



# wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 25, 2024 – 04:12 PM EDT

PDB ID : 7UGW  
Title : M. tuberculosis DNA gyrase cleavage core bound to DNA and evybactin  
Authors : Hauk, G.; Imai, Y.; Lewis, K.; Berger, J.M.  
Deposited on : 2022-03-25  
Resolution : 3.00 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>.

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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 : 3.0  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.002 (Gargrove)  
Density-Fitness : 1.0.11  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.38.3

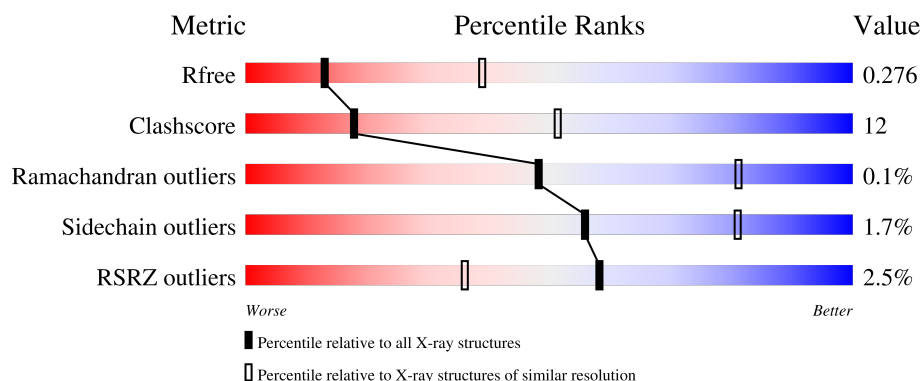
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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.



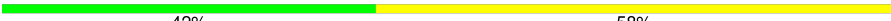
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	164625	2511 (3.00-3.00)
Clashscore	180529	2866 (3.00-3.00)
Ramachandran outliers	177936	2778 (3.00-3.00)
Sidechain outliers	177891	2781 (3.00-3.00)
RSRZ outliers	164620	2523 (3.00-3.00)

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	500	
1	C	500	
2	B	251	
2	D	251	
3	V	46	

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Mol	Chain	Length	Quality of chain
4	E	12	 42% 58%

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 24266 atoms, of which 11892 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 DNA gyrase subunit A.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	485	Total	C	H	N	O	S	0	0	0
			7469	2342	3719	676	719	13			
1	C	487	Total	C	H	N	O	S	0	0	0
			7640	2377	3822	700	728	13			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	129	PHE	TYR	engineered mutation	UNP P9WG47
C	129	PHE	TYR	engineered mutation	UNP P9WG47

- Molecule 2 is a protein called DNA gyrase subunit B.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	248	Total	C	H	N	O	S	0	0	0
			3905	1222	1963	348	365	7			
2	D	232	Total	C	H	N	O	S	0	0	0
			3598	1138	1787	320	346	7			

- Molecule 3 is a DNA chain called DNA (46-MER).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	V	46	Total	C	H	N	O	P	0	0	0
			1459	446	514	184	270	45			

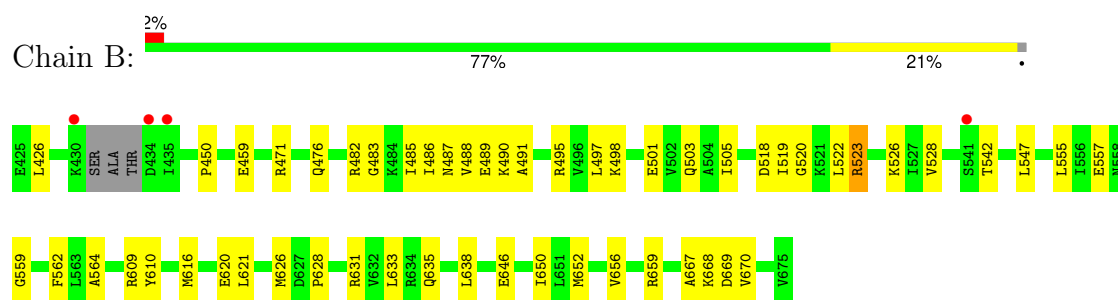
- Molecule 4 is a protein called evybactin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	12	Total	C	H	N	O	0	0	0
			193	64	87	21	21			

