



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 28, 2025 – 08:54 PM JST

PDB ID : 8Z1P / pdb_00008z1p
Title : Crystal structure of *Saccharomyces cerevisiae* isoleucyl-tRNA synthetase in complex with a mimic tRNA(Met) and isoleucine
Authors : Chen, B.; Yi, F.; Zhou, H.
Deposited on : 2024-04-11
Resolution : 2.83 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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 Phenix2.0rc1
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 2.0rc1
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.006 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.43.1

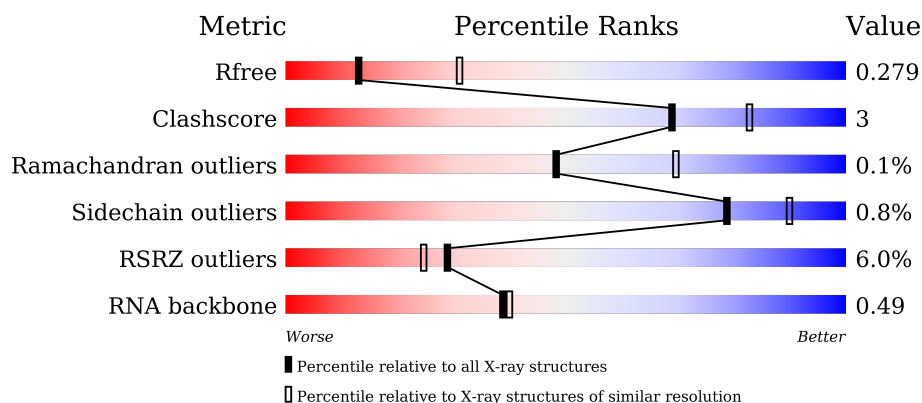
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.83 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}	164625	1367 (2.86-2.82)
Clashscore	180529	1455 (2.86-2.82)
Ramachandran outliers	177936	1422 (2.86-2.82)
Sidechain outliers	177891	1423 (2.86-2.82)
RSRZ outliers	164620	1368 (2.86-2.82)
RNA backbone	3690	1096 (3.08-2.60)

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	1080	<div> <div>6%</div> <div>89%</div> <div>9%</div> </div>
2	B	76	<div> <div>8%</div> <div>72%</div> <div>12%</div> <div>14%</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8988 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 isoleucine-tRNA ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1060	Total	C	N	O	S	0	0	0
			7607	4855	1259	1470	23			

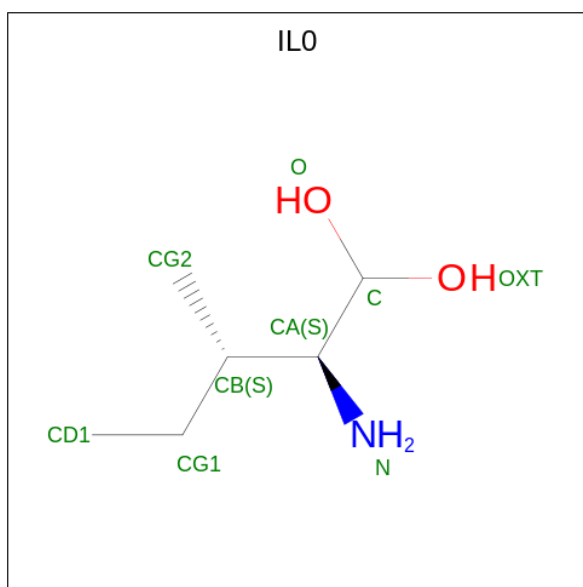
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1073	LEU	-	expression tag	UNP A0A6A5Q0L4
A	1074	GLU	-	expression tag	UNP A0A6A5Q0L4
A	1075	HIS	-	expression tag	UNP A0A6A5Q0L4
A	1076	HIS	-	expression tag	UNP A0A6A5Q0L4
A	1077	HIS	-	expression tag	UNP A0A6A5Q0L4
A	1078	HIS	-	expression tag	UNP A0A6A5Q0L4
A	1079	HIS	-	expression tag	UNP A0A6A5Q0L4
A	1080	HIS	-	expression tag	UNP A0A6A5Q0L4

- Molecule 2 is a RNA chain called tRNA(Met).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	65	Total	C	N	O	P	0	0	0
			1365	607	244	449	65			

- Molecule 3 is (2S,3S)-2-amino-3-methylpentane-1,1-diol (CCD ID: IL0) (formula: C₆H₁₅NO₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			9	6	1	2		

