Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 07:03 am BST

PDB ID	:	4DDJ
Title	:	Crystal structure of saposin A in complex with lauryldimethylamine-N-oxide (LDAO)
Authors	:	Popovic, K.; Prive, G.G.
Deposited on	:	2012-01-18
Resolution	:	1.90 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 ⓘ symbol.

The following versions of software and data (see references ①) were used in the production of this report:

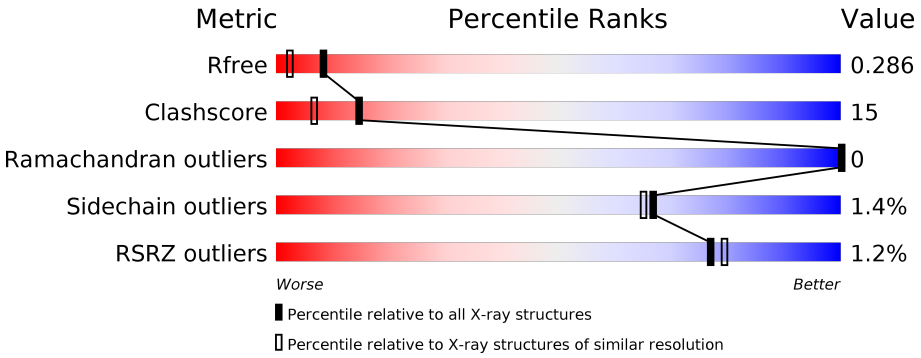
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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 on 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	A	83	% 84% 11%

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
2	LDA	A	119	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 991 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.

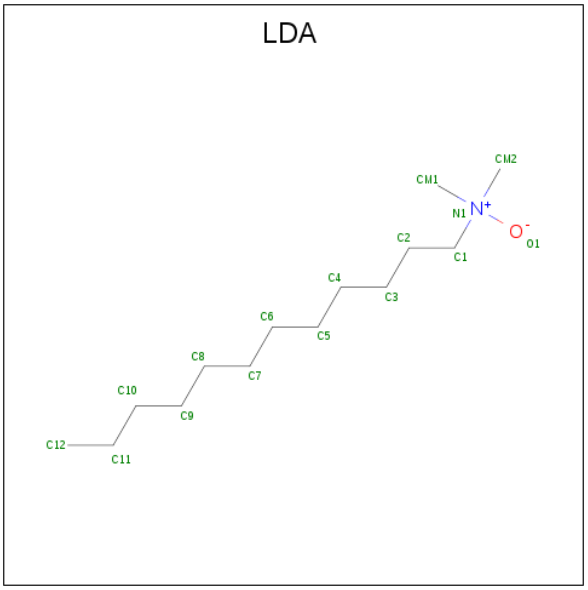
- Molecule 1 is a protein called Saposin-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	80	Total	C	N	O	S	0	0	0
			606	380	93	124	9			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	expression tag	UNP P07602
A	0	GLY	-	expression tag	UNP P07602

- Molecule 2 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula: $C_{14}H_{31}NO$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			16	14	1	1		
2	A	1	Total	C	N	O	0	0
			16	14	1	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C N O 16 14 1 1	0	0
2	A	1	Total C N O 16 14 1 1	0	0
2	A	1	Total C N O 16 14 1 1	0	0
2	A	1	Total C N O 16 14 1 1	0	0
2	A	1	Total C N O 16 14 1 1	0	0
2	A	1	Total C N O 16 14 1 1	0	0
2	A	1	Total C N O 16 14 1 1	0	0
2	A	1	Total C N O 16 14 1 1	0	0
2	A	1	Total C N O 16 14 1 1	0	0
2	A	1	Total C N O 16 14 1 1	0	0
2	A	1	Total C N O 16 14 1 1	0	0
2	A	1	Total C N O 16 14 1 1	0	0
2	A	1	Total C N O 16 14 1 1	0	0
2	A	1	Total C N O 16 14 1 1	0	0
2	A	1	Total C N O 16 14 1 1	0	0
2	A	1	Total C N O 16 14 1 1	0	0
2	A	1	Total C N O 16 14 1 1	0	0
2	A	1	Total C N O 16 14 1 1	0	0

