



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 11:03 PM UTC

PDB ID : 1SKU / pdb_00001sku
Title : E. coli Aspartate Transcarbamylase 240's Loop Mutant (K244N)
Authors : Alam, N.; Stieglitz, K.A.; Caban, M.D.; Gourinath, S.; Tsuruta, H.;
Kantrowitz, E.R.
Deposited on : 2004-03-05
Resolution : 2.60 Å(reported)

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

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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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

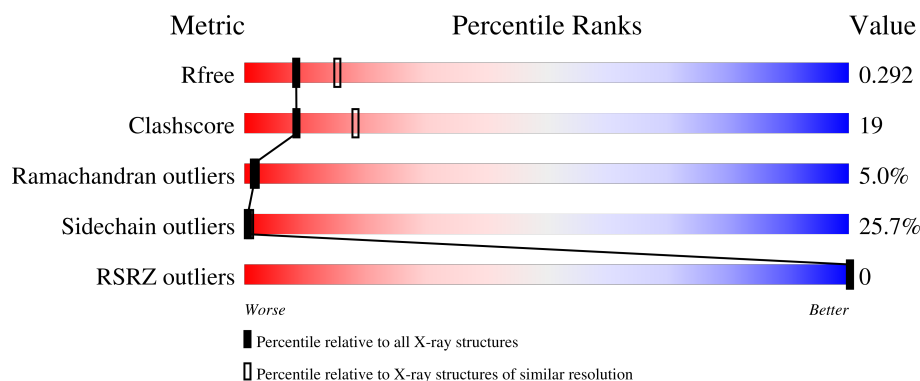
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	310	
1	C	310	
2	B	153	
2	D	153	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7229 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 Aspartate carbamoyltransferase catalytic chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	310	Total	C	N	O	S	0	0	0
			2414	1525	423	457	9			
1	C	310	Total	C	N	O	S	0	0	0
			2414	1525	423	457	9			

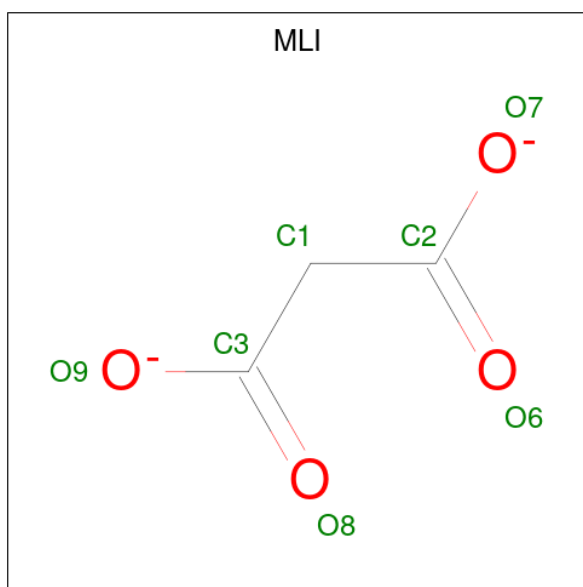
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	244	ASN	LYS	engineered mutation	UNP P0A786
C	244	ASN	LYS	engineered mutation	UNP P0A786

- Molecule 2 is a protein called Aspartate carbamoyltransferase regulatory chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	148	Total	C	N	O	S	0	0	0
			1160	729	205	221	5			
2	D	148	Total	C	N	O	S	0	0	0
			1159	729	205	220	5			

- Molecule 3 is MALONATE ION (CCD ID: MLI) (formula: C₃H₂O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			7	3	4		
3	C	1	Total	C	O	0	0
			7	3	4		

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Zn	0	0
			1	1		
4	D	1	Total	Zn	0	0
			1	1		

