



wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 3LQQ
Title : Structure of the CED-4 Apoptosome
Authors : Qi, S.; Pang, Y.; Shi, Y.; Yan, N.; Liu, Q.
Deposited on : 2010-02-09
Resolution : 3.53 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

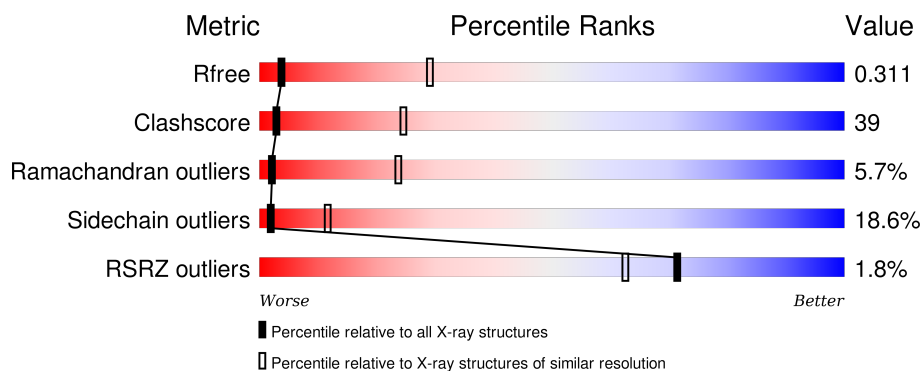
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.53 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	1136 (3.68-3.40)
Clashscore	102246	1248 (3.68-3.40)
Ramachandran outliers	100387	1208 (3.68-3.40)
Sidechain outliers	100360	1208 (3.68-3.40)
RSRZ outliers	91569	1143 (3.68-3.40)

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	549	<div> <div> <div>2%</div> <div>37%</div> <div>42%</div> <div>12%</div> <div>8%</div> </div> </div>
1	B	549	<div> <div>2%</div> <div>36%</div> <div>41%</div> <div>13%</div> <div>9%</div> </div>

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 8124 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.

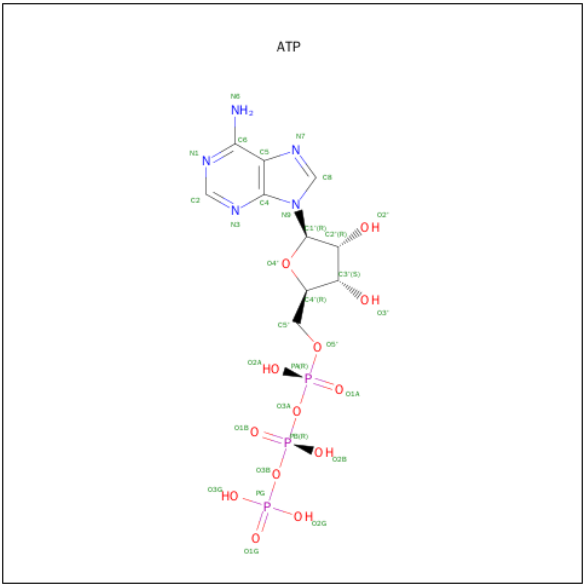
- Molecule 1 is a protein called Cell death protein 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	503	Total	C	N	O	S	0	0	0
			4039	2575	676	759	29			
1	B	501	Total	C	N	O	S	0	0	0
			4021	2565	673	754	29			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mg	0	0
			1	1		
2	A	1	Total	Mg	0	0
			1	1		

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).

