

Full wwPDB X-ray Structure Validation Report (i)

Oct 5, 2023 - 06:05 AM EDT

PDB ID	:	6VYP
Title	:	Crystal structure of the LSD1/CoREST histone demethylase bound to its nu-
		cleosome substrate
Authors	:	Kim, S.; Zhu, J.; Eek, P.; Yennawar, N.; Song, T.
Deposited on		
Resolution	:	4.99 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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	:	FAILED
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.99 Å.

There are no overall percentile quality scores available for this entry.

MolProbity and EDS failed to run properly - the sequence quality summary graphics cannot be shown.



2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 52996 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.

Mol	Chain	Residues		At	oms		ZeroOcc	AltConf	Trace	
1	А	110	Total	С	Ν	0	S	0	0	0
	A	110	893	559	174	156	4	0	0	0
1	Е	110	Total	С	Ν	0	S	0	0	0
	Ľ	110	889	557	174	154	4	0	0	0
1	9	94	Total	С	Ν	0	S	0	0	0
	a	94	774	489	147	135	3	0	0	0
1	0	103	Total	С	Ν	0	S	0	0	0
	е	105	836	525	158	149	4	0	U	0

• Molecule 1 is a protein called Histone H3.

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	4	MET	LYS	engineered mutation	UNP A0A310TTQ1
Е	4	MET	LYS	engineered mutation	UNP A0A310TTQ1
a	4	MET	LYS	engineered mutation	UNP A0A310TTQ1
е	4	MET	LYS	engineered mutation	UNP A0A310TTQ1

• Molecule 2 is a protein called Histone H4.

Mol	Chain	Residues		At	oms		ZeroOcc	AltConf	Trace	
2	В	81	Total	С	Ν	0	S	0	0	0
	D	01	648	410	126	111	1	0	0	0
2	F	78	Total	С	Ν	0	S	0	0	0
	Г	10	619	391	120	107	1	0	0	0
2	h	80	Total	С	Ν	0	S	0	0	0
	b	80	638	401	125	111	1	0	0	0
2	f	78	Total	С	Ν	0	S	0	0	0
	1	10	619	391	120	107	1	0	0	0

• Molecule 3 is a protein called Histone H2A type 1.



Mol	Chain	Residues		Ato	ms		ZeroOcc	AltConf	Trace	
3	С	103	Total	С	Ν	Ο	0	0	0	
0	U	100	795	501	155	139	0	0	0	
3	G	105	Total	С	Ν	Ο	0	0	0	
0	G	105	809	510	158	141	0	0	U	
3		103	Total	С	Ν	Ο	0	0	0	
0	с	105	795	501	155	139	0	0	0	
3	ŝ	104	Total	С	Ν	Ο	0	0	0	
0	g 1	104	804	507	157	140		0	U	

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
С	99	ARG	GLY	engineered mutation	UNP P06897
С	123	SER	ALA	engineered mutation	UNP P06897
G	99	ARG	GLY	engineered mutation	UNP P06897
G	123	SER	ALA	engineered mutation	UNP P06897
с	99	ARG	GLY	engineered mutation	UNP P06897
с	123	SER	ALA	engineered mutation	UNP P06897
g	99	ARG	GLY	engineered mutation	UNP P06897
g	123	SER	ALA	engineered mutation	UNP P06897

• Molecule 4 is a protein called Histone H2B 1.1.

Mol	Chain	Residues		At	oms		ZeroOcc	AltConf	Trace	
4	Л	92	Total	С	Ν	0	S	0	0	0
4	D	92	719	453	129	135	2	0	0	0
4	Н	93	Total	С	Ν	0	S	0	0	0
4	11	90	726	457	130	137	2	0	0	0
4	d	91	Total	С	Ν	0	S	0	0	0
4	d	91	708	447	125	134	2	0	0	0
4	h	93	Total	С	Ν	Ο	S	0	0	0
4	h	90	726	457	130	137	2	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	29	THR	SER	engineered mutation	UNP P02281
Н	29	THR	SER	engineered mutation	UNP P02281
d	29	THR	SER	engineered mutation	UNP P02281
h	29	THR	SER	engineered mutation	UNP P02281

• Molecule 5 is a DNA chain called DNA (191-MER).



Mol	Chain	Residues		А	toms		ZeroOcc	AltConf	Trace	
5	Ι	191	Total 3895		N 710	0 1145	Р 191	0	0	0
5	i	191	Total 3895	-	N 710	0 1145	Р 191	0	0	0

• Molecule 6 is a DNA chain called DNA (191-MER).

Mol	Chain	Residues		А	toms		ZeroOcc	AltConf	Trace	
6	J	191	Total 3936	C 1863		0 1147	Р 191	0	0	0
6	j	191	Total 3936	C 1863		0 1147	Р 191	0	0	0

• Molecule 7 is a protein called Lysine-specific histone demethylase 1A.

Mol	Chain	Residues		At	oms		ZeroOcc	AltConf	Trace	
7	М	666	Total	С	Ν	0	S	0	0	0
1	111	000	5205	3319	902	964	20	0	0	0
7	m	666	Total	С	Ν	0	S	0	0	0
1	m	000	5205	3319	902	964	20	0	0	0
7	K	666	Total	С	Ν	0	S	0	0	0
1	Γ	000	5205	3319	902	964	20	0	0	0
7	ŀ	666	Total	С	Ν	Ο	S	0	0	0
1	k	000	5205	3319	902	964	20	0	0	0

There are 20 discrepancies between the modelled and reference sequences:

Residue	Modelled	Actual	Comment	Reference
169	GLY	-	expression tag	UNP O60341
170	SER	-	expression tag	UNP O60341
608	ALA	ARG	engineered mutation	UNP O60341
717	ALA	ASN	engineered mutation	UNP O60341
721	ALA	ASP	engineered mutation	UNP O60341
169	GLY	-	expression tag	UNP O60341
170	SER	-	expression tag	UNP O60341
608	ALA	ARG	engineered mutation	UNP O60341
717	ALA	ASN	engineered mutation	UNP O60341
721	ALA	ASP	engineered mutation	UNP O60341
169	GLY	-	expression tag	UNP O60341
170	SER	-	expression tag	UNP O60341
608	ALA	ARG	engineered mutation	UNP O60341
717	ALA	ASN	engineered mutation	UNP O60341
721	ALA	ASP	engineered mutation	UNP O60341
	$ \begin{array}{r} 169 \\ 170 \\ 608 \\ 717 \\ 721 \\ 169 \\ 170 \\ 608 \\ 717 \\ 721 \\ 169 \\ 170 \\ 608 \\ 717 \\ 721 \\ 169 \\ 170 \\ 608 \\ 717 \\ 717 \\ 721 \\ $	169 GLY 170 SER 608 ALA 717 ALA 721 ALA 169 GLY 170 SER 608 ALA 721 ALA 169 GLY 170 SER 608 ALA 717 ALA 721 ALA 721 ALA 169 GLY 170 SER 608 ALA 717 ALA 169 GLY 170 SER 608 ALA 717 ALA	169 GLY - 170 SER - 608 ALA ARG 717 ALA ASN 721 ALA ASP 169 GLY - 170 SER - 608 ALA ASP 169 GLY - 170 SER - 608 ALA ARG 717 ALA ASN 721 ALA ASN 169 GLY - 170 SER - 608 ALA ARG 717 ALA ASN	169GLY-expression tag170SER-expression tag608ALAARGengineered mutation717ALAASNengineered mutation721ALAASPengineered mutation169GLY-expression tag170SER-expression tag608ALAARGengineered mutation717ALAASNengineered mutation717ALAASNengineered mutation711ALAASNengineered mutation721ALAASPengineered mutation710SER-expression tag169GLY-expression tag170SER-expression tag170ALAARGengineered mutation717ALAARGengineered mutation717ALAARGengineered mutation717ALAARGengineered mutation

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Chain	Residue	Modelled	Actual	Comment	Reference					
k	169	GLY	-	expression tag	UNP O60341					
k	170	SER	-	expression tag	UNP O60341					
k	608	ALA	ARG	engineered mutation	UNP O60341					
k	717	ALA	ASN	engineered mutation	UNP O60341					
k	721	ALA	ASP	engineered mutation	UNP O60341					

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• Molecule 8 is a protein called REST corepressor 1.