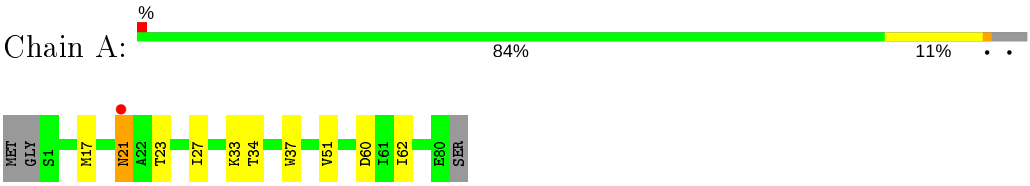
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	65	Total O 65 65	0	0

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 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: Saposin-A



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α, β, γ	39.79Å 39.79Å 247.28Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	10.00 – 1.90 9.96 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.3 (10.00-1.90) 99.3 (9.96-1.90)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.31 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.230 , 0.280 0.244 , 0.286	Depositor DCC
R_{free} test set	478 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å^2)	30.8	Xtriage
Anisotropy	0.074	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 44.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	991	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.68% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: LDA

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	0.96	1/614 (0.2%)	0.82	0/833

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	33	LYS	CE-NZ	5.86	1.63	1.49

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	A	606	0	605	13	1
2	A	320	0	620	29	0
3	A	65	0	0	0	3
All	All	991	0	1225	33	3

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 15.

All (33) 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:A:17:MET:HE2	2:A:119:LDA:H91	1.56	0.86
1:A:17:MET:CE	2:A:119:LDA:H91	2.09	0.82
2:A:119:LDA:H81	2:A:119:LDA:C12	2.20	0.71
2:A:119:LDA:H81	2:A:119:LDA:H122	1.73	0.69
2:A:112:LDA:C12	2:A:119:LDA:H111	2.26	0.65
2:A:112:LDA:H121	2:A:119:LDA:C11	2.27	0.64
2:A:105:LDA:HM22	2:A:110:LDA:H41	1.79	0.64
2:A:102:LDA:H123	2:A:109:LDA:H111	1.79	0.63
2:A:119:LDA:C8	2:A:119:LDA:H122	2.28	0.63
1:A:34:THR:CG2	2:A:117:LDA:H81	2.30	0.62
2:A:112:LDA:H121	2:A:119:LDA:H121	1.82	0.59
1:A:21:ASN:H	1:A:21:ASN:HD22	1.51	0.59
2:A:112:LDA:H123	2:A:119:LDA:H111	1.84	0.58
2:A:112:LDA:C12	2:A:119:LDA:C11	2.86	0.54
2:A:113:LDA:H72	2:A:119:LDA:H72	1.90	0.54
2:A:101:LDA:H52	2:A:108:LDA:H61	1.91	0.53
2:A:112:LDA:H121	2:A:119:LDA:C12	2.40	0.51
1:A:34:THR:HG21	2:A:117:LDA:H81	1.93	0.50
2:A:101:LDA:H91	2:A:108:LDA:H91	1.94	0.50
2:A:102:LDA:H101	2:A:109:LDA:H102	1.95	0.49
2:A:119:LDA:C8	2:A:119:LDA:C12	2.87	0.47
1:A:34:THR:HG22	2:A:117:LDA:H81	1.97	0.46
2:A:120:LDA:H81	2:A:120:LDA:H112	1.84	0.45
2:A:112:LDA:H122	2:A:112:LDA:H92	1.69	0.45
2:A:120:LDA:HM22	2:A:120:LDA:H22	1.49	0.44
1:A:21:ASN:H	1:A:21:ASN:ND2	2.14	0.43
1:A:62:ILE:HD13	2:A:102:LDA:H121	2.01	0.43
1:A:51:VAL:HG22	2:A:117:LDA:H111	2.00	0.43
2:A:113:LDA:H22	2:A:113:LDA:HM21	1.75	0.42
1:A:37:TRP:HE3	2:A:117:LDA:H41	1.85	0.42
1:A:17:MET:HE2	2:A:119:LDA:C9	2.38	0.42
1:A:23:THR:O	1:A:27:ILE:HG13	2.19	0.41
1:A:21:ASN:N	1:A:21:ASN:ND2	2.68	0.41