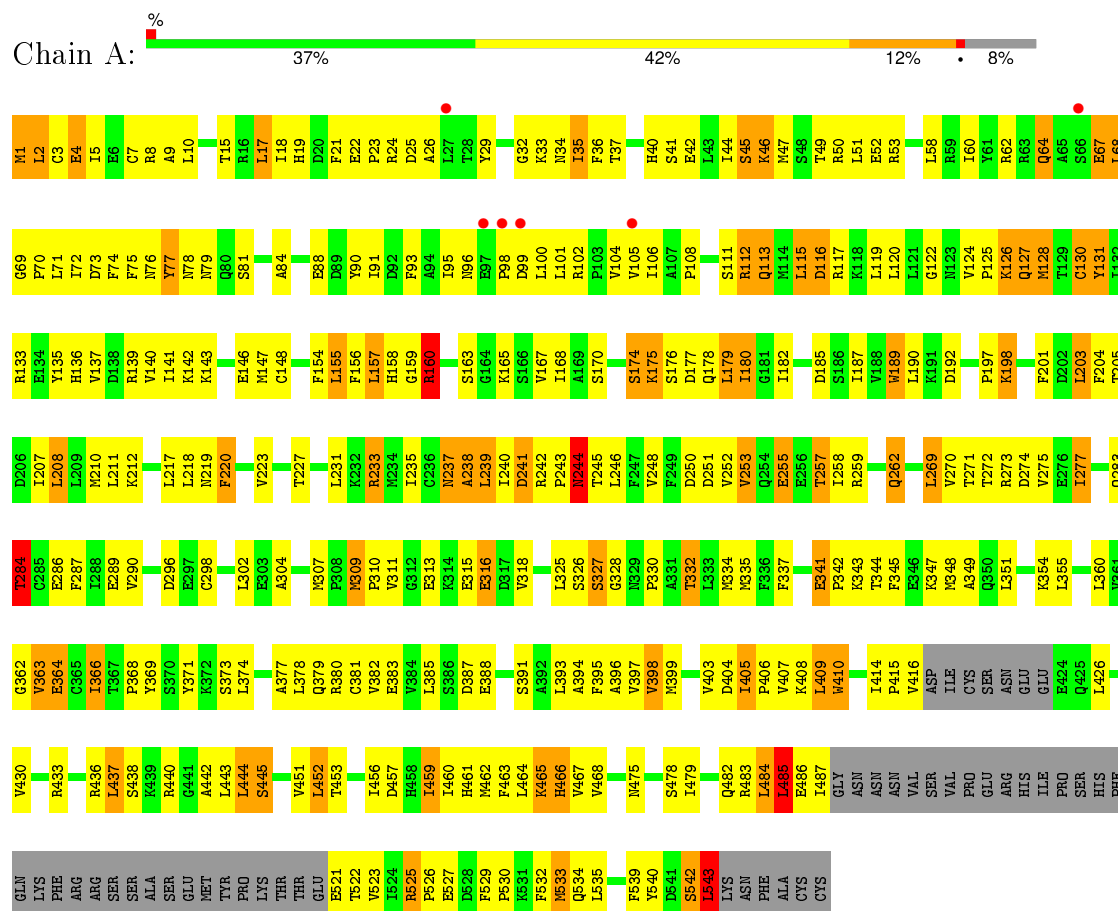


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

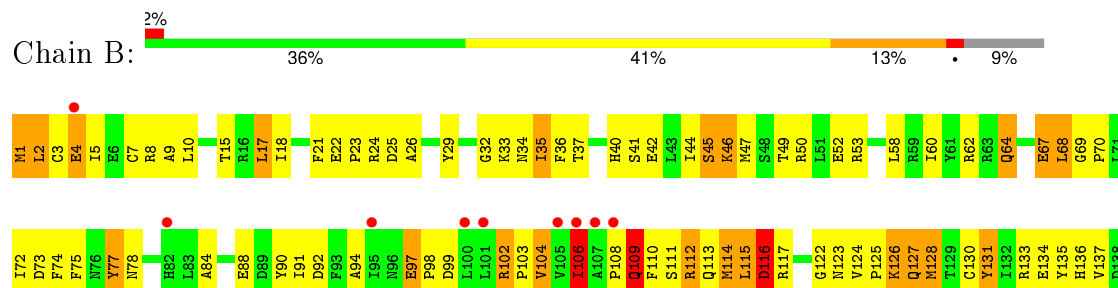
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 ($\text{RSRZ} > 2$). 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: Cell death protein 4



• Molecule 1: Cell death protein 4



PHE	GLN	LYS	PHE	ARG	SER	SER	ALA	SER	GLU	MET	TYR	PRO	LYS	THR	THR	GLU	E521	T522	V523	R524	R525	P526	E527	P528	P529	P530	K531	F532	K533	Q534	L535	F539	V540	D541	S542	L543	LYS	ASN	PHE	ALA	CYS	CYS																
V430	R433	R436	R437	S438	R439	R440	G441	A442	L443	I444	S445	V451	L452	T453	I456	D457	H458	I459	I460	H461	M462	F463	L464	K465	H466	V467	V468	M475	S478	I479	L480	E481	Q482	R483	L484	L485	E486	I487	GLY	ASN	ASN	ASN	VAL	SER	VAL	PRO	GLU	ARG	HIS	ILE	PRO	HIS						
G362	V363	E364	C365	I366	T367	P368	Y369	S370	Y371	K372	S373	L374	A377	L378	Q379	R380	C381	V382	L385	E388	S391	A392	L393	A394	F395	A396	V397	V398	M399	P400	P401	G402	V403	D404	P406	V407	K408	L409	W410	I414	P415	V416	ASP	ILE	VAL	ASN	PRO	GLU	ARG	HIS	ILE	PRO	L426					
S282	Q283	T284	C285	E286	F287	I288	E289	Y290	D296	E297	C298	L302	M307	R308	M309	P310	V311	G312	E313	V314	E315	E316	D317	V318	L325	S326	S327	G328	M329	P330	A331	T332	L333	M334	F337	E341	P342	K343	T344	F345	E346	K347	M348	A349	Q350	L351	K354	L355	L360	V361								
R139	V140	I141	K142	K143	E146	M147	C148	F153	F154	L155	F156	L157	H158	G159	R160	A161	G162	S163	G164	K165	S166	V167	I168	A169	S170	S174	K175	S176	D177	Q178	L179	V253	I180	G181	I182	D185	S186	I187	V188	H189	L190	K191	D192	R265	L266	R267	C268	L269	V270	T271	T272	R273	D274	V275	E276	L277	S278	N279

