

wwPDB X-ray Structure Validation Summary Report (i)

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PDB ID	:	5GKI
Title	:	Structure of EndoMS-dsDNA3 complex
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Deposited on	:	2016-07-04
Resolution	:	2.90 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:

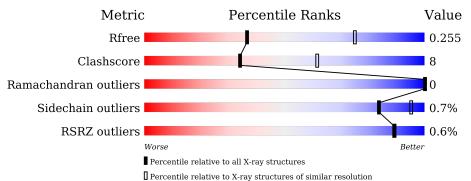
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.90 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R _{free}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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	252	79%	15%	5%
1	В	252	% 74%	21%	5%
2	С	15	40% 60%		
3	D	15	40% 60%		



2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 5075 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 Endonuclease EndoMS.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	Δ	239	Total	С	Ν	0	S	0	0	0
	A	239	1900	1202	337	357	4	0	0	0
1	р	239	Total	С	Ν	0	S	0	0	0
	D	239	1900	1202	337	357	4	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	165	ALA	ASP	engineered mutation	UNP Q5JER9
В	165	ALA	ASP	engineered mutation	UNP Q5JER9

• Molecule 2 is a DNA chain called DNA (5'-D(*GP*CP*CP*TP*AP*GP*GP*TP*CP*CP* CP*GP*TP*CP*C)-3').

Mol	Chain	Residues		A	toms			ZeroOcc	AltConf	Trace
2	С	15	Total 598	C 286	N 104	0 180	Р 28	0	15	0

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

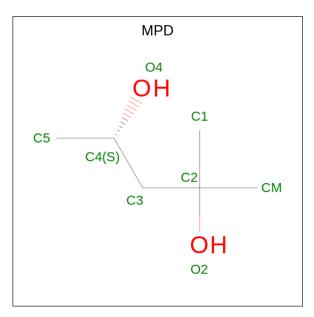
Mol	Chain	Residues		A	toms			ZeroOcc	AltConf	Trace
3	D	15	Total 622	C 292	N 128	0 174	Р 28	0	15	0

• Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	1	Total Mg 1 1	0	0
4	В	1	Total Mg 1 1	0	0



• Molecule 5 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 8 & 6 & 2 \end{array}$	0	0
5	С	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 8 & 6 & 2 \end{array}$	0	0
5	С	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 8 & 6 & 2 \end{array}$	0	0
5	С	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 8 6 2 \end{array}$	0	0

• Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	А	6	Total O 6 6	0	0
6	В	11	Total O 11 11	0	0
6	С	1	Total O 1 1	0	0
6	D	3	Total O 3 3	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.

Chain A:	79%	15%	5%
MET 22 120 121 131 140 140 140 140 144 140	K71 W77 Q78 Q78 B81 E87 E88 R89 P101 P101 P101 F113 V115 F113 F115 F115	N142 F154 F154 F157 V164 V164 V164 V166 N174 V166	E178 E178 K181 K194 K194 S195
Y196 Y197 E199 1199 X207 X207 X207 X207 X207 X207 X207 X203 1298 C228 C228 C228 C228 C228 C228 C228 C	R240 R240 SER LYS LYS GLY GLY GLY LYS LYS LYS LEU PHE		
• Molecule 1: Endon	uclease EndoMS		
Chain B:	74%	21%	5%
MET 82 83 17 17 19 12 813 813 813 813 813	R44 D42 D42 S47 E48 S61 S63 S63 S63 S63 F74 M77 P74 P77 P77 P77 P77 P77 P78 P80	L86 E87 E87 E87 E87 E87 C98 K100 K100 E10 E110	M114 V115 S116 F123 E132 E132
A133 E134 E134 E144 L153 L167 C168 C168 C168 C168 E179 E179	4192 1193 1194 1195 195 195 1200 1228 420 1228 420 1228 420 1228 4240 1228 1228 1228 1228 1228 1228 1228 122	LYS GLY ARG CLN CLN CLN LYS LLU LLU PHE	
• Molecule 2: DNA)	(5'-D(*GP*CP*CP*TP*AI	P*GP*GP*TP*CP*(CP*CP*GP*TP*CP*C)-3'
Chain C:	40%	60%	
01 05 06 07 01 113 113 113 011 113 011 113 011 113 011 113 011 113 011 113 011 113 011 113 011 113 011 113 01 01 01 01 01 01 01 01 01 01 01 01 01			
• Molecule 3: DNA ((5'-D(*GP*GP*AP*CP*GI	P*GP*GP*GP*CP*(CP*TP*AP*GP*GP*C)-3'
Chain D:	40%	60%	
61 65 66 66 66 61 710 613 711 613 711 613 711 613			

