



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 28, 2016 – 11:42 AM EDT

PDB ID : 5AX8
Title : Recombinant expression, purification and preliminary crystallographic studies of the mature form of human mitochondrial aspartate aminotransferase
Authors : Jiang, X.; Wang, J.; Chang, H.; Zhou, Y.
Deposited on : 2015-07-20
Resolution : 2.99 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 : unknown
Xtriage (Phenix) : 1.9-1692
EDS : rb-20027107
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) : rb-20027107

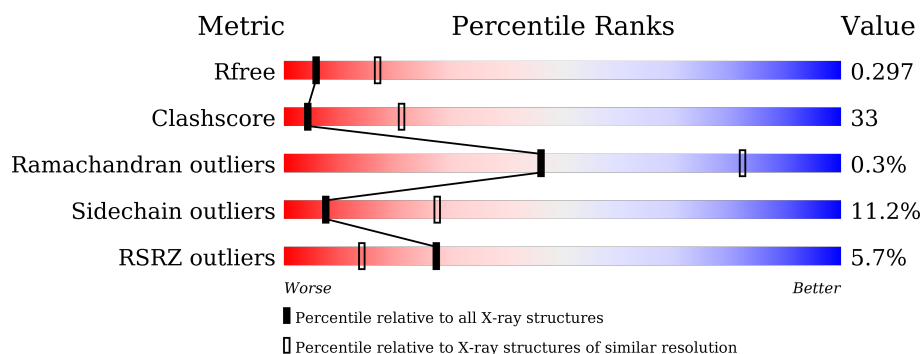
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.99 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	1992 (3.00-2.96)
Clashscore	102246	2349 (3.00-2.96)
Ramachandran outliers	100387	2274 (3.00-2.96)
Sidechain outliers	100360	2277 (3.00-2.96)
RSRZ outliers	91569	2007 (3.00-2.96)

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	407	
1	B	407	
1	C	407	
1	D	407	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 12580 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 aminotransferase, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	401	Total	C	N	O	S	0	0	0
			3145	2001	552	574	18			
1	B	401	Total	C	N	O	S	0	0	0
			3145	2001	552	574	18			
1	C	401	Total	C	N	O	S	0	0	0
			3145	2001	552	574	18			
1	D	401	Total	C	N	O	S	0	0	0
			3145	2001	552	574	18			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	346	GLY	VAL	engineered mutation	UNP P00505
A	431	HIS	-	expression tag	UNP P00505
A	432	HIS	-	expression tag	UNP P00505
A	433	HIS	-	expression tag	UNP P00505
A	434	HIS	-	expression tag	UNP P00505
A	435	HIS	-	expression tag	UNP P00505
A	436	HIS	-	expression tag	UNP P00505
B	346	GLY	VAL	engineered mutation	UNP P00505
B	431	HIS	-	expression tag	UNP P00505
B	432	HIS	-	expression tag	UNP P00505
B	433	HIS	-	expression tag	UNP P00505
B	434	HIS	-	expression tag	UNP P00505
B	435	HIS	-	expression tag	UNP P00505
B	436	HIS	-	expression tag	UNP P00505
C	346	GLY	VAL	engineered mutation	UNP P00505
C	431	HIS	-	expression tag	UNP P00505
C	432	HIS	-	expression tag	UNP P00505
C	433	HIS	-	expression tag	UNP P00505
C	434	HIS	-	expression tag	UNP P00505
C	435	HIS	-	expression tag	UNP P00505
C	436	HIS	-	expression tag	UNP P00505