All (3) 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)
3:A:261:HOH:O	3:A:263:HOH:O[8_565]	1.86	0.34
3:A:232:HOH:O	3:A:233:HOH:O[10_554]	1.91	0.29
1:A:60:ASP:OD2	3:A:242:HOH:O[8_665]	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	A	78/83 (94%)	78 (100%)	0	0	100 100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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	A	72/74 (97%)	71 (99%)	1 (1%)	67 65

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	ASN

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

Mol	Chain	Res	Type
1	A	21	ASN

5.3.3 RNA

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)

20 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 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	$\#\|Z\| > 2$
2	LDA	A	111	-	12,15,15	2.02	1 (8%)	14,17,17	0.60	0
2	LDA	A	104	-	12,15,15	2.01	1 (8%)	14,17,17	1.14	1 (7%)
2	LDA	A	110	-	12,15,15	1.91	1 (8%)	14,17,17	0.60	0
2	LDA	A	117	-	12,15,15	2.01	1 (8%)	14,17,17	0.74	0
2	LDA	A	108	-	12,15,15	2.03	1 (8%)	14,17,17	0.69	0
2	LDA	A	116	-	12,15,15	1.98	1 (8%)	14,17,17	0.63	0
2	LDA	A	101	-	12,15,15	1.93	1 (8%)	14,17,17	1.04	1 (7%)
2	LDA	A	113	-	12,15,15	2.13	1 (8%)	14,17,17	0.59	0
2	LDA	A	118	-	12,15,15	2.13	1 (8%)	14,17,17	0.80	0
2	LDA	A	105	-	12,15,15	2.07	1 (8%)	14,17,17	0.61	0
2	LDA	A	109	-	12,15,15	2.00	1 (8%)	14,17,17	0.68	0
2	LDA	A	102	-	12,15,15	2.05	1 (8%)	14,17,17	0.85	0
2	LDA	A	112	-	12,15,15	2.06	1 (8%)	14,17,17	0.89	0
2	LDA	A	103	-	12,15,15	1.99	1 (8%)	14,17,17	0.71	0
2	LDA	A	106	-	12,15,15	1.92	1 (8%)	14,17,17	0.66	0
2	LDA	A	107	-	12,15,15	1.94	1 (8%)	14,17,17	0.61	0
2	LDA	A	120	-	12,15,15	2.06	1 (8%)	14,17,17	0.54	0
2	LDA	A	115	-	12,15,15	1.99	1 (8%)	14,17,17	0.54	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	LDA	A	119	-	12,15,15	2.03	1 (8%)	14,17,17	0.63	0
2	LDA	A	114	-	12,15,15	1.98	1 (8%)	14,17,17	0.51	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
2	LDA	A	111	-	-	5/13/13/13	-
2	LDA	A	104	-	-	8/13/13/13	-
2	LDA	A	110	-	-	8/13/13/13	-
2	LDA	A	117	-	-	9/13/13/13	-
2	LDA	A	108	-	-	9/13/13/13	-
2	LDA	A	116	-	-	6/13/13/13	-
2	LDA	A	101	-	-	5/13/13/13	-
2	LDA	A	113	-	-	6/13/13/13	-
2	LDA	A	118	-	-	10/13/13/13	-
2	LDA	A	105	-	-	4/13/13/13	-
2	LDA	A	109	-	-	11/13/13/13	-
2	LDA	A	102	-	-	6/13/13/13	-
2	LDA	A	112	-	-	11/13/13/13	-
2	LDA	A	103	-	-	11/13/13/13	-
2	LDA	A	106	-	-	6/13/13/13	-
2	LDA	A	107	-	-	7/13/13/13	-
2	LDA	A	120	-	-	7/13/13/13	-
2	LDA	A	115	-	-	9/13/13/13	-
2	LDA	A	119	-	-	11/13/13/13	-
2	LDA	A	114	-	-	4/13/13/13	-

