



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 27, 2020 – 01:32 PM BST

PDB ID : 6KJ9
Title : E. coli ATCase catalytic subunit mutant - G128/130A
Authors : Lei, Z.; Zheng, J.; Jia, Z.C.
Deposited on : 2019-07-22
Resolution : 2.50 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
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

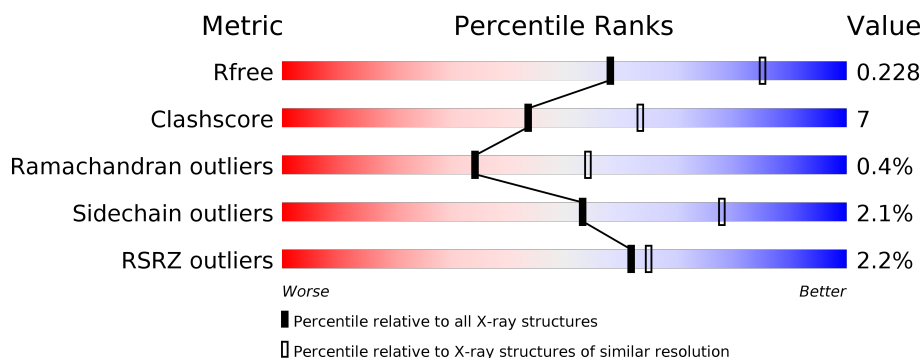
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	310	<div> <div style="width: 100%;">%</div> <div> <div style="width: 7%;"></div> <div style="width: 86%;"></div> <div style="width: 10%;"></div> <div style="width: 3%;"></div> </div> <div>86% 10% . .</div> </div>
1	B	310	<div> <div style="width: 100%;">%</div> <div> <div style="width: 7%;"></div> <div style="width: 80%;"></div> <div style="width: 15%;"></div> <div style="width: 3%;"></div> </div> <div>80% 15% . .</div> </div>
1	C	310	<div> <div style="width: 100%;">%</div> <div> <div style="width: 7%;"></div> <div style="width: 76%;"></div> <div style="width: 15%;"></div> <div style="width: 2%;"></div> </div> <div>76% 15% . 6%</div> </div>
1	D	310	<div> <div style="width: 100%;">%</div> <div> <div style="width: 7%;"></div> <div style="width: 79%;"></div> <div style="width: 12%;"></div> <div style="width: 2%;"></div> </div> <div>79% 12% . 8%</div> </div>
1	E	310	<div> <div style="width: 100%;">%</div> <div> <div style="width: 7%;"></div> <div style="width: 71%;"></div> <div style="width: 18%;"></div> <div style="width: 4%;"></div> </div> <div>71% 18% . 9%</div> </div>
1	F	310	<div> <div style="width: 100%;">%</div> <div> <div style="width: 7%;"></div> <div style="width: 85%;"></div> <div style="width: 10%;"></div> <div style="width: 3%;"></div> </div> <div>85% 10% . .</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 14188 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 subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	301	Total	C	N	O	S	0	0	0
			2339	1482	406	442	9			
1	B	301	Total	C	N	O	S	0	0	0
			2331	1480	405	437	9			
1	C	291	Total	C	N	O	S	0	0	0
			2243	1423	388	423	9			
1	D	284	Total	C	N	O	S	0	0	0
			2216	1407	386	414	9			
1	E	283	Total	C	N	O	S	0	0	0
			2163	1377	370	408	8			
1	F	298	Total	C	N	O	S	0	0	0
			2313	1469	396	439	9			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	128	ALA	GLY	engineered mutation	UNP P0A786
A	130	ALA	GLY	engineered mutation	UNP P0A786
B	128	ALA	GLY	engineered mutation	UNP P0A786
B	130	ALA	GLY	engineered mutation	UNP P0A786
C	128	ALA	GLY	engineered mutation	UNP P0A786
C	130	ALA	GLY	engineered mutation	UNP P0A786
D	128	ALA	GLY	engineered mutation	UNP P0A786
D	130	ALA	GLY	engineered mutation	UNP P0A786
E	128	ALA	GLY	engineered mutation	UNP P0A786
E	130	ALA	GLY	engineered mutation	UNP P0A786
F	128	ALA	GLY	engineered mutation	UNP P0A786
F	130	ALA	GLY	engineered mutation	UNP P0A786

