



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 19, 2016 – 07:19 AM EDT

PDB ID : 5IWM  
Title : 2.5A structure of GSK945237 with S.aureus DNA gyrase and DNA.  
Authors : Bax, B.D.; Miles, T.J.  
Deposited on : 2016-03-22  
Resolution : 2.50 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  
<http://wwpdb.org/validation/2016/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 : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20027790  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20027790

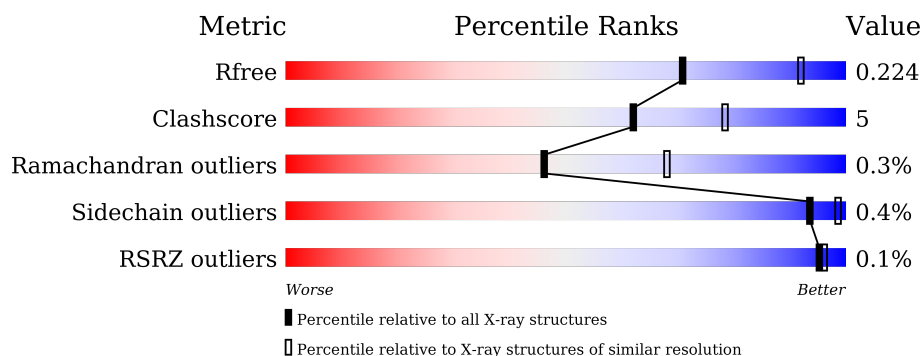
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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))
$R_{free}$	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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. 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	B	202	
1	D	202	
2	A	490	
2	C	490	
3	E	20	
4	F	20	

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
6	GOL	C	501	-	-	-	X
7	6EJ	F	101[A]	-	-	-	X

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 12686 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 DNA gyrase subunit B,DNA gyrase subunit B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	189	Total	C	N	O	S	0	1	0
			1492	937	259	287	9			
1	D	189	Total	C	N	O	S	0	2	0
			1496	938	259	290	9			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	409	MET	-	expression tag	UNP P66937
B	544	THR	-	linker	UNP P66937
B	545	GLY	-	linker	UNP P66937
D	409	MET	-	expression tag	UNP P66937
D	544	THR	-	linker	UNP P66937
D	545	GLY	-	linker	UNP P66937

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	483	Total	C	N	O	S	0	11	0
			3923	2434	720	752	17			
2	C	481	Total	C	N	O	S	0	4	0
			3847	2389	703	739	16			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	123	PHE	TYR	conflict	UNP Q99XG5
C	123	PHE	TYR	conflict	UNP Q99XG5

- Molecule 3 is a DNA chain called DNA (5'-D(\*AP\*GP\*CP\*CP\*GP\*TP\*AP\*GP\*GP\*TP\*TP\*CP\*AP\*CP\*CP\*GP\*CP\*AP\*CP\*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	20	Total	C	N	O	P	0	20	0
			794	377	149	230	38			

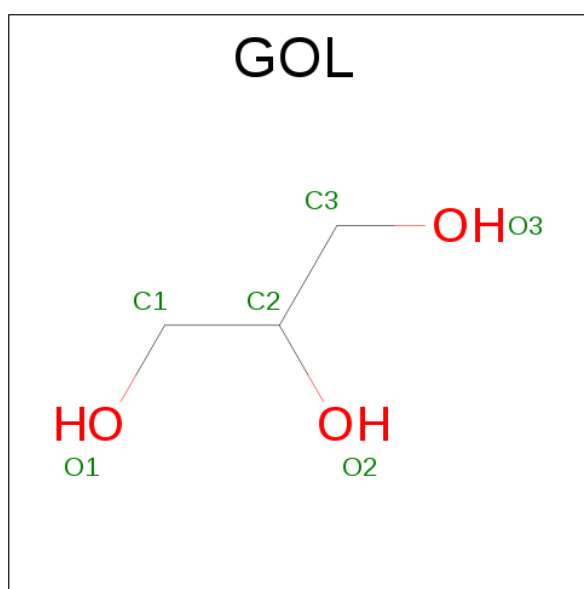
- Molecule 4 is a DNA chain called DNA (5'-D(\*TP\*GP\*TP\*GP\*CP\*GP\*GP\*TP\*GP\*AP\*AP\*CP\*CP\*TP\*AP\*CP\*GP\*GP\*CP\*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	20	Total	C	N	O	P	0	20	0
			798	380	148	233	37			