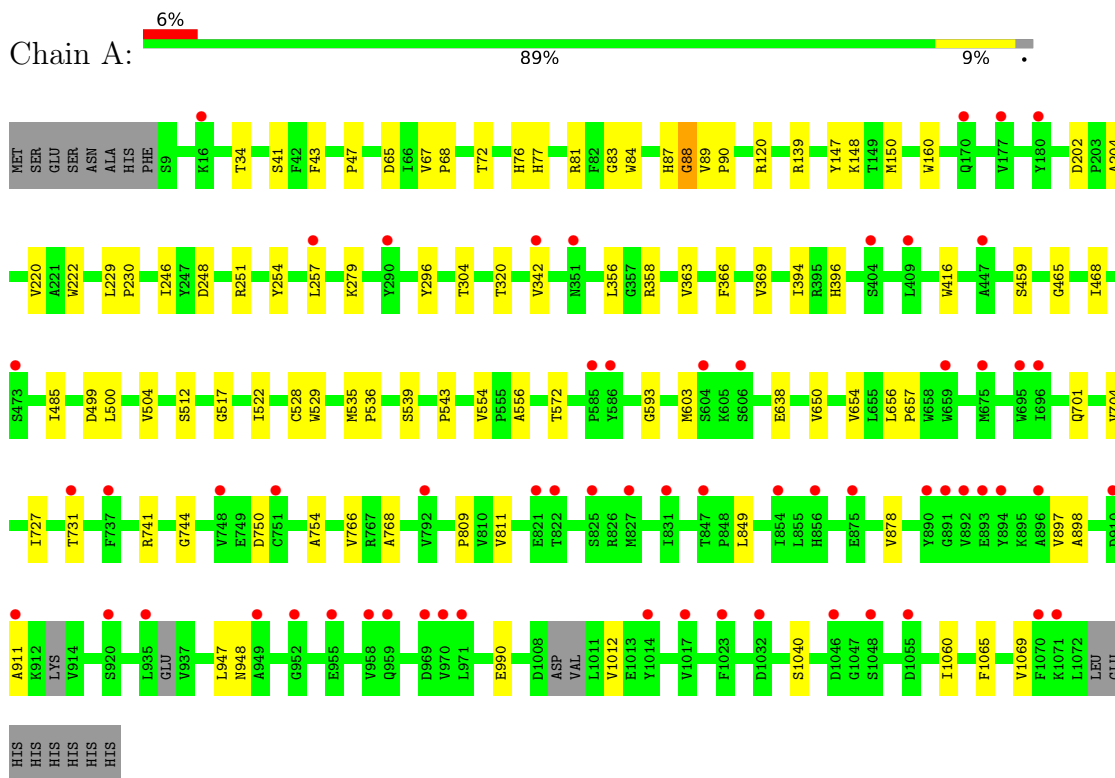
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	7	Total	O	0	0
			7	7		

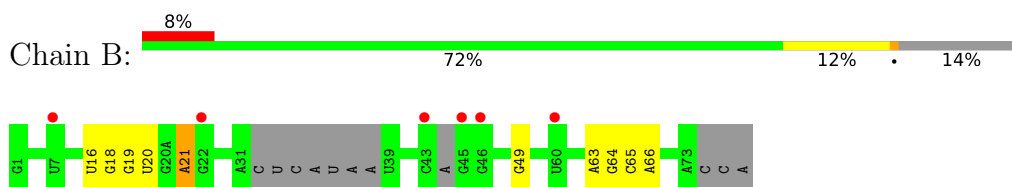
3 Residue-property plots

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: isoleucine-tRNA ligase



• Molecule 2: tRNA(Met)



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	52.66Å 81.21Å 106.17Å 78.39° 83.65° 71.78°	Depositor
Resolution (Å)	75.92 – 2.83 75.92 – 2.83	Depositor EDS
% Data completeness (in resolution range)	76.4 (75.92-2.83) 76.4 (75.92-2.83)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.84 (at 2.82Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.237 , 0.278 0.239 , 0.279	Depositor DCC
R_{free} test set	1845 reflections (4.68%)	wwPDB-VP
Wilson B-factor (Å ²)	79.5	Xtriage
Anisotropy	0.442	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 74.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8988	wwPDB-VP
Average B, all atoms (Å ²)	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.84% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: IL0

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	1.03	1/7801 (0.0%)	1.39	3/10703 (0.0%)
2	B	0.56	0/1523	0.75	0/2368
All	All	0.97	1/9324 (0.0%)	1.29	3/13071 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	911	ALA	C-O	6.05	1.28	1.23

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	88	GLY	CA-C-N	10.38	126.78	120.24
1	A	88	GLY	C-N-CA	10.38	126.78	120.24
1	A	147	TYR	CB-CA-C	5.16	119.23	109.37

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	7607	0	6343	51	0
2	B	1365	0	693	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	9	0	12	0	0
4	A	7	0	0	0	0
All	All	8988	0	7048	54	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 3.