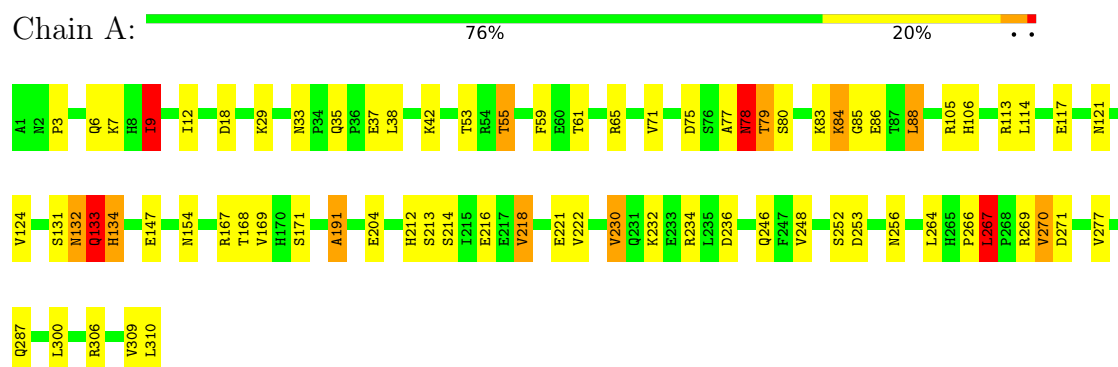
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	22	Total	O	0	0
			22	22		
5	B	10	Total	O	0	0
			10	10		
5	C	27	Total	O	0	0
			27	27		
5	D	7	Total	O	0	0
			7	7		

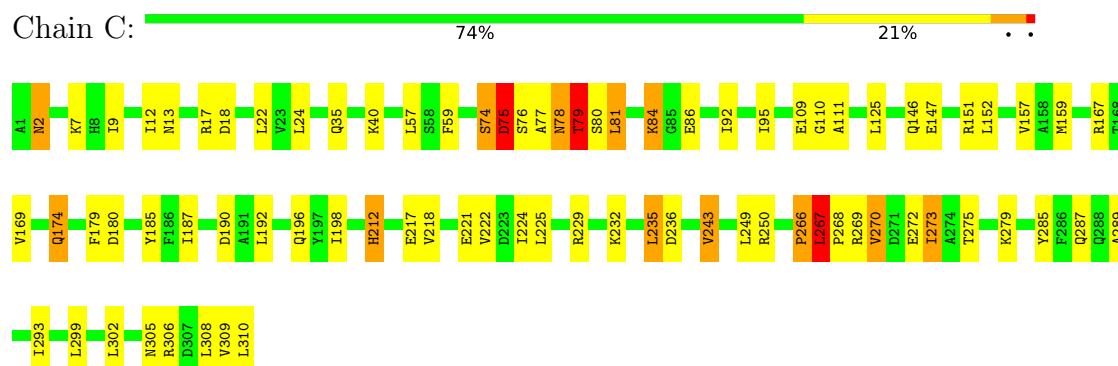
3 Residue-property plots

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.

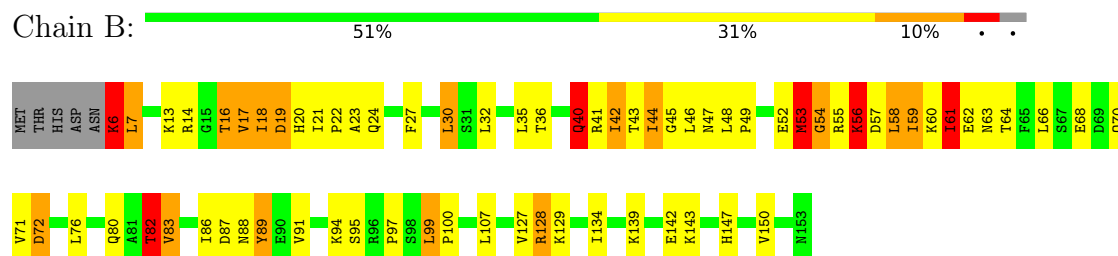
- Molecule 1: Aspartate carbamoyltransferase catalytic chain