- Molecule 5 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

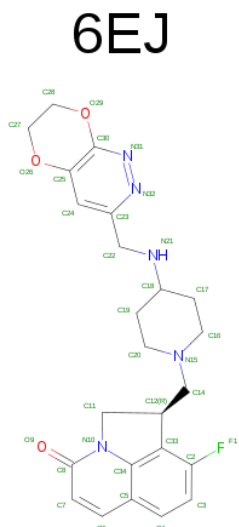
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Mn	0	0
			1	1		
5	D	1	Total	Mn	0	0
			1	1		

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	C	1	Total	C	O	0	0
			6	3	3		

- Molecule 7 is (1R)-1-[(4-{[(6,7-dihydro[1,4]dioxino[2,3-c]pyridazin-3-yl)methyl]amino}piperidin-1-yl)methyl]-9-fluoro-1,2-dihydro-4H-pyrrolo[3,2,1-ij]quinolin-4-one (three-letter code: 6EJ) (formula: C<sub>24</sub>H<sub>26</sub>FN<sub>5</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	F	1	Total	C	F	N	O	0	1
			66	48	2	10	6		


- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	35	Total O 35 35	0	0
8	A	86	Total O 87 87	0	1
8	D	29	Total O 29 29	0	0
8	C	74	Total O 75 75	0	1
8	E	15	Total O 16 16	0	1
8	F	19	Total O 20 20	0	1

### 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 errors 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.

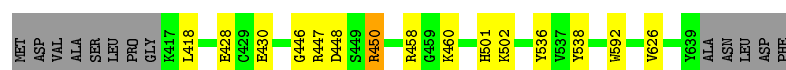
- Molecule 1: DNA gyrase subunit B,DNA gyrase subunit B

Chain B: 




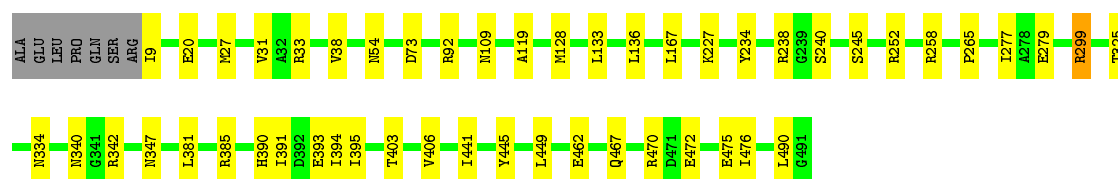
- Molecule 1: DNA gyrase subunit B,DNA gyrase subunit B

Chain D: 




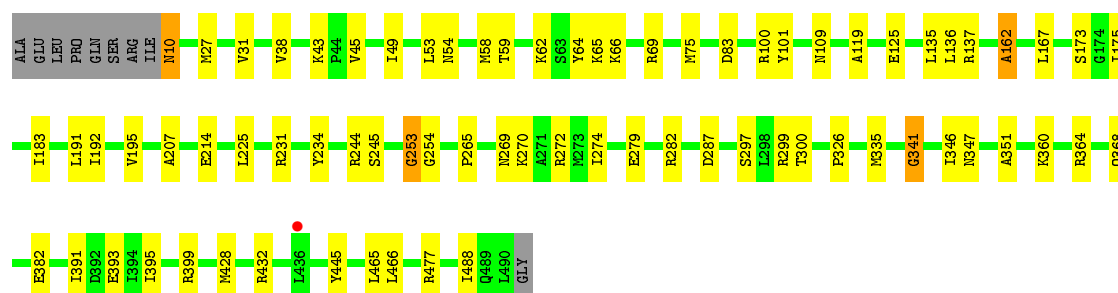
- Molecule 2: DNA gyrase subunit A

Chain A: 



- Molecule 2: DNA gyrase subunit A

Chain C: 



