



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 10:57 PM UTC

PDB ID : 3VBA / pdb_00003vba
Title : Crystal structure of methanogen 3-isopropylmalate isomerase small subunit
Authors : Hwang, K.Y.; Lee, E.H.
Deposited on : 2012-01-02
Resolution : 2.00 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Xtrriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

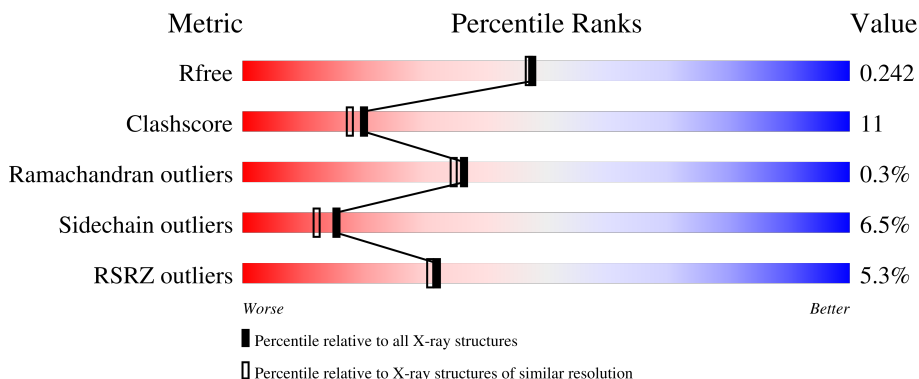
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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.



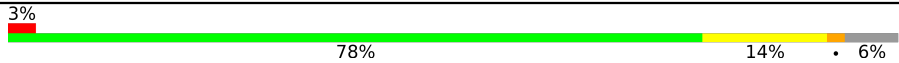
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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 of 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	176	 4% 74% 18% . .
1	B	176	 5% 74% 19% . .
1	C	176	 9% 70% 22% . 6%
1	D	176	 6% 73% 15% 5% 7%
1	E	176	 4% 77% 14% . . 6%

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Mol	Chain	Length	Quality of chain
1	F	176	 <p>A horizontal bar chart representing the quality of chain. The bar is divided into four segments: a small red segment on the left labeled '3%', a large green segment labeled '78%', a yellow segment labeled '14%', and a small grey segment on the right labeled '6%'.</p>

2 Entry composition i

There are 2 unique types of molecules in this entry. The entry contains 8356 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 Isopropylmalate/citramalate isomerase small subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	169	1295	828	217	241	9	0	0	0
1	B	169	1295	828	217	241	9	0	0	0
1	C	166	1269	812	213	236	8	0	0	0
1	D	163	1250	801	210	231	8	0	0	0
1	E	165	1263	809	212	233	9	0	0	0
1	F	165	1263	809	212	233	9	0	0	0

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	169	LEU	-	expression tag	UNP Q58673
A	170	GLU	-	expression tag	UNP Q58673
A	171	HIS	-	expression tag	UNP Q58673
A	172	HIS	-	expression tag	UNP Q58673
A	173	HIS	-	expression tag	UNP Q58673
A	174	HIS	-	expression tag	UNP Q58673
A	175	HIS	-	expression tag	UNP Q58673
A	176	HIS	-	expression tag	UNP Q58673
B	169	LEU	-	expression tag	UNP Q58673
B	170	GLU	-	expression tag	UNP Q58673
B	171	HIS	-	expression tag	UNP Q58673
B	172	HIS	-	expression tag	UNP Q58673
B	173	HIS	-	expression tag	UNP Q58673
B	174	HIS	-	expression tag	UNP Q58673
B	175	HIS	-	expression tag	UNP Q58673
B	176	HIS	-	expression tag	UNP Q58673
C	169	LEU	-	expression tag	UNP Q58673

