



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 06:47 PM GMT

PDB ID : 4MRS
Title : Structure of a bacterial Atm1-family ABC transporter
Authors : Lee, J.Y.; Yang, J.G.; Zhitnitsky, D.; Lewinson, O.; Rees, D.C.
Deposited on : 2013-09-17
Resolution : 2.35 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

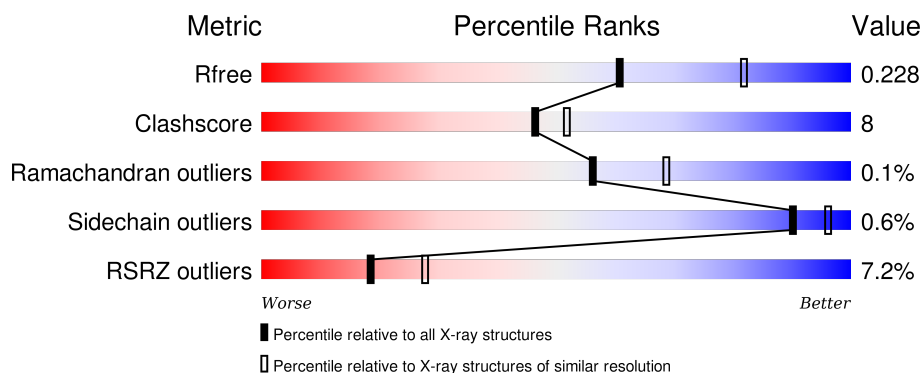
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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}	91344	1352 (2.38-2.34)
Clashscore	102246	1456 (2.38-2.34)
Ramachandran outliers	100387	1435 (2.38-2.34)
Sidechain outliers	100360	1436 (2.38-2.34)
RSRZ outliers	91569	1358 (2.38-2.34)

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. 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 $\leq 5\%$. 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	614	<div> <div>6%</div> <div> <div></div> <div>83%</div> <div>14%</div> <div>.</div> </div> </div>
1	B	614	<div> <div>8%</div> <div> <div></div> <div>82%</div> <div>15%</div> <div>.</div> </div> </div>

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	701	-	-	-	X
2	LDA	A	702	-	-	-	X
2	LDA	A	706	-	-	-	X
2	LDA	A	707	-	-	-	X
2	LDA	A	708	-	-	-	X
2	LDA	B	701	-	-	-	X
2	LDA	B	702	-	-	-	X
2	LDA	B	706	-	-	-	X
3	GDS	A	703	-	-	-	X
3	GDS	B	703	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9931 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.

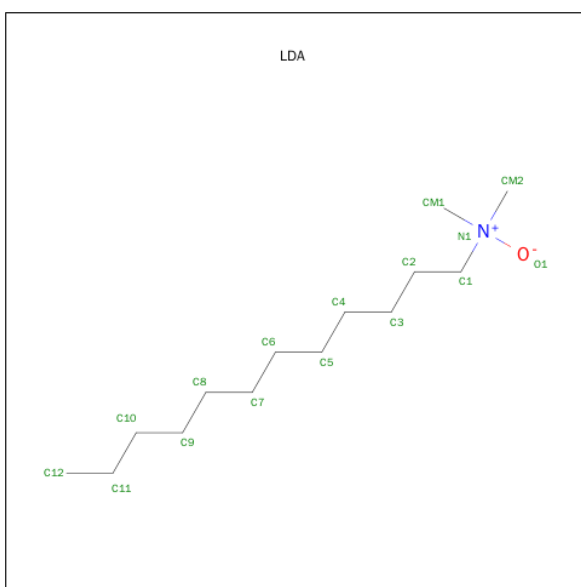
- Molecule 1 is a protein called ABC transporter related protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	600	Total	C	N	O	Se	0	0	0
			4658	2970	828	848	12			
1	B	598	Total	C	N	O	Se	0	0	0
			4645	2963	825	845	12			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	609	HIS	-	EXPRESSION TAG	UNP Q2G506
A	610	HIS	-	EXPRESSION TAG	UNP Q2G506
A	611	HIS	-	EXPRESSION TAG	UNP Q2G506
A	612	HIS	-	EXPRESSION TAG	UNP Q2G506
A	613	HIS	-	EXPRESSION TAG	UNP Q2G506
A	614	HIS	-	EXPRESSION TAG	UNP Q2G506
B	609	HIS	-	EXPRESSION TAG	UNP Q2G506
B	610	HIS	-	EXPRESSION TAG	UNP Q2G506
B	611	HIS	-	EXPRESSION TAG	UNP Q2G506
B	612	HIS	-	EXPRESSION TAG	UNP Q2G506
B	613	HIS	-	EXPRESSION TAG	UNP Q2G506
B	614	HIS	-	EXPRESSION TAG	UNP Q2G506