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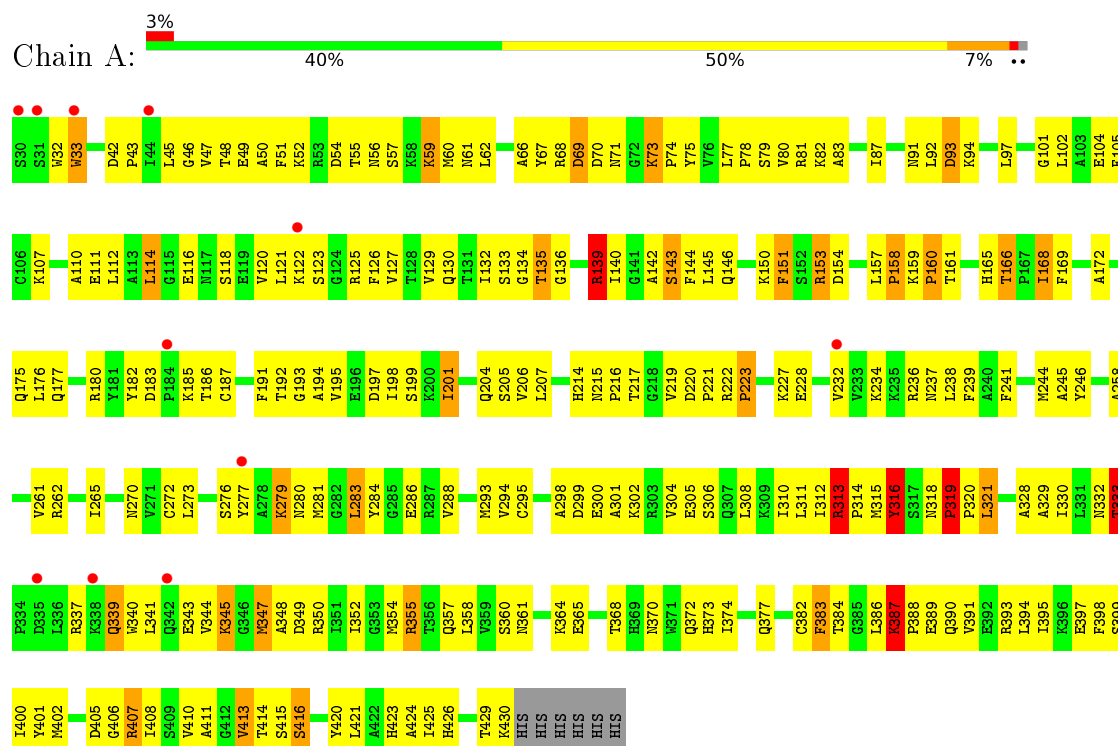
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Chain	Residue	Modelled	Actual	Comment	Reference
D	346	GLY	VAL	engineered mutation	UNP P00505
D	431	HIS	-	expression tag	UNP P00505
D	432	HIS	-	expression tag	UNP P00505
D	433	HIS	-	expression tag	UNP P00505
D	434	HIS	-	expression tag	UNP P00505
D	435	HIS	-	expression tag	UNP P00505
D	436	HIS	-	expression tag	UNP P00505

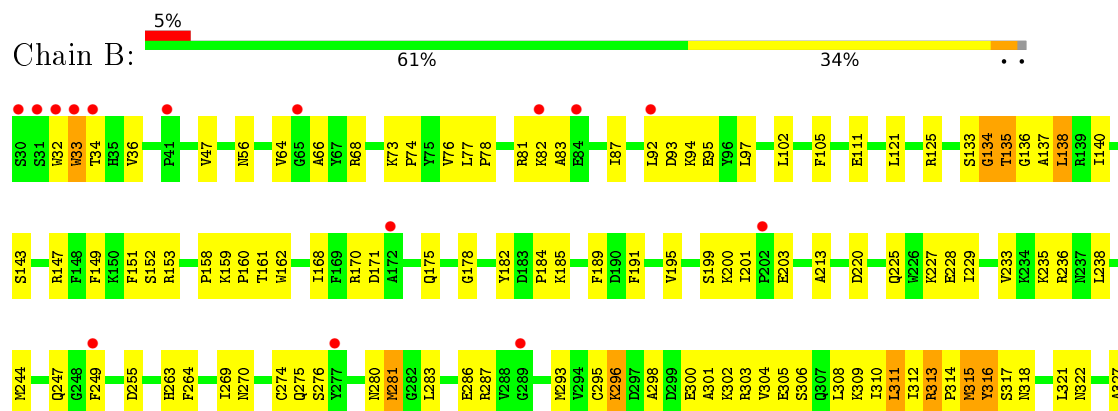
3 Residue-property plots

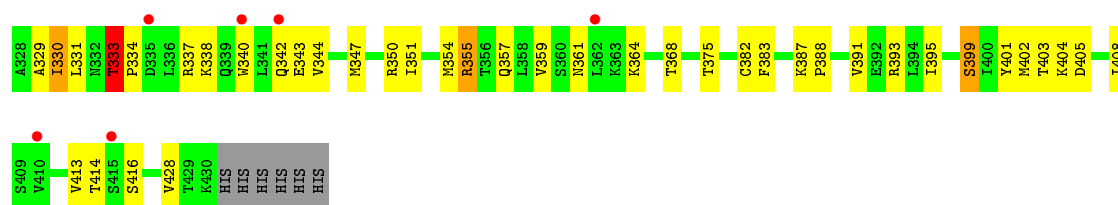
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 ($RSRZ > 2$). 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 aminotransferase, mitochondrial



