

wwPDB X-ray Structure Validation Summary Report (i)

Oct 14, 2024 - 10:15 pm BST

PDB ID	:	9FZ6
Title	:	A 2.58A crystal structure of S. aureus DNA gyrase and DNA with metals
		identified through anomalous scattering
Authors	:	Morgan, H.; Duman, R.; Bax, B.D.; Warren, A.J.
Deposited on	:	2024-07-04
Resolution	:	2.58 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 A user guide is available at https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) 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 (1)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as 541 be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
buster-report	:	1.1.7(2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 2.58 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.



Motric	Whole archive	Similar resolution
	$(\# { m Entries})$	$(\# { m Entries}, { m resolution} { m range}({ m \AA}))$
R_{free}	164625	4456 (2.60-2.56)
Clashscore	180529	4905 (2.60-2.56)
Ramachandran outliers	177936	4847 (2.60-2.56)
Sidechain outliers	177891	4847 (2.60-2.56)
RSRZ outliers	164620	4456 (2.60-2.56)

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 >=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	А	483	83%	16%	•
1	С	483	82%	17%	•
2	В	190	88%	12%	
2	D	190	79%	19%	••
3	Е	8	62% 38%		_

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Mol	Chain	Length	Quality of chain						
3	F	8	75% 25%						
4	G	14	43%	36%	7%	14%			
4	Н	14	57%	29%		14%			



2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 11963 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 A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	А	483	Total 3870	C 2405	N 708	0 741	S 16	0	4	0
1	С	481	Total 3891	С 2417	N 713	0 744	S 17	0	8	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	123	PHE	TYR	engineered mutation	UNP P20831
А	457	THR	ALA	conflict	UNP P20831
С	123	PHE	TYR	engineered mutation	UNP P20831
С	457	THR	ALA	conflict	UNP P20831

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	2 B	100	Total	С	Ν	0	S	0	0	0
		190	1486	933	256	288	9	0	0	
0	р	190	Total	С	Ν	0	S	0	2	0
2 D	169	1492	935	257	291	9	0		0	

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
В	544	THR	-	linker	UNP P0A0K8
В	545	GLY	-	linker	UNP P0A0K8
D	544	THR	-	linker	UNP P0A0K8
D	545	GLY	-	linker	UNP P0A0K8

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	3 E	0	Total	С	Ν	Ο	Р	0	0	0
J		0	163	78	33	45	$\overline{7}$	0	0	
2	Б	0	Total	С	Ν	Ο	Р	0	0	0
J	3 F	0	163	78	33	45	7	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	4 G	19	Total	С	Ν	0	Р	0	1	0
4		12	266	126	48	79	13			
4	4 H	12	Total	С	Ν	0	Р	0	0	0
4			219	101	37	69	12	0	0	

• Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0
5	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0
5	С	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0
5	С	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 6 3 3 \end{array}$	0	0
5	С	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 6 3 3 \end{array}$	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	С	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0
5	Е	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0

• Molecule 6 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	В	1	Total Mn 1 1	0	0
6	С	1	Total Mn 1 1	0	1
6	D	1	Total Mn 1 1	0	0
6	G	1	Total Mn 1 1	0	0
6	Н	1	Total Mn 1 1	0	0

• Molecule 7 is 2-[BIS-(2-HYDROXY-ETHYL)-AMINO]-2-HYDROXYMETHYL-PROPAN E-1,3-DIOL (three-letter code: BTB) (formula: C₈H₁₉NO₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	C	1	Total	С	Ν	0	0	1
	1	28	16	2	10	0	1	



• Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	А	107	Total O 107 107	0	0
8	В	27	TotalO2727	0	0
8	С	137	Total O 137 137	0	0
8	D	29	TotalO2929	0	0
8	Е	6	Total O 6 6	0	0
8	F	9	Total O 9 9	0	0
8	G	11	Total O 12 12	0	1
8	Н	11	Total O 11 11	0	0



3 Residue-property plots (i)

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: DNA gyrase subunit A



D610 A611

DA DG G200 A201 C201: C201:

K417 R629 Y639 ALA



Chain E:	62%	38%	
A1 65 65			
• Molecule 3: D	NA (5'-D(*AP*GP*CP*CP*G	P*TP*AP*G)-3')	
Chain F:	75%	25%	
A1 68 68			
• Molecule 4: D	NA $(5'-D(*AP*GP*TP*AP*C$	P*CP*TP*AP*CP*GP*GP	*CP*T)-3')
Chain G:	43%	36% 7% 14%	