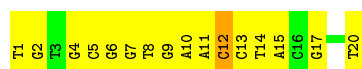
- Molecule 3: DNA (5'-D(\*AP\*GP\*CP\*CP\*GP\*TP\*AP\*GP\*GP\*TP\*TP\*CP\*AP\*CP\*CP\*GP\*CP\*AP\*CP\*A)-3')

Chain E:  25% 75%



- Molecule 4: DNA (5'-D(\*TP\*GP\*TP\*GP\*CP\*GP\*GP\*TP\*GP\*AP\*AP\*CP\*CP\*TP\*AP\*CP\*GP\*GP\*CP\*T)-3')

Chain F:  20% 75% 5%





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	93.78Å 93.78Å 413.35Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	24.99 – 2.50 24.99 – 2.50	Depositor EDS
% Data completeness (in resolution range)	92.5 (24.99-2.50) 92.5 (24.99-2.50)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.14 (at 2.50Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, $R_{free}$	0.180 , 0.224 0.180 , 0.224	Depositor DCC
$R_{free}$ test set	2625 reflections (4.19%)	DCC
Wilson B-factor (Å <sup>2</sup> )	20.3	Xtriage
Anisotropy	0.278	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , -1.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.39$ , $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	0.168 for h,-h-k,-l	Xtriage
Reported twinning fraction	0.831 for H, K, L 0.169 for K, H, -L	Depositor
Outliers	0 of 65320 reflections	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	12686	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.14% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, MN, 6EJ

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	B	0.61	2/1519 (0.1%)	0.73	2/2049 (0.1%)
1	D	0.71	8/1520 (0.5%)	0.72	2/2052 (0.1%)
2	A	0.56	2/3974 (0.1%)	0.64	0/5347
2	C	0.58	1/3895 (0.0%)	0.67	3/5248 (0.1%)
3	E	0.44	0/908	0.86	2/1396 (0.1%)
4	F	0.40	0/893	0.85	2/1374 (0.1%)
All	All	0.58	13/12709 (0.1%)	0.71	11/17466 (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
2	C	0	3

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	341	GLY	C-N	-8.93	1.13	1.34
1	D	592	TRP	CD1-NE1	-7.52	1.25	1.38
1	D	446	GLY	C-O	-7.11	1.12	1.23
2	A	20[A]	GLU	CA-C	6.41	1.69	1.52
2	A	20[B]	GLU	CA-C	6.41	1.69	1.52

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	341	GLY	O-C-N	-10.58	105.77	122.70
1	D	447	ARG	NE-CZ-NH2	9.22	124.91	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	447	ARG	NE-CZ-NH1	-8.25	116.18	120.30
4	F	12[A]	DC	C1'-O4'-C4'	-6.41	103.69	110.10
4	F	12[B]	DC	C1'-O4'-C4'	-6.41	103.69	110.10

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	287[B]	ASP	Mainchain
2	C	341	GLY	Mainchain

## 5.2 Too-close contacts

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	B	1492	0	1474	14	0
1	D	1496	0	1461	12	0
2	A	3923	0	3975	36	0
2	C	3847	0	3886	43	1
3	E	794	0	410	16	1
4	F	798	0	401	21	0
5	B	1	0	0	0	0
5	D	1	0	0	0	0
6	C	6	0	8	0	0
7	F	66	0	0	0	0
8	A	87	0	0	7	0
8	B	35	0	0	0	0
8	C	75	0	0	7	0
8	D	29	0	0	2	0
8	E	16	0	0	2	0
8	F	20	0	0	0	0
All	All	12686	0	11615	128	1

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 5.