- Molecule 2 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula: C₁₄H₃₁NO).



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		
2	A	1	Total	C	N	O	0	0
			16	14	1	1		
2	A	1	Total	C			0	0
			6	6				
2	A	1	Total	C			0	0
			5	5				
2	A	1	Total	C			0	0
			6	6				
2	A	1	Total	C			0	0
			4	4				
2	B	1	Total	C	N	O	0	0
			16	14	1	1		
2	B	1	Total	C	N	O	0	0
			16	14	1	1		
2	B	1	Total	C			0	0
			7	7				
2	B	1	Total	C			0	0
			6	6				
2	B	1	Total	C	N	O	0	0
			11	9	1	1		
2	B	1	Total	C			0	0
			5	5				

- Molecule 3 is OXIDIZED GLUTATHIONE DISULFIDE (three-letter code: GDS) (formula:

GDS

Chemical structure of GDS (Glycyl-L-glutamate-L-glutamate-L-glutamate-L-glutamate) showing the repeating units of the peptide chain. The structure is a linear chain of four L-glutamate residues linked by amide bonds. The residues are labeled with atom names: C1, C2, C3, C4 for the alpha-carbons; N1, N2, N3, N4 for the amide nitrogens; O1, O2, O3, O4 for the carboxylate oxygens; and H1, H2, H3, H4 for the amide hydrogens. The chain is shown in a zig-zag conformation with various bond angles and lengths indicated by numbers in parentheses.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 40	C 20	N 6	O 12	S 2	0	0
3	B	1	Total 40	C 20	N 6	O 12	S 2	0	0

-
- The diagram shows the Lewis structure of the phosphate ion (PO_4^{3-}). A central phosphorus atom (P) is bonded to four oxygen atoms (O). The top oxygen atom is labeled '03' and has a negative charge (O^-). The right oxygen atom is labeled '01' and is double-bonded to the phosphorus. The bottom oxygen atom is labeled '04' and has a negative charge (O^-). The left oxygen atom is labeled '02' and has a negative charge (O^-). The phosphorus atom is labeled 'P' and has a green '0' next to it. The entire structure is enclosed in a black rectangular box.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	P	0	0
			5	4	1		



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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	P	0	0
			5	4	1		
4	B	1	Total	O	P	0	0
			5	4	1		
4	B	1	Total	O	P	0	0
			5	4	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	197	Total	O	0	0
			197	197		
5	B	201	Total	O	0	0
			201	201		

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	322.17Å 95.40Å 79.40Å 90.00° 101.81° 90.00°	Depositor
Resolution (Å)	39.66 – 2.35 39.66 – 2.34	Depositor EDS
% Data completeness (in resolution range)	96.1 (39.66-2.35) 83.7 (39.66-2.34)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.22 (at 2.34Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.193 , 0.223 0.200 , 0.228	Depositor DCC
R_{free} test set	4781 reflections (6.09%)	DCC
Wilson B-factor (Å ²)	48.9	Xtriage
Anisotropy	0.357	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 48.5	EDS
Estimated twinning fraction	0.024 for -h-2*k,l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 95159 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9931	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.26% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: PO4, GDS, 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	0.45	0/4732	0.60	0/6408
1	B	0.45	0/4719	0.63	0/6389
All	All	0.45	0/9451	0.62	0/12797

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

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	4658	0	4733	70	0
1	B	4645	0	4723	75	0
2	A	69	0	119	8	0
2	B	61	0	104	7	0
3	A	40	0	28	11	0
3	B	40	0	28	5	0
4	A	10	0	0	0	0
4	B	10	0	0	1	0
5	A	197	0	0	12	0
5	B	201	0	0	6	0
All	All	9931	0	9735	146	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 8.