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Chain	Residue	Modelled	Actual	Comment	Reference
C	170	GLU	-	expression tag	UNP Q58673
C	171	HIS	-	expression tag	UNP Q58673
C	172	HIS	-	expression tag	UNP Q58673
C	173	HIS	-	expression tag	UNP Q58673
C	174	HIS	-	expression tag	UNP Q58673
C	175	HIS	-	expression tag	UNP Q58673
C	176	HIS	-	expression tag	UNP Q58673
D	169	LEU	-	expression tag	UNP Q58673
D	170	GLU	-	expression tag	UNP Q58673
D	171	HIS	-	expression tag	UNP Q58673
D	172	HIS	-	expression tag	UNP Q58673
D	173	HIS	-	expression tag	UNP Q58673
D	174	HIS	-	expression tag	UNP Q58673
D	175	HIS	-	expression tag	UNP Q58673
D	176	HIS	-	expression tag	UNP Q58673
E	169	LEU	-	expression tag	UNP Q58673
E	170	GLU	-	expression tag	UNP Q58673
E	171	HIS	-	expression tag	UNP Q58673
E	172	HIS	-	expression tag	UNP Q58673
E	173	HIS	-	expression tag	UNP Q58673
E	174	HIS	-	expression tag	UNP Q58673
E	175	HIS	-	expression tag	UNP Q58673
E	176	HIS	-	expression tag	UNP Q58673
F	169	LEU	-	expression tag	UNP Q58673
F	170	GLU	-	expression tag	UNP Q58673
F	171	HIS	-	expression tag	UNP Q58673
F	172	HIS	-	expression tag	UNP Q58673
F	173	HIS	-	expression tag	UNP Q58673
F	174	HIS	-	expression tag	UNP Q58673
F	175	HIS	-	expression tag	UNP Q58673
F	176	HIS	-	expression tag	UNP Q58673

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	140	Total O 140 140	0	0
2	B	122	Total O 122 122	0	0
2	C	117	Total O 117 117	0	0
2	D	125	Total O 125 125	0	0

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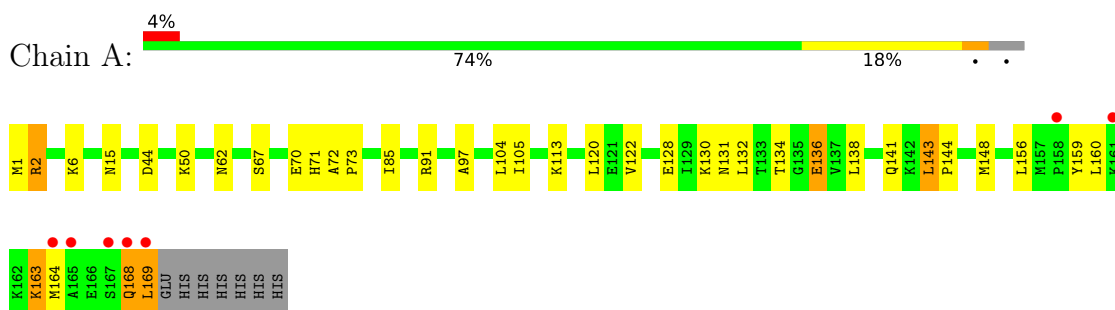
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	E	105	Total 105	O 105	0	0
2	F	112	Total 112	O 112	0	0

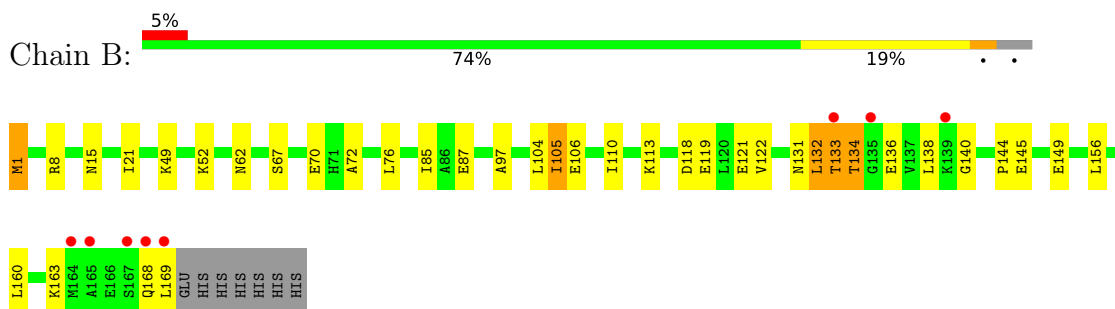
3 Residue-property plots [i](#)

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.