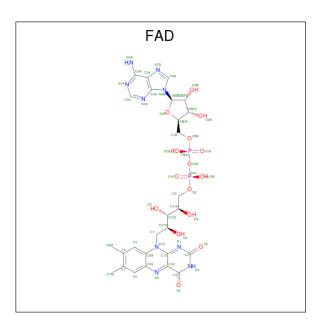
Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
8	Ν	133	Total	С	Ν	Ο	\mathbf{S}	0	0	0
0	IN	155	1076	676	194	203	3	0	0	0
8	n	133	Total	С	Ν	0	S	0	0	0
0	n	100	1076	676	194	203	3	0	0	0
8	т	133	Total	С	Ν	0	S	0	0	0
0		199	1076	676	194	203	3	0	0	0
8	1	133	Total	С	Ν	0	S	0	0	0
0	I	133	1076	676	194	203	3	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
N	284	GLY	-	expression tag	UNP Q9UKL0
N	285	SER	-	expression tag	UNP Q9UKL0
n	284	GLY	-	expression tag	UNP Q9UKL0
n	285	SER	-	expression tag	UNP Q9UKL0
L	284	GLY	-	expression tag	UNP Q9UKL0
L	285	SER	-	expression tag	UNP Q9UKL0
1	284	GLY	-	expression tag	UNP Q9UKL0
1	285	SER	-	expression tag	UNP Q9UKL0

• Molecule 9 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).





Mol	Chain	Residues		Atoms				ZeroOcc	AltConf	
9	М	1	Total	С	Ν	Ο	Р	0	0	
9	IVI	1	53	27	9	15	2	0	0	
9	m	1	Total	С	Ν	Ο	Р	0	0	
9	m	1	53	27	9	15	2	0	0	
9	K	1	Total	С	Ν	Ο	Р	0	0	
9	Λ	1	53	27	9	15	2	0	0	
0	1-	1	Total	С	Ν	Ο	Р	0	0	
9	k	1	53	27	9	15	2	0	0	

MolProbity and EDS failed to run properly - this section is therefore empty.



3 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	103.77Å 335.77Å 174.63Å	Depositor
a, b, c, α , β , γ	90.00° 91.07° 90.00°	Depositor
Resolution (Å)	20.17 - 4.99	Depositor
% Data completeness	99.3 (20.17-4.99)	Depositor
(in resolution range)	· · · · · · · · · · · · · · · · · · ·	-
R_{merge}	0.08	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.25 (at 4.97 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.15.2_3472	Depositor
R, R_{free}	0.229 , 0.277	Depositor
Wilson B-factor $(Å^2)$	309.0	Xtriage
Anisotropy	0.119	Xtriage
L-test for twinning ²	$< L > = 0.42, < L^2 > = 0.25$	Xtriage
Estimated twinning fraction	0.165 for h,-k,-l	Xtriage
Total number of atoms	52996	wwPDB-VP
Average B, all atoms $(Å^2)$	415.0	wwPDB-VP

EDS failed to run properly - this section is therefore incomplete.

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 2.43% 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.

4 Model quality (i)

4.1 Standard geometry (i)

MolProbity failed to run properly - this section is therefore empty.

4.2 Too-close contacts (i)

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles (i)

4.3.1 Protein backbone (i)

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains (i)

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA (i)

MolProbity failed to run properly - this section is therefore empty.

4.4 Non-standard residues in protein, DNA, RNA chains (i)

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

4.5 Carbohydrates (i)

There are no monosaccharides in this entry.

4.6 Ligand geometry (i)

4 ligands 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



Mol	Turne	Chain	Res	Link	Bond lengths			Bond angles		
10101	Type	Chain	nes	LIIIK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
9	FAD	К	900	-	53,58,58	0.48	0	68,89,89	0.54	2 (2%)
9	FAD	m	900	-	53,58,58	0.46	0	68,89,89	0.53	2 (2%)
9	FAD	k	900	-	53,58,58	0.54	0	68,89,89	0.60	1 (1%)
9	FAD	М	900	-	53,58,58	0.45	0	68,89,89	0.51	2 (2%)

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).

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
9	FAD	К	900	-	-	13/30/50/50	0/6/6/6
9	FAD	m	900	-	-	15/30/50/50	0/6/6/6
9	FAD	k	900	-	-	18/30/50/50	0/6/6/6
9	FAD	М	900	-	-	15/30/50/50	0/6/6/6

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
9	m	900	FAD	P-O3P-PA	-2.60	123.90	132.83
9	Κ	900	FAD	P-O3P-PA	-2.52	124.17	132.83
9	М	900	FAD	P-O3P-PA	-2.43	124.50	132.83
9	М	900	FAD	C5A-C6A-N6A	2.29	123.83	120.35
9	Κ	900	FAD	C5A-C6A-N6A	2.28	123.82	120.35
9	k	900	FAD	C5A-C6A-N6A	2.28	123.82	120.35
9	m	900	FAD	C5A-C6A-N6A	2.27	123.80	120.35

There are no chirality outliers.

All (61) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	М	900	FAD	C5B-O5B-PA-O1A
9	М	900	FAD	C5B-O5B-PA-O2A
9	М	900	FAD	C3'-C4'-C5'-O5'

Continued on next page...