4 Data and refinement statistics

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, α , β , γ	181.64Å 181.64Å 203.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.66 – 3.53 28.66 – 3.53	Depositor EDS
% Data completeness (in resolution range)	98.7 (28.66-3.53) 98.8 (28.66-3.53)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.54 (at 3.55Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.5_2)	Depositor
R, R_{free}	0.275 , 0.311 0.271 , 0.311	Depositor DCC
R_{free} test set	1032 reflections (5.21%)	DCC
Wilson B-factor (Å ²)	112.9	Xtriage
Anisotropy	0.540	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 89.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 20854 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	8124	wwPDB-VP
Average B, all atoms (Å ²)	151.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.89% 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: MG, ATP

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	0.48	0/4113	0.67	2/5558 (0.0%)
1	B	0.47	0/4095	0.67	1/5534 (0.0%)
All	All	0.47	0/8208	0.67	3/11092 (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	B	0	1
All	All	0	2

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	409	LEU	CA-CB-CG	5.59	128.16	115.30
1	A	409	LEU	CA-CB-CG	5.44	127.82	115.30
1	A	543	LEU	CA-CB-CG	5.16	127.16	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	485	LEU	Peptide
1	B	485	LEU	Peptide

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	4039	0	4066	328	0
1	B	4021	0	4052	321	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	31	0	12	6	0
3	B	31	0	12	5	0
All	All	8124	0	8142	642	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 39.

The worst 5 of 642 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:160:ARG:HG3	1:A:160:ARG:HH11	1.10	1.12
1:B:160:ARG:HG3	1:B:160:ARG:HH11	1.03	1.11
1:A:93:PHE:HE1	1:A:100:LEU:HD23	1.24	1.01
1:A:41:SER:O	1:A:45:SER:HB3	1.61	1.00
1:B:41:SER:O	1:B:45:SER:HB3	1.62	0.98

There are no symmetry-related clashes.

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	497/549 (90%)	399 (80%)	73 (15%)	25 (5%)	3 27

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	495/549 (90%)	388 (78%)	75 (15%)	32 (6%)	1	20
All	All	992/1098 (90%)	787 (79%)	148 (15%)	57 (6%)	2	24

5 of 57 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	127	GLN
1	A	327	SER
1	A	341	GLU
1	A	398	VAL
1	A	445	SER

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	458/501 (91%)	376 (82%)	82 (18%)	2	13
1	B	456/501 (91%)	368 (81%)	88 (19%)	2	11
All	All	914/1002 (91%)	744 (81%)	170 (19%)	2	12

5 of 170 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	485	LEU
1	B	104	VAL
1	B	451	VAL
1	A	539	PHE
1	B	45	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	534	GLN
1	B	34	ASN

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Mol	Chain	Res	Type
1	B	219	ASN
1	A	244	ASN
1	A	471	GLN

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 carbohydrates 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	ATP	A	602	2	24,33,33	1.18	2 (8%)	31,52,52	2.08	8 (25%)
3	ATP	B	602	2	24,33,33	1.15	1 (4%)	31,52,52	2.58	11 (35%)

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	ATP	A	602	2	-	0/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ATP	B	602	2	-	0/18/38/38	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	602	ATP	O4'-C1'	3.06	1.45	1.41
3	B	602	ATP	C5-C4	3.55	1.48	1.40
3	A	602	ATP	C5-C4	3.67	1.48	1.40

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	602	ATP	C2'-C1'-N9	-7.67	102.58	114.29
3	B	602	ATP	N3-C2-N1	-6.61	123.83	128.89
3	A	602	ATP	N3-C2-N1	-5.54	124.65	128.89
3	A	602	ATP	PB-O3B-PG	-5.52	114.16	132.67
3	B	602	ATP	PA-O3A-PB	-4.85	119.10	132.73

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	602	ATP	6	0
3	B	602	ATP	5	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	503/549 (91%)	-0.21	6 (1%) 81 73	93, 139, 207, 267	0
1	B	501/549 (91%)	-0.19	12 (2%) 62 52	92, 140, 214, 339	0
All	All	1004/1098 (91%)	-0.20	18 (1%) 71 62	92, 140, 211, 339	0

The worst 5 of 18 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	100	LEU	4.9
1	B	105	VAL	4.2
1	B	521	GLU	4.0
1	B	107	ALA	2.8
1	B	95	ILE	2.8

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
3	ATP	A	602	31/31	0.91	0.34	1.04	92,118,143,313	0
3	ATP	B	602	31/31	0.92	0.28	0.47	105,118,136,278	0
2	MG	B	601	1/1	0.95	0.46	-	80,80,80,80	0
2	MG	A	601	1/1	0.75	1.97	-	313,313,313,313	0

6.5 Other polymers [i](#)

There are no such residues in this entry.