



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 12:09 AM GMT

PDB ID : 1MLX
Title : Crystal Structure Analysis of a 2'-O-[2-(Methylthio)-ethyl]-Modified Oligodeoxynucleotide Duplex
Authors : Prakash, T.P.; Manoharan, M.; Kawasaki, A.M.; Fraser, A.S.; Lesnik, E.A.; Sioufi, N.; Leeds, J.M.; Teplova, M.; Egli, M.
Deposited on : 2002-08-31
Resolution : 1.25 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

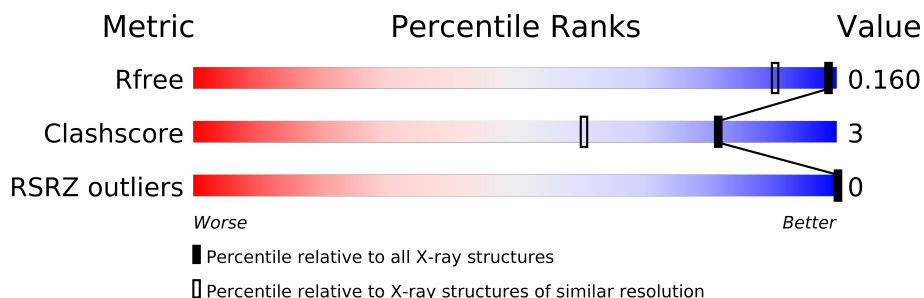
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 1.25 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}	66092	1021 (1.30-1.22)
Clashscore	79885	1125 (1.30-1.22)
RSRZ outliers	66119	1021 (1.30-1.22)

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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	10	
1	B	10	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 781 atoms, of which 224 are hydrogens and 0 are deuterium.

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 DNA chain called 5'-D(*GP*CP*GP*TP*AP*SMTP*AP*CP*GP*C)-3'.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	10	Total	C	H	N	O	P	0	0	0
			316	98	112	38	59	9			
1	B	10	Total	C	H	N	O	P	S	0	0
			319	100	112	38	59	9	1		

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	84	Total	O	0	0
			84	84		
2	B	62	Total	O	0	0
			62	62		

3 Residue-property plots

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: 5'-D(*GP*CP*GP*TP*AP*SMTP*AP*CP*GP*C)-3'

Chain A: 

G1	C2	G3	T4	A5	T6	A7	C8	G9	C10
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- Molecule 1: 5'-D(*GP*CP*GP*TP*AP*SMTP*AP*CP*GP*C)-3'

Chain B: 

G111	C112	G113	T114	A115	T116	A117	G118	G119	C120
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4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	24.73Å 44.47Å 46.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 1.25 19.58 – 1.25	Depositor EDS
% Data completeness (in resolution range)	(Not available) (15.00-1.25) 93.3 (19.58-1.25)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.70 (at 1.25Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.141 , (Not available) 0.149 , 0.160	Depositor DCC
R_{free} test set	1360 reflections (11.05%)	DCC
Wilson B-factor (Å ²)	16.2	Xtriage
Anisotropy	0.202	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.43 , 68.3	EDS
Estimated twinning fraction	0.018 for -h,l,k	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	1 of 14080 reflections (0.007%)	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	781	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.26% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SMT

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	2.83	18/203 (8.9%)	2.99	31/309 (10.0%)
1	B	2.87	18/203 (8.9%)	2.94	29/309 (9.4%)
All	All	2.85	36/406 (8.9%)	2.97	60/618 (9.7%)

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	114	DT	C5-C6	-9.91	1.27	1.34
1	B	111	DG	N9-C8	8.87	1.44	1.37
1	A	8	DC	C5-C6	-7.99	1.27	1.34
1	A	4	DT	C5-C7	-7.82	1.45	1.50
1	B	115	DA	N1-C2	-7.74	1.27	1.34
1	A	3	DG	O4'-C1'	7.03	1.50	1.42
1	A	9	DG	C6-N1	6.87	1.44	1.39
1	B	119	DG	C2'-C1'	-6.75	1.45	1.52
1	A	8	DC	C4-N4	-6.68	1.27	1.33
1	B	117	DA	C8-N7	6.61	1.36	1.31
1	B	117	DA	C6-N1	6.56	1.40	1.35
1	B	111	DG	N3-C4	-6.51	1.30	1.35
1	B	119	DG	N7-C5	6.51	1.43	1.39
1	A	5	DA	N1-C2	6.50	1.40	1.34
1	A	2	DC	C4-C5	6.26	1.48	1.43
1	A	7	DA	C6-N1	-6.26	1.31	1.35
1	A	10	DC	C2-N3	6.24	1.40	1.35
1	B	120	DC	C4-C5	6.24	1.48	1.43
1	A	10	DC	C2-O2	-6.18	1.18	1.24
1	B	113	DG	C2-N3	-6.01	1.27	1.32
1	A	9	DG	C8-N7	5.75	1.34	1.30
1	A	7	DA	C6-N6	5.66	1.38	1.33
1	B	113	DG	C8-N7	-5.65	1.27	1.30
1	B	111	DG	N7-C5	5.64	1.42	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1	DG	O4'-C1'	5.63	1.49	1.42
1	B	119	DG	N9-C4	-5.62	1.33	1.38
1	B	113	DG	N1-C2	5.61	1.42	1.37
1	B	115	DA	N7-C5	5.59	1.42	1.39
1	B	111	DG	O4'-C1'	5.58	1.49	1.42
1	A	1	DG	N9-C4	-5.53	1.33	1.38
1	B	119	DG	O4'-C1'	5.44	1.48	1.42
1	A	3	DG	C2'-C1'	-5.29	1.47	1.52
1	A	9	DG	C2-N3	-5.21	1.28	1.32
1	A	9	DG	C2-N2	5.08	1.39	1.34
1	B	115	DA	C6-N1	5.06	1.39	1.35
1	A	9	DG	N9-C4	-5.03	1.33	1.38