The worst 5 of 146 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:365:ASN:ND2	5:A:903:HOH:O	2.00	0.93
1:B:130:ARG:NH2	1:B:370:TYR:O	2.07	0.87
3:A:703:GDS:HA31	3:A:703:GDS:HB21	1.63	0.79
3:A:703:GDS:HB22	1:B:320:MSE:HE1	1.66	0.78
1:B:358:ARG:NH2	5:B:920:HOH:O	2.16	0.78

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	Percentiles	
1	A	598/614 (97%)	587 (98%)	11 (2%)	0	100	100
1	B	596/614 (97%)	588 (99%)	7 (1%)	1 (0%)	52	63
All	All	1194/1228 (97%)	1175 (98%)	18 (2%)	1 (0%)	56	69

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	74	GLN

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	A	478/478 (100%)	474 (99%)	4 (1%)	86	94
1	B	477/478 (100%)	475 (100%)	2 (0%)	93	97
All	All	955/956 (100%)	949 (99%)	6 (1%)	90	96

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	154	MSE
1	B	154	MSE
1	A	242	ARG
1	A	123	ARG
1	B	123	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

19 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	701	-	15,15,15	3.86	2 (13%)	16,17,17	0.41	0
2	LDA	A	702	-	15,15,15	3.87	1 (6%)	16,17,17	0.82	1 (6%)
3	GDS	A	703	-	27,39,39	2.60	6 (22%)	32,50,50	1.60	8 (25%)
4	PO4	A	704	-	4,4,4	0.42	0	6,6,6	0.28	0
4	PO4	A	705	-	4,4,4	0.49	0	6,6,6	0.28	0
2	LDA	A	706	-	15,15,15	3.84	2 (13%)	16,17,17	0.39	0
2	LDA	A	707	-	5,5,15	0.36	0	4,4,17	0.27	0
2	LDA	A	708	-	4,4,15	0.35	0	3,3,17	0.28	0
2	LDA	A	709	-	5,5,15	0.35	0	4,4,17	0.27	0
2	LDA	A	710	-	3,3,15	0.53	0	2,2,17	0.63	0
2	LDA	B	701	-	15,15,15	3.84	2 (13%)	16,17,17	0.49	0
2	LDA	B	702	-	15,15,15	3.83	2 (13%)	16,17,17	0.60	0
3	GDS	B	703	-	27,39,39	2.42	6 (22%)	32,50,50	1.41	4 (12%)
4	PO4	B	704	-	4,4,4	0.45	0	6,6,6	0.27	0
4	PO4	B	705	-	4,4,4	0.44	0	6,6,6	0.28	0
2	LDA	B	706	-	6,6,15	0.36	0	5,5,17	0.25	0
2	LDA	B	707	-	5,5,15	0.31	0	4,4,17	0.29	0
2	LDA	B	708	-	10,10,15	4.54	2 (20%)	11,12,17	0.51	0
2	LDA	B	709	-	4,4,15	0.32	0	3,3,17	0.35	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	701	-	-	0/13/13/13	0/0/0/0
2	LDA	A	702	-	-	0/13/13/13	0/0/0/0
3	GDS	A	703	-	-	0/39/51/51	0/0/0/0
4	PO4	A	704	-	-	0/0/0/0	0/0/0/0
4	PO4	A	705	-	-	0/0/0/0	0/0/0/0
2	LDA	A	706	-	-	0/13/13/13	0/0/0/0
2	LDA	A	707	-	-	0/3/3/13	0/0/0/0
2	LDA	A	708	-	-	0/2/2/13	0/0/0/0
2	LDA	A	709	-	-	0/3/3/13	0/0/0/0
2	LDA	A	710	-	-	0/1/1/13	0/0/0/0
2	LDA	B	701	-	-	0/13/13/13	0/0/0/0
2	LDA	B	702	-	-	0/13/13/13	0/0/0/0
3	GDS	B	703	-	-	0/39/51/51	0/0/0/0
4	PO4	B	704	-	-	0/0/0/0	0/0/0/0
4	PO4	B	705	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	LDA	B	706	-	-	0/4/4/13	0/0/0/0
2	LDA	B	707	-	-	0/3/3/13	0/0/0/0
2	LDA	B	708	-	-	0/8/8/13	0/0/0/0
2	LDA	B	709	-	-	0/2/2/13	0/0/0/0