9 M 900 FAD $O4'-C4'-C5'-O5'$ 9 M 900 FAD $C5'-O5'-P-O1P$ 9 M 900 FAD $C5'-O5'-P-O2P$ 9 M 900 FAD $C5'-O5'-P-O3P$ 9 m 900 FAD $C5B-O5B-PA-O1A$ 9 m 900 FAD $C3'-C4'-C5'-O5'$ 9 m 900 FAD $C3'-C4'-C5'-O5'$ 9 m 900 FAD $C5'-O5'-P-O1P$ 9 m 900 FAD $C5'-O5'-P-O3P$ 9 M 900 FAD $C5'-O5'-P-O3P$ 9 M 900 FAD C5B-O5B-PA-O2A 9 K 900 FAD C5B-O5B-PA-O2A 9 K 900 FAD N10-C1'-C2'-C2' 9 K 900 FAD C5B-O5B-PA-O3P 9 k 900 FAD C1'-C2'-C3'-C3' 9 k	Mol	nued fron Chain	Res	Type	Atoms
9 M 900 FAD $C5'-O5'-P-O1P$ 9 M 900 FAD $C5'-O5'-P-O3P$ 9 m 900 FAD $C5B-O5B-PA-O1A$ 9 m 900 FAD $C5B-O5B-PA-O2A$ 9 m 900 FAD $C3'-C4'-C5'-O5'$ 9 m 900 FAD $C3'-C4'-C5'-O5'$ 9 m 900 FAD $C5'-O5'-P-O1P$ 9 m 900 FAD $C5'-O5'-P-O2P$ 9 m 900 FAD $C5'-O5'-P-O3P$ 9 M 900 FAD $C5'-O5'-P-O3P$ 9 M 900 FAD C5B-O5B-PA-O2A 9 K 900 FAD C4B-C5B-O5B-PA-O3P 9 K 900 FAD N10-C1'-C2'-C3' 9 K 900 FAD C5B-O5B-PA-O3P 9 k 900 FAD C1'-C2'-C3' 9 K 9					
9 M 900 FAD $C5^{\circ}-O5^{\circ}-P-O2P$ 9 M 900 FAD $C5^{\circ}-O5^{\circ}-P-O3P$ 9 m 900 FAD $C5B-O5B-PA-O1A$ 9 m 900 FAD $C3^{\circ}-C4^{\circ}-C5^{\circ}-O5^{\circ}$ 9 m 900 FAD $C3^{\circ}-C4^{\circ}-C5^{\circ}-O5^{\circ}$ 9 m 900 FAD $C5^{\circ}-O5^{\circ}-P-O1P$ 9 m 900 FAD $C5^{\circ}-O5^{\circ}-P-O2P$ 9 m 900 FAD $C5^{\circ}-O5^{\circ}-P-O2P$ 9 M 900 FAD $C5^{\circ}-O5^{\circ}-P-O3P$ 9 K 900 FAD C5B-O5B-PA-O2A 9 K 900 FAD N10-C1^{\circ}-C2^{\circ}-O3^{\circ} 9 K 900 FAD N10-C1^{\circ}-C2^{\circ}-O3^{\circ} 9 K 900 FAD C5B-O5B-PA-O3P 9 k 900 FAD C1^{\circ}-C2^{\circ}-C3^{\circ} 9 k 900 FAD C1^{\circ					
9 M 900 FAD $C5^{\circ}-O5^{\circ}-P-O3P$ 9 m 900 FAD $C5B-O5B-PA-O1A$ 9 m 900 FAD $C3^{\circ}-C4^{\circ}-C5^{\circ}-O5^{\circ}$ 9 m 900 FAD $C3^{\circ}-C4^{\circ}-C5^{\circ}-O5^{\circ}$ 9 m 900 FAD $C5^{\circ}-O5^{\circ}-P-O1P$ 9 m 900 FAD $C5^{\circ}-O5^{\circ}-P-O2P$ 9 m 900 FAD $C5^{\circ}-O5^{\circ}-P-O3P$ 9 M 900 FAD $C5B-O5B-PA-O2A$ 9 M 900 FAD C5B-O5B-PA-O3P 9 K 900 FAD C4B-C5B-O5B-PA 9 K 900 FAD N10-C1^{\circ}-C2^{\circ}-O3^{\circ} 9 K 900 FAD C5B-O5B-PA-O3P 9 k 900 FAD C10-C1^{\circ}-C2^{\circ}-O3^{\circ} 9 k 900 FAD C1^{\circ}-C2^{\circ}-O3^{\circ} 9 k 900 FAD C1^{\circ}-C2^{\circ}-C3^		-			
9 m 900 FAD C5B-05B-PA-01A 9 m 900 FAD C5B-05B-PA-02A 9 m 900 FAD C3'-C4'-C5'-O5' 9 m 900 FAD O4'-C4'-C5'-O5' 9 m 900 FAD C5'-O5'-P-01P 9 m 900 FAD C5'-O5'-P-03P 9 M 900 FAD C5B-05B-PA-02A 9 M 900 FAD C5B-05B-PA-03P 9 K 900 FAD C4B-C5B-05B-PA 9 K 900 FAD N10-C1'-C2'-02' 9 K 900 FAD N10-C1'-C2'-C3' 9 k 900 FAD N10-C1'-C2'-C3' 9 k 900 FAD N10-C1'-C2'-C3' 9 k 900 FAD N10-C1'-C2'-C3'-C3' 9 k 900 FAD N10-C1'-C2'-C3'-C3' 9 k 900 </td <td></td> <td></td> <td></td> <td></td> <td></td>					
9 m 900 FAD C5B-05B-PA-02A 9 m 900 FAD C3'-C4'-C5'-O5' 9 m 900 FAD C4'-C5'-O5' 9 m 900 FAD C5'-O5'-P-O1P 9 m 900 FAD C5'-O5'-P-O3P 9 M 900 FAD C5B-05B-PA-02A 9 K 900 FAD C5B-05B-PA-02A 9 K 900 FAD C4B-C5B-05B-PA-03P 9 K 900 FAD N10-C1'-C2'-C3' 9 K 900 FAD N10-C1'-C2'-C3' 9 k 900 FAD C5B-05B-PA-03P 9 k 900 FAD C1'-C2'-C3' 9 k 900 FAD N10-C1'-C2'-C3' 9 k 900 FAD N10-C1'-C2'-C3'-C3' 9 k 900 FAD C1'-C2'-C3'-C4'-O4' 9 k 900					
9 m 900 FAD $O4'-C4'-C5'-O5'$ 9 m 900 FAD $C5'-O5'-P-O1P$ 9 m 900 FAD $C5'-O5'-P-O2P$ 9 m 900 FAD $C5'-O5'-P-O3P$ 9 K 900 FAD $C5B-O5B-PA-O2A$ 9 K 900 FAD $C5B-O5B-PA-O3P$ 9 K 900 FAD $C4B-C5B-O5B-PA-O3P$ 9 K 900 FAD N10-C1'-C2'-C3' 9 K 900 FAD N10-C1'-C2'-C3' 9 k 900 FAD C5B-O5B-PA-O3P 9 k 900 FAD C1'-C2'-C3' 9 k 900 FAD C1'-C2'-C3' 9 k 900 FAD N10-C1'-C2'-C3' 9 k 900 FAD C1'-C2'-C3'-C4'-O4' 9 k 900 FAD C1'-C2'-C3'-C4'-O4' 9 k	9	m		FAD	C5B-O5B-PA-O2A
9 m 900 FAD $C5'-O5'-P-O1P$ 9 m 900 FAD $C5'-O5'-P-O2P$ 9 m 900 FAD $C5B-O5B-PA-O2A$ 9 K 900 FAD $C5B-O5B-PA-O2A$ 9 K 900 FAD $C5B-O5B-PA-O3P$ 9 K 900 FAD $C4B-C5B-O5B-PA-O2A$ 9 K 900 FAD N10-C1'-C2'-C3' 9 K 900 FAD N10-C1'-C2'-C3' 9 k 900 FAD C5B-O5B-PA-O2A 9 k 900 FAD C5B-O5B-PA-O2A 9 k 900 FAD C1'-C2'-C3' 9 k 900 FAD N10-C1'-C2'-C3' 9 k 900 FAD N10-C1'-C2'-C3'-O4' 9 k 900 FAD C1'-C2'-C3'-C4'-O4' 9 k 900 FAD O3'-C3'-C4'-O4' 9 k	9	m			C3'-C4'-C5'-O5'
9m900FAD $C5'-O5'-P-O2P$ 9m900FAD $C5B-O5B-PA-O2A$ 9K900FAD $C5B-O5B-PA-O3P$ 9K900FAD $C4B-C5B-O5B-PA-O3P$ 9K900FAD $N10-C1'-C2'-O2'$ 9K900FAD $N10-C1'-C2'-O2'$ 9K900FAD $N10-C1'-C2'-C3'$ 9k900FAD $C5B-O5B-PA-O2A$ 9k900FAD $C5B-O5B-PA-O2A$ 9k900FAD $C2'-C1'-N10-C10$ 9k900FAD $C2'-C1'-N10-C10$ 9k900FAD $N10-C1'-C2'-C3'$ 9k900FAD $N10-C1'-C2'-C3'$ 9k900FAD $C1'-C2'-C3'-C4'$ 9k900FAD $C1'-C2'-C3'-C4'-C4'$ 9k900FAD $C2'-C3'-C4'-C4'$ 9k900FAD $O3'-C3'-C4'-C4'$ 9k900FAD $O3'-C3'-C4'-C4'$ 9M900FAD $O4B-C4B-C5B-O5B$ 9K900FAD $O4B-C4B-C5B-O5B$ 9K900FAD $C2'-C3'-C4'-O4'$ 9M900FAD $O4B-C4B-C5B-O5B$ 9K900FAD $O3'-C3'-C4'-O4'$ 9M900FAD $O3'-C3'-C4'-C5'$ 9M900FAD $O3'-C3'-C4'-C5'$ 9M900FAD $O3'-C3'-$	9	m	900	FAD	O4'-C4'-C5'-O5'