- Molecule 1: Aspartate carbamoyltransferase catalytic chain



- Molecule 2: Aspartate carbamoyltransferase regulatory chain



- Molecule 2: Aspartate carbamoyltransferase regulatory chain

F125	E62	ME1
A126	N63	THR
V127	T64	HIS
R128	F65	ASP
K129		ASN
L130	E68	K6
A131	D69	L7
M132	Q70	Q8
D133	V71	V9
I134	D72	E10
A135	Q73	A11
L136	L74	I12
K137	A75	K13
C138	L76	R14
K139	Y77	G15
V140	A78	T16
C141	P79	V17
E142	Q80	I18
K143	A81	D19
E144	T82	H20
F145	V83	I21
S146	N84	P22
H147	R85	A23
N148	I86	Q24
V149	D87	I25
L150	N88	G26
L151	Y89	F27
A152	E90	X28
M153	V91	L29
	V92	L30
	G93	S31
	K94	L32
	S95	F33
	R96	K34
	P97	L35
	S98	T36
	L99	E37
	P100	T38
	E101	D39
	I102	Q40
	I103	R41
	D104	L42
	M105	T43
	V106	L44
	L107	G45
	V108	L46
	C109	N47
	P110	L48
	M111	P49
	S112	
	M113	E52
	C114	M53
	I115	G54
		R55
	E119	K56
	P120	D57
	V121	L58
	S122	F59
	S123	K60
		T61

4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	125.67Å 125.67Å 198.20Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.55 – 2.60 29.55 – 2.60	Depositor EDS
% Data completeness (in resolution range)	89.4 (29.55-2.60) 89.5 (29.55-2.60)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.80 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.201 , 0.231 0.303 , 0.292	Depositor DCC
R_{free} test set	1720 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	46.1	Xtriage
Anisotropy	0.174	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 39.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.480 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7229	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.80% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.85	9/2460 (0.4%)	0.91	12/3339 (0.4%)
1	C	0.57	3/2460 (0.1%)	0.88	13/3339 (0.4%)
2	B	0.82	4/1177 (0.3%)	1.22	12/1590 (0.8%)
2	D	0.80	9/1176 (0.8%)	1.19	9/1590 (0.6%)
All	All	0.75	25/7273 (0.3%)	1.00	46/9858 (0.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	C	0	1
2	B	0	2
2	D	0	2
All	All	0	7

The worst 5 of 25 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	134	HIS	C-N	23.08	1.62	1.34
1	A	191	ALA	C-N	11.96	1.49	1.33
2	B	83	VAL	C-N	11.81	1.49	1.33
1	C	75	ASP	C-N	-10.97	1.18	1.33
1	A	78	ASN	C-N	-9.88	1.19	1.33

The worst 5 of 46 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	89	TYR	CA-C-N	-15.38	101.31	123.00
2	B	89	TYR	C-N-CA	-15.38	101.31	123.00
1	C	75	ASP	O-C-N	-10.96	108.01	122.59
2	D	14	ARG	O-C-N	-10.85	107.82	122.36
1	A	78	ASN	O-C-N	-10.74	108.39	122.14

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	133	GLN	Mainchain
1	A	78	ASN	Mainchain
2	B	6	LYS	Mainchain
2	B	87	ASP	Mainchain
1	C	75	ASP	Mainchain

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	2414	0	2415	23	0
1	C	2414	0	2415	32	0
2	B	1160	0	1185	44	0
2	D	1159	0	1183	189	0
3	A	7	0	2	0	0
3	C	7	0	2	0	0
4	B	1	0	0	0	0
4	D	1	0	0	0	0
5	A	22	0	0	1	0
5	B	10	0	0	3	0
5	C	27	0	0	1	0
5	D	7	0	0	0	0
All	All	7229	0	7202	272	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 19.