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	118	LDA	O1-N1	-7.34	1.25	1.42
2	A	113	LDA	O1-N1	-7.31	1.25	1.42
2	A	105	LDA	O1-N1	-7.09	1.25	1.42
2	A	112	LDA	O1-N1	-7.09	1.25	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	120	LDA	O1-N1	-7.06	1.25	1.42
2	A	102	LDA	O1-N1	-7.06	1.25	1.42
2	A	119	LDA	O1-N1	-6.97	1.25	1.42
2	A	108	LDA	O1-N1	-6.97	1.25	1.42
2	A	117	LDA	O1-N1	-6.94	1.25	1.42
2	A	104	LDA	O1-N1	-6.93	1.26	1.42
2	A	111	LDA	O1-N1	-6.91	1.26	1.42
2	A	109	LDA	O1-N1	-6.87	1.26	1.42
2	A	103	LDA	O1-N1	-6.85	1.26	1.42
2	A	115	LDA	O1-N1	-6.83	1.26	1.42
2	A	116	LDA	O1-N1	-6.80	1.26	1.42
2	A	114	LDA	O1-N1	-6.77	1.26	1.42
2	A	107	LDA	O1-N1	-6.66	1.26	1.42
2	A	101	LDA	O1-N1	-6.63	1.26	1.42
2	A	106	LDA	O1-N1	-6.62	1.26	1.42
2	A	110	LDA	O1-N1	-6.55	1.26	1.42

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	104	LDA	CM2-N1-C1	-2.92	104.09	110.23
2	A	101	LDA	CM2-N1-C1	-2.68	104.61	110.23

There are no chirality outliers.

All (153) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	104	LDA	C2-C1-N1-CM1
2	A	104	LDA	C2-C1-N1-CM2
2	A	108	LDA	C2-C1-N1-CM1
2	A	108	LDA	C2-C1-N1-CM2
2	A	113	LDA	N1-C1-C2-C3
2	A	118	LDA	N1-C1-C2-C3
2	A	109	LDA	C2-C1-N1-CM1
2	A	109	LDA	C2-C1-N1-CM2
2	A	102	LDA	N1-C1-C2-C3
2	A	112	LDA	C2-C1-N1-O1
2	A	112	LDA	C2-C1-N1-CM2
2	A	103	LDA	C2-C1-N1-CM1
2	A	115	LDA	C2-C1-N1-CM2
2	A	119	LDA	C2-C1-N1-O1
2	A	119	LDA	C2-C1-N1-CM2

