



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 7, 2020 – 02:04 AM BST

PDB ID : 6LB8
Title : Crystal structure of the Ca²⁺-free T4L-MICU1-MICU2 complex
Authors : Wu, W.; Shen, Q.; Zheng, J.; Jia, Z.
Deposited on : 2019-11-13
Resolution : 3.28 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
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)	:	2.13.1

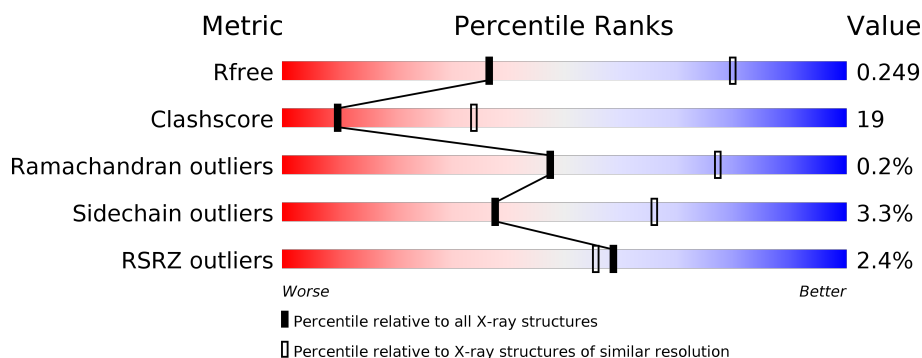
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.28 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	1177 (3.32-3.24)
Clashscore	141614	1044 (3.30-3.26)
Ramachandran outliers	138981	1026 (3.30-3.26)
Sidechain outliers	138945	1025 (3.30-3.26)
RSRZ outliers	127900	1141 (3.32-3.24)

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	527	<div> <div>3%</div> <div> <div></div> <div>54%</div> <div>33%</div> <div>12%</div> </div> </div>
1	C	527	<div> <div>%</div> <div> <div></div> <div>53%</div> <div>37%</div> <div>8%</div> </div> </div>
2	B	330	<div> <div>4%</div> <div> <div></div> <div>57%</div> <div>34%</div> <div>7%</div> </div> </div>
2	D	330	<div> <div>2%</div> <div> <div></div> <div>65%</div> <div>26%</div> <div>8%</div> </div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 12694 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 Endolysin, Calcium uptake protein 1, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	462	Total	C	N	O	S	0	0	0
			3715	2359	640	696	20			
1	C	483	Total	C	N	O	S	0	0	0
			3896	2470	678	729	19			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	993	MET	-	expression tag	UNP D9IEF7
A	994	GLY	-	expression tag	UNP D9IEF7
A	995	HIS	-	expression tag	UNP D9IEF7
A	996	HIS	-	expression tag	UNP D9IEF7
A	997	HIS	-	expression tag	UNP D9IEF7
A	998	HIS	-	expression tag	UNP D9IEF7
A	999	HIS	-	expression tag	UNP D9IEF7
A	1000	HIS	-	expression tag	UNP D9IEF7
A	1054	THR	CYS	engineered mutation	UNP D9IEF7
A	1097	ALA	CYS	engineered mutation	UNP D9IEF7
A	1162	HIS	-	linker	UNP D9IEF7
A	1163	MET	-	linker	UNP D9IEF7
A	445	GLY	-	expression tag	UNP Q9BPX6
A	446	SER	-	expression tag	UNP Q9BPX6
A	447	GLY	-	expression tag	UNP Q9BPX6
A	448	SER	-	expression tag	UNP Q9BPX6
A	449	GLY	-	expression tag	UNP Q9BPX6
A	450	SER	-	expression tag	UNP Q9BPX6
A	451	GLY	-	expression tag	UNP Q9BPX6
A	452	SER	-	expression tag	UNP Q9BPX6
C	993	MET	-	expression tag	UNP D9IEF7
C	994	GLY	-	expression tag	UNP D9IEF7
C	995	HIS	-	expression tag	UNP D9IEF7
C	996	HIS	-	expression tag	UNP D9IEF7
C	997	HIS	-	expression tag	UNP D9IEF7

