



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 02:37 PM GMT

PDB ID : 3ZZI
Title : Crystal structure of a tetrameric acetylglutamate kinase from *Saccharomyces cerevisiae*
Authors : De Cima, S.; Gil-Ortiz, F.; Crabeel, M.; Fita, I.; Rubio, V.
Deposited on : 2011-09-01
Resolution : 3.80 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

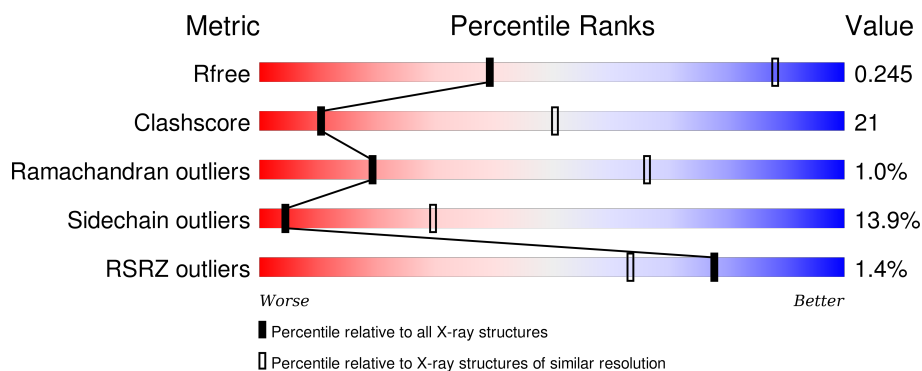
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.80 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	1317 (4.10-3.50)
Clashscore	102246	1458 (4.10-3.50)
Ramachandran outliers	100387	1397 (4.10-3.50)
Sidechain outliers	100360	1392 (4.10-3.50)
RSRZ outliers	91569	1325 (4.10-3.50)

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. 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	464	<div> <div></div> <div>59% 29% 6% 6%</div> </div>
1	B	464	<div> <div></div> <div>59% 29% 6% 6%</div> </div>
1	C	464	<div> <div>2%</div> <div>58% 29% 6% 6%</div> </div>
1	D	464	<div> <div>%</div> <div>55% 32% 6% 6%</div> </div>
1	E	464	<div> <div>%</div> <div>53% 32% 8% 6%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	464	<div><div>%</div><div><div></div><div>56%</div><div>31%</div><div>7%</div><div>6%</div></div></div>
1	G	464	<div><div>3%</div><div><div></div><div>61%</div><div>26%</div><div>6%</div><div>6%</div></div></div>
1	H	464	<div><div>%</div><div><div></div><div>53%</div><div>34%</div><div>7%</div><div>6%</div></div></div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 27248 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 ACETYLGLUTAMATE KINASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	436	Total	C	N	O	S	0	0	0
			3402	2167	571	655	9			
1	B	436	Total	C	N	O	S	0	0	0
			3402	2167	571	655	9			
1	C	436	Total	C	N	O	S	0	0	0
			3408	2170	574	655	9			
1	D	436	Total	C	N	O	S	0	0	0
			3404	2167	573	655	9			
1	E	436	Total	C	N	O	S	0	0	0
			3408	2170	574	655	9			
1	F	436	Total	C	N	O	S	0	0	0
			3408	2170	574	655	9			
1	G	436	Total	C	N	O	S	0	0	0
			3408	2170	574	655	9			
1	H	436	Total	C	N	O	S	0	0	0
			3408	2170	574	655	9			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	50	MET	-	EXPRESSION TAG	UNP Q01217
A	51	GLY	-	EXPRESSION TAG	UNP Q01217
A	52	HIS	-	EXPRESSION TAG	UNP Q01217
A	53	HIS	-	EXPRESSION TAG	UNP Q01217
A	54	HIS	-	EXPRESSION TAG	UNP Q01217
A	55	HIS	-	EXPRESSION TAG	UNP Q01217
A	56	HIS	-	EXPRESSION TAG	UNP Q01217
A	57	HIS	-	EXPRESSION TAG	UNP Q01217
B	50	MET	-	EXPRESSION TAG	UNP Q01217
B	51	GLY	-	EXPRESSION TAG	UNP Q01217
B	52	HIS	-	EXPRESSION TAG	UNP Q01217
B	53	HIS	-	EXPRESSION TAG	UNP Q01217
B	54	HIS	-	EXPRESSION TAG	UNP Q01217

