



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 7, 2024 – 02:23 PM EDT

PDB ID : 4MRR
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 : 2.97 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

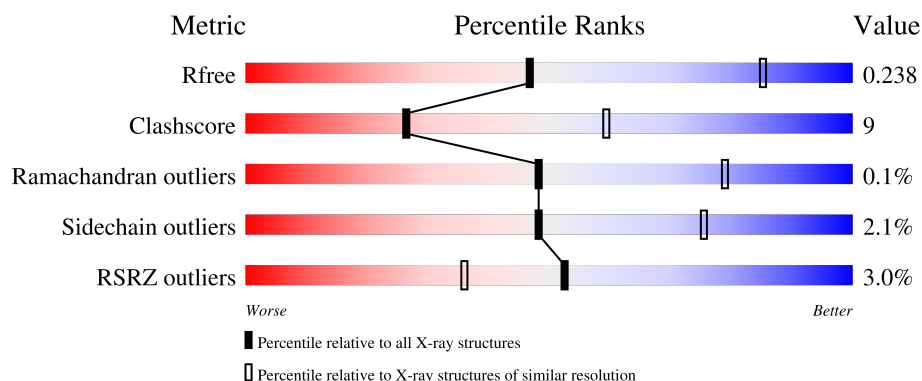
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.97 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}	164625	3360 (3.00-2.96)
Clashscore	180529	3751 (3.00-2.96)
Ramachandran outliers	177936	3628 (3.00-2.96)
Sidechain outliers	177891	3631 (3.00-2.96)
RSRZ outliers	164620	3372 (3.00-2.96)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	 2% 77% 20% ..
1	B	614	 4% 76% 21% .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9415 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.

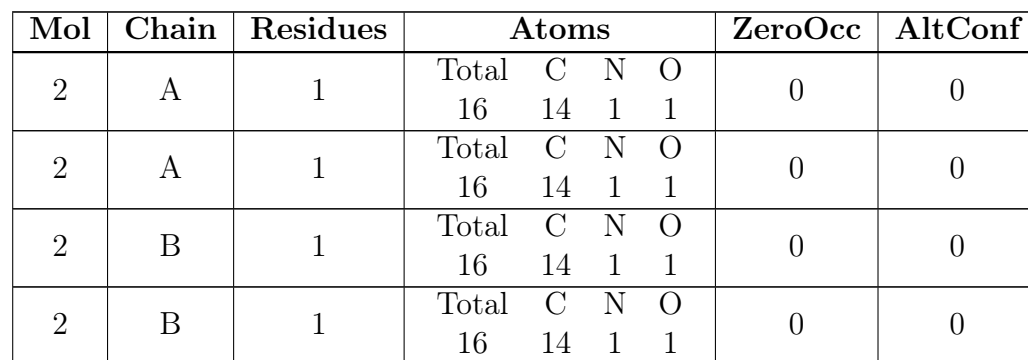
- Molecule 1 is a protein called ABC transporter related protein.

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			

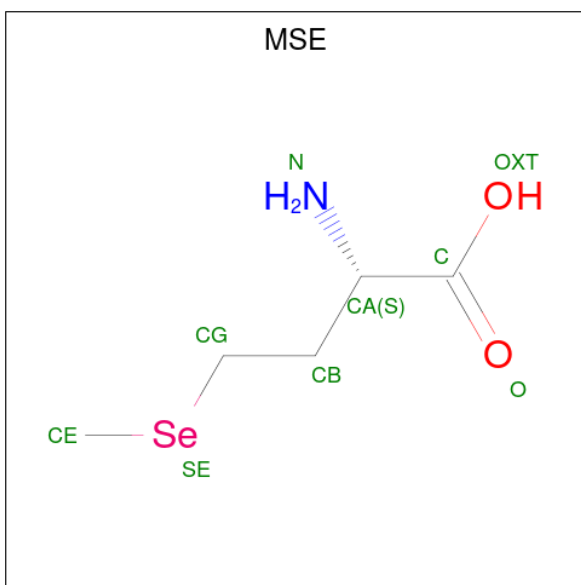
There are 12 discrepancies between the modelled and reference sequences:

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).