• Molecule 1: Endonuclease EndoMS



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants	92.03Å 92.03Å 405.35Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 120.00°	Depositor
Resolution (Å)	24.72 - 2.90	Depositor
Resolution (A)	24.72 - 2.90	EDS
% Data completeness	96.5 (24.72-2.90)	Depositor
(in resolution range)	93.6 (24.72-2.90)	EDS
R _{merge}	(Not available)	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$9.10 (at 2.89 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
D D.	0.182 , 0.255	Depositor
R, R_{free}	0.186 , 0.255	DCC
R_{free} test set	1212 reflections (5.12%)	wwPDB-VP
Wilson B-factor $(Å^2)$	38.0	Xtriage
Anisotropy	0.377	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.37, 54.4	EDS
L-test for twinning ²	$ < L >=0.47, < L^2>=0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5075	wwPDB-VP
Average B, all atoms $(Å^2)$	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.20% 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: MG, MPD

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
	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.47	0/1929	0.65	0/2599
1	В	0.49	0/1929	0.68	0/2599
2	С	0.77	0/666	0.93	0/1022
3	D	0.78	0/700	0.82	0/1080
All	All	0.57	0/5224	0.73	0/7300

There are no bond length outliers.

There are no bond angle outliers.

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	А	1900	0	1969	31	0
1	В	1900	0	1969	35	0
2	С	598	0	318	10	0
3	D	622	0	309	14	0
4	А	1	0	0	0	0
4	В	1	0	0	0	0
5	А	8	0	14	0	0
5	С	24	0	42	4	0
6	А	6	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	В	11	0	0	0	0
6	С	1	0	0	0	0
6	D	3	0	0	0	0
All	All	5075	0	4621	74	0

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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 8.

The worst 5 of 74 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:B:13:SER:HB3	1:B:16:GLU:HG3	1.65	0.78
1:B:179:GLU:OE2	1:B:192:GLN:NE2	2.20	0.74
1:A:77:TRP:O	3:D:8[B]:DG:N1	2.28	0.66
1:A:181:LYS:NZ	2:C:6[B]:DG:OP1	2.30	0.64
1:B:194:LYS:HD2	1:B:228:GLU:HG3	1.80	0.64

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	237/252~(94%)	224 (94%)	13~(6%)	0	100	100
1	В	237/252~(94%)	226~(95%)	11 (5%)	0	100	100
All	All	474/504~(94%)	450 (95%)	24~(5%)	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 side chain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles		
1	А	210/222~(95%)	209 (100%)	1 (0%)	88 96		
1	В	210/222~(95%)	208~(99%)	2(1%)	76 92		
All	All	420/444~(95%)	417 (99%)	3 (1%)	84 95		

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	100	LYS
1	В	63	SER
1	В	132	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	В	192	GLN

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 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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	Turne	Chain	Res	Link	B	ond leng	gths	B	ond ang	gles
IVIOI	Type	Unam	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2
5	MPD	С	101	-	7,7,7	0.57	0	9,10,10	1.33	2 (22%)
5	MPD	С	103	-	7,7,7	0.42	0	9,10,10	0.63	0
5	MPD	С	102	-	7,7,7	0.44	0	9,10,10	0.95	0
5	MPD	А	302	-	7,7,7	0.51	0	9,10,10	0.63	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	MPD	С	101	-	-	2/5/5/5	-
5	MPD	С	103	-	-	4/5/5/5	-
5	MPD	С	102	-	-	0/5/5/5	-
5	MPD	А	302	-	-	3/5/5/5	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
5	С	101	MPD	CM-C2-C1	-2.55	105.27	110.57
5	С	101	MPD	CM-C2-C3	2.26	120.49	109.96

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	А	302	MPD	C2-C3-C4-O4
5	С	101	MPD	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
5	С	103	MPD	O2-C2-C3-C4
5	А	302	MPD	O2-C2-C3-C4
5	С	103	MPD	C1-C2-C3-C4

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	С	101	MPD	2	0
5	С	103	MPD	1	0
5	С	102	MPD	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^{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	$\langle RSRZ \rangle$	#RSRZ>2	$\mathbf{OWAB}(\mathrm{\AA}^2)$	$\mathbf{Q} \! < \! 0.9$
1	А	239/252~(94%)	-0.54	1 (0%) 92 93	11, 26, 54, 107	0
1	В	239/252~(94%)	-0.53	2 (0%) 86 86	6, 24, 57, 95	0
2	С	15/15~(100%)	-0.41	0 100 100	16, 21, 46, 47	0
3	D	15/15~(100%)	-0.40	0 100 100	16, 20, 46, 47	0
All	All	508/534~(95%)	-0.53	3 (0%) 89 89	6, 25, 54, 107	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	А	2	SER	9.4
1	В	2	SER	7.6
1	В	123	TYR	2.6

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.



Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\operatorname{B-factors}(\operatorname{\AA}^2)$	Q < 0.9
5	MPD	С	103	8/8	0.91	0.21	22,46,62,64	0
5	MPD	А	302	8/8	0.92	0.15	7,24,35,56	0
5	MPD	С	102	8/8	0.93	0.18	$9,\!22,\!50,\!52$	0
5	MPD	С	101	8/8	0.93	0.15	$13,\!31,\!35,\!58$	0
4	MG	А	301	1/1	0.96	0.26	13,13,13,13	0
4	MG	В	301	1/1	0.96	0.24	9,9,9,9	0

6.5 Other polymers (i)

There are no such residues in this entry.