9 m 900 FAD C5'-O5'-P-O3P 9 K 900 FAD C5B-O5B-PA-O2A 9 K 900 FAD C5B-O5B-PA-O3P 9 K 900 FAD C4B-C5B-O5B-PA 9 K 900 FAD N10-C1'-C2'-O2' 9 K 900 FAD N10-C1'-C2'-C3' 9 k 900 FAD C5B-O5B-PA-O2A 9 k 900 FAD C5B-O5B-PA-O2A 9 k 900 FAD C2'-C1'-N10-C10 9 k 900 FAD N10-C1'-C2'-C3' 9 k 900 FAD N10-C1'-C2'-C3' 9 k 900 FAD C1'-C2'-C3'-C4' 9 k 900 FAD C2'-C3'-C4'-O4' 9 k 900 FAD O3'-C3'-C4'-O4' 9 k 900 FAD O3'-C3'-C4'-O4' 9 M 900	9	m	900	FAD	C5'-O5'-P-O1P
9 K 900 FAD C5B-O5B-PA-O2A 9 K 900 FAD C4B-C5B-O5B-PA 9 K 900 FAD N10-C1'-C2'-O2' 9 K 900 FAD N10-C1'-C2'-C3' 9 K 900 FAD N10-C1'-C2'-C3' 9 k 900 FAD C5B-O5B-PA-O2A 9 k 900 FAD C5B-O5B-PA-O2A 9 k 900 FAD C5B-O5B-PA-O3P 9 k 900 FAD C2'-C1'-N10-C10 9 k 900 FAD N10-C1'-C2'-C3' 9 k 900 FAD N10-C1'-C2'-C3'-C4' 9 k 900 FAD C1'-C2'-C3'-C4'-O4' 9 k 900 FAD C2'-C3'-C4'-C5' 9 k 900 FAD O3'-C3'-C4'-O4' 9 k 900 FAD O3'-C3'-C4'-O4' 9 M 90	9	m	900	FAD	C5'-O5'-P-O2P
9 K 900 FAD C5B-O5B-PA-O2A 9 K 900 FAD C4B-C5B-O5B-PA 9 K 900 FAD N10-C1'-C2'-O2' 9 K 900 FAD N10-C1'-C2'-C3' 9 K 900 FAD N10-C1'-C2'-C3' 9 k 900 FAD C5B-O5B-PA-O2A 9 k 900 FAD C5B-O5B-PA-O2A 9 k 900 FAD C5B-O5B-PA-O3P 9 k 900 FAD C2'-C1'-N10-C10 9 k 900 FAD N10-C1'-C2'-C3' 9 k 900 FAD N10-C1'-C2'-C3'-C4' 9 k 900 FAD C1'-C2'-C3'-C4'-O4' 9 k 900 FAD C2'-C3'-C4'-C5' 9 k 900 FAD O3'-C3'-C4'-O4' 9 k 900 FAD O3'-C3'-C4'-O4' 9 M 90	9	m	900	FAD	C5'-O5'-P-O3P
9K900FADC4B-C5B-O5B-PA9K900FADN10-C1'-C2'-O2'9K900FADN10-C1'-C2'-C3'9k900FADC5B-O5B-PA-O2A9k900FADC5B-O5B-PA-O3P9k900FADC2'-C1'-N10-C109k900FADN10-C1'-C2'-C3'9k900FADN10-C1'-C2'-C3'9k900FADN10-C1'-C2'-C3'-C4'9k900FADC1'-C2'-C3'-C4'9k900FADC2'-C3'-C4'-C4'9k900FADC2'-C3'-C4'-C5'9k900FADO3'-C3'-C4'-C5'9k900FADO3'-C3'-C4'-C4'9k900FADO3'-C3'-C4'-C4'9M900FADO4B-C4B-C5B-O5B9K900FADC2'-C3'-C4'-C4'9M900FADC2'-C3'-C4'-C4'9M900FADC2'-C3'-C4'-C4'9M900FADC2'-C3'-C4'-C5'9M900FADC2'-C3'-C4'-C5'9M900FADC2'-C3'-C4'-C5'9M900FADC2'-C3'-C4'-C5'9M900FADC2'-C3'-C4'-C5'9M900FADC2'-C3'-C4'-C5'9M900FADC2'-C3'-C4'-C5'9M900 <td>9</td> <td></td> <td>900</td> <td></td> <td>C5B-O5B-PA-O2A</td>	9		900		C5B-O5B-PA-O2A
9K900FADC4B-C5B-O5B-PA9K900FADN10-C1'-C2'-O2'9K900FADN10-C1'-C2'-C3'9k900FADC5B-O5B-PA-O2A9k900FADC5B-O5B-PA-O3P9k900FADC2'-C1'-N10-C109k900FADN10-C1'-C2'-C3'9k900FADN10-C1'-C2'-C3'9k900FADN10-C1'-C2'-C3'-C4'9k900FADC1'-C2'-C3'-C4'9k900FADC2'-C3'-C4'-O4'9k900FADC2'-C3'-C4'-C5'9k900FADO3'-C3'-C4'-C5'9k900FADO3'-C3'-C4'-O4'9k900FADO3'-C3'-C4'-O4'9M900FADO4B-C4B-C5B-O5B9K900FADC2'-C3'-C4'-O4'9M900FADC2'-C3'-C4'-O4'9M900FADC2'-C3'-C4'-O4'9M900FADC2'-C3'-C4'-O4'9M900FADC2'-C3'-C4'-O4'9M900FADC2'-C3'-C4'-O4'9M900FADC2'-C3'-C4'-C5'9M900FADC2'-C3'-C4'-C5'9M900FADC2'-C3'-C4'-C5'9M900FADC2'-C3'-C4'-C5'9M900 <td>9</td> <td>K</td> <td></td> <td></td> <td>C5B-O5B-PA-O3P</td>	9	K			C5B-O5B-PA-O3P
9 K 900 FAD N10-C1'-C2'-O2' 9 K 900 FAD N10-C1'-C2'-C3' 9 k 900 FAD C5B-O5B-PA-O2A 9 k 900 FAD C5B-O5B-PA-O3P 9 k 900 FAD C2'-C1'-N10-C10 9 k 900 FAD N10-C1'-C2'-C3' 9 k 900 FAD N10-C1'-C2'-C3' 9 k 900 FAD C1'-C2'-C3'-C4' 9 k 900 FAD C1'-C2'-C3'-C4'-O4' 9 k 900 FAD C2'-C3'-C4'-C5' 9 k 900 FAD C2'-C3'-C4'-C4' 9 k 900 FAD O3'-C3'-C4'-C4' 9 k 900 FAD O3'-C3'-C4'-C4' 9 M 900 FAD O3'-C3'-C4'-O4' 9 M 900 FAD O4B-C4B-C5B-O5B 9 K 900	9	K			C4B-C5B-O5B-PA
9 k 900 FAD C5B-05B-PA-02A 9 k 900 FAD C5B-05B-PA-03P 9 k 900 FAD C2'-C1'-N10-C10 9 k 900 FAD N10-C1'-C2'-O2' 9 k 900 FAD N10-C1'-C2'-C3' 9 k 900 FAD C1'-C2'-C3'-O4' 9 k 900 FAD C1'-C2'-C3'-C4'-Q4' 9 k 900 FAD C2'-C3'-C4'-O4' 9 k 900 FAD O3'-C3'-C4'-O4' 9 k 900 FAD O3'-C3'-C4'-O4' 9 k 900 FAD O3'-C3'-C4'-O4' 9 M 900 FAD O3'-C3'-C4'-O4' 9 M 900 FAD O3'-C3'-C4'-O4' 9 M 900 FAD O4B-C4B-C5B-O5B 9 K 900 FAD C3B-C4B-C5B-O5B 9 M 900	9	K	900	FAD	N10-C1'-C2'-O2'
9k900FADC5B-O5B-PA-O3P9k900FADC2'-C1'-N10-C109k900FADN10-C1'-C2'-O2'9k900FADN10-C1'-C2'-C3'9k900FADC1'-C2'-C3'-O3'9k900FADC1'-C2'-C3'-C4'9k900FADC2'-C3'-C4'-O4'9k900FADC2'-C3'-C4'-C5'9k900FADO3'-C3'-C4'-C5'9k900FADO3'-C3'-C4'-C5'9k900FADO3'-C3'-C4'-O4'9m900FADO3'-C3'-C4'-O4'9m900FADO4B-C4B-C5B-O5B9M900FADO4B-C4B-C5B-O5B9K900FADC2'-C3'-C4'-O4'9M900FADC2'-C3'-C4'-O4'9M900FADC2'-C3'-C4'-O4'9M900FADC2'-C3'-C4'-O4'9M900FADC2'-C3'-C4'-O4'9M900FADO3'-C3'-C4'-C5'9M900FADO3'-C3'-C4'-C5'9M900FADC2'-C3'-C4'-C5'9M900FADC2'-C3'-C4'-C5'9M900FADC2'-C3'-C4'-C5'9M900FADC2'-C3'-C4'-C5'9M900FADC2'-C3'-C4'-C5'9M900	9	K	900	FAD	N10-C1'-C2'-C3'