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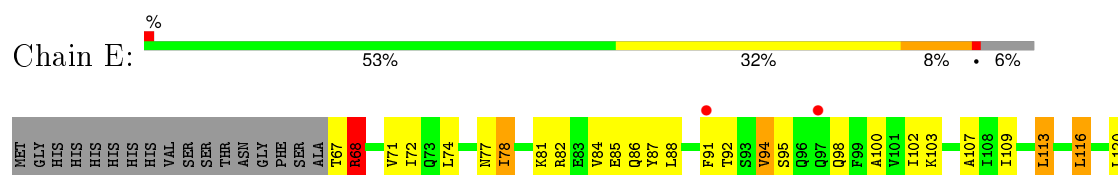
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Chain	Residue	Modelled	Actual	Comment	Reference
B	55	HIS	-	EXPRESSION TAG	UNP Q01217
B	56	HIS	-	EXPRESSION TAG	UNP Q01217
B	57	HIS	-	EXPRESSION TAG	UNP Q01217
C	50	MET	-	EXPRESSION TAG	UNP Q01217
C	51	GLY	-	EXPRESSION TAG	UNP Q01217
C	52	HIS	-	EXPRESSION TAG	UNP Q01217
C	53	HIS	-	EXPRESSION TAG	UNP Q01217
C	54	HIS	-	EXPRESSION TAG	UNP Q01217
C	55	HIS	-	EXPRESSION TAG	UNP Q01217
C	56	HIS	-	EXPRESSION TAG	UNP Q01217
C	57	HIS	-	EXPRESSION TAG	UNP Q01217
D	50	MET	-	EXPRESSION TAG	UNP Q01217
D	51	GLY	-	EXPRESSION TAG	UNP Q01217
D	52	HIS	-	EXPRESSION TAG	UNP Q01217
D	53	HIS	-	EXPRESSION TAG	UNP Q01217
D	54	HIS	-	EXPRESSION TAG	UNP Q01217
D	55	HIS	-	EXPRESSION TAG	UNP Q01217
D	56	HIS	-	EXPRESSION TAG	UNP Q01217
D	57	HIS	-	EXPRESSION TAG	UNP Q01217
E	50	MET	-	EXPRESSION TAG	UNP Q01217
E	51	GLY	-	EXPRESSION TAG	UNP Q01217
E	52	HIS	-	EXPRESSION TAG	UNP Q01217
E	53	HIS	-	EXPRESSION TAG	UNP Q01217
E	54	HIS	-	EXPRESSION TAG	UNP Q01217
E	55	HIS	-	EXPRESSION TAG	UNP Q01217
E	56	HIS	-	EXPRESSION TAG	UNP Q01217
E	57	HIS	-	EXPRESSION TAG	UNP Q01217
F	50	MET	-	EXPRESSION TAG	UNP Q01217
F	51	GLY	-	EXPRESSION TAG	UNP Q01217
F	52	HIS	-	EXPRESSION TAG	UNP Q01217
F	53	HIS	-	EXPRESSION TAG	UNP Q01217
F	54	HIS	-	EXPRESSION TAG	UNP Q01217
F	55	HIS	-	EXPRESSION TAG	UNP Q01217
F	56	HIS	-	EXPRESSION TAG	UNP Q01217
F	57	HIS	-	EXPRESSION TAG	UNP Q01217
G	50	MET	-	EXPRESSION TAG	UNP Q01217
G	51	GLY	-	EXPRESSION TAG	UNP Q01217
G	52	HIS	-	EXPRESSION TAG	UNP Q01217
G	53	HIS	-	EXPRESSION TAG	UNP Q01217
G	54	HIS	-	EXPRESSION TAG	UNP Q01217
G	55	HIS	-	EXPRESSION TAG	UNP Q01217
G	56	HIS	-	EXPRESSION TAG	UNP Q01217