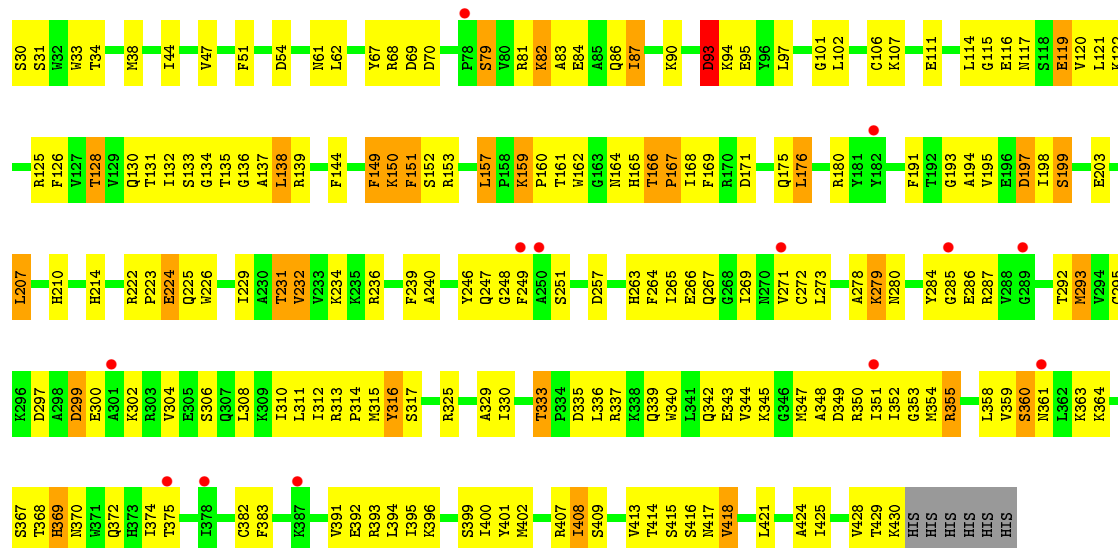
- Molecule 1: Aspartate aminotransferase, mitochondrial





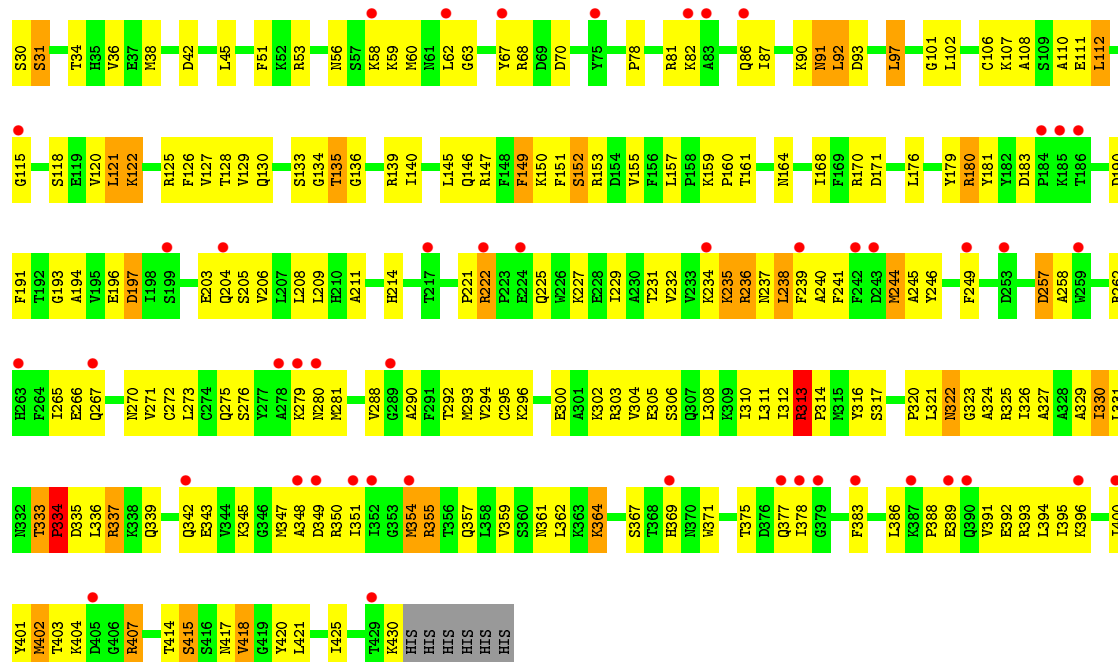
• Molecule 1: Aspartate aminotransferase, mitochondrial