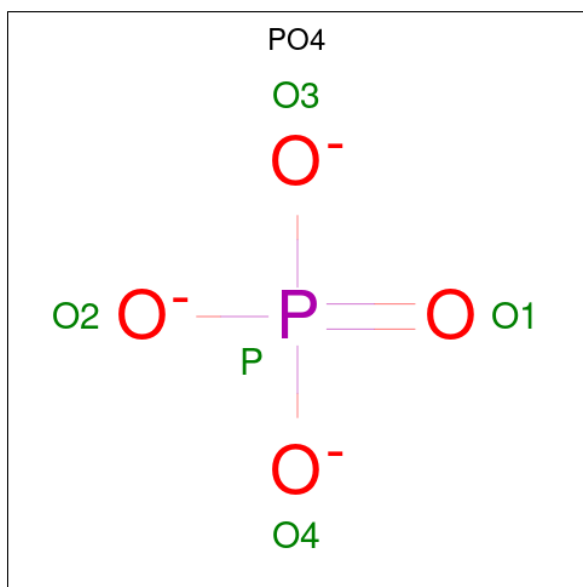


- Molecule 3 is SELENOMETHIONINE (three-letter code: MSE) (formula: $\text{C}_5\text{H}_{11}\text{NO}_2\text{Se}$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	Se	0	0
			9	5	1	2	1		
3	B	1	Total	C	N	O	Se	0	0
			9	5	1	2	1		

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).

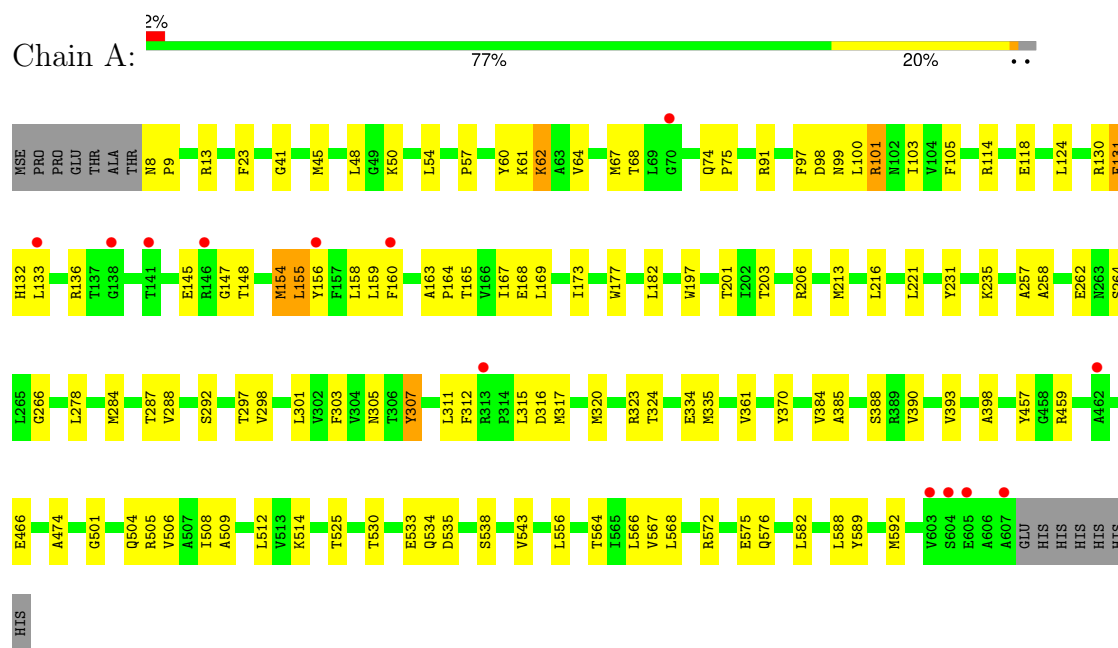


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	P	0	0
			5	4	1		
4	A	1	Total	O	P	0	0
			5	4	1		
4	A	1	Total	O	P	0	0
			5	4	1		
4	B	1	Total	O	P	0	0
			5	4	1		
4	B	1	Total	O	P	0	0
			5	4	1		
4	B	1	Total	O	P	0	0
			5	4	1		