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

Chain H:	57%	29%	14%
DA DG C2009 A2011 A2011 C2012 C2013 C2013 T2020			



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61	Depositor
Cell constants	93.63Å 93.63Å 410.87Å	Deperitor
a, b, c, α , β , γ	90.00° 90.00° 120.00°	Depositor
$\mathbf{P}_{\text{acclution}}(\hat{\mathbf{A}})$	57.72 - 2.58	Depositor
Resolution (A)	57.72 - 2.58	EDS
% Data completeness	99.9 (57.72-2.58)	Depositor
(in resolution range)	99.8(57.72-2.58)	EDS
R_{merge}	0.23	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.64 (at 2.58 \text{\AA})$	Xtriage
Refinement program	PHENIX (1.21_5207: ???), REFMAC 5.8.0425	Depositor
D D.	0.140 , 0.200	Depositor
n, n_{free}	0.133 , 0.198	DCC
R_{free} test set	3166 reflections $(4.98%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	68.5	Xtriage
Anisotropy	0.037	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.29, 35.2	EDS
L-test for twinning ²	$< L >=0.40, < L^2>=0.23$	Xtriage
Estimated twinning fraction	0.479 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	11963	wwPDB-VP
Average B, all atoms $(Å^2)$	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 2.82% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



¹Intensities 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: MN, BTB, GOL

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).

Mal	Chain	Bond lengths		Bond angles		
	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.37	0/3918	0.65	0/5274	
1	С	0.35	0/3940	0.64	0/5304	
2	В	0.33	0/1510	0.63	0/2037	
2	D	0.32	0/1515	0.57	0/2045	
3	Е	0.61	0/183	1.11	0/281	
3	F	0.60	0/183	1.08	1/281~(0.4%)	
4	G	0.65	0/297	1.14	1/456~(0.2%)	
4	Н	0.59	0/243	1.14	0/373	
All	All	0.38	0/11789	0.69	2/16051~(0.0%)	

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	А	0	1
1	С	0	1
All	All	0	2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
3	F	4	DC	O4'-C4'-C3'	-6.94	101.72	104.50
4	G	2017	DG	O5'-P-OP2	-5.71	100.56	105.70

There are no chirality outliers.

All (2) planarity outliers are listed below:



Mol	Chain	Res	Type	Group
1	А	364	ARG	Sidechain
1	С	429	ARG	Sidechain

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	А	3870	0	3927	50	0
1	С	3891	0	3941	50	0
2	В	1486	0	1460	13	0
2	D	1492	0	1451	21	0
3	Е	163	0	91	3	0
3	F	163	0	91	1	0
4	G	266	0	147	7	0
4	Н	219	0	119	4	0
5	А	12	0	16	0	0
5	С	24	0	32	0	0
5	Е	6	0	8	1	0
6	В	1	0	0	0	0
6	С	1	0	0	0	0
6	D	1	0	0	0	0
6	G	1	0	0	0	0
6	Н	1	0	0	0	0
7	С	28	0	34	2	0
8	А	107	0	0	5	0
8	В	27	0	0	3	0
8	С	137	0	0	8	0
8	D	29	0	0	1	0
8	Е	6	0	0	0	0
8	F	9	0	0	0	0
8	G	12	0	0	2	0
8	Н	11	0	0	0	0
All	All	11963	0	11317	142	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 6.

The worst 5 of 142 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:D:460:LYS:NZ	8:D:801:HOH:O	2.02	0.85
1:C:94:ALA:O	8:C:1001:HOH:O	2.05	0.74
1:C:358:HIS:HD2	8:C:1087:HOH:O	1.71	0.74
1:C:62:LYS:O	1:C:127:ARG:NH1	2.24	0.70
2:D:447:ARG:NH1	2:D:452:GLN:O	2.24	0.70

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	ntiles
1	А	485/483~(100%)	460 (95%)	25~(5%)	0	100	100
1	С	487/483~(101%)	465~(96%)	22~(4%)	0	100	100
2	В	188/190~(99%)	182 (97%)	6 (3%)	0	100	100
2	D	187/190~(98%)	170 (91%)	15 (8%)	2 (1%)	12	25
All	All	1347/1346 (100%)	1277 (95%)	68 (5%)	2 (0%)	44	69

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	490	GLY
2	D	610	ASP

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	А	420/417~(101%)	416 (99%)	4 (1%)	73	87	
1	\mathbf{C}	423/417~(101%)	407~(96%)	16 (4%)	28	52	
2	В	156/158~(99%)	153~(98%)	3~(2%)	52	74	
2	D	157/158~(99%)	156~(99%)	1 (1%)	84	93	
All	All	1156/1150~(100%)	1132 (98%)	24 (2%)	52	71	

5 of 24 residues with a non-rotameric sidechain are listed below:

Mol	Chain	\mathbf{Res}	Type
1	С	284	LYS
1	С	299	ARG
1	С	287[B]	ASP
1	С	392	ASP
2	В	615	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	79	HIS
1	С	56	GLN
1	С	340	ASN
2	D	463	ASN
2	D	475	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 oligosaccharides in this entry.