9k900FAD $C2'-C1'-N10-C10$ 9k900FAD $N10-C1'-C2'-O2'$ 9k900FAD $N10-C1'-C2'-C3'$ 9k900FAD $C1'-C2'-C3'-O3'$ 9k900FAD $C1'-C2'-C3'-C4'$ 9k900FAD $C2'-C3'-C4'-O4'$ 9k900FAD $C2'-C3'-C4'-O4'$ 9k900FAD $O3'-C3'-C4'-O4'$ 9k900FAD $O3'-C3'-C4'-O4'$ 9k900FAD $O3'-C3'-C4'-O4'$ 9M900FAD $O3'-C3'-C4'-O4'$ 9M900FAD $O3'-C3'-C4'-O4'$ 9M900FAD $O4B-C4B-C5B-O5B$ 9K900FAD $O4B-C4B-C5B-O5B$ 9K900FAD $C2'-C3'-C4'-O4'$ 9M900FAD $C2'-C3'-C4'-O4'$ 9M900FAD $C2'-C3'-C4'-O4'$ 9M900FAD $C2'-C3'-C4'-O4'$ 9M900FAD $O3'-C3'-C4'-C5'$ 9M900FAD $O3'-C3'-C$	9	k	900	FAD	C5B-O5B-PA-O2A
9k900FADN10-C1'-C2'-O2'9k900FADN10-C1'-C2'-C3'9k900FADC1'-C2'-C3'-O3'9k900FADC1'-C2'-C3'-C4'9k900FADC2'-C3'-C4'-O4'9k900FADC2'-C3'-C4'-O4'9k900FADC2'-C3'-C4'-O4'9k900FADO3'-C3'-C4'-O4'9k900FADO3'-C3'-C4'-O4'9M900FADO3'-C3'-C4'-O4'9M900FADO3'-C3'-C4'-O4'9M900FADO4B-C4B-C5B-O5B9K900FADO4B-C4B-C5B-O5B9K900FADC2'-C3'-C4'-O4'9M900FADC2'-C3'-C4'-O4'9M900FADC2'-C3'-C4'-O4'9M900FADC2'-C3'-C4'-O4'9M900FADC2'-C3'-C4'-O4'9M900FADO3'-C3'-C4'-C5'9M900FADO3'-C3'-C4'-C5'9M900FADO3'-C3'-C4'-C5'9M900FADO3'-C3'-C4'-C5'9M900FADO3'-C3'-C4'-C5'9M900FADC2'-C3'-C4'-C5'9M900FADC2'-C3'-C4'-C5'9M900FADC3B-C4B-C5B-O5B9M900 <td>9</td> <td>k</td> <td>900</td> <td>FAD</td> <td>C5B-O5B-PA-O3P</td>	9	k	900	FAD	C5B-O5B-PA-O3P
9 k 900 FAD N10-C1'-C2'-C3' 9 k 900 FAD C1'-C2'-C3'-O3' 9 k 900 FAD C1'-C2'-C3'-C4' 9 k 900 FAD C2'-C3'-C4'-O4' 9 k 900 FAD C2'-C3'-C4'-O4' 9 k 900 FAD C2'-C3'-C4'-C5' 9 k 900 FAD O3'-C3'-C4'-O4' 9 k 900 FAD O3'-C3'-C4'-O4' 9 k 900 FAD O3'-C3'-C4'-O4' 9 M 900 FAD O3'-C3'-C4'-O4' 9 m 900 FAD O3'-C3'-C4'-O4' 9 M 900 FAD O4B-C4B-C5B-O5B 9 K 900 FAD C3B-C4B-C5B-O5B 9 K 900 FAD O4B-C4B-C5B-O5B 9 M 900 FAD C2'-C3'-C4'-O4' 9 M 900 </td <td>9</td> <td>k</td> <td>900</td> <td>FAD</td> <td>C2'-C1'-N10-C10</td>	9	k	900	FAD	C2'-C1'-N10-C10
9 k 900 FAD C1'-C2'-C3'-O3' 9 k 900 FAD C1'-C2'-C3'-C4' 9 k 900 FAD C2'-C3'-C4'-O4' 9 k 900 FAD C2'-C3'-C4'-O4' 9 k 900 FAD C2'-C3'-C4'-C5' 9 k 900 FAD O3'-C3'-C4'-C4' 9 k 900 FAD O3'-C3'-C4'-O4' 9 M 900 FAD O4B-C4B-C5B-O5B 9 K 900 FAD C4B-C4B-C5B-O5B 9 K 900 FAD O4B-C4B-C5B-O5B 9 M 900 FAD C2'-C3'-C4'-O4' 9 M 900 FAD O3'-C3'-C4'-C5' 9 M 900 </td <td>9</td> <td>k</td> <td>900</td> <td>FAD</td> <td>N10-C1'-C2'-O2'</td>	9	k	900	FAD	N10-C1'-C2'-O2'
9 k 900 FAD C1'-C2'-C3'-C4' 9 k 900 FAD C2'-C3'-C4'-O4' 9 k 900 FAD C2'-C3'-C4'-O4' 9 k 900 FAD C2'-C3'-C4'-C5' 9 k 900 FAD O3'-C3'-C4'-O4' 9 k 900 FAD O3'-C3'-C4'-O4' 9 M 900 FAD O4B-C4B-C5B-O5B 9 K 900 FAD C3B-C4B-C5B-O5B 9 K 900 FAD C3B-C4B-C5B-O5B 9 M 900 FAD C2'-C3'-C4'-O4' 9 M 900 FAD C2'-C3'-C4'-O4' 9 M 900 FAD O3'-C3'-C4'-C5' 9 M 900 </td <td>9</td> <td>k</td> <td>900</td> <td>FAD</td> <td>N10-C1'-C2'-C3'</td>	9	k	900	FAD	N10-C1'-C2'-C3'
9 k 900 FAD C2'-C3'-C4'-O4' 9 k 900 FAD C2'-C3'-C4'-C5' 9 k 900 FAD O3'-C3'-C4'-O4' 9 k 900 FAD O3'-C3'-C4'-O4' 9 k 900 FAD O3'-C3'-C4'-O4' 9 M 900 FAD O4B-C4B-C5B-O5B 9 K 900 FAD C3B-C4B-C5B-O5B 9 K 900 FAD C3B-C4B-C5B-O5B 9 M 900 FAD C2'-C3'-C4'-O4' 9 M 900 FAD C2'-C3'-C4'-C5' 9 M 900 FAD O3'-C3'-C4'-C5' 9 M 900 </td <td>9</td> <td>k</td> <td>900</td> <td>FAD</td> <td>C1'-C2'-C3'-O3'</td>	9	k	900	FAD	C1'-C2'-C3'-O3'
9 k 900 FAD C2'-C3'-C4'-C5' 9 k 900 FAD O3'-C3'-C4'-O4' 9 k 900 FAD O3'-C3'-C4'-O4' 9 M 900 FAD O4B-C4B-C5B-O5B 9 K 900 FAD C3B-C4B-C5B-O5B 9 K 900 FAD C3B-C4B-C5B-O5B 9 K 900 FAD C3B-C4B-C5B-O5B 9 M 900 FAD C2'-C3'-C4'-O4' 9 m 900 FAD C2'-C3'-C4'-C5' 9 M 900 FAD O3'-C3'-C4'-C5' 9 M 900 FAD O3'-C3'-C4'-C5' 9 M 900 </td <td>9</td> <td>k</td> <td>900</td> <td>FAD</td> <td>C1'-C2'-C3'-C4'</td>	9	k	900	FAD	C1'-C2'-C3'-C4'
9 k 900 FAD O3'-C3'-C4'-O4' 9 k 900 FAD O3'-C3'-C4'-C5' 9 M 900 FAD O3'-C3'-C4'-O4' 9 m 900 FAD O3'-C3'-C4'-O4' 9 m 900 FAD O3'-C3'-C4'-O4' 9 m 900 FAD O4B-C4B-C5B-O5B 9 K 900 FAD O4B-C4B-C5B-O5B 9 K 900 FAD C3B-C4B-C5B-O5B 9 K 900 FAD O4B-C4B-C5B-O5B 9 K 900 FAD C3B-C4B-C5B-O5B 9 M 900 FAD C2'-C3'-C4'-O4' 9 m 900 FAD C2'-C3'-C4'-O4' 9 M 900 FAD O3'-C3'-C4'-C5' 9 M 900 FAD O4B-C4B-C5B-O5B 9 M 900 FAD O4B-C4B-C5B-O5B 9 m 900 </td <td>9</td> <td>k</td> <td>900</td> <td>FAD</td> <td>C2'-C3'-C4'-O4'</td>	9	k	900	FAD	C2'-C3'-C4'-O4'
9 k 900 FAD O3'-C3'-C4'-C5' 9 M 900 FAD O3'-C3'-C4'-O4' 9 m 900 FAD O3'-C3'-C4'-O4' 9 M 900 FAD O3'-C3'-C4'-O4' 9 M 900 FAD O4B-C4B-C5B-O5B 9 K 900 FAD O4B-C4B-C5B-O5B 9 K 900 FAD C3B-C4B-C5B-O5B 9 K 900 FAD C3B-C4B-C5B-O5B 9 K 900 FAD O4B-C4B-C5B-O5B 9 M 900 FAD C2'-C3'-C4'-O4' 9 m 900 FAD C2'-C3'-C4'-O4' 9 m 900 FAD O3'-C3'-C4'-C5' 9 M 900 FAD O4B-C4B-C5B-O5B 9 M 900 FAD O4B-C4B-C5B-O5B 9 m 900 FAD O3'-C3'-C4'-C5' 9 m 900 </td <td>9</td> <td>k</td> <td>900</td> <td>FAD</td> <td>C2'-C3'-C4'-C5'</td>	9	k	900	FAD	C2'-C3'-C4'-C5'
