



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 13, 2020 – 11:39 AM BST

PDB ID : 3MI3
Title : Homocitrate Synthase Lys4 bound to Lysine
Authors : Bulfer, S.L.; Scott, E.M.; Pillus, L.; Trievel, R.C.
Deposited on : 2010-04-09
Resolution : 2.38 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 ⓘ](#)) 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 : 2.14.4.dev1
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) : 2.14.4.dev1

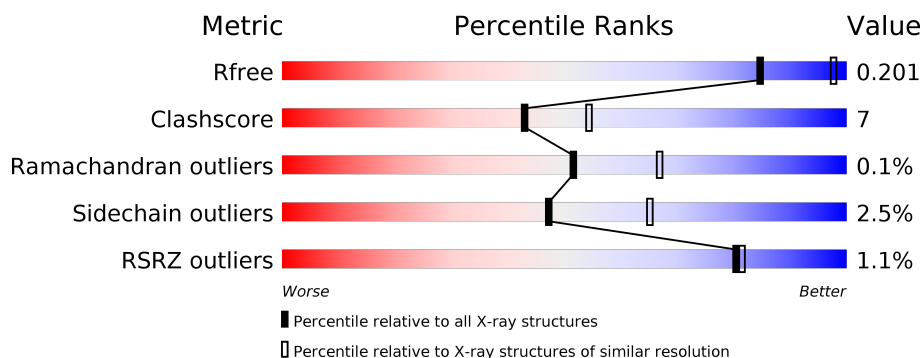
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.38 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	5509 (2.40-2.36)
Clashscore	141614	6082 (2.40-2.36)
Ramachandran outliers	138981	5973 (2.40-2.36)
Sidechain outliers	138945	5975 (2.40-2.36)
RSRZ outliers	127900	5397 (2.40-2.36)

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 $\leq 5\%$. 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	423	<div> <div>%</div> <div> <div></div> <div>77%</div> <div>10%</div> <div>13%</div> </div> </div>
1	B	423	<div> <div>%</div> <div> <div></div> <div>74%</div> <div>12%</div> <div>13%</div> </div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6107 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 Homocitrate synthase, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	370	Total	C	N	O	S	0	9	0
			2885	1802	503	563	17			
1	B	369	Total	C	N	O	S	0	13	0
			2914	1822	515	561	16			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	EXPRESSION TAG	UNP Q9Y823
A	-3	ALA	-	EXPRESSION TAG	UNP Q9Y823
A	-2	MET	-	EXPRESSION TAG	UNP Q9Y823
A	-1	GLY	-	EXPRESSION TAG	UNP Q9Y823
A	0	SER	-	EXPRESSION TAG	UNP Q9Y823
B	-4	GLY	-	EXPRESSION TAG	UNP Q9Y823
B	-3	ALA	-	EXPRESSION TAG	UNP Q9Y823
B	-2	MET	-	EXPRESSION TAG	UNP Q9Y823
B	-1	GLY	-	EXPRESSION TAG	UNP Q9Y823
B	0	SER	-	EXPRESSION TAG	UNP Q9Y823

- Molecule 2 is LYSINE (three-letter code: LYS) (formula: C₆H₁₅N₂O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			10	6	2	2		
2	B	1	Total	C	N	O	0	0
			10	6	2	2		

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Zn	0	0
			1	1		
3	A	1	Total	Zn	0	0
			1	1		

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Na	0	0
			1	1		
4	A	1	Total	Na	0	0
			1	1		

- Molecule 5 is water.