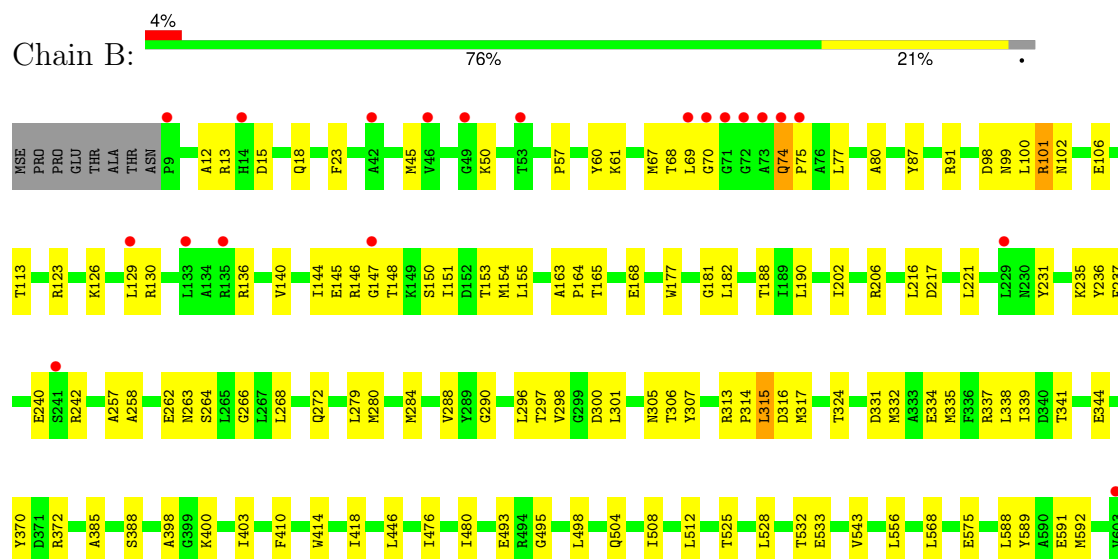
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: ABC transporter related protein



• Molecule 1: ABC transporter related protein



5604	
5605	
5606	
ALA	
GLU	
HIS	
HIS	
HIS	
HIS	
HIS	
HIS	

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Deposition
Cell constants a, b, c, α , β , γ	322.76Å 95.95Å 81.13Å 90.00° 101.78° 90.00°	Deposition
Resolution (Å)	39.50 – 2.97 39.50 – 2.97	Deposition EDS
% Data completeness (in resolution range)	97.7 (39.50-2.97) 86.6 (39.50-2.97)	Deposition EDS
R_{merge}	(Not available)	Deposition
R_{sym}	(Not available)	Deposition
$\langle I/\sigma(I) \rangle$ ¹	0.59 (at 2.95Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309), REFMAC (rigid body)	Deposition
R, R_{free}	0.203 , 0.236 0.206 , 0.238	Deposition DCC
R_{free} test set	2527 reflections (5.06%)	wwPDB
Wilson B-factor (Å ²)	86.7	Xtriage
Anisotropy	0.478	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 40.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.026 for -h-2*1,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9415	wwPDB
Average B, all atoms (Å ²)	64.0	wwPDB

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.03% 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, 0.333 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: PO4, 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	0.51	0/4732	0.64	0/6408
1	B	0.51	0/4719	0.66	0/6389
All	All	0.51	0/9451	0.65	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	95	1
1	B	4645	0	4723	97	1
2	A	32	0	62	6	0
2	B	32	0	62	6	0
3	A	9	0	8	3	0
3	B	9	0	8	5	0
4	A	15	0	0	2	0
4	B	15	0	0	0	0
All	All	9415	0	9596	175	1

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 9.

The worst 5 of 175 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:147:GLY:HA3	2:A:701:LDA:H51	1.53	0.91
1:A:154:MSE:HE3	1:A:158:LEU:HD12	1.56	0.87
1:B:61:LYS:NZ	1:B:300:ASP:OD1	2.09	0.85
1:B:45:MSE:HB2	1:B:101:ARG:HB3	1.60	0.83
1:A:334:GLU:HG2	2:A:701:LDA:H22	1.66	0.78

All (1) 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)
1:A:13:ARG:NH2	1:B:591:GLU:OE1[4_547]	2.10	0.10

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%)	578 (97%)	20 (3%)	0	100	100
1	B	596/614 (97%)	580 (97%)	15 (2%)	1 (0%)	44	74
All	All	1194/1228 (97%)	1158 (97%)	35 (3%)	1 (0%)	48	79

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%)	465 (97%)	13 (3%)	40	69
1	B	477/478 (100%)	470 (98%)	7 (2%)	60	82
All	All	955/956 (100%)	935 (98%)	20 (2%)	48	75

5 of 20 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	101	ARG
1	B	297	THR
1	B	418	ILE
1	B	315	LEU
1	A	203	THR

