16

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:312:ACT:CH3	5:D:522:HOH:O[1_545]	1.63	0.57
1:A:256:LYS:NZ	1:D:202:ASN:OD1[2_5411]	1.69	0.51

## 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	277/276 (100%)	274 (99%)	3 (1%)	0	100 100
1	B	277/276 (100%)	273 (99%)	4 (1%)	0	100 100
1	C	279/276 (101%)	275 (99%)	4 (1%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	278/276 (101%)	275 (99%)	3 (1%)	0	100	100
All	All	1111/1104 (101%)	1097 (99%)	14 (1%)	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	250/247 (101%)	239 (96%)	11 (4%)	28	35
1	B	250/247 (101%)	243 (97%)	7 (3%)	43	56
1	C	252/247 (102%)	243 (96%)	9 (4%)	35	45
1	D	251/247 (102%)	243 (97%)	8 (3%)	39	50
All	All	1003/988 (102%)	968 (96%)	35 (4%)	41	46

5 of 35 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	72[A]	TYR
1	D	72[B]	TYR
1	D	154	LYS
1	B	72[A]	TYR
1	B	70	SER

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

Mol	Chain	Res	Type
1	C	88	ASN
1	C	245	ASN

### 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](#)

Of 75 ligands modelled in this entry, 8 are monoatomic - leaving 67 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	$\# Z  > 2$
4	ACT	D	316	-	3,3,3	0.87	0	3,3,3	2.04	2 (66%)
2	SO4	C	302	-	4,4,4	0.18	0	6,6,6	0.16	0
2	SO4	C	303	-	4,4,4	0.21	0	6,6,6	0.26	0
2	SO4	D	306	-	4,4,4	0.39	0	6,6,6	0.35	0
4	ACT	B	311	-	3,3,3	1.24	1 (33%)	3,3,3	0.36	0
4	ACT	C	317	-	3,3,3	0.91	0	3,3,3	1.79	2 (66%)
4	ACT	C	319	-	3,3,3	0.95	0	3,3,3	0.95	0
4	ACT	D	314	-	3,3,3	1.01	0	3,3,3	1.50	1 (33%)
4	ACT	B	309	-	3,3,3	0.88	0	3,3,3	1.48	1 (33%)
2	SO4	C	307	-	4,4,4	0.18	0	6,6,6	0.06	0
4	ACT	A	312	-	3,3,3	1.22	0	3,3,3	1.80	1 (33%)
2	SO4	A	306	-	4,4,4	0.37	0	6,6,6	0.42	0
4	ACT	A	314	-	3,3,3	0.77	0	3,3,3	1.70	1 (33%)
4	ACT	D	312	-	3,3,3	0.93	0	3,3,3	1.27	0
2	SO4	C	301	-	4,4,4	0.15	0	6,6,6	0.20	0
4	ACT	A	313	-	3,3,3	0.73	0	3,3,3	1.06	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	ACT	B	313	-	3,3,3	1.07	0	3,3,3	0.90	0
4	ACT	B	314	-	3,3,3	0.83	0	3,3,3	1.79	1 (33%)
4	ACT	D	313	-	3,3,3	0.99	0	3,3,3	0.94	0
4	ACT	D	315	-	3,3,3	1.08	0	3,3,3	1.88	2 (66%)
4	ACT	A	318	-	3,3,3	0.69	0	3,3,3	1.46	0
4	ACT	C	320	-	3,3,3	0.87	0	3,3,3	0.75	0
4	ACT	B	312	-	3,3,3	1.07	0	3,3,3	1.08	0
2	SO4	B	306	-	4,4,4	0.14	0	6,6,6	0.22	0