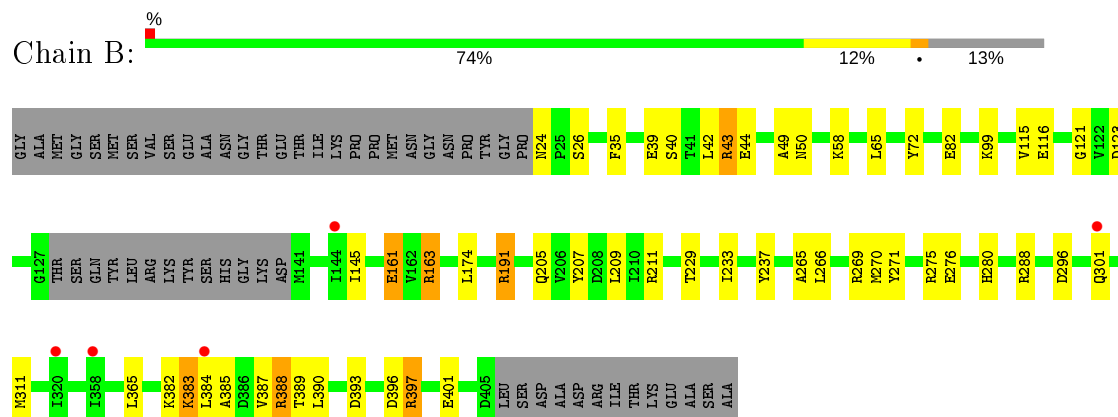
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	147	Total	O	0	0
			147	147		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	137	Total	O	0	0
			137	137		

- Molecule 1: Homocitrate synthase, mitochondrial



4 Data and refinement statistics

Property	Value	Source
Space group	P 62	Depositor
Cell constants a, b, c, α , β , γ	135.64Å 135.64Å 122.93Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	38.69 – 2.38 38.69 – 2.38	Depositor EDS
% Data completeness (in resolution range)	98.0 (38.69-2.38) 98.0 (38.69-2.38)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.05 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.170 , 0.203 0.169 , 0.201	Depositor DCC
R_{free} test set	2556 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	49.0	Xtriage
Anisotropy	0.002	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 53.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.489 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	6107	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.87% 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: NA, 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	0.62	0/2946	0.70	1/3995 (0.0%)
1	B	0.61	0/2978	0.70	1/4034 (0.0%)
All	All	0.62	0/5924	0.70	2/8029 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	191	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	A	163	ARG	NE-CZ-NH2	-5.35	117.62	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	2885	0	2797	41	0
1	B	2914	0	2852	48	0
2	A	10	0	12	0	0
2	B	10	0	12	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	1	0	0	0	0
5	A	147	0	0	0	0
5	B	137	0	0	2	0
All	All	6107	0	5673	78	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 7.