Chain C: 3% 50% 41% 7%



• Molecule 1: Aspartate aminotransferase, mitochondrial

Chain D: 12% 48% 43% 7%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	56.71Å 76.14Å 94.25Å 78.00° 85.65° 78.41°	Depositor
Resolution (Å)	48.31 – 2.99 48.31 – 2.99	Depositor EDS
% Data completeness (in resolution range)	88.2 (48.31-2.99) 80.6 (48.31-2.99)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.45 (at 3.01Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.273 , 0.291 0.281 , 0.297	Depositor DCC
R_{free} test set	1893 reflections (7.36%)	DCC
Wilson B-factor (Å ²)	53.1	Xtriage
Anisotropy	0.055	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 19.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 26960 reflections	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	12580	wwPDB-VP
Average B, all atoms (Å ²)	52.0	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 46.57 % 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 1.1230e-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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	1.41	4/3218 (0.1%)	1.03	14/4348 (0.3%)
1	B	0.66	2/3218 (0.1%)	0.69	2/4348 (0.0%)
1	C	0.70	1/3218 (0.0%)	0.72	3/4348 (0.1%)
1	D	0.62	1/3218 (0.0%)	0.72	3/4348 (0.1%)
All	All	0.91	8/12872 (0.1%)	0.80	22/17392 (0.1%)

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	334	PRO	N-CD	5.36	1.55	1.47
1	A	388	PRO	N-CD	5.35	1.55	1.47
1	A	319	PRO	N-CD	5.20	1.55	1.47
1	C	167	PRO	N-CD	5.19	1.55	1.47
1	B	314	PRO	N-CD	5.17	1.55	1.47

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	313	ARG	C-N-CD	6.00	140.99	128.40
1	A	333	THR	C-N-CD	5.93	140.86	128.40
1	A	201	ILE	C-N-CD	5.89	140.78	128.40
1	A	183	ASP	C-N-CD	5.89	140.78	128.40
1	D	333	THR	C-N-CD	5.84	140.67	128.40

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	3145	0	3133	294	0
1	B	3145	0	3133	160	0
1	C	3145	0	3133	220	0
1	D	3145	0	3133	250	0
All	All	12580	0	12532	833	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 33.

The worst 5 of 833 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:32:TRP:CE3	1:D:151:PHE:CZ	2.21	1.29
1:D:333:THR:HG21	1:D:336:LEU:CD1	1.63	1.28
1:D:333:THR:HG23	1:D:336:LEU:CB	1.65	1.26
1:D:333:THR:CG2	1:D:336:LEU:HB2	1.65	1.25
1:B:33:TRP:HH2	1:D:149:PHE:CD1	1.54	1.24

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	399/407 (98%)	391 (98%)	7 (2%)	1 (0%)	46	82
1	B	399/407 (98%)	387 (97%)	10 (2%)	2 (0%)	34	75
1	C	399/407 (98%)	387 (97%)	10 (2%)	2 (0%)	34	75
1	D	399/407 (98%)	390 (98%)	9 (2%)	0	100	100
All	All	1596/1628 (98%)	1555 (97%)	36 (2%)	5 (0%)	46	82

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	116	GLU
1	B	281	MET
1	C	93	ASP
1	B	134	GLY
1	A	160	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	333/339 (98%)	290 (87%)	43 (13%)	5	21
1	B	333/339 (98%)	309 (93%)	24 (7%)	18	52
1	C	333/339 (98%)	295 (89%)	38 (11%)	7	27
1	D	333/339 (98%)	289 (87%)	44 (13%)	5	20
All	All	1332/1356 (98%)	1183 (89%)	149 (11%)	7	27

5 of 149 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	30	SER
1	C	197	ASP
1	D	337	ARG
1	C	79	SER
1	C	133	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	339	GLN
1	A	423	HIS
1	C	86	GLN
1	A	322	ASN
1	B	322	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 carbohydrates 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	401/407 (98%)	0.16	11 (2%) 58 35	38, 44, 58, 65	0
1	B	401/407 (98%)	0.51	21 (5%) 31 16	41, 49, 64, 77	0
1	C	401/407 (98%)	0.49	13 (3%) 51 30	41, 51, 58, 65	0
1	D	401/407 (98%)	0.77	47 (11%) 6 3	45, 62, 70, 75	0
All	All	1604/1628 (98%)	0.48	92 (5%) 27 14	38, 51, 68, 77	0

The worst 5 of 92 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	32	TRP	6.4
1	B	31	SER	6.3
1	A	31	SER	6.3
1	B	33	TRP	5.6
1	D	351	ILE	4.7

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.