9 M 900 FAD O3'-C3'-C4'-O4' 9 m 900 FAD O3'-C3'-C4'-O4' 9 M 900 FAD O4B-C4B-C5B-O5B 9 K 900 FAD O4B-C4B-C5B-O5B 9 K 900 FAD C3B-C4B-C5B-O5B 9 K 900 FAD C3B-C4B-C5B-O5B 9 k 900 FAD O4B-C4B-C5B-O5B 9 k 900 FAD C2'-C3'-C4'-O4' 9 M 900 FAD C2'-C3'-C4'-O4' 9 M 900 FAD C2'-C3'-C4'-O4' 9 M 900 FAD C2'-C3'-C4'-C5' 9 M 900 FAD O3'-C3'-C4'-C5' 9 M 900 FAD O4B-C4B-C5B-O5B 9 m 900 FAD O3'-C3'-C4'-C5' 9 m 900 FAD O3'-C3'-C4'-C5' 9 m 900 FAD C2'-C3'-C4'-C5' 9 m 900 FAD	9	k	900	FAD	O3'-C3'-C4'-O4'
9 m 900 FAD O3'-C3'-C4'-O4' 9 M 900 FAD O4B-C4B-C5B-O5B 9 K 900 FAD O4B-C4B-C5B-O5B 9 K 900 FAD C3B-C4B-C5B-O5B 9 K 900 FAD C3B-C4B-C5B-O5B 9 k 900 FAD C3B-C4B-C5B-O5B 9 k 900 FAD C4B-C4B-C5B-O5B 9 M 900 FAD C2'-C3'-C4'-O4' 9 m 900 FAD C2'-C3'-C4'-O4' 9 M 900 FAD C2'-C3'-C4'-C5' 9 M 900 FAD C2'-C3'-C4'-C5' 9 M 900 FAD O4B-C4B-C5B-O5B 9 m 900 FAD O4B-C4B-C5B-O5B 9 m 900 FAD O3'-C3'-C4'-C5' 9 m 900 FAD C2'-C3'-C4'-C5' 9 m 900 </td <td>9</td> <td>k</td> <td>900</td> <td>FAD</td> <td>O3'-C3'-C4'-C5'</td>	9	k	900	FAD	O3'-C3'-C4'-C5'
9 M 900 FAD O4B-C4B-C5B-O5B 9 K 900 FAD O4B-C4B-C5B-O5B 9 K 900 FAD C3B-C4B-C5B-O5B 9 k 900 FAD O4B-C4B-C5B-O5B 9 k 900 FAD O4B-C4B-C5B-O5B 9 k 900 FAD O4B-C4B-C5B-O5B 9 M 900 FAD C2'-C3'-C4'-O4' 9 m 900 FAD C2'-C3'-C4'-O4' 9 M 900 FAD O3'-C3'-C4'-C5' 9 M 900 FAD O4B-C4B-C5B-O5B 9 M 900 FAD O4B-C4B-C5B-O5B 9 m 900 FAD O4B-C4B-C5B-O5B 9 m 900 FAD O3'-C3'-C4'-C5' 9 m 900 FAD O3'-C3'-C4'-C5' 9 m 900 FAD C2'-C3'-C4'-C5' 9 M 900 FAD C2'-C3'-C4'-C5' 9 M 900 FAD	9	М	900	FAD	O3'-C3'-C4'-O4'
9 K 900 FAD O4B-C4B-C5B-O5B 9 K 900 FAD C3B-C4B-C5B-O5B 9 k 900 FAD O4B-C4B-C5B-O5B 9 M 900 FAD O4B-C4B-C5B-O5B 9 M 900 FAD C2'-C3'-C4'-O4' 9 m 900 FAD C2'-C3'-C4'-O4' 9 M 900 FAD O3'-C3'-C4'-C5' 9 M 900 FAD C2'-C3'-C4'-C5' 9 M 900 FAD O4B-C4B-C5B-O5B 9 M 900 FAD O2'-C3'-C4'-C5' 9 m 900 FAD O4B-C4B-C5B-O5B 9 m 900 FAD O4B-C4B-C5B-O5B 9 m 900 FAD O3'-C3'-C4'-C5' 9 m 900 FAD C2'-C3'-C4'-C5' 9 M 900 FAD C2'-C3'-C4'-C5' 9 M 900 FAD C3B-C4B-C5B-O5B	9	m	900	FAD	O3'-C3'-C4'-O4'
9 K 900 FAD C3B-C4B-C5B-O5B 9 k 900 FAD O4B-C4B-C5B-O5B 9 M 900 FAD C2'-C3'-C4'-O4' 9 m 900 FAD C2'-C3'-C4'-O4' 9 M 900 FAD C2'-C3'-C4'-O4' 9 M 900 FAD O3'-C3'-C4'-C5' 9 M 900 FAD C2'-C3'-C4'-C5' 9 M 900 FAD O4B-C4B-C5B-O5B 9 m 900 FAD O4B-C4B-C5B-O5B 9 m 900 FAD O3'-C3'-C4'-C5' 9 m 900 FAD C2'-C3'-C4'-C5' 9 M 900 FAD C3'-C3'-C4'-C5' 9 M 900 FAD C2'-C3'-C4'-C5' 9 M 900 FAD C2'-C3'-C4'-C5' 9 M 900 FAD C3B-C4B-C5B-O5B	9	М	900	FAD	O4B-C4B-C5B-O5B
9 k 900 FAD O4B-C4B-C5B-O5B 9 M 900 FAD C2'-C3'-C4'-O4' 9 m 900 FAD C2'-C3'-C4'-O4' 9 m 900 FAD C2'-C3'-C4'-O4' 9 M 900 FAD O3'-C3'-C4'-C5' 9 M 900 FAD C2'-C3'-C4'-C5' 9 m 900 FAD O4B-C4B-C5B-O5B 9 m 900 FAD O3'-C3'-C4'-C5' 9 m 900 FAD O4B-C4B-C5B-O5B 9 m 900 FAD C2'-C3'-C4'-C5' 9 m 900 FAD C2'-C3'-C4'-C5' 9 M 900 FAD C2'-C3'-C4'-C5' 9 M 900 FAD C3B-C4B-C5B-O5B	9	K	900	FAD	
9 M 900 FAD C2'-C3'-C4'-O4' 9 m 900 FAD C2'-C3'-C4'-O4' 9 M 900 FAD C2'-C3'-C4'-O4' 9 M 900 FAD O3'-C3'-C4'-C5' 9 M 900 FAD C2'-C3'-C4'-C5' 9 m 900 FAD O4B-C4B-C5B-O5B 9 m 900 FAD O3'-C3'-C4'-C5' 9 m 900 FAD C2'-C3'-C4'-C5' 9 m 900 FAD C3'-C3'-C4'-C5' 9 M 900 FAD C2'-C3'-C4'-C5' 9 M 900 FAD C2'-C3'-C4'-C5' 9 M 900 FAD C3B-C4B-C5B-O5B	9	K	900	FAD	C3B-C4B-C5B-O5B
9 m 900 FAD C2'-C3'-C4'-O4' 9 M 900 FAD O3'-C3'-C4'-C5' 9 M 900 FAD C2'-C3'-C4'-C5' 9 M 900 FAD C2'-C3'-C4'-C5' 9 m 900 FAD O4B-C4B-C5B-O5B 9 m 900 FAD O3'-C3'-C4'-C5' 9 m 900 FAD C2'-C3'-C4'-C5' 9 m 900 FAD C2'-C3'-C4'-C5' 9 M 900 FAD C2'-C3'-C4'-C5' 9 M 900 FAD C3B-C4B-C5B-O5B	9	k	900	FAD	
9 M 900 FAD O3'-C3'-C4'-C5' 9 M 900 FAD C2'-C3'-C4'-C5' 9 M 900 FAD O4B-C4B-C5B-O5B 9 m 900 FAD O3'-C3'-C4'-C5' 9 m 900 FAD O4B-C4B-C5B-O5B 9 m 900 FAD C2'-C3'-C4'-C5' 9 m 900 FAD C2'-C3'-C4'-C5' 9 M 900 FAD C3B-C4B-C5B-O5B	9	М	900	FAD	C2'-C3'-C4'-O4'
9 M 900 FAD C2'-C3'-C4'-C5' 9 m 900 FAD O4B-C4B-C5B-O5B 9 m 900 FAD O3'-C3'-C4'-C5' 9 m 900 FAD C2'-C3'-C4'-C5' 9 m 900 FAD C2'-C3'-C4'-C5' 9 M 900 FAD C3B-C4B-C5B-O5B	9	m	900		
9 m 900 FAD O4B-C4B-C5B-O5B 9 m 900 FAD O3'-C3'-C4'-C5' 9 m 900 FAD C2'-C3'-C4'-C5' 9 M 900 FAD C3B-C4B-C5B-O5B	9	М	900	FAD	
9 m 900 FAD O3'-C3'-C4'-C5' 9 m 900 FAD C2'-C3'-C4'-C5' 9 M 900 FAD C3B-C4B-C5B-O5B	9	М	900	FAD	C2'-C3'-C4'-C5'
9 m 900 FAD C2'-C3'-C4'-C5' 9 M 900 FAD C3B-C4B-C5B-O5B	9	m	900	FAD	
9 M 900 FAD C3B-C4B-C5B-O5B	9	m	900	FAD	O3'-C3'-C4'-C5'
	9	m	900	FAD	C2'-C3'-C4'-C5'
9 k 900 FAD C3B-C4B-C5B-O5B	9	М	900		
	9	k	900	FAD	C3B-C4B-C5B-O5B