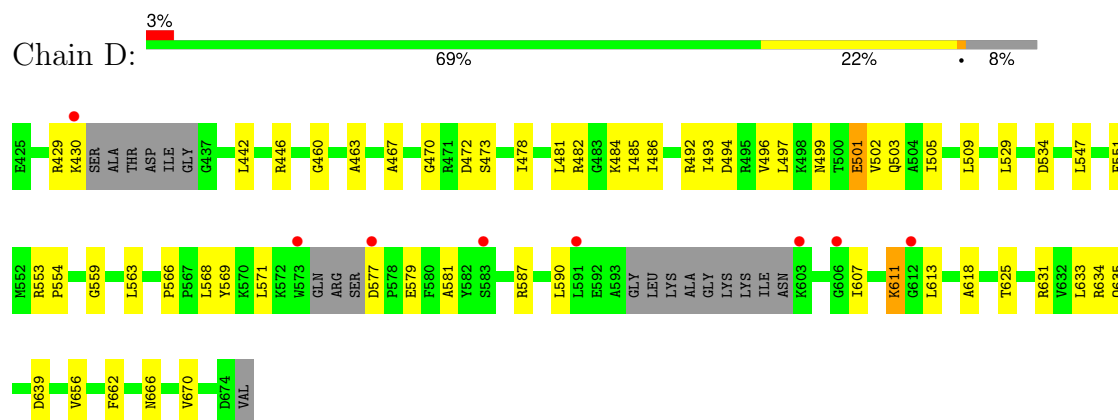
- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total 1	Mg 1	0	0
5	V	1	Total 1	Mg 1	0	0

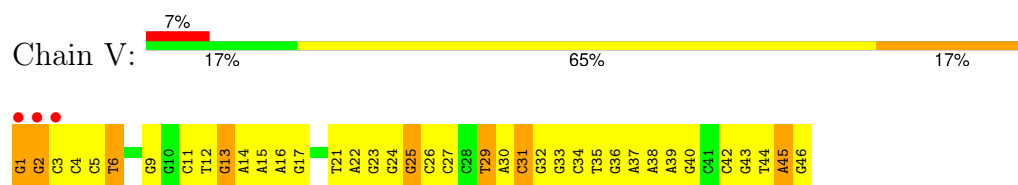




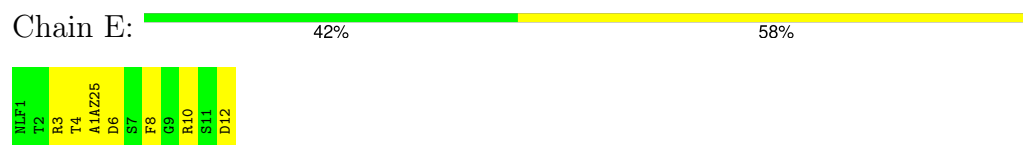
• Molecule 2: DNA gyrase subunit B



• Molecule 3: DNA (46-MER)



• Molecule 4: evybactin



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	83.08Å 105.09Å 250.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.44 – 3.00 48.44 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.7 (48.44-3.00) 99.6 (48.44-3.00)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.53 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, $R_{free}$	0.218 , 0.276 0.218 , 0.276	Depositor DCC
$R_{free}$ test set	42931 reflections (4.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	59.1	Xtriage
Anisotropy	0.682	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 30.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	24266	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.26% 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: NLF, MG, DAR, DSN, IAS, A1AZ2

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	0.58	0/3808	0.85	3/5168 (0.1%)
1	C	0.63	0/3877	0.88	5/5253 (0.1%)
2	B	0.62	0/1970	0.89	1/2648 (0.0%)
2	D	0.60	0/1837	0.92	3/2475 (0.1%)
3	V	1.57	7/1062 (0.7%)	1.40	16/1638 (1.0%)
4	E	4.46	7/32 (21.9%)	0.87	0/37
All	All	0.77	14/12586 (0.1%)	0.94	28/17219 (0.2%)

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	8	PHE	CG-CD1	10.98	1.55	1.38
4	E	8	PHE	CE1-CZ	9.50	1.55	1.37
4	E	8	PHE	CG-CD2	9.43	1.52	1.38
4	E	8	PHE	CD2-CE2	8.54	1.56	1.39
4	E	8	PHE	CE2-CZ	7.80	1.52	1.37

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	437	ASP	CB-CG-OD2	10.35	127.62	118.30
3	V	23	DG	O4'-C4'-C3'	-9.11	100.54	106.00
3	V	24	DG	O4'-C4'-C3'	-8.86	100.68	106.00
3	V	2	DG	O4'-C1'-N9	8.12	113.69	108.00
3	V	31	DC	O4'-C4'-C3'	-7.71	101.37	106.00

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	3750	3719	3719	78	0
1	C	3818	3822	3822	62	0
2	B	1942	1963	1963	54	0
2	D	1811	1787	1786	47	0
3	V	945	514	514	75	0
4	E	106	87	68	0	0
5	B	1	0	0	0	0
5	V	1	0	0	0	0
All	All	12374	11892	11872	292	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 12.