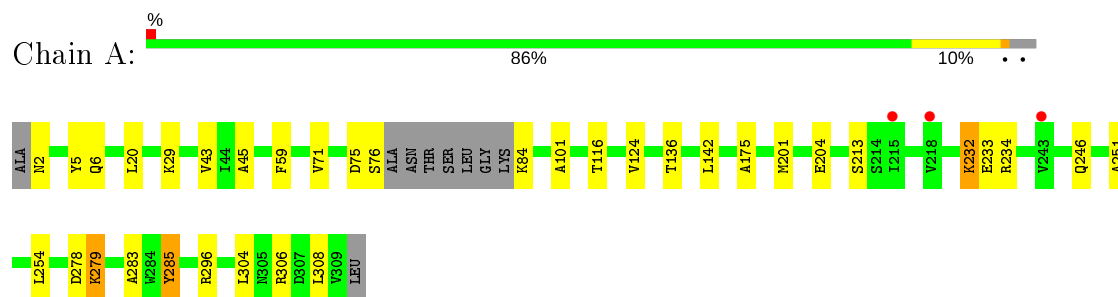
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	69	Total 69	O 69	0	0
2	B	120	Total 120	O 120	0	0
2	C	89	Total 89	O 89	0	0
2	D	120	Total 120	O 120	0	0
2	E	47	Total 47	O 47	0	0
2	F	138	Total 138	O 138	0	0

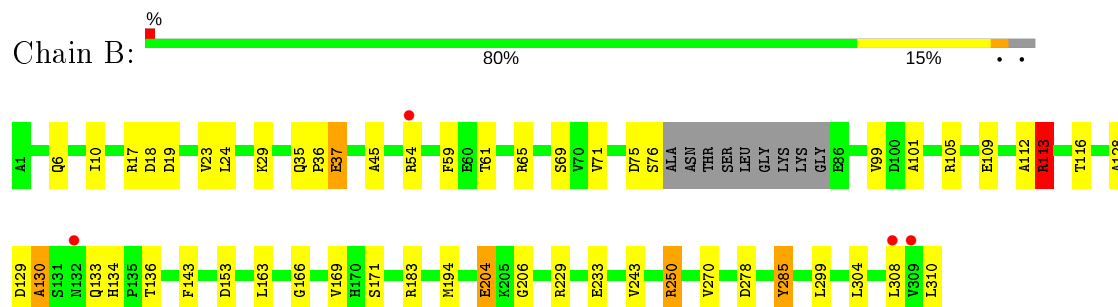
3 Residue-property plots [i](#)

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.

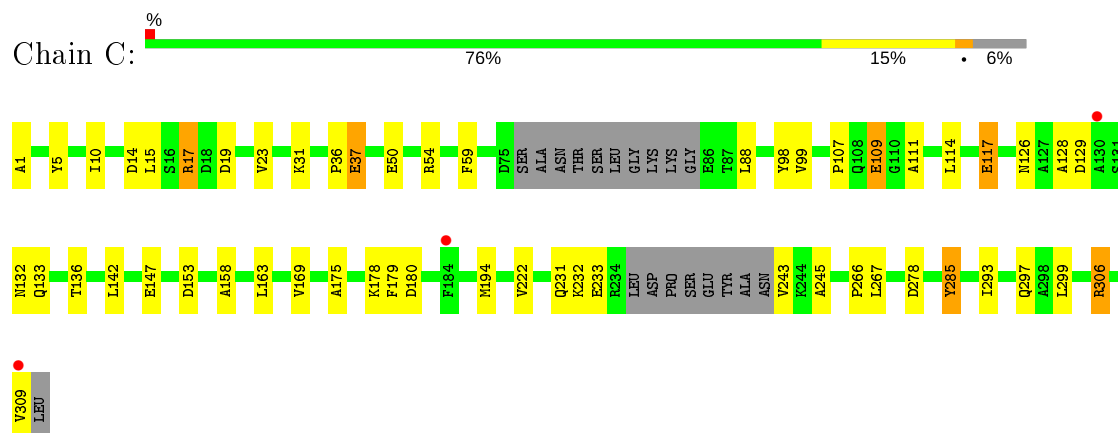
- Molecule 1: Aspartate carbamoyltransferase catalytic subunit