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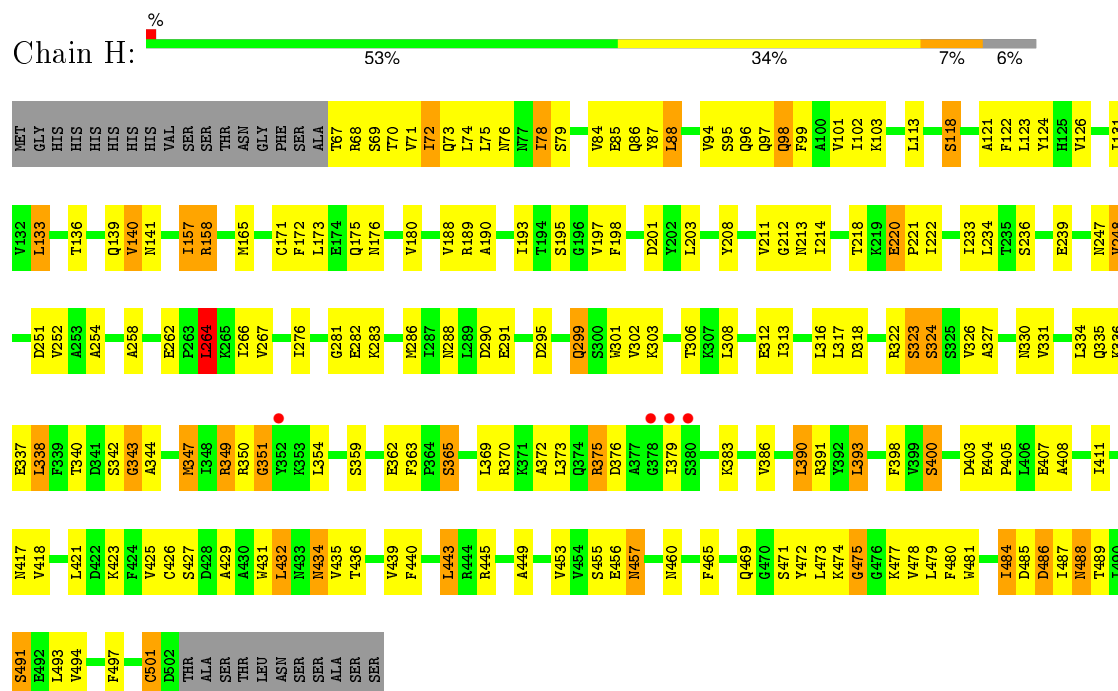
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Chain	Residue	Modelled	Actual	Comment	Reference
G	57	HIS	-	EXPRESSION TAG	UNP Q01217
H	50	MET	-	EXPRESSION TAG	UNP Q01217
H	51	GLY	-	EXPRESSION TAG	UNP Q01217
H	52	HIS	-	EXPRESSION TAG	UNP Q01217
H	53	HIS	-	EXPRESSION TAG	UNP Q01217
H	54	HIS	-	EXPRESSION TAG	UNP Q01217
H	55	HIS	-	EXPRESSION TAG	UNP Q01217
H	56	HIS	-	EXPRESSION TAG	UNP Q01217
H	57	HIS	-	EXPRESSION TAG	UNP Q01217





- Molecule 1: ACETYLGLUTAMATE KINASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	95.24Å 111.29Å 113.14Å 75.77° 89.29° 69.12°	Depositor
Resolution (Å)	109.11 – 3.80 66.22 – 3.80	Depositor EDS
% Data completeness (in resolution range)	95.3 (109.11-3.80) 88.1 (66.22-3.80)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.35 (at 3.77Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.197 , 0.236 0.200 , 0.245	Depositor DCC
R_{free} test set	2003 reflections (5.30%)	DCC
Wilson B-factor (Å ²)	136.5	Xtriage
Anisotropy	0.142	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 81.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 39772 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	27248	wwPDB-VP
Average B, all atoms (Å ²)	127.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.48% 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

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	0.86	3/3460 (0.1%)	0.95	9/4686 (0.2%)
1	B	0.86	3/3460 (0.1%)	0.92	3/4686 (0.1%)
1	C	0.77	0/3466	0.89	9/4693 (0.2%)
1	D	0.80	2/3462 (0.1%)	0.93	8/4689 (0.2%)
1	E	0.94	6/3466 (0.2%)	1.00	12/4693 (0.3%)
1	F	0.86	5/3466 (0.1%)	0.92	2/4693 (0.0%)
1	G	0.75	2/3466 (0.1%)	0.84	1/4693 (0.0%)
1	H	0.83	4/3466 (0.1%)	0.99	11/4693 (0.2%)
All	All	0.83	25/27712 (0.1%)	0.93	55/37526 (0.1%)

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
1	E	0	2
1	G	0	2
1	H	0	1
All	All	0	7

The worst 5 of 25 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	239	GLU	CD-OE1	8.55	1.35	1.25
1	H	239	GLU	CD-OE1	7.00	1.33	1.25
1	H	282	GLU	CG-CD	6.51	1.61	1.51
1	H	481	TRP	CD2-CE2	6.05	1.48	1.41
1	E	223	GLU	CD-OE1	6.04	1.32	1.25