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Chain	Residue	Modelled	Actual	Comment	Reference
C	998	HIS	-	expression tag	UNP D9IEF7
C	999	HIS	-	expression tag	UNP D9IEF7
C	1000	HIS	-	expression tag	UNP D9IEF7
C	1054	THR	CYS	engineered mutation	UNP D9IEF7
C	1097	ALA	CYS	engineered mutation	UNP D9IEF7
C	1162	HIS	-	linker	UNP D9IEF7
C	1163	MET	-	linker	UNP D9IEF7
C	445	GLY	-	expression tag	UNP Q9BPX6
C	446	SER	-	expression tag	UNP Q9BPX6
C	447	GLY	-	expression tag	UNP Q9BPX6
C	448	SER	-	expression tag	UNP Q9BPX6
C	449	GLY	-	expression tag	UNP Q9BPX6
C	450	SER	-	expression tag	UNP Q9BPX6
C	451	GLY	-	expression tag	UNP Q9BPX6
C	452	SER	-	expression tag	UNP Q9BPX6

- Molecule 2 is a protein called Calcium uptake protein 2, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	308	Total	C	N	O	S	0	0	0
			2566	1650	433	467	16			
2	D	303	Total	C	N	O	S	0	0	0
			2517	1616	426	459	16			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	77	GLY	-	expression tag	UNP Q8IYU8
B	78	SER	-	expression tag	UNP Q8IYU8
B	79	GLY	-	expression tag	UNP Q8IYU8
B	80	SER	-	expression tag	UNP Q8IYU8
B	81	GLY	-	expression tag	UNP Q8IYU8
B	82	SER	-	expression tag	UNP Q8IYU8
B	83	GLY	-	expression tag	UNP Q8IYU8
D	77	GLY	-	expression tag	UNP Q8IYU8
D	78	SER	-	expression tag	UNP Q8IYU8
D	79	GLY	-	expression tag	UNP Q8IYU8
D	80	SER	-	expression tag	UNP Q8IYU8
D	81	GLY	-	expression tag	UNP Q8IYU8
D	82	SER	-	expression tag	UNP Q8IYU8
D	83	GLY	-	expression tag	UNP Q8IYU8

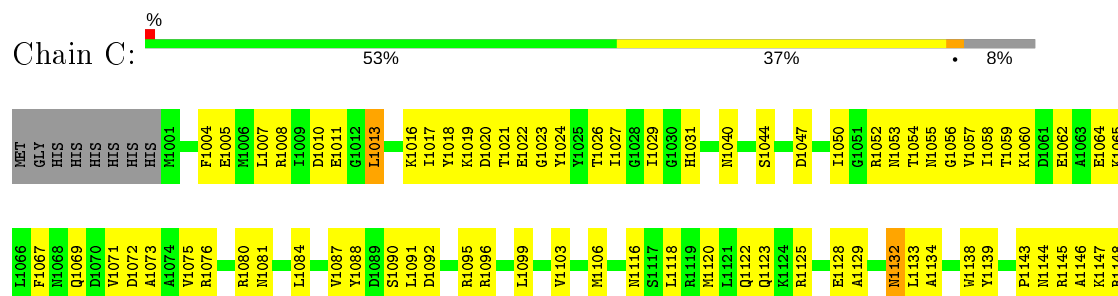
3 Residue-property plots [i](#)

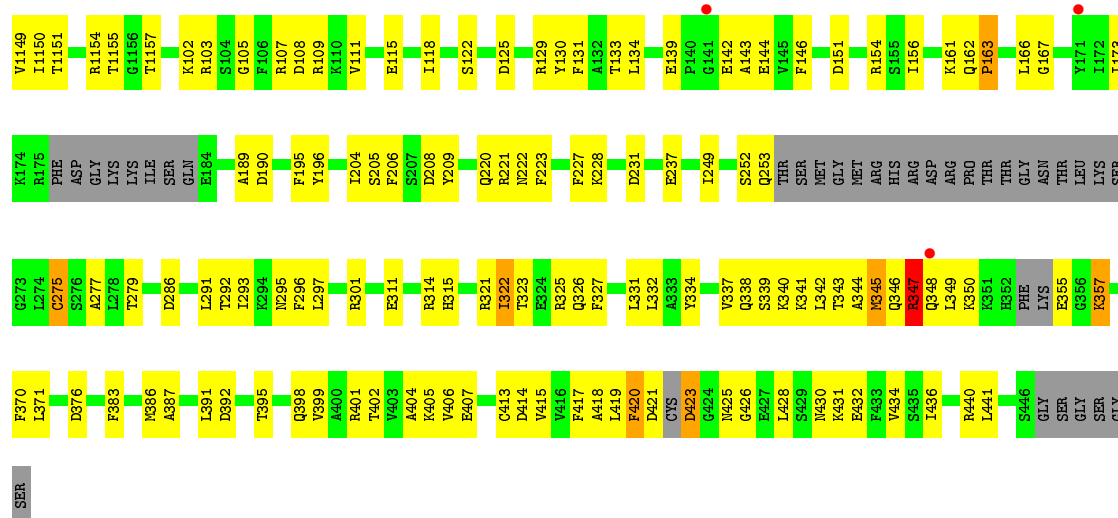
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Endolysin, Calcium uptake protein 1, mitochondrial