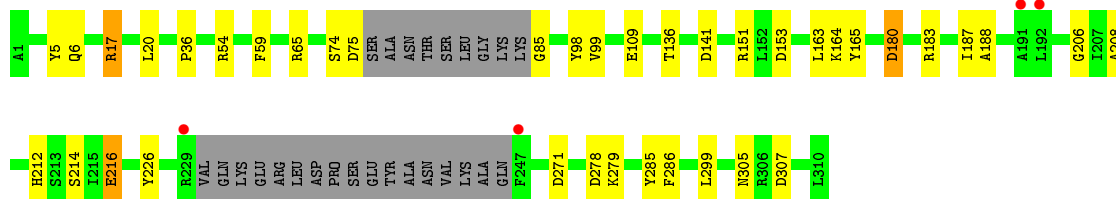
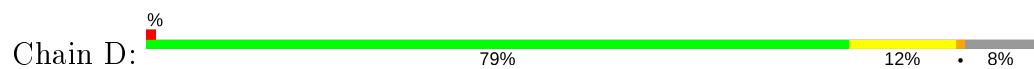
- Molecule 1: Aspartate carbamoyltransferase catalytic subunit



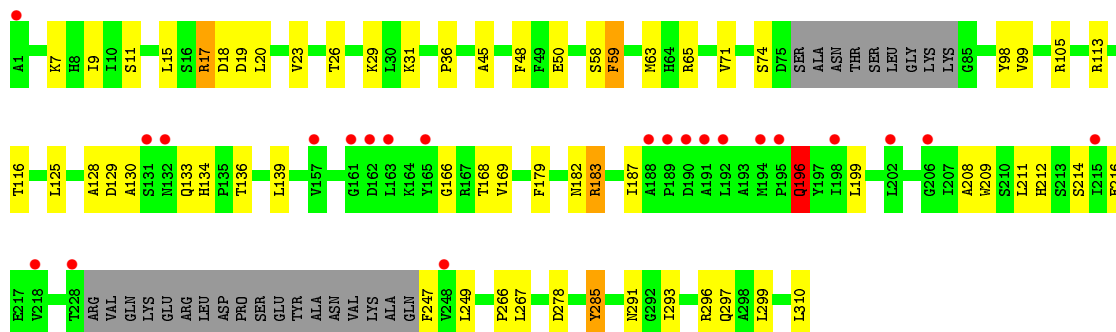
- Molecule 1: Aspartate carbamoyltransferase catalytic subunit



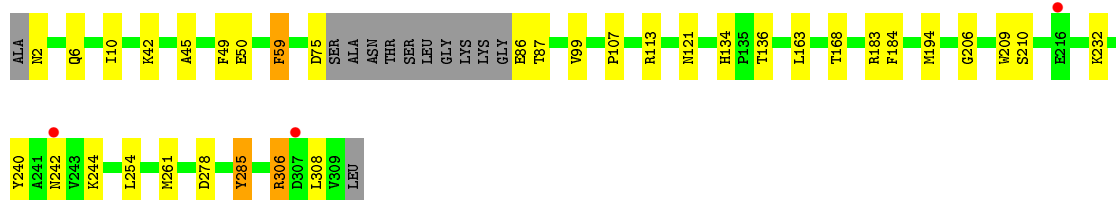
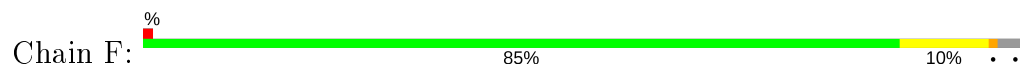
- Molecule 1: Aspartate carbamoyltransferase catalytic subunit



- Molecule 1: Aspartate carbamoyltransferase catalytic subunit



- Molecule 1: Aspartate carbamoyltransferase catalytic subunit



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	81.76 Å 96.73 Å 121.69 Å 90.00° 94.16° 90.00°	Depositor
Resolution (Å)	48.36 – 2.50 48.36 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.2 (48.36-2.50) 93.3 (48.36-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.38 (at 2.51 Å)	Xtriage
Refinement program	PHENIX 1.14-3260	Depositor
R, R_{free}	0.192 , 0.228 0.191 , 0.228	Depositor DCC
R_{free} test set	2005 reflections (3.08%)	wwPDB-VP
Wilson B-factor (Å ²)	32.5	Xtriage
Anisotropy	0.017	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 46.4	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	0.94	EDS
Total number of atoms	14188	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 40.52 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.7037e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical 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	0.36	0/2384	0.58	0/3240
1	B	0.49	4/2376 (0.2%)	0.76	8/3231 (0.2%)
1	C	0.48	3/2285 (0.1%)	0.69	5/3109 (0.2%)
1	D	0.43	0/2258	0.71	7/3066 (0.2%)
1	E	0.38	0/2205	0.70	6/3004 (0.2%)
1	F	0.40	0/2358	0.64	3/3207 (0.1%)
All	All	0.43	7/13866 (0.1%)	0.68	29/18857 (0.2%)