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	112	DC	C6-N1-C2	-14.21	114.61	120.30
1	A	9	DG	N1-C2-N3	13.09	131.75	123.90
1	B	112	DC	C5-C6-N1	12.20	127.10	121.00
1	A	9	DG	C6-N1-C2	-10.09	119.05	125.10
1	B	111	DG	C2-N3-C4	9.95	116.88	111.90
1	A	3	DG	N1-C2-N3	9.93	129.85	123.90
1	A	5	DA	N1-C2-N3	-9.22	124.69	129.30
1	A	8	DC	O4'-C4'-C3'	-8.66	100.81	106.00
1	A	9	DG	N3-C2-N2	-8.32	114.08	119.90
1	B	112	DC	C4-C5-C6	-8.12	113.34	117.40
1	A	9	DG	N1-C6-O6	-7.93	115.14	119.90
1	A	3	DG	C6-N1-C2	-7.92	120.35	125.10
1	A	1	DG	C6-N1-C2	-7.92	120.35	125.10
1	A	1	DG	C5-N7-C8	-7.70	100.45	104.30
1	B	113	DG	O4'-C4'-C3'	-7.62	101.43	106.00
1	B	114	DT	C5-C6-N1	7.60	128.26	123.70
1	B	117	DA	C8-N9-C4	7.56	108.82	105.80
1	A	1	DG	N1-C2-N3	7.25	128.25	123.90
1	A	3	DG	C2-N3-C4	-7.22	108.29	111.90
1	A	1	DG	P-O3'-C3'	7.08	128.19	119.70
1	B	114	DT	O4'-C4'-C3'	-7.02	101.69	104.50
1	A	3	DG	C8-N9-C4	6.98	109.19	106.40
1	B	113	DG	N7-C8-N9	6.91	116.56	113.10
1	A	3	DG	N7-C8-N9	-6.87	109.67	113.10
1	B	111	DG	N1-C2-N3	-6.85	119.79	123.90
1	B	113	DG	C8-N9-C4	-6.84	103.66	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1	DG	N7-C8-N9	6.84	116.52	113.10
1	B	111	DG	O4'-C1'-N9	-6.83	103.22	108.00
1	B	119	DG	P-O5'-C5'	6.65	131.54	120.90
1	A	5	DA	N7-C8-N9	-6.54	110.53	113.80
1	A	1	DG	N3-C4-C5	-6.35	125.42	128.60
1	A	5	DA	C5-N7-C8	6.33	107.06	103.90
1	A	7	DA	C6-N1-C2	6.29	122.37	118.60
1	B	111	DG	C6-C5-N7	-6.26	126.64	130.40
1	B	117	DA	N9-C4-C5	-6.11	103.36	105.80
1	A	3	DG	O4'-C1'-N9	-6.05	103.77	108.00
1	A	9	DG	C5-C6-O6	6.01	132.20	128.60
1	B	111	DG	C5-C6-N1	-5.98	108.51	111.50
1	B	119	DG	C1'-O4'-C4'	-5.85	104.25	110.10
1	B	119	DG	O4'-C4'-C3'	-5.85	102.16	104.50
1	A	8	DC	C2-N3-C4	-5.84	116.98	119.90
1	A	3	DG	C5-C6-N1	5.80	114.40	111.50
1	A	1	DG	O4'-C1'-N9	-5.79	103.94	108.00
1	A	3	DG	C5-N7-C8	5.76	107.18	104.30
1	B	114	DT	C6-N1-C2	-5.69	118.45	121.30
1	A	7	DA	C2-N3-C4	-5.69	107.76	110.60
1	B	112	DC	N1-C2-N3	5.63	123.14	119.20
1	A	7	DA	O4'-C4'-C3'	-5.54	102.29	104.50
1	B	111	DG	N7-C8-N9	-5.46	110.37	113.10
1	B	112	DC	N1-C2-O2	-5.44	115.63	118.90
1	A	4	DT	C4-C5-C6	-5.43	114.74	118.00
1	B	117	DA	N3-C4-C5	5.42	130.59	126.80
1	B	115	DA	N9-C4-C5	5.27	107.91	105.80
1	B	114	DT	N3-C4-O4	-5.23	116.76	119.90
1	B	119	DG	N1-C2-N3	-5.21	120.77	123.90
1	A	9	DG	C4-C5-N7	-5.20	108.72	110.80
1	A	9	DG	O4'-C1'-N9	-5.19	104.36	108.00
1	B	119	DG	C5-C6-O6	5.14	131.69	128.60
1	B	117	DA	C2-N3-C4	-5.14	108.03	110.60
1	B	119	DG	N1-C6-O6	-5.11	116.84	119.90