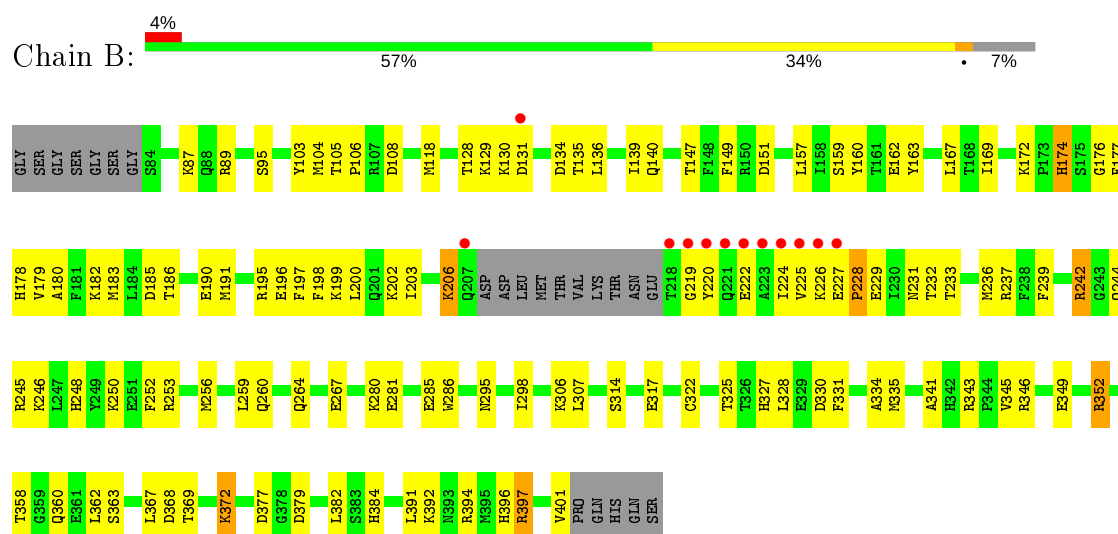


- Molecule 1: Endolysin, Calcium uptake protein 1, mitochondrial

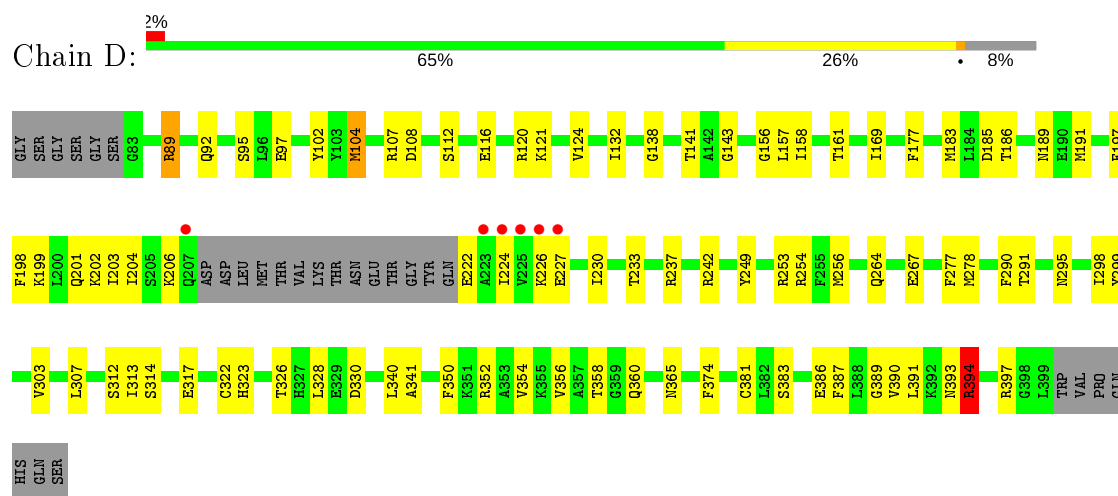




• Molecule 2: Calcium uptake protein 2, mitochondrial



• Molecule 2: Calcium uptake protein 2, mitochondrial



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	79.34Å 133.30Å 178.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.06 – 3.28 49.06 – 3.28	Depositor EDS
% Data completeness (in resolution range)	98.9 (49.06-3.28) 98.9 (49.06-3.28)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.73 (at 3.25Å)	Xtriage
Refinement program	PHENIX 1.10.1 _2155	Depositor
R, R_{free}	0.183 , 0.249 0.183 , 0.249	Depositor DCC
R_{free} test set	1992 reflections (6.81%)	wwPDB-VP
Wilson B-factor (Å ²)	55.3	Xtriage
Anisotropy	0.073	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 44.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	12694	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.77% 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