2	SO4	C	306	-	4,4,4	0.13	0	6,6,6	0.16	0
4	ACT	D	319	-	3,3,3	1.01	0	3,3,3	1.04	0
4	ACT	A	316	-	3,3,3	0.76	0	3,3,3	1.43	0
4	ACT	A	311	-	3,3,3	0.96	0	3,3,3	0.71	0
2	SO4	A	305	-	4,4,4	0.26	0	6,6,6	0.17	0
2	SO4	C	304	-	4,4,4	0.17	0	6,6,6	0.09	0
2	SO4	D	302	-	4,4,4	0.15	0	6,6,6	0.19	0
2	SO4	B	304	-	4,4,4	0.15	0	6,6,6	0.13	0
2	SO4	C	309	-	4,4,4	0.39	0	6,6,6	0.67	0
4	ACT	C	318	-	3,3,3	0.75	0	3,3,3	1.85	1 (33%)
2	SO4	D	305	-	4,4,4	0.11	0	6,6,6	0.21	0
2	SO4	B	302	-	4,4,4	0.16	0	6,6,6	0.11	0
4	ACT	A	309	-	3,3,3	0.60	0	3,3,3	1.10	0
4	ACT	B	310	-	3,3,3	1.07	0	3,3,3	1.54	1 (33%)
2	SO4	B	307	-	4,4,4	0.15	0	6,6,6	0.14	0
2	SO4	C	310	-	4,4,4	0.38	0	6,6,6	0.73	0
4	ACT	C	321	-	3,3,3	0.84	0	3,3,3	1.69	1 (33%)
2	SO4	B	301	-	4,4,4	0.14	0	6,6,6	0.17	0
4	ACT	A	320	-	3,3,3	0.93	0	3,3,3	1.32	1 (33%)
4	ACT	D	320	-	3,3,3	1.11	0	3,3,3	1.43	1 (33%)
4	ACT	D	310	-	3,3,3	1.00	0	3,3,3	1.69	1 (33%)
2	SO4	B	303	-	4,4,4	0.17	0	6,6,6	0.09	0
4	ACT	A	315	-	3,3,3	0.96	0	3,3,3	1.45	0
2	SO4	C	305	-	4,4,4	0.18	0	6,6,6	0.13	0
2	SO4	A	302	-	4,4,4	0.21	0	6,6,6	0.18	0
2	SO4	A	303	-	4,4,4	0.16	0	6,6,6	0.14	0
2	SO4	C	308	-	4,4,4	0.64	0	6,6,6	0.68	0
2	SO4	D	303	-	4,4,4	0.15	0	6,6,6	0.14	0
2	SO4	A	304	-	4,4,4	0.14	0	6,6,6	0.29	0
2	SO4	D	304	-	4,4,4	0.14	0	6,6,6	0.15	0
4	ACT	C	316	-	3,3,3	1.01	0	3,3,3	1.80	1 (33%)
4	ACT	A	310	-	3,3,3	1.30	1 (33%)	3,3,3	1.43	1 (33%)
4	ACT	D	318	-	3,3,3	1.06	0	3,3,3	1.13	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	ACT	D	317	-	3,3,3	1.02	0	3,3,3	0.85	0
2	SO4	D	301	-	4,4,4	0.21	0	6,6,6	0.19	0
4	ACT	D	309	-	3,3,3	0.77	0	3,3,3	0.85	0
2	SO4	A	301	-	4,4,4	0.07	0	6,6,6	0.19	0
2	SO4	B	305	-	4,4,4	0.15	0	6,6,6	0.19	0
4	ACT	A	317	-	3,3,3	0.95	0	3,3,3	1.14	0
4	ACT	A	319	-	3,3,3	0.97	0	3,3,3	1.96	2 (66%)
4	ACT	C	315	-	3,3,3	1.19	1 (33%)	3,3,3	0.98	0
4	ACT	D	311	-	3,3,3	1.09	0	3,3,3	0.82	0
2	SO4	A	307	-	4,4,4	0.45	0	6,6,6	0.54	0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	310	ACT	OXT-C	-2.15	1.20	1.30
4	B	311	ACT	OXT-C	-2.12	1.20	1.30
4	C	315	ACT	OXT-C	-2.07	1.20	1.30

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	319	ACT	OXT-C-O	-2.57	112.59	122.05
4	A	312	ACT	OXT-C-O	-2.52	112.75	122.05
4	B	314	ACT	OXT-C-CH3	2.47	125.39	115.18
4	C	318	ACT	OXT-C-CH3	2.47	125.37	115.18
4	D	314	ACT	OXT-C-O	-2.46	113.00	122.05