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens

added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	204	112	0	1	0
1	B	207	112	0	1	0
2	A	84	0	0	0	0
2	B	62	0	0	0	0
All	All	557	224	0	2	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 3.

All (2) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:116:SMT:SC	1:B:116:SMT:CD	2.13	1.35
1:A:1:DG:H3'	1:A:1:DG:HO5'	1.81	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

There are no protein chains in this entry.

5.3.2 Protein sidechains ⓘ

There are no protein chains in this entry.

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

2 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
1	SMT	A	6	1	20,23,27	2.37	7 (35%)	25,33,39	3.10	7 (28%)
1	SMT	B	116	1	24,26,27	2.18	8 (33%)	29,36,39	4.45	10 (34%)

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
1	SMT	A	6	1	-	0/8/27/31	0/2/2/2
1	SMT	B	116	1	-	0/11/30/31	0/2/2/2

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	6	SMT	O2'-C2'	-6.99	1.38	1.46
1	B	116	SMT	CD-SC	5.54	2.13	1.78
1	B	116	SMT	O2'-CA'	4.43	1.55	1.42
1	A	6	SMT	P-OP1	4.09	1.51	1.46
1	A	6	SMT	O4'-C1'	3.76	1.47	1.41
1	B	116	SMT	C6-C5	-3.23	1.31	1.40
1	B	116	SMT	C2-N3	-3.01	1.31	1.37
1	B	116	SMT	P-OP1	2.99	1.50	1.46
1	B	116	SMT	C2-N1	-2.67	1.35	1.38
1	A	6	SMT	C4-N3	2.63	1.41	1.37
1	B	116	SMT	O4'-C1'	2.45	1.45	1.41
1	A	6	SMT	C5A-C5	-2.16	1.46	1.51
1	B	116	SMT	O4'-C4'	2.13	1.50	1.45
1	A	6	SMT	C2'-C1'	-2.06	1.49	1.52
1	A	6	SMT	C2-N3	-2.00	1.33	1.37

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	116	SMT	C6-N1-C2	-16.13	117.83	122.41
1	B	116	SMT	CD-SC-CB	14.59	154.67	100.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	6	SMT	C6-N1-C2	-11.39	119.17	122.41
1	A	6	SMT	C5-C6-N1	7.25	128.64	121.59
1	B	116	SMT	C5-C6-N1	5.28	126.72	121.59
1	B	116	SMT	N3-C2-N1	4.04	119.35	115.97
1	A	6	SMT	C2-N1-C1'	-3.73	115.87	118.21
1	A	6	SMT	O2'-C2'-C1'	3.71	117.29	107.39
1	B	116	SMT	O2'-CA'-CB	-3.37	95.19	109.50
1	B	116	SMT	C5A-C5-C6	3.31	125.63	118.59
1	A	6	SMT	C5A-C5-C6	2.75	124.43	118.59
1	B	116	SMT	C5A-C5-C4	-2.70	118.29	121.04
1	B	116	SMT	C2-N1-C1'	2.67	119.88	118.21
1	B	116	SMT	C4'-O4'-C1'	-2.42	107.12	109.75
1	A	6	SMT	C6-N1-C1'	2.23	124.87	119.33
1	A	6	SMT	C4'-O4'-C1'	-2.19	107.37	109.75
1	B	116	SMT	O2'-C2'-C1'	2.10	112.66	108.78

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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 ⓘ

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, 95th 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 ²)	Q<0.9
1	A	10/10 (100%)	-0.44	0 100 100	15, 17, 20, 24	0
1	B	10/10 (100%)	-0.60	0 100 100	17, 19, 20, 27	0
All	All	20/20 (100%)	-0.52	0 100 100	15, 18, 24, 27	0

There are no RSRZ outliers to report.

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

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, 95th 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
1	SMT	A	6	22/26	0.06	1.15	14,20,29,29	0
1	SMT	B	116	25/26	0.06	0.65	14,18,27,51	0

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.