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Mol	Chain	Res	Type	Atoms
9	k	900	FAD	C4'-C5'-O5'-P
9	k	900	FAD	P-O3P-PA-O5B
9	М	900	FAD	C4B-C5B-O5B-PA
9	М	900	FAD	C5B-O5B-PA-O3P
9	m	900	FAD	C5B-O5B-PA-O3P
9	m	900	FAD	C4B-C5B-O5B-PA
9	k	900	FAD	C4B-C5B-O5B-PA
9	k	900	FAD	O2'-C2'-C3'-O3'
9	m	900	FAD	C3B-C4B-C5B-O5B
9	Κ	900	FAD	C2'-C3'-C4'-O4'
9	Κ	900	FAD	O2'-C2'-C3'-O3'
9	Κ	900	FAD	O2'-C2'-C3'-C4'
9	Κ	900	FAD	O4'-C4'-C5'-O5'
9	k	900	FAD	O2'-C2'-C3'-C4'
9	Κ	900	FAD	C1'-C2'-C3'-O3'
9	Κ	900	FAD	O3'-C3'-C4'-O4'

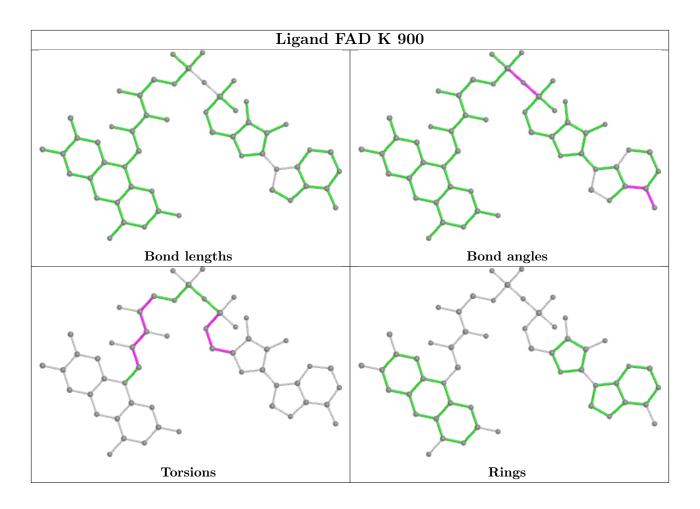
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There are no ring outliers.