The worst 5 of 292 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)
3:V:25:DG:H5''	3:V:25:DG:H8	1.27	0.95
3:V:35:DT:H2'	3:V:36:DG:O4'	1.70	0.92
1:A:275:PRO:HG2	1:A:278:VAL:HG21	1.55	0.89
3:V:25:DG:H5''	3:V:25:DG:C8	2.14	0.82
3:V:21:DT:H2''	3:V:22:DA:O5'	1.80	0.82

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	481/500 (96%)	449 (93%)	32 (7%)	0	100	100
1	C	485/500 (97%)	449 (93%)	35 (7%)	1 (0%)	44	77
2	B	244/251 (97%)	228 (93%)	16 (7%)	0	100	100
2	D	224/251 (89%)	206 (92%)	18 (8%)	0	100	100
4	E	5/12 (42%)	5 (100%)	0	0	100	100
All	All	1439/1514 (95%)	1337 (93%)	101 (7%)	1 (0%)	48	81

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	39	ARG

### 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	393/419 (94%)	385 (98%)	8 (2%)	50	78
1	C	405/419 (97%)	396 (98%)	9 (2%)	47	76
2	B	204/210 (97%)	204 (100%)	0	100	100
2	D	189/210 (90%)	187 (99%)	2 (1%)	70	87
4	E	4/4 (100%)	3 (75%)	1 (25%)	0	2
All	All	1195/1262 (95%)	1175 (98%)	20 (2%)	56	81

5 of 20 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	340	SER
2	D	494	ASP
4	E	4	THR
2	D	501	GLU
1	A	306	SER

Sometimes 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 ⓘ

6 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	$\# Z  > 2$
4	IAS	E	12	4	6,7,8	1.49	1 (16%)	3,8,10	1.74	1 (33%)
4	DAR	E	10	4	9,10,11	3.19	3 (33%)	5,11,13	0.23	0
4	A1AZ2	E	5	4	7,11,12	2.32	1 (14%)	7,14,16	1.65	2 (28%)
4	IAS	E	6	4	6,7,8	2.15	1 (16%)	3,8,10	1.46	1 (33%)
4	DAR	E	3	4	9,10,11	3.60	4 (44%)	5,11,13	0.45	0
4	DSN	E	7	4	4,5,6	0.28	0	1,5,7	0.33	0

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
4	IAS	E	12	4	-	2/7/7/8	-
4	DAR	E	10	4	-	3/8/9/11	-
4	A1AZ2	E	5	4	-	2/5/6/8	0/1/1/1
4	IAS	E	6	4	-	2/7/7/8	-
4	DAR	E	3	4	-	3/8/9/11	-
4	DSN	E	7	4	-	2/2/4/6	-

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	3	DAR	CZ-NE	8.35	1.49	1.33
4	E	10	DAR	CZ-NE	7.05	1.46	1.33
4	E	5	A1AZ2	CB-CG	5.92	1.60	1.50
4	E	3	DAR	CZ-NH2	5.17	1.50	1.32
4	E	6	IAS	CB-CG	4.59	1.62	1.50

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	5	A1AZ2	NE2-CE1-ND1	-2.73	108.21	112.26
4	E	5	A1AZ2	CM-ND1-CG	2.43	127.68	124.44
4	E	12	IAS	OD1-CG-CB	-2.31	118.64	125.38
4	E	6	IAS	OXT-C-O	-2.06	119.42	124.08

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	E	3	DAR	N-CA-CB-CG
4	E	3	DAR	C-CA-CB-CG
4	E	7	DSN	N-CA-CB-OG
4	E	7	DSN	C-CA-CB-OG
4	E	10	DAR	NE-CD-CG-CB

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	485/500 (97%)	0.03	21 (4%) 40 23	42, 63, 120, 147	0
1	C	487/500 (97%)	-0.13	2 (0%) 89 77	41, 59, 100, 152	0
2	B	248/251 (98%)	0.15	4 (1%) 70 49	46, 69, 102, 122	0
2	D	232/251 (92%)	0.27	8 (3%) 48 28	54, 73, 106, 140	0
3	V	46/46 (100%)	0.42	3 (6%) 26 15	46, 74, 121, 135	0
4	E	5/12 (41%)	0.45	0 100 100	52, 53, 54, 54	0
All	All	1503/1560 (96%)	0.05	38 (2%) 58 36	41, 66, 108, 152	0

The worst 5 of 38 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	14	ARG	4.4
2	B	434	ASP	4.3
1	A	288	ALA	3.6
1	A	316	ILE	3.3
1	A	292	ARG	3.2

### 6.2 Non-standard residues in protein, DNA, RNA chains [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(Å <sup>2</sup> )	Q<0.9
4	DSN	E	7	6/7	0.54	0.17	49,51,62,63	0
4	IAS	E	6	8/9	0.71	0.13	48,49,59,59	0
4	DAR	E	10	11/12	0.78	0.15	49,53,63,64	0
4	IAS	E	12	8/9	0.79	0.13	47,48,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	DAR	E	3	11/12	0.81	0.15	46,50,58,61	0
4	A1AZ2	E	5	11/12	0.87	0.13	47,48,58,58	0

### 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
5	MG	B	701	1/1	0.80	0.40	43,43,43,43	0
5	MG	V	101	1/1	0.86	0.53	63,63,63,63	0

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

There are no such residues in this entry.