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	0/3776	0.71	2/5064 (0.0%)
1	C	0.68	1/3962 (0.0%)	0.70	2/5314 (0.0%)
2	B	0.69	1/2621 (0.0%)	0.69	0/3504
2	D	0.68	1/2569 (0.0%)	0.72	1/3431 (0.0%)
All	All	0.67	3/12928 (0.0%)	0.71	5/17313 (0.0%)

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	1
1	C	0	1
All	All	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	163	PRO	N-CD	-15.84	1.25	1.47
2	B	322	CYS	CB-SG	-7.36	1.69	1.82
2	D	381	CYS	CB-SG	-5.29	1.73	1.81

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	394	ARG	NE-CZ-NH1	-8.02	116.29	120.30
1	A	140	PRO	N-CA-C	-7.11	93.62	112.10
1	C	322	ILE	CG1-CB-CG2	-6.63	96.81	111.40
1	C	163	PRO	CA-N-CD	6.53	120.84	111.70
1	A	1063	ALA	O-C-N	5.70	131.83	122.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	109	ARG	Sidechain
1	C	347	ARG	Sidechain

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	3715	0	3685	132	6
1	C	3896	0	3888	209	9
2	B	2566	0	2541	90	7
2	D	2517	0	2498	66	4
All	All	12694	0	12612	485	13

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 485 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:C:345:MET:HE2	1:C:419:LEU:HG	1.24	1.19
1:C:339:SER:O	1:C:343:THR:HG22	1.42	1.16
1:C:345:MET:CE	1:C:419:LEU:HG	1.75	1.14
1:C:346:GLN:O	1:C:347:ARG:HG3	1.46	1.13
1:C:131:PHE:HA	1:C:162:GLN:NE2	1.63	1.13

The worst 5 of 13 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:1137:ARG:NH1	2:D:237:ARG:NH1[1_655]	1.32	0.88
1:A:176:PHE:CE1	1:C:1075:VAL:CG1[2_455]	1.42	0.78
1:A:1137:ARG:NH1	2:D:237:ARG:CZ[1_655]	1.43	0.77
1:A:1137:ARG:NH2	2:D:143:GLY:O[1_655]	1.64	0.56
2:B:346:ARG:NE	1:C:139:GLU:OE2[4_555]	1.73	0.47

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	446/527 (85%)	419 (94%)	27 (6%)	0	100	100
1	C	473/527 (90%)	440 (93%)	31 (7%)	2 (0%)	34	67
2	B	304/330 (92%)	284 (93%)	19 (6%)	1 (0%)	41	72
2	D	299/330 (91%)	283 (95%)	16 (5%)	0	100	100
All	All	1522/1714 (89%)	1426 (94%)	93 (6%)	3 (0%)	47	77

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	345	MET
1	C	347	ARG
2	B	228	PRO

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	399/456 (88%)	389 (98%)	10 (2%)	47	72
1	C	419/456 (92%)	404 (96%)	15 (4%)	35	63
2	B	280/298 (94%)	266 (95%)	14 (5%)	24	55
2	D	275/298 (92%)	269 (98%)	6 (2%)	52	74
All	All	1373/1508 (91%)	1328 (97%)	45 (3%)	38	66

5 of 45 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	352	ARG
1	C	1055	ASN
2	D	199	LYS
2	B	382	LEU
1	C	1060	LYS

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	304	GLN
1	A	362	GLN
1	C	162	GLN
2	D	393	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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	462/527 (87%)	0.01	17 (3%) 41 39	14, 39, 81, 97	0
1	C	483/527 (91%)	-0.07	3 (0%) 89 90	13, 40, 74, 101	0
2	B	308/330 (93%)	-0.13	12 (3%) 39 37	10, 33, 83, 111	0
2	D	303/330 (91%)	-0.23	6 (1%) 65 63	9, 29, 62, 104	0
All	All	1556/1714 (90%)	-0.09	38 (2%) 59 55	9, 37, 78, 111	0

The worst 5 of 38 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	219	GLY	6.9
2	B	221	GLN	5.6
2	B	218	THR	5.4
2	D	225	VAL	5.2
2	D	223	ALA	5.2

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.