All (78) 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:B:301[A]:GLN:HE22	1:B:397:ARG:HD2	1.10	1.11
1:A:237:TYR:HD1	1:A:270:MET:HE1	1.23	1.01
1:B:301[A]:GLN:NE2	1:B:397:ARG:HD2	1.92	0.85
1:B:276[A]:GLU:OE2	1:B:280[A]:HIS:CE1	2.32	0.82
1:A:388:ARG:HG2	1:A:388:ARG:HH11	1.46	0.80
1:A:163:ARG:HD3	1:A:191:ARG:HH21	1.46	0.79
1:A:237:TYR:CD1	1:A:270:MET:HE1	2.15	0.77
1:B:388:ARG:HG2	1:B:389:THR:N	2.02	0.73
1:A:351:ARG:HD3	1:B:50:ASN:OD1	1.89	0.73
1:B:43:ARG:HG3	1:B:44:GLU:H	1.56	0.71
1:A:392:MET:CE	1:B:50:ASN:HB2	2.21	0.70
1:A:163:ARG:HD3	1:A:191:ARG:NH2	2.05	0.70
1:B:43:ARG:HG3	1:B:44:GLU:N	2.07	0.69
1:A:123:ASP:HB2	1:A:163:ARG:CZ	2.22	0.69
1:B:266:LEU:HD11	1:B:270:MET:HE3	1.78	0.65
1:A:229:THR:HB	1:B:269:ARG:HD2	1.79	0.64
1:A:191:ARG:HD2	1:A:222:GLU:HB3	1.81	0.63
1:A:269:ARG:HD2	1:B:229:THR:HB	1.80	0.62
1:A:392:MET:HE1	1:B:50:ASN:HB2	1.81	0.61
1:B:301[B]:GLN:CD	1:B:393:ASP:HB3	2.22	0.60
1:B:123:ASP:HB2	1:B:163:ARG:CZ	2.32	0.59
1:A:123:ASP:HB2	1:A:163:ARG:NH2	2.17	0.59
1:A:39:GLU:HG3	1:A:65:LEU:HD22	1.84	0.59
1:A:24:ASN:HB3	1:A:25:PRO:HD3	1.86	0.58
1:A:392:MET:HE2	1:B:50:ASN:HB2	1.85	0.57
1:A:392:MET:CE	1:B:50:ASN:CB	2.83	0.56
1:B:123:ASP:HB2	1:B:163:ARG:NH1	2.21	0.56
1:B:26:SER:HB3	1:B:211:ARG:NH2	2.21	0.56
1:B:382:LYS:C	1:B:384:LEU:H	2.10	0.55
1:B:163:ARG:HD2	1:B:191:ARG:NH2	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:237:TYR:HD1	1:A:270:MET:CE	2.08	0.55
1:B:383:LYS:HG2	1:B:383:LYS:O	2.07	0.54
1:A:112:ARG:O	1:A:116:GLU:HG2	2.08	0.53
1:B:387:VAL:O	1:B:388:ARG:CB	2.56	0.53
1:B:174:LEU:HD21	1:B:209:LEU:HD13	1.91	0.53
1:B:40:SER:OG	1:B:43:ARG:HG3	2.09	0.52
1:A:271:TYR:CE1	1:A:275[B]:ARG:HG3	2.46	0.51
1:A:392:MET:HE2	1:B:50:ASN:CB	2.41	0.51
1:A:163:ARG:HD2	1:A:222:GLU:OE1	2.11	0.50
1:B:39:GLU:HG3	1:B:65:LEU:HD22	1.93	0.50
1:B:276[A]:GLU:OE2	1:B:280[A]:HIS:ND1	2.44	0.50
1:A:65:LEU:HD21	1:A:251:ILE:HD11	1.94	0.50
1:A:312[A]:CYS:SG	1:A:392:MET:SD	3.09	0.49
1:B:207:TYR:O	1:B:211:ARG:HB2	2.13	0.49
1:A:161[B]:GLU:HG2	1:A:190:ASN:ND2	2.28	0.48
1:A:336:LYS:HE2	1:A:338:GLU:HG2	1.95	0.48
1:A:328:ASN:HD22	1:A:330:SER:H	1.62	0.48
1:B:82:GLU:OE2	5:B:689:HOH:O	2.20	0.48
1:B:385:ALA:HA	1:B:388:ARG:O	2.13	0.47
1:A:26:SER:HB3	1:A:211:ARG:NH2	2.29	0.47
1:B:72:TYR:CD1	1:B:99:LYS:HB2	2.50	0.47
1:A:355:TRP:HB2	1:A:378:THR:HG21	1.97	0.46
1:B:43:ARG:CG	1:B:44:GLU:N	2.77	0.46
1:A:266:LEU:O	1:A:270:MET:HG2	2.17	0.45
1:B:237:TYR:HD1	1:B:270:MET:HE1	1.81	0.45
1:B:266:LEU:CD1	1:B:270:MET:HE3	2.46	0.45
1:B:311:MET:CE	1:B:396:ASP:CG	2.86	0.44
1:B:115:VAL:HG23	1:B:116:GLU:OE2	2.18	0.43
1:A:338:GLU:H	1:A:338:GLU:CD	2.22	0.43
1:A:351:ARG:HH11	1:B:50:ASN:ND2	2.16	0.43
1:A:392:MET:HE1	1:B:50:ASN:CB	2.47	0.43
1:B:288:ARG:HD2	1:B:365:LEU:HD22	2.01	0.42
1:A:207:TYR:O	1:A:211:ARG:HB2	2.20	0.42
1:A:265:ALA:HB2	1:A:307:TYR:CD2	2.55	0.42
1:B:271:TYR:CE1	1:B:275:ARG:HG3	2.54	0.42
1:A:233:ILE:HD13	1:A:265:ALA:HB1	2.01	0.42
1:B:401[A]:GLU:CD	1:B:401[A]:GLU:H	2.22	0.42
1:A:385:ALA:HA	1:A:388:ARG:O	2.20	0.42
1:B:121:GLY:HA3	1:B:161[A]:GLU:HG2	2.01	0.42
1:A:26:SER:HB3	1:A:211:ARG:HH21	1.84	0.42
1:B:35:PHE:CZ	1:B:270:MET:HG3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:42:LEU:HD22	1:B:58:LYS:HG2	2.02	0.41
1:A:388:ARG:HH11	1:A:388:ARG:CG	2.24	0.41
1:B:233:ILE:HD13	1:B:265:ALA:HB1	2.01	0.41
1:B:26:SER:HB3	1:B:211:ARG:HH21	1.84	0.41
1:A:352:LEU:O	1:A:357:ALA:HB2	2.22	0.40
1:A:348:VAL:HG11	1:B:49:ALA:O	2.21	0.40
1:B:301[B]:GLN:NE2	5:B:622:HOH:O	2.55	0.40