The worst 5 of 55 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	316	LEU	CB-CG-CD1	-8.74	96.14	111.00
1	C	68	ARG	CB-CA-C	-7.61	95.19	110.40
1	A	316	LEU	CB-CG-CD1	-7.41	98.41	111.00
1	E	334	LEU	CB-CG-CD2	-7.02	99.06	111.00
1	H	295	ASP	CB-CG-OD2	6.83	124.45	118.30

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	94	VAL	Peptide
1	B	417	ASN	Peptide
1	E	94	VAL	Peptide
1	E	95	SER	Peptide
1	G	95	SER	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	3402	0	3429	130	0
1	B	3402	0	3429	147	1
1	C	3408	0	3440	143	0
1	D	3404	0	3429	142	0
1	E	3408	0	3440	197	0
1	F	3408	0	3440	183	0
1	G	3408	0	3440	140	1
1	H	3408	0	3440	180	0
All	All	27248	0	27487	1169	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 21.

The worst 5 of 1169 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:E:354:LEU:HD11	1:E:438:ASN:ND2	1.54	1.22

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:327:ALA:HB2	1:B:347:MET:CE	1.75	1.14
1:B:327:ALA:HB2	1:B:347:MET:HE3	1.29	1.12
1:E:418:VAL:HG21	1:E:493:LEU:HD11	1.25	1.11
1:D:418:VAL:HG21	1:D:493:LEU:HD11	1.12	1.11

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:B:304:TYR:OH	1:G:495:GLU:OE2[1_546]	2.15	0.05

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	434/464 (94%)	386 (89%)	44 (10%)	4 (1%)	21	68
1	B	434/464 (94%)	386 (89%)	44 (10%)	4 (1%)	21	68
1	C	434/464 (94%)	385 (89%)	45 (10%)	4 (1%)	21	68
1	D	434/464 (94%)	386 (89%)	44 (10%)	4 (1%)	21	68
1	E	434/464 (94%)	387 (89%)	43 (10%)	4 (1%)	21	68
1	F	434/464 (94%)	387 (89%)	43 (10%)	4 (1%)	21	68
1	G	434/464 (94%)	388 (89%)	42 (10%)	4 (1%)	21	68
1	H	434/464 (94%)	381 (88%)	46 (11%)	7 (2%)	12	58
All	All	3472/3712 (94%)	3086 (89%)	351 (10%)	35 (1%)	19	66

5 of 35 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	343	GLY

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Mol	Chain	Res	Type
1	H	343	GLY
1	C	434	ASN
1	D	434	ASN
1	E	434	ASN

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	372/397 (94%)	322 (87%)	50 (13%)	5	30
1	B	372/397 (94%)	322 (87%)	50 (13%)	5	30
1	C	373/397 (94%)	322 (86%)	51 (14%)	4	30
1	D	372/397 (94%)	316 (85%)	56 (15%)	3	25
1	E	373/397 (94%)	324 (87%)	49 (13%)	5	31
1	F	373/397 (94%)	323 (87%)	50 (13%)	5	30
1	G	373/397 (94%)	321 (86%)	52 (14%)	4	30
1	H	373/397 (94%)	316 (85%)	57 (15%)	3	25
All	All	2981/3176 (94%)	2566 (86%)	415 (14%)	4	30

5 of 415 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	383	LYS
1	E	349	ARG
1	H	290	ASP
1	D	440	PHE
1	E	113	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 78 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	374	GLN

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Mol	Chain	Res	Type
1	E	213	ASN
1	H	213	ASN
1	D	438	ASN
1	E	77	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 ⓘ

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	436/464 (93%)	-0.19	1 (0%) 95 91	52, 102, 194, 258	0
1	B	436/464 (93%)	-0.15	2 (0%) 91 85	63, 107, 191, 268	0
1	C	436/464 (93%)	-0.07	10 (2%) 64 48	76, 126, 279, 425	0
1	D	436/464 (93%)	-0.12	4 (0%) 85 74	72, 124, 202, 273	0
1	E	436/464 (93%)	-0.17	6 (1%) 78 63	49, 101, 184, 260	0
1	F	436/464 (93%)	-0.14	6 (1%) 78 63	54, 117, 194, 296	0
1	G	436/464 (93%)	0.00	15 (3%) 49 34	74, 139, 214, 274	0
1	H	436/464 (93%)	-0.13	4 (0%) 85 74	70, 134, 211, 284	0
All	All	3488/3712 (93%)	-0.12	48 (1%) 78 63	49, 118, 210, 425	0

The worst 5 of 48 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	383	LYS	5.7
1	G	384	GLU	5.6
1	H	379	ILE	5.4
1	G	382	GLY	4.3
1	G	376	ASP	4.1

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

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.