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

34 monomers are involved in 77 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	316	ACT	2	0
4	B	311	ACT	1	0
4	C	317	ACT	3	0
4	C	319	ACT	2	0
4	D	314	ACT	6	0
4	B	309	ACT	4	0
4	A	312	ACT	4	1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	314	ACT	4	0
4	D	312	ACT	3	0
2	C	301	SO4	1	0
4	A	313	ACT	2	0
4	B	313	ACT	1	0
4	D	315	ACT	3	0
4	A	318	ACT	3	0
4	C	320	ACT	2	0
4	B	312	ACT	1	0
2	B	306	SO4	1	0
4	D	319	ACT	5	0
4	A	309	ACT	3	0
4	B	310	ACT	1	0
2	C	310	SO4	1	0
4	A	320	ACT	3	0
4	D	320	ACT	1	0
4	D	310	ACT	3	0
2	C	308	SO4	1	0
2	A	304	SO4	1	0
4	C	316	ACT	1	0
4	A	310	ACT	3	0
4	D	318	ACT	3	0
4	D	309	ACT	2	0
4	A	317	ACT	3	0
4	C	315	ACT	2	0
4	D	311	ACT	2	0
2	A	307	SO4	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 [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	276/276 (100%)	-0.71	0 <a href="#">100</a> <a href="#">100</a>	26, 35, 52, 81	0
1	B	276/276 (100%)	-0.72	0 <a href="#">100</a> <a href="#">100</a>	27, 36, 53, 84	0
1	C	276/276 (100%)	-0.70	2 (0%) <a href="#">87</a> <a href="#">86</a>	26, 36, 53, 86	0
1	D	276/276 (100%)	-0.69	1 (0%) <a href="#">92</a> <a href="#">91</a>	26, 36, 53, 85	0
All	All	1104/1104 (100%)	-0.70	3 (0%) <a href="#">94</a> <a href="#">93</a>	26, 36, 53, 86	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	24	LYS	3.4
1	C	25	GLY	2.2
1	D	24	LYS	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 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
4	ACT	B	314	4/4	0.80	0.15	47,68,69,75	0
4	ACT	D	310	4/4	0.80	0.17	54,66,78,79	0
4	ACT	B	312	4/4	0.83	0.10	31,63,65,65	0
4	ACT	D	317	4/4	0.86	0.12	65,66,72,81	0
4	ACT	D	309	4/4	0.88	0.12	56,57,64,73	0
4	ACT	A	313	4/4	0.88	0.12	39,54,64,69	0
4	ACT	C	320	4/4	0.88	0.12	63,74,78,84	0
4	ACT	D	312	4/4	0.89	0.10	50,59,59,68	0
4	ACT	A	320	4/4	0.91	0.14	52,63,69,83	0
4	ACT	D	319	4/4	0.91	0.08	57,67,74,81	0
4	ACT	A	318	4/4	0.92	0.16	44,47,48,58	0
4	ACT	C	318	4/4	0.92	0.16	42,61,65,69	0
4	ACT	C	321	4/4	0.93	0.09	52,62,69,70	0
2	SO4	B	304	5/5	0.93	0.11	71,77,96,102	0
4	ACT	D	318	4/4	0.93	0.13	58,76,77,81	0
4	ACT	A	314	4/4	0.93	0.09	36,54,57,70	0
4	ACT	D	320	4/4	0.93	0.15	48,53,54,64	0
4	ACT	A	309	4/4	0.94	0.18	53,59,62,73	0
4	ACT	D	311	4/4	0.95	0.17	54,62,68,69	0
4	ACT	A	312	4/4	0.95	0.10	44,45,52,65	0
4	ACT	A	316	4/4	0.95	0.11	49,62,63,71	0
4	ACT	B	313	4/4	0.95	0.07	52,52,56,62	0
4	ACT	A	311	4/4	0.95	0.15	48,49,52,52	0
4	ACT	C	316	4/4	0.95	0.10	45,49,60,65	0
4	ACT	C	317	4/4	0.96	0.10	40,49,57,64	0
4	ACT	A	315	4/4	0.96	0.09	62,71,75,76	0
4	ACT	C	319	4/4	0.96	0.07	53,61,78,78	0
2	SO4	D	305	5/5	0.96	0.15	65,67,89,111	0
4	ACT	A	317	4/4	0.96	0.12	47,55,55,65	0
3	CL	C	314	1/1	0.96	0.06	56,56,56,56	0
2	SO4	B	302	5/5	0.96	0.13	58,65,80,91	0
4	ACT	B	309	4/4	0.96	0.07	54,74,74,84	0
4	ACT	B	311	4/4	0.96	0.12	50,50,60,62	0
4	ACT	D	314	4/4	0.96	0.12	50,50,57,62	0
2	SO4	A	306	5/5	0.96	0.32	68,75,95,96	0
2	SO4	B	307	5/5	0.96	0.26	78,81,87,89	0
2	SO4	C	306	5/5	0.96	0.13	61,66,85,95	0
2	SO4	C	310	5/5	0.96	0.13	58,63,79,83	0
2	SO4	B	303	5/5	0.97	0.12	64,64,87,105	0
4	ACT	D	313	4/4	0.97	0.07	53,54,57,60	0
2	SO4	C	307	5/5	0.97	0.12	70,74,87,100	0
4	ACT	D	315	4/4	0.97	0.11	48,48,50,61	0
4	ACT	D	316	4/4	0.97	0.12	45,52,54,65	0