The worst 5 of 128 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)
2:C:58:MET:HG2	2:C:65:LYS:HG3	1.44	0.99
3:E:12[B]:DC:H2"	3:E:13[B]:DA:OP2	1.72	0.88
1:B:447:ARG:HD3	1:B:454:ILE:HD11	1.58	0.83
2:A:238:ARG:HH11	2:A:238:ARG:HG2	1.48	0.78
2:C:66:LYS:HD2	8:C:639:HOH:O	1.85	0.74

All (1) 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)
2:C:393:GLU:OE1	3:E:1[A]:DA:N1[1_445]	2.10	0.10

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	B	188/202 (93%)	185 (98%)	3 (2%)	0	100	100
1	D	189/202 (94%)	183 (97%)	6 (3%)	0	100	100
2	A	492/490 (100%)	483 (98%)	8 (2%)	1 (0%)	52	75
2	C	483/490 (99%)	471 (98%)	9 (2%)	3 (1%)	30	50
All	All	1352/1384 (98%)	1322 (98%)	26 (2%)	4 (0%)	46	68

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	33	ARG
2	C	162	ALA
2	C	253	GLY
2	C	326	PRO

### 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	B	158/168 (94%)	158 (100%)	0	100	100
1	D	157/168 (94%)	155 (99%)	2 (1%)	76	92
2	A	426/423 (101%)	424 (100%)	2 (0%)	92	98
2	C	417/423 (99%)	416 (100%)	1 (0%)	95	99
All	All	1158/1182 (98%)	1153 (100%)	5 (0%)	93	98

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	299	ARG
2	A	334	ASN
1	D	418	LEU
1	D	450	ARG
2	C	10	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
2	A	368	GLN
1	D	476	ASN
2	C	10	ASN
2	A	354	HIS
1	D	501	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](#)

Of 5 ligands modelled in this entry, 2 are monoatomic - leaving 3 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	$\# Z  > 2$
6	GOL	C	501	-	5,5,5	0.30	0	5,5,5	0.52	0
7	6EJ	F	101[A]	-	31,38,38	1.04	2 (6%)	33,55,55	1.69	10 (30%)
7	6EJ	F	101[B]	-	31,38,38	0.97	2 (6%)	33,55,55	1.51	7 (21%)

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
6	GOL	C	501	-	-	0/4/4/4	0/0/0/0
7	6EJ	F	101[A]	-	-	0/9/34/34	0/5/6/6
7	6EJ	F	101[B]	-	-	0/9/34/34	0/5/6/6

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	F	101[A]	6EJ	C5-C34	-2.32	1.37	1.42
7	F	101[B]	6EJ	C5-C34	-2.29	1.37	1.42
7	F	101[B]	6EJ	C30-N31	2.08	1.34	1.32
7	F	101[A]	6EJ	C30-N31	2.36	1.34	1.32

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	F	101[B]	6EJ	C3-C2-C33	-3.17	121.41	124.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	F	101[A]	6EJ	F1-C2-C33	-2.50	115.46	118.03
7	F	101[A]	6EJ	C3-C2-C33	-2.40	122.08	124.16
7	F	101[A]	6EJ	C30-N31-N32	-2.23	117.86	119.42
7	F	101[B]	6EJ	C30-N31-N32	-2.15	117.91	119.42

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 [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	C	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	341:GLY	C	342[A]:ARG	N	1.13
1	C	341:GLY	C	342[B]:ARG	N	1.12

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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	B	189/202 (93%)	-0.46	0	100   100	11, 21, 37, 46	0
1	D	189/202 (93%)	-0.31	0	100   100	11, 26, 45, 58	0
2	A	483/490 (98%)	-0.54	0	100   100	7, 18, 34, 49	0
2	C	481/490 (98%)	-0.59	1 (0%)	95   96	8, 17, 33, 51	0
3	E	20/20 (100%)	-0.77	0	100   100	9, 19, 31, 36	1 (5%)
4	F	20/20 (100%)	-0.77	0	100   100	12, 21, 41, 53	1 (5%)
All	All	1382/1424 (97%)	-0.52	1 (0%)	95   96	7, 19, 38, 58	2 (0%)

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	436	LEU	2.3

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

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
7	6EJ	F	101[A]	33/33	0.95	0.16	3.20	21,23,34,34	33
6	GOL	C	501	6/6	0.91	0.16	3.14	27,30,36,39	0
7	6EJ	F	101[B]	33/33	0.95	0.16	1.50	19,21,23,25	33
5	MN	B	701	1/1	0.99	0.07	-2.04	14,14,14,14	0
5	MN	D	1001	1/1	0.99	0.06	-3.14	17,17,17,17	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.