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

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

12 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	$\# Z > 2$
4	PO4	B	706	-	4,4,4	0.97	0	6,6,6	0.61	0
3	MSE	B	703	-	5,8,8	1.32	0	3,9,9	1.57	1 (33%)
2	LDA	B	702	-	13,15,15	1.60	2 (15%)	14,17,17	0.88	0
4	PO4	A	704	-	4,4,4	0.88	0	6,6,6	0.61	0
2	LDA	A	702	-	13,15,15	1.61	2 (15%)	14,17,17	1.04	1 (7%)
4	PO4	A	706	-	4,4,4	0.80	0	6,6,6	0.49	0
2	LDA	B	701	-	13,15,15	1.57	2 (15%)	14,17,17	0.81	0
4	PO4	B	704	-	4,4,4	0.97	0	6,6,6	0.47	0
3	MSE	A	703	-	5,8,8	1.38	0	3,9,9	1.40	1 (33%)
4	PO4	B	705	-	4,4,4	0.98	0	6,6,6	0.43	0
4	PO4	A	705	-	4,4,4	0.94	0	6,6,6	0.48	0
2	LDA	A	701	-	13,15,15	1.56	2 (15%)	14,17,17	0.58	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
3	MSE	B	703	-	-	2/7/8/8	-
2	LDA	B	702	-	-	7/13/13/13	-
2	LDA	A	702	-	-	8/13/13/13	-
2	LDA	B	701	-	-	9/13/13/13	-
3	MSE	A	703	-	-	2/7/8/8	-
2	LDA	A	701	-	-	10/13/13/13	-

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	702	LDA	O1-N1	-5.31	1.29	1.42
2	B	701	LDA	O1-N1	-4.88	1.30	1.42
2	B	702	LDA	O1-N1	-4.80	1.30	1.42
2	A	701	LDA	O1-N1	-4.67	1.30	1.42
2	A	701	LDA	C1-N1	-3.01	1.48	1.51

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	703	MSE	OXT-C-O	-2.54	118.32	124.08
2	A	702	LDA	C1-C2-C3	2.31	120.75	110.81
3	A	703	MSE	OXT-C-O	-2.27	118.93	124.08

There are no chirality outliers.

5 of 38 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	701	LDA	C2-C1-N1-CM1
2	A	701	LDA	C2-C1-N1-CM2
2	A	702	LDA	C2-C1-N1-O1
2	A	702	LDA	C2-C1-N1-CM1
2	B	701	LDA	C2-C1-N1-O1

There are no ring outliers.

7 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	703	MSE	5	0
2	B	702	LDA	4	0
4	A	704	PO4	1	0
4	A	706	PO4	1	0
2	B	701	LDA	2	0
3	A	703	MSE	3	0
2	A	701	LDA	6	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%)	-0.48	13 (2%)	62 45	21, 62, 114, 179	0
1	B	586/614 (95%)	-0.40	22 (3%)	44 30	21, 58, 111, 161	0
All	All	1174/1228 (95%)	-0.44	35 (2%)	52 36	21, 61, 112, 179	0

The worst 5 of 35 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	71	GLY	6.8
1	B	14	HIS	6.3
1	B	73	ALA	5.3
1	A	133	LEU	5.2
1	B	133	LEU	5.1

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	B-factors(\AA^2)	Q<0.9
4	PO4	A	704	5/5	0.31	0.13	129,129,135,142	5
4	PO4	B	704	5/5	0.73	0.12	92,93,100,103	5
4	PO4	A	705	5/5	0.79	0.09	73,82,84,85	5
2	LDA	B	702	16/16	0.79	0.31	25,54,93,103	0
4	PO4	B	706	5/5	0.80	0.16	119,120,123,127	0
3	MSE	A	703	9/9	0.81	0.18	25,63,88,101	9
4	PO4	A	706	5/5	0.81	0.12	97,101,102,103	5
2	LDA	A	701	16/16	0.86	0.29	51,57,90,90	16
4	PO4	B	705	5/5	0.88	0.06	98,103,106,110	0
3	MSE	B	703	9/9	0.91	0.16	35,55,86,94	9
2	LDA	B	701	16/16	0.92	0.23	48,58,77,77	16
2	LDA	A	702	16/16	0.93	0.18	35,43,52,52	16

6.5 Other polymers [i](#)

There are no such residues in this entry.