No monomer is involved in short contacts.

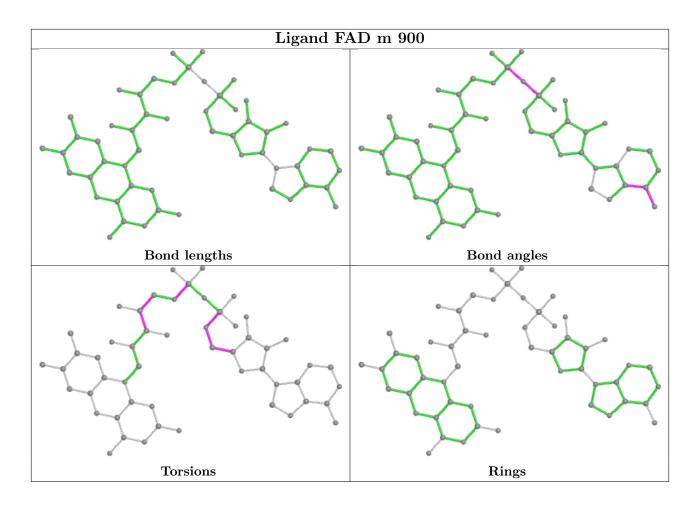
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



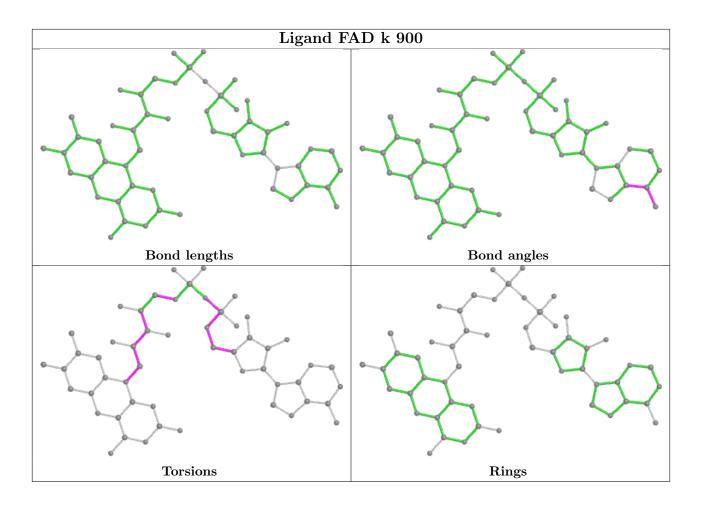




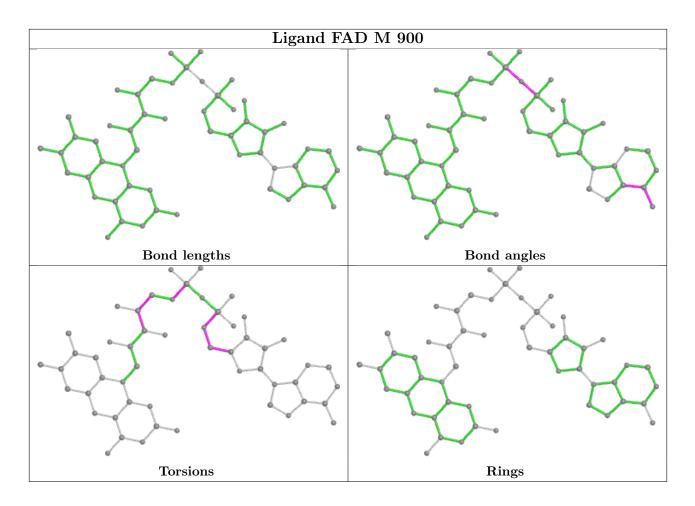












4.7 Other polymers (i)

There are no such residues in this entry.

4.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



5 Fit of model and data (i)

5.1 Protein, DNA and RNA chains (i)

EDS failed to run properly - this section is therefore empty.

5.2 Non-standard residues in protein, DNA, RNA chains (i)

EDS failed to run properly - this section is therefore empty.

5.3 Carbohydrates (i)

EDS failed to run properly - this section is therefore empty.

5.4 Ligands (i)

EDS failed to run properly - this section is therefore empty.

5.5 Other polymers (i)

EDS failed to run properly - this section is therefore empty.