The worst 5 of 23 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	702	LDA	O1-N1	-14.68	1.25	1.39
2	A	701	LDA	O1-N1	-14.57	1.25	1.39
2	A	706	LDA	O1-N1	-14.53	1.25	1.39
2	B	702	LDA	O1-N1	-14.51	1.25	1.39
2	B	701	LDA	O1-N1	-14.51	1.25	1.39

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	703	GDS	O1-CD1-CG1	-2.57	117.56	121.98
3	A	703	GDS	O5-C5-N4	-2.50	118.07	123.08
3	B	703	GDS	CA4-N4-C5	-2.40	119.04	122.34
2	A	702	LDA	CM2-N1-CM1	-2.34	106.19	108.83
3	A	703	GDS	CB6-CG6-CD6	-2.22	107.99	113.27

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

11 monomers are involved in 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	701	LDA	4	0
2	A	702	LDA	3	0
3	A	703	GDS	11	0
2	A	706	LDA	1	0
2	B	702	LDA	3	0
3	B	703	GDS	5	0
4	B	705	PO4	1	0
2	B	706	LDA	2	0
2	B	707	LDA	1	0
2	B	708	LDA	2	0
2	B	709	LDA	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, 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	588/614 (95%)	0.45	38 (6%)	22 33	33, 60, 104, 146	0
1	B	586/614 (95%)	0.54	47 (8%)	15 23	31, 56, 107, 165	0
All	All	1174/1228 (95%)	0.49	85 (7%)	18 28	31, 58, 106, 165	0

The worst 5 of 85 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	71	GLY	15.8
1	B	70	GLY	11.1
1	A	138	GLY	9.2
1	B	72	GLY	9.0
1	A	137	THR	8.3

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 carbohydrates 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. 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	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	LDA	A	707	6/16	0.85	0.46	16.35	63,72,74,74	0
2	LDA	B	706	7/16	0.82	0.39	11.77	60,69,74,76	0
2	LDA	A	708	5/16	0.82	0.50	10.45	68,72,77,78	0
2	LDA	B	701	16/16	0.95	0.36	10.34	58,72,82,86	0
2	LDA	B	702	16/16	0.78	0.37	9.62	60,78,101,108	0
2	LDA	A	701	16/16	0.87	0.45	9.05	55,66,101,111	0
3	GDS	A	703	40/40	0.65	0.44	5.98	79,117,136,137	0
3	GDS	B	703	40/40	0.87	0.42	5.57	42,84,111,133	0
2	LDA	A	706	16/16	0.81	0.38	4.58	57,80,111,118	0
2	LDA	A	702	16/16	0.93	0.32	3.50	55,67,89,92	0
4	PO4	B	704	5/5	0.93	0.14	0.33	134,136,137,140	0
2	LDA	B	708	11/16	0.89	0.20	0.09	61,71,89,89	0
4	PO4	A	705	5/5	0.93	0.14	-0.01	79,80,85,88	5
2	LDA	A	709	6/16	0.88	0.20	-	56,59,64,65	0
2	LDA	B	709	5/16	0.90	0.22	-	53,58,62,64	0
2	LDA	B	707	6/16	0.75	0.22	-	84,89,91,91	0
4	PO4	B	705	5/5	0.87	0.15	-	133,136,138,140	0
4	PO4	A	704	5/5	0.78	0.13	-	150,151,151,151	0
2	LDA	A	710	4/16	0.94	0.15	-	49,55,58,61	0

6.5 Other polymers [i](#)

There are no such residues in this entry.