The worst 5 of 272 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)
2:D:59:ILE:CD1	2:D:59:ILE:CG1	1.75	1.61
1:C:267:LEU:HD11	1:C:289:ALA:CB	1.51	1.37
1:A:75:ASP:HB3	1:A:78:ASN:ND2	1.45	1.28
1:C:267:LEU:CD1	1:C:289:ALA:HB2	1.73	1.17
2:D:21:ILE:HB	2:D:57:ASP:O	1.47	1.14

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	308/310 (99%)	276 (90%)	22 (7%)	10 (3%)	3	5
1	C	308/310 (99%)	283 (92%)	18 (6%)	7 (2%)	5	9
2	B	146/153 (95%)	104 (71%)	30 (20%)	12 (8%)	0	0
2	D	146/153 (95%)	102 (70%)	28 (19%)	16 (11%)	0	0
All	All	908/926 (98%)	765 (84%)	98 (11%)	45 (5%)	1	2

5 of 45 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	85	GLY
1	A	133	GLN
2	B	17	VAL
2	B	56	LYS
1	C	79	THR

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	261/261 (100%)	209 (80%)	52 (20%)	1	2
1	C	261/261 (100%)	208 (80%)	53 (20%)	1	2
2	B	132/137 (96%)	93 (70%)	39 (30%)	0	0
2	D	132/137 (96%)	74 (56%)	58 (44%)	0	0
All	All	786/796 (99%)	584 (74%)	202 (26%)	0	1

5 of 202 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	180	ASP
1	C	310	LEU
2	D	149	VAL
1	C	198	ILE
1	C	250	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 27 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	126	ASN
1	C	231	GLN
2	D	84	ASN
1	C	196	GLN
1	C	244	ASN

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

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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	$\# Z > 2$
3	MLI	C	312	-	6,6,6	2.27	2 (33%)	7,7,7	1.02	0
3	MLI	A	311	-	6,6,6	1.96	2 (33%)	7,7,7	1.22	1 (14%)

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	MLI	C	312	-	-	4/4/4/4	-
3	MLI	A	311	-	-	2/4/4/4	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	312	MLI	C1-C2	3.80	1.57	1.51
3	A	311	MLI	C1-C3	3.06	1.55	1.51
3	C	312	MLI	C1-C3	2.79	1.55	1.51
3	A	311	MLI	C1-C2	2.77	1.55	1.51

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	311	MLI	O7-C2-C1	2.09	120.98	114.51

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	312	MLI	C3-C1-C2-O7
3	C	312	MLI	C3-C1-C2-O6
3	C	312	MLI	C2-C1-C3-O9
3	A	311	MLI	C2-C1-C3-O9
3	C	312	MLI	C2-C1-C3-O8

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	3
2	D	2
1	C	1

The worst 5 of 6 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	134:HIS	C	135:PRO	N	1.62
1	A	78:ASN	C	79:THR	N	1.19
1	A	83:LYS	C	84:LYS	N	1.19
1	D	14:ARG	C	15:GLY	N	1.19
1	D	28:LYS	C	29:LEU	N	1.19

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	310/310 (100%)	-1.51	0 100 100	2, 19, 55, 79	0
1	C	310/310 (100%)	-1.48	0 100 100	4, 22, 55, 104	0
2	B	148/153 (96%)	-1.15	0 100 100	3, 55, 119, 151	0
2	D	148/153 (96%)	-1.21	0 100 100	2, 49, 95, 107	0
All	All	916/926 (98%)	-1.39	0 100 100	2, 25, 87, 151	0

There are no RSRZ outliers to report.

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 oligosaccharides 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(Å ²)	Q<0.9
3	MLI	C	312	7/7	0.98	0.06	68,72,73,74	0
3	MLI	A	311	7/7	0.99	0.06	55,61,63,66	0
4	ZN	B	315	1/1	1.00	0.03	84,84,84,84	0
4	ZN	D	314	1/1	1.00	0.01	59,59,59,59	0

6.5 Other polymers [i](#)

There are no such residues in this entry.