5.6 Ligand geometry (i)

Of 14 ligands modelled in this entry, 5 are monoatomic - leaving 9 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).

Mal	Turne	Chain	Dec. Lin	Tink	Bo	ond leng	sths	B	ond ang	gles
1VIOI	туре	Unam	nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2
5	GOL	С	905	-	$5,\!5,\!5$	0.18	0	$5,\!5,\!5$	0.40	0
5	GOL	А	501	-	$5,\!5,\!5$	0.12	0	$5,\!5,\!5$	0.37	0
5	GOL	С	906	-	$5,\!5,\!5$	0.10	0	$5,\!5,\!5$	0.23	0
5	GOL	Е	101	-	$5,\!5,\!5$	0.06	0	$5,\!5,\!5$	0.19	0
5	GOL	С	903	-	$5,\!5,\!5$	0.12	0	$5,\!5,\!5$	0.37	0
5	GOL	А	502	-	$5,\!5,\!5$	0.12	0	$5,\!5,\!5$	0.24	0
7	BTB	С	902[B]	-	13,13,13	0.88	0	7,16,16	0.32	0
5	GOL	С	904	-	$5,\!5,\!5$	0.13	0	$5,\!5,\!5$	0.37	0
7	BTB	С	902[A]	6	13,13,13	0.83	0	7,16,16	0.37	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
5	GOL	С	905	-	-	2/4/4/4	-
5	GOL	А	501	-	-	2/4/4/4	-
5	GOL	С	906	-	-	0/4/4/4	-
5	GOL	Е	101	-	-	0/4/4/4	-
5	GOL	С	903	-	-	1/4/4/4	-
5	GOL	А	502	-	-	0/4/4/4	-
7	BTB	С	902[B]	-	-	2/21/21/21	-
5	GOL	С	904	-	-	2/4/4/4	-
7	BTB	С	902[A]	6	-	4/21/21/21	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.



Mol	Chain	Res	Type	Atoms
5	А	501	GOL	O1-C1-C2-C3
5	С	904	GOL	C1-C2-C3-O3
7	С	902[A]	BTB	O1-C1-C2-C3
7	С	902[A]	BTB	O1-C1-C2-C4
7	С	902[A]	BTB	O1-C1-C2-N

5 of 13 torsion outliers are listed below:

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	Е	101	GOL	1	0
7	С	902[A]	BTB	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









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	D	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	545:GLY	С	580:TYR	N	3.31



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 $>$	#RSRZ>2			$\mathbf{OWAB}(\mathrm{\AA}^2)$	Q<0.9
1	А	483/483~(100%)	-1.63	0	100	100	25, 59, 82, 106	4 (0%)
1	С	481/483~(99%)	-1.63	0	100	100	24,60,81,97	8 (1%)
2	В	190/190~(100%)	-1.59	0	100	100	47, 68, 91, 123	0
2	D	189/190~(99%)	-1.42	0	100	100	52, 83, 116, 155	2(1%)
3	Е	8/8~(100%)	-2.03	0	100	100	54, 60, 62, 67	0
3	F	8/8~(100%)	-2.08	0	100	100	54,62,73,76	0
4	G	12/14~(85%)	-1.90	0	100	100	49, 60, 109, 127	1 (8%)
4	Н	12/14~(85%)	-1.87	0	100	100	41, 66, 131, 132	0
All	All	1383/1390 (99%)	-1.61	0	100	100	24, 63, 93, 155	15 (1%)

There are no RSRZ outliers to report.

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^{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.



$9F_{2}$	Z6
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	GOL	С	906	6/6	0.96	0.05	104,110,121,126	0
5	GOL	С	905	6/6	0.98	0.06	62,69,78,80	0
5	GOL	С	903	6/6	0.99	0.06	76,84,92,98	0
5	GOL	С	904	6/6	0.99	0.05	117,122,126,129	0
5	GOL	А	501	6/6	0.99	0.03	68,84,85,90	0
5	GOL	А	502	6/6	0.99	0.07	68,74,82,89	0
5	GOL	Е	101	6/6	0.99	0.06	94,99,105,109	0
6	MN	С	901[A]	1/1	0.99	0.05	60,60,60,60	1
6	MN	G	2101	1/1	0.99	0.03	89,89,89,89	1
7	BTB	С	902[A]	14/14	0.99	0.07	57,59,61,63	14
7	BTB	С	902[B]	14/14	0.99	0.07	160,182,187,190	14
6	MN	Н	2101	1/1	1.00	0.02	98,98,98,98	1
6	MN	D	701	1/1	1.00	0.01	59, 59, 59, 59, 59	0
6	MN	В	701	1/1	1.00	0.03	50, 50, 50, 50	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.





























6.5 Other polymers (i)

There are no such residues in this entry.