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Mol	Chain	Res	Type	Atoms
2	A	119	LDA	N1-C1-C2-C3
2	A	120	LDA	C11-C10-C9-C8
2	A	112	LDA	C1-C2-C3-C4
2	A	101	LDA	C2-C3-C4-C5
2	A	118	LDA	C2-C3-C4-C5
2	A	118	LDA	C5-C6-C7-C8
2	A	109	LDA	C11-C10-C9-C8
2	A	106	LDA	C7-C8-C9-C10
2	A	119	LDA	C2-C3-C4-C5
2	A	103	LDA	C7-C8-C9-C10
2	A	106	LDA	C5-C6-C7-C8
2	A	114	LDA	C3-C4-C5-C6
2	A	118	LDA	C4-C5-C6-C7
2	A	110	LDA	C7-C8-C9-C10
2	A	101	LDA	C3-C4-C5-C6
2	A	110	LDA	C5-C6-C7-C8
2	A	113	LDA	C6-C7-C8-C9
2	A	104	LDA	C7-C8-C9-C10
2	A	113	LDA	C11-C10-C9-C8
2	A	118	LDA	C6-C7-C8-C9
2	A	115	LDA	C4-C5-C6-C7
2	A	106	LDA	C3-C4-C5-C6
2	A	117	LDA	C3-C4-C5-C6
2	A	116	LDA	C2-C3-C4-C5
2	A	101	LDA	C4-C5-C6-C7
2	A	113	LDA	C3-C4-C5-C6
2	A	112	LDA	C11-C10-C9-C8
2	A	115	LDA	C11-C10-C9-C8
2	A	114	LDA	C11-C10-C9-C8
2	A	117	LDA	C4-C5-C6-C7
2	A	112	LDA	C5-C6-C7-C8
2	A	119	LDA	C4-C5-C6-C7
2	A	117	LDA	C2-C3-C4-C5
2	A	106	LDA	C6-C7-C8-C9
2	A	114	LDA	C6-C7-C8-C9
2	A	104	LDA	C4-C5-C6-C7
2	A	118	LDA	C3-C4-C5-C6
2	A	103	LDA	C11-C10-C9-C8
2	A	102	LDA	C3-C4-C5-C6
2	A	116	LDA	C1-C2-C3-C4
2	A	103	LDA	C2-C3-C4-C5
2	A	102	LDA	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
2	A	119	LDA	C5-C6-C7-C8
2	A	104	LDA	C6-C7-C8-C9
2	A	117	LDA	C5-C6-C7-C8
2	A	107	LDA	C4-C5-C6-C7
2	A	119	LDA	C1-C2-C3-C4
2	A	110	LDA	C11-C10-C9-C8
2	A	103	LDA	C6-C7-C8-C9
2	A	120	LDA	C5-C6-C7-C8
2	A	119	LDA	C3-C4-C5-C6
2	A	120	LDA	C3-C4-C5-C6
2	A	107	LDA	C7-C8-C9-C10
2	A	117	LDA	C1-C2-C3-C4
2	A	102	LDA	C7-C8-C9-C10
2	A	113	LDA	C5-C6-C7-C8
2	A	109	LDA	C3-C4-C5-C6
2	A	108	LDA	C11-C10-C9-C8
2	A	116	LDA	C3-C4-C5-C6
2	A	103	LDA	C5-C6-C7-C8
2	A	115	LDA	C3-C4-C5-C6
2	A	116	LDA	C11-C10-C9-C8
2	A	115	LDA	C1-C2-C3-C4
2	A	104	LDA	C9-C10-C11-C12
2	A	108	LDA	C9-C10-C11-C12
2	A	109	LDA	C1-C2-C3-C4
2	A	120	LDA	C9-C10-C11-C12
2	A	107	LDA	C9-C10-C11-C12
2	A	104	LDA	C11-C10-C9-C8
2	A	106	LDA	C4-C5-C6-C7
2	A	108	LDA	C6-C7-C8-C9
2	A	118	LDA	C1-C2-C3-C4
2	A	109	LDA	C7-C8-C9-C10
2	A	114	LDA	C1-C2-C3-C4
2	A	110	LDA	C3-C4-C5-C6
2	A	112	LDA	C6-C7-C8-C9
2	A	111	LDA	C1-C2-C3-C4
2	A	111	LDA	N1-C1-C2-C3
2	A	120	LDA	N1-C1-C2-C3
2	A	116	LDA	N1-C1-C2-C3
2	A	109	LDA	N1-C1-C2-C3
2	A	103	LDA	N1-C1-C2-C3
2	A	107	LDA	N1-C1-C2-C3
2	A	120	LDA	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
2	A	107	LDA	C11-C10-C9-C8
2	A	107	LDA	C1-C2-C3-C4
2	A	110	LDA	C9-C10-C11-C12
2	A	117	LDA	C7-C8-C9-C10
2	A	116	LDA	C7-C8-C9-C10
2	A	117	LDA	C6-C7-C8-C9
2	A	107	LDA	C3-C4-C5-C6
2	A	111	LDA	C9-C10-C11-C12
2	A	115	LDA	C9-C10-C11-C12
2	A	117	LDA	C9-C10-C11-C12
2	A	110	LDA	C1-C2-C3-C4
2	A	111	LDA	C2-C3-C4-C5
2	A	118	LDA	C2-C1-N1-CM1
2	A	118	LDA	C2-C1-N1-CM2
2	A	112	LDA	C2-C1-N1-CM1
2	A	103	LDA	C2-C1-N1-CM2
2	A	115	LDA	C2-C1-N1-CM1
2	A	119	LDA	C2-C1-N1-CM1
2	A	105	LDA	C1-C2-C3-C4
2	A	101	LDA	C9-C10-C11-C12
2	A	112	LDA	C9-C10-C11-C12
2	A	104	LDA	C2-C1-N1-O1
2	A	108	LDA	C2-C1-N1-O1
2	A	118	LDA	C2-C1-N1-O1
2	A	105	LDA	C11-C10-C9-C8
2	A	120	LDA	C2-C3-C4-C5
2	A	119	LDA	C7-C8-C9-C10
2	A	113	LDA	C9-C10-C11-C12
2	A	101	LDA	C5-C6-C7-C8
2	A	112	LDA	C4-C5-C6-C7
2	A	109	LDA	C9-C10-C11-C12
2	A	111	LDA	C11-C10-C9-C8
2	A	108	LDA	C5-C6-C7-C8
2	A	117	LDA	N1-C1-C2-C3
2	A	106	LDA	N1-C1-C2-C3
2	A	115	LDA	N1-C1-C2-C3
2	A	102	LDA	C6-C7-C8-C9
2	A	103	LDA	C1-C2-C3-C4
2	A	105	LDA	C9-C10-C11-C12
2	A	115	LDA	C6-C7-C8-C9
2	A	108	LDA	C2-C3-C4-C5
2	A	119	LDA	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
2	A	108	LDA	C7-C8-C9-C10
2	A	110	LDA	C6-C7-C8-C9
2	A	109	LDA	C6-C7-C8-C9
2	A	110	LDA	C2-C1-N1-CM1
2	A	103	LDA	C3-C4-C5-C6
2	A	112	LDA	N1-C1-C2-C3
2	A	105	LDA	C6-C7-C8-C9
2	A	109	LDA	C2-C1-N1-O1
2	A	103	LDA	C2-C1-N1-O1
2	A	109	LDA	C2-C3-C4-C5
2	A	102	LDA	C5-C6-C7-C8
2	A	112	LDA	C7-C8-C9-C10