All (54) 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:485:ILE:HG12	1:A:500:LEU:HD21	1.75	0.68
1:A:897:VAL:O	1:A:948:ASN:N	2.27	0.68
1:A:593:GLY:HA3	1:A:638:GLU:O	2.00	0.61
1:A:87:HIS:CG	1:A:465:GLY:HA2	2.36	0.61
1:A:528:CYS:HG	1:A:529:TRP:CD1	2.20	0.59
1:A:84:TRP:HB2	1:A:148:LYS:HG2	1.85	0.56
1:A:990:GLU:HG3	1:A:1060:ILE:HG12	1.88	0.55
1:A:67:VAL:HB	1:A:68:PRO:HD3	1.88	0.54
1:A:120:ARG:HG3	1:A:150:MET:HE1	1.90	0.54
1:A:65:ASP:HB2	1:A:139:ARG:HG3	1.90	0.52
1:A:468:ILE:HB	1:A:522:ILE:HD11	1.92	0.52
1:A:160:TRP:CD2	1:A:543:PRO:HD3	2.46	0.50
1:A:89:VAL:N	1:A:90:PRO:CD	2.75	0.49
1:A:41:SER:HB3	1:A:556:ALA:HA	1.95	0.48
1:A:656:LEU:HB3	1:A:657:PRO:HD3	1.94	0.48
1:A:499:ASP:HB3	1:A:504:VAL:HG21	1.95	0.48
1:A:1012:VAL:HG22	1:A:1069:VAL:HG12	1.95	0.48
1:A:229:LEU:N	1:A:230:PRO:CD	2.76	0.48
1:A:204:ALA:HB1	1:A:222:TRP:HE1	1.78	0.47
1:A:741:ARG:HD2	1:A:754:ALA:HB2	1.96	0.47
1:A:535:MET:HG3	1:A:536:PRO:HD3	1.96	0.47
1:A:1060:ILE:HG13	1:A:1065:PHE:HE1	1.80	0.47
1:A:148:LYS:HB3	1:A:150:MET:HG2	1.96	0.46
1:A:47:PRO:HD2	1:A:83:GLY:O	2.16	0.46
1:A:65:ASP:CG	1:A:139:ARG:HA	2.39	0.46
1:A:220:VAL:HG12	1:A:320:THR:HG21	1.96	0.46
1:A:529:TRP:HB3	1:A:572:THR:HG21	1.97	0.46
2:B:65:C:H2'	2:B:66:A:C8	2.51	0.45
1:A:650:VAL:O	1:A:654:VAL:HB	2.16	0.45
1:A:898:ALA:HA	1:A:947:LEU:HA	1.98	0.45
1:A:81:ARG:NH2	1:A:539:SER:O	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1012:VAL:HG23	1:A:1040:SER:HB2	1.98	0.45
1:A:296:TYR:CE2	1:A:363:VAL:HG13	2.52	0.44
1:A:366:PHE:O	1:A:369:VAL:HG23	2.18	0.44
1:A:43:PHE:HZ	1:A:554:VAL:HG22	1.81	0.44
1:A:416:TRP:HB2	1:A:459:SER:HB3	2.00	0.44
1:A:768:ALA:HB2	1:A:809:PRO:HG2	2.00	0.44
1:A:535:MET:C	1:A:535:MET:SD	3.01	0.43
2:B:63:A:H2'	2:B:64:G:C8	2.53	0.43
1:A:248:ASP:HB3	1:A:251:ARG:HB2	2.00	0.43
1:A:88:GLY:C	1:A:90:PRO:HD2	2.44	0.42
1:A:727:ILE:O	1:A:731:THR:HG22	2.19	0.42
1:A:849:LEU:O	1:A:878:VAL:HA	2.20	0.42
1:A:202:ASP:HB2	1:A:396:HIS:NE2	2.36	0.41
1:A:72:THR:HA	1:A:76:HIS:O	2.20	0.41
1:A:246:ILE:O	1:A:254:TYR:HA	2.21	0.41
1:A:34:THR:O	1:A:77:HIS:HB2	2.20	0.41
1:A:257:LEU:C	1:A:257:LEU:HD12	2.46	0.41
1:A:603:MET:HE2	1:A:603:MET:HB2	1.86	0.41
2:B:21:A:H8	2:B:21:A:H5''	1.84	0.41
1:A:304:THR:O	1:A:342:VAL:HA	2.21	0.40
1:A:704:VAL:HG23	1:A:811:VAL:HG22	2.02	0.40
1:A:512:SER:HB3	1:A:517:GLY:O	2.21	0.40
1:A:356:LEU:HD23	1:A:358:ARG:HH21	1.86	0.40