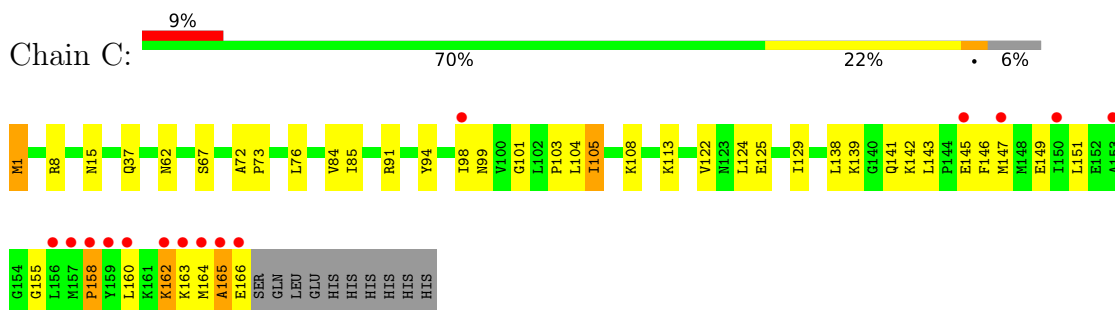
- Molecule 1: Isopropylmalate/citramalate isomerase small subunit



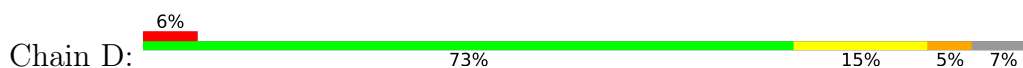
- Molecule 1: Isopropylmalate/citramalate isomerase small subunit

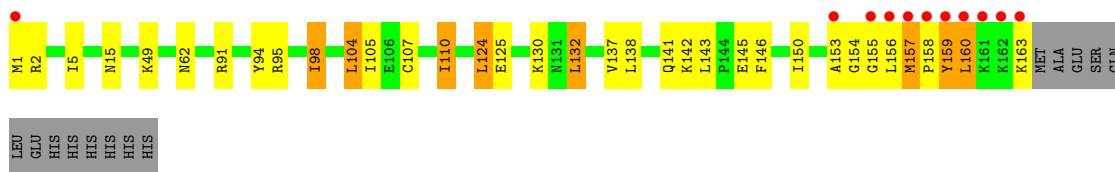


- Molecule 1: Isopropylmalate/citramalate isomerase small subunit

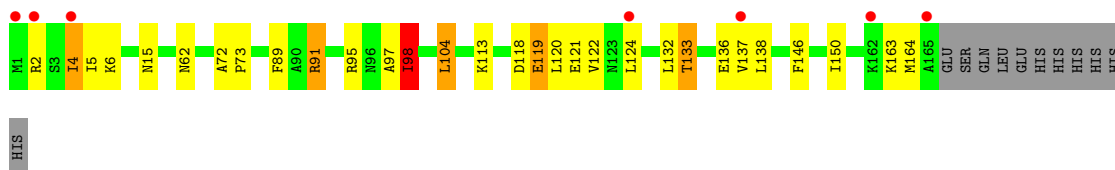
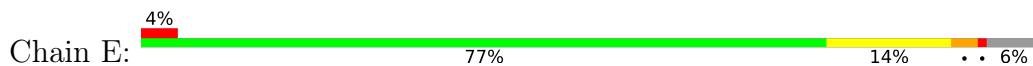


- Molecule 1: Isopropylmalate/citramalate isomerase small subunit

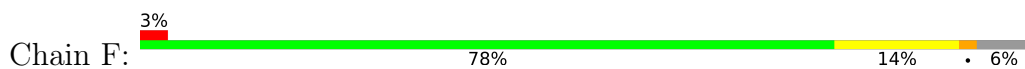




• Molecule 1: Isopropylmalate/citramalate isomerase small subunit



• Molecule 1: Isopropylmalate/citramalate isomerase small subunit



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	33.84Å 107.14Å 288.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.90 – 2.00 43.90 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.0 (43.90-2.00) 99.1 (43.90-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.25 (at 1.81Å)	Xtrriage
Refinement program	PHENIX 1.6.4_486	Depositor
R, R_{free}	0.197 , 0.244 0.193 , 0.242	Depositor DCC
R_{free} test set	4877 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	18.2	Xtrriage
Anisotropy	0.167	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 51.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8356	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 56.86 % 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 2.5737e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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](#)