*Continued on next page...*

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	ACT	C	315	4/4	0.97	0.22	49,56,57,66	0
2	SO4	C	309	5/5	0.97	0.13	69,70,74,82	0
2	SO4	C	305	5/5	0.97	0.14	60,62,81,94	0
2	SO4	D	304	5/5	0.97	0.16	61,65,77,88	0
4	ACT	A	319	4/4	0.98	0.12	53,53,57,76	0
2	SO4	D	303	5/5	0.98	0.15	61,70,71,73	0
2	SO4	A	307	5/5	0.98	0.12	60,67,72,84	0
4	ACT	B	310	4/4	0.98	0.09	39,48,62,64	0
2	SO4	A	305	5/5	0.98	0.12	43,53,58,69	0
2	SO4	D	306	5/5	0.98	0.22	78,79,83,89	0
2	SO4	C	304	5/5	0.98	0.20	62,69,74,76	0
2	SO4	A	304	5/5	0.98	0.14	54,60,75,77	0
2	SO4	D	302	5/5	0.98	0.11	49,50,54,55	0
2	SO4	C	301	5/5	0.99	0.09	41,41,48,52	0
2	SO4	D	301	5/5	0.99	0.11	42,45,50,56	0
2	SO4	C	302	5/5	0.99	0.09	46,46,52,56	0
2	SO4	C	303	5/5	0.99	0.10	39,56,59,76	0
2	SO4	A	303	5/5	0.99	0.16	60,65,71,72	0
2	SO4	B	301	5/5	0.99	0.12	63,71,72,77	0
2	SO4	B	305	5/5	0.99	0.12	47,50,52,58	0
3	CL	A	308	1/1	0.99	0.06	39,39,39,39	0
3	CL	B	308	1/1	0.99	0.07	38,38,38,38	0
3	CL	C	311	1/1	0.99	0.10	66,66,66,66	0
3	CL	C	312	1/1	0.99	0.05	53,53,53,53	0
3	CL	C	313	1/1	0.99	0.09	41,41,41,41	0
2	SO4	B	306	5/5	0.99	0.12	41,44,49,57	0
3	CL	D	307	1/1	0.99	0.05	57,57,57,57	0
2	SO4	C	308	5/5	0.99	0.09	43,53,62,71	0
4	ACT	A	310	4/4	0.99	0.08	33,38,40,45	0
2	SO4	A	302	5/5	0.99	0.11	49,51,54,57	0
3	CL	D	308	1/1	1.00	0.08	39,39,39,39	0
2	SO4	A	301	5/5	1.00	0.12	45,46,49,50	0

## 6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.