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	1052/1080 (97%)	985 (94%)	66 (6%)	1 (0%)	48 69

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	744	GLY

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	650/967 (67%)	645 (99%)	5 (1%)	79 90

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	279	LYS
1	A	394	ILE
1	A	701	GLN
1	A	750	ASP
1	A	766	VAL

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

Mol	Chain	Res	Type
1	A	232	ASN
1	A	461	ASN
1	A	668	GLN
1	A	701	GLN
1	A	708	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	62/76 (81%)	6 (9%)	1 (1%)

All (6) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	16	U
2	B	18	G
2	B	19	G
2	B	20	U
2	B	21	A
2	B	49	G

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	B	21	A

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](#)

1 ligand is modelled in this entry.

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	IL0	A	1101	-	7,8,8	4.28	2 (28%)	5,10,10	3.06	1 (20%)

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	IL0	A	1101	-	-	4/10/10/10	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1101	IL0	O-C	-8.16	1.22	1.40
3	A	1101	IL0	OXT-C	-7.69	1.23	1.40

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1101	IL0	OXT-C-O	6.83	123.29	111.27

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1101	IL0	OXT-C-CA-N
3	A	1101	IL0	OXT-C-CA-CB
3	A	1101	IL0	O-C-CA-N
3	A	1101	IL0	O-C-CA-CB

There are no ring outliers.

No monomer is involved in short contacts.

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

6.1 Protein, DNA and RNA chains

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	1060/1080 (98%)	0.42	61 (5%)	30 25	41, 72, 119, 159	0
2	B	65/76 (85%)	0.70	6 (9%)	16 14	69, 97, 121, 144	0
All	All	1125/1156 (97%)	0.44	67 (5%)	29 24	41, 73, 120, 159	0

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	890	TYR	5.6
1	A	935	LEU	4.5
1	A	959	GLN	4.1
1	A	910	ASP	4.0
2	B	45	G	4.0
1	A	896	ALA	3.8
1	A	958	VAL	3.3
1	A	891	GLY	3.3
1	A	955	GLU	3.1
1	A	748	VAL	3.0
1	A	751	CYS	2.9
1	A	854	ILE	2.9
1	A	875	GLU	2.9
1	A	969	ASP	2.9
1	A	1023	PHE	2.8
1	A	920	SER	2.8
1	A	847	THR	2.8
1	A	911	ALA	2.8
1	A	894	TYR	2.8
1	A	404	SER	2.8
1	A	825	SER	2.7
1	A	827	MET	2.7
1	A	893	GLU	2.7
1	A	892	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	821	GLU	2.7
1	A	257	LEU	2.6
1	A	586	TYR	2.6
1	A	731	THR	2.6
1	A	695	TRP	2.6
1	A	606	SER	2.5
2	B	7	U	2.5
1	A	342	VAL	2.5
1	A	473	SER	2.5
1	A	831	ILE	2.5
1	A	16	LYS	2.4
1	A	1014	TYR	2.4
1	A	696	ILE	2.4
1	A	351	ASN	2.4
1	A	585	PRO	2.3
2	B	60	U	2.3
1	A	409	LEU	2.3
2	B	43	C	2.3
1	A	177	VAL	2.3
1	A	1046	ASP	2.3
2	B	22	G	2.3
1	A	949	ALA	2.2
1	A	1070	PHE	2.2
1	A	952	GLY	2.2
1	A	737	PHE	2.2
1	A	1032	ASP	2.2
1	A	180	TYR	2.1
1	A	447	ALA	2.1
1	A	971	LEU	2.1
1	A	970	VAL	2.1
1	A	1017	VAL	2.1
1	A	856	HIS	2.1
2	B	46	G	2.1
1	A	170	GLN	2.1
1	A	1071	LYS	2.1
1	A	604	SER	2.1
1	A	1048	SER	2.1
1	A	659	TRP	2.1
1	A	822	THR	2.0
1	A	1055	ASP	2.0
1	A	290	TYR	2.0
1	A	675	MET	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	792	VAL	2.0

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](#)

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. 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	B-factors(\AA^2)	Q<0.9
3	IL0	A	1101	9/9	0.89	0.16	47,50,55,55	0

6.5 Other polymers [i](#)

There are no such residues in this entry.