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	375/423 (89%)	362 (96%)	13 (4%)	0	100	100
1	B	378/423 (89%)	362 (96%)	15 (4%)	1 (0%)	41	53
All	All	753/846 (89%)	724 (96%)	28 (4%)	1 (0%)	51	67

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	383	LYS

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	307/356 (86%)	302 (98%)	5 (2%)	62	78
1	B	311/356 (87%)	300 (96%)	11 (4%)	36	52
All	All	618/712 (87%)	602 (97%)	16 (3%)	47	64

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	ARG
1	A	174	LEU
1	A	296	ASP
1	A	328	ASN
1	A	389	THR
1	B	24	ASN
1	B	43	ARG
1	B	145	ILE
1	B	161[A]	GLU
1	B	161[B]	GLU
1	B	163	ARG
1	B	205	GLN
1	B	296	ASP
1	B	388	ARG
1	B	390	LEU
1	B	397	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	286	GLN
1	A	328	ASN
1	B	24	ASN
1	B	107	HIS

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 [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 4 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	$\# Z > 2$
2	LYS	A	1000	3	5,9,9	0.62	0	4,10,10	0.75	0
2	LYS	B	1000	3	5,9,9	0.54	0	4,10,10	0.59	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	LYS	A	1000	3	-	0/5/9/9	-
2	LYS	B	1000	3	-	0/5/9/9	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

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

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	370/423 (87%)	0.27	3 (0%) 86 86	43, 51, 67, 97	0
1	B	369/423 (87%)	0.35	5 (1%) 75 77	45, 53, 76, 85	1 (0%)
All	All	739/846 (87%)	0.31	8 (1%) 80 81	43, 52, 72, 97	1 (0%)

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	301[A]	GLN	4.8
1	A	379	VAL	3.3
1	A	320	ILE	2.9
1	B	320	ILE	2.8
1	B	144	ILE	2.5
1	B	358	ILE	2.4
1	B	384	LEU	2.0
1	A	144	ILE	2.0

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
2	LYS	A	1000	10/10	0.96	0.15	48,49,50,52	0
2	LYS	B	1000	10/10	0.97	0.14	48,48,53,53	0
4	NA	B	501	1/1	1.00	0.09	25,25,25,25	1
3	ZN	B	500	1/1	1.00	0.15	43,43,43,43	0
3	ZN	A	500	1/1	1.00	0.13	44,44,44,44	0
4	NA	A	501	1/1	1.00	0.07	28,28,28,28	1

6.5 Other polymers [i](#)

There are no such residues in this entry.