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	0.49	0/1317	0.78	0/1770
1	B	0.49	0/1317	0.83	2/1770 (0.1%)
1	C	0.46	0/1291	0.80	0/1736
1	D	0.48	0/1272	0.85	1/1710 (0.1%)
1	E	0.43	0/1285	0.79	1/1727 (0.1%)
1	F	0.45	0/1285	0.77	0/1727
All	All	0.47	0/7767	0.80	4/10440 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	72	ALA	CA-C-N	-6.11	113.39	119.56
1	B	72	ALA	C-N-CA	-6.11	113.39	119.56
1	D	2	ARG	N-CA-C	5.69	115.62	108.45
1	E	98	ILE	CB-CA-C	-5.09	105.19	112.22

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	1295	0	1335	39	1
1	B	1295	0	1335	43	1
1	C	1269	0	1304	40	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1250	0	1291	41	0
1	E	1263	0	1305	22	0
1	F	1263	0	1305	20	0
2	A	140	0	0	1	0
2	B	122	0	0	1	0
2	C	117	0	0	2	0
2	D	125	0	0	2	0
2	E	105	0	0	0	0
2	F	112	0	0	2	0
All	All	8356	0	7875	177	1

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 11.

The worst 5 of 177 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:D:105:ILE:HG22	1:D:143:LEU:HD11	1.44	1.00
1:B:134:THR:HG22	1:B:136:GLU:H	1.29	0.94
1:A:134:THR:HG21	2:A:245:HOH:O	1.82	0.79
1:A:85:ILE:HD11	1:A:122:VAL:HG21	1.67	0.76
1:D:153:ALA:HB3	1:D:159:TYR:HB2	1.67	0.75

All (1) 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:1:MET:O	1:B:1:MET:O[1_455]	1.93	0.27

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	167/176 (95%)	164 (98%)	2 (1%)	1 (1%)	21	17
1	B	167/176 (95%)	167 (100%)	0	0	100	100
1	C	164/176 (93%)	158 (96%)	4 (2%)	2 (1%)	10	6
1	D	161/176 (92%)	157 (98%)	4 (2%)	0	100	100
1	E	163/176 (93%)	160 (98%)	3 (2%)	0	100	100
1	F	163/176 (93%)	161 (99%)	2 (1%)	0	100	100
All	All	985/1056 (93%)	967 (98%)	15 (2%)	3 (0%)	36	35

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	165	ALA
1	A	168	GLN
1	C	158	PRO

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	139/146 (95%)	130 (94%)	9 (6%)	15	12
1	B	139/146 (95%)	132 (95%)	7 (5%)	22	20
1	C	135/146 (92%)	128 (95%)	7 (5%)	21	18
1	D	134/146 (92%)	123 (92%)	11 (8%)	10	7
1	E	135/146 (92%)	124 (92%)	11 (8%)	11	7
1	F	135/146 (92%)	127 (94%)	8 (6%)	18	14
All	All	817/876 (93%)	764 (94%)	53 (6%)	15	12

5 of 53 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	137	VAL
1	E	4	ILE

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Mol	Chain	Res	Type
1	F	132	LEU
1	D	138	LEU
1	D	159	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	15	ASN
1	E	15	ASN
1	F	141	GLN
1	F	62	ASN
1	F	99	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 oligosaccharides 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	169/176 (96%)	-0.12	7 (4%) 41 40	10, 17, 38, 59	0
1	B	169/176 (96%)	0.09	8 (4%) 36 35	9, 19, 40, 56	0
1	C	166/176 (94%)	0.22	15 (9%) 15 14	10, 19, 51, 75	0
1	D	163/176 (92%)	0.20	11 (6%) 24 22	9, 19, 46, 70	0
1	E	165/176 (93%)	0.20	7 (4%) 40 39	13, 22, 45, 69	0
1	F	165/176 (93%)	0.15	5 (3%) 52 51	11, 21, 44, 73	0
All	All	997/1056 (94%)	0.12	53 (5%) 32 31	9, 19, 46, 75	0

The worst 5 of 53 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	158	PRO	4.9
1	D	159	TYR	4.2
1	D	162	LYS	4.0
1	F	165	ALA	3.8
1	D	1	MET	3.8

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 oligosaccharides 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.