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	117	GLU	CB-CG	7.30	1.66	1.52
1	C	17	ARG	CZ-NH1	-6.29	1.24	1.33
1	C	117	GLU	CG-CD	6.16	1.61	1.51
1	B	37	GLU	CD-OE2	6.05	1.32	1.25
1	B	37	GLU	CG-CD	-5.72	1.43	1.51

The worst 5 of 29 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	17	ARG	NE-CZ-NH2	-12.31	114.14	120.30
1	B	37	GLU	CA-CB-CG	-12.12	86.72	113.40
1	B	250	ARG	NE-CZ-NH2	-11.93	114.33	120.30
1	D	17	ARG	NE-CZ-NH2	-9.19	115.70	120.30
1	D	180	ASP	CB-CG-OD1	-9.17	110.04	118.30

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	2339	0	2319	26	0
1	B	2331	0	2319	34	0
1	C	2243	0	2211	46	0
1	D	2216	0	2219	19	0
1	E	2163	0	2124	38	0
1	F	2313	0	2291	22	0
2	A	69	0	0	6	0
2	B	120	0	0	7	0
2	C	89	0	0	4	1
2	D	120	0	0	4	0
2	E	47	0	0	5	1
2	F	138	0	0	4	1
All	All	14188	0	13483	180	2

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.

The worst 5 of 180 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:17:ARG:NH2	1:C:179:PHE:HA	1.50	1.25
1:C:17:ARG:HH22	1:C:179:PHE:HA	0.87	0.99
1:C:17:ARG:HH22	1:C:179:PHE:CA	1.80	0.90
1:F:75:ASP:OD2	2:F:401:HOH:O	1.91	0.87
1:E:182:ASN:O	2:E:401:HOH:O	1.93	0.87

All (2) 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)
2:E:439:HOH:O	2:F:474:HOH:O[1_565]	1.90	0.30
2:C:481:HOH:O	2:C:484:HOH:O[2_557]	2.11	0.09

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	297/310 (96%)	286 (96%)	11 (4%)	0	100	100
1	B	297/310 (96%)	283 (95%)	12 (4%)	2 (1%)	22	39
1	C	285/310 (92%)	274 (96%)	9 (3%)	2 (1%)	22	39
1	D	278/310 (90%)	265 (95%)	12 (4%)	1 (0%)	34	54
1	E	277/310 (89%)	267 (96%)	9 (3%)	1 (0%)	34	54
1	F	294/310 (95%)	281 (96%)	12 (4%)	1 (0%)	41	61
All	All	1728/1860 (93%)	1656 (96%)	65 (4%)	7 (0%)	34	54

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	232	LYS
1	E	130	ALA
1	B	206	GLY
1	C	109	GLU
1	D	206	GLY

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	251/261 (96%)	247 (98%)	4 (2%)	62	84
1	B	249/261 (95%)	242 (97%)	7 (3%)	43	70
1	C	238/261 (91%)	235 (99%)	3 (1%)	69	87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	239/261 (92%)	233 (98%)	6 (2%)	47	73
1	E	228/261 (87%)	221 (97%)	7 (3%)	40	67
1	F	249/261 (95%)	245 (98%)	4 (2%)	62	84
All	All	1454/1566 (93%)	1423 (98%)	31 (2%)	53	78

5 of 31 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	20	LEU
1	D	75	ASP
1	F	244	LYS
1	D	54	ARG
1	D	151	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	132	ASN
1	C	21	ASN
1	F	41	HIS
1	F	146	GLN
1	F	297	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 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	301/310 (97%)	-0.08	3 (0%) 82 84	27, 49, 83, 100	0
1	B	301/310 (97%)	-0.30	4 (1%) 77 79	24, 38, 66, 92	0
1	C	291/310 (93%)	-0.13	3 (1%) 82 84	23, 42, 68, 100	0
1	D	284/310 (91%)	-0.25	4 (1%) 75 77	19, 32, 60, 78	0
1	E	283/310 (91%)	0.26	22 (7%) 13 13	31, 55, 101, 114	0
1	F	298/310 (96%)	-0.28	3 (1%) 82 84	23, 35, 73, 110	0
All	All	1758/1860 (94%)	-0.13	39 (2%) 62 65	19, 41, 83, 114	0

The worst 5 of 39 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	161	GLY	5.6
1	E	165	TYR	4.9
1	D	247	PHE	4.6
1	E	189	PRO	4.6
1	E	191	ALA	4.4

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.