There are no ring outliers.

11 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	110	LDA	1	0
2	A	117	LDA	5	0
2	A	108	LDA	2	0
2	A	101	LDA	2	0
2	A	113	LDA	2	0
2	A	105	LDA	1	0
2	A	109	LDA	2	0
2	A	102	LDA	3	0
2	A	112	LDA	7	0
2	A	120	LDA	2	0
2	A	119	LDA	14	0

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, 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			OWAB(Å^2)	Q<0.9
1	A	80/83 (96%)	0.18	1 (1%)	77	79	19, 26, 40, 57	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	21	ASN	4.5

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. 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	B-factors(Å^2)	Q<0.9
2	LDA	A	110	16/16	0.47	0.36	61,77,95,95	0
2	LDA	A	112	16/16	0.48	0.25	69,72,88,89	0
2	LDA	A	115	16/16	0.52	0.21	66,70,88,89	0
2	LDA	A	116	16/16	0.53	0.28	83,92,99,99	0
2	LDA	A	114	16/16	0.65	0.23	60,72,83,84	0
2	LDA	A	106	16/16	0.66	0.17	39,47,69,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	LDA	A	111	16/16	0.66	0.21	54,60,80,80	0
2	LDA	A	117	16/16	0.66	0.24	58,60,72,72	0
2	LDA	A	107	16/16	0.69	0.21	52,60,72,74	0
2	LDA	A	120	16/16	0.74	0.21	48,51,53,53	16
2	LDA	A	109	16/16	0.77	0.19	65,76,93,93	0
2	LDA	A	108	16/16	0.79	0.17	59,66,79,79	0
2	LDA	A	113	16/16	0.81	0.15	48,58,74,76	0
2	LDA	A	119	16/16	0.82	0.20	65,77,92,93	0
2	LDA	A	103	16/16	0.82	0.19	44,50,67,67	0
2	LDA	A	102	16/16	0.83	0.15	55,60,69,69	0
2	LDA	A	104	16/16	0.84	0.14	39,49,63,63	0
2	LDA	A	118	16/16	0.84	0.13	46,56,59,59	0
2	LDA	A	105	16/16	0.84	0.15	36,41,61,62	0
2	LDA	A	101	16/16	0.85	0.13	45,51,55,56	0

6.5 Other polymers (i)

There are no such residues in this entry.