



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 07:54 PM UTC

PDB ID : 2Q5R / pdb_00002q5r
Title : Structure of apo Staphylococcus aureus D-tagatose-6-phosphate kinase
Authors : McGrath, T.E.; Soloveychik, M.; Romanov, V.; Thambipillai, D.; Dharamsi, A.; Virag, C.; Domagala, M.; Pai, E.F.; Edwards, A.M.; Battaile, K.; Chirgadze, N.Y.
Deposited on : 2007-06-01
Resolution : 2.30 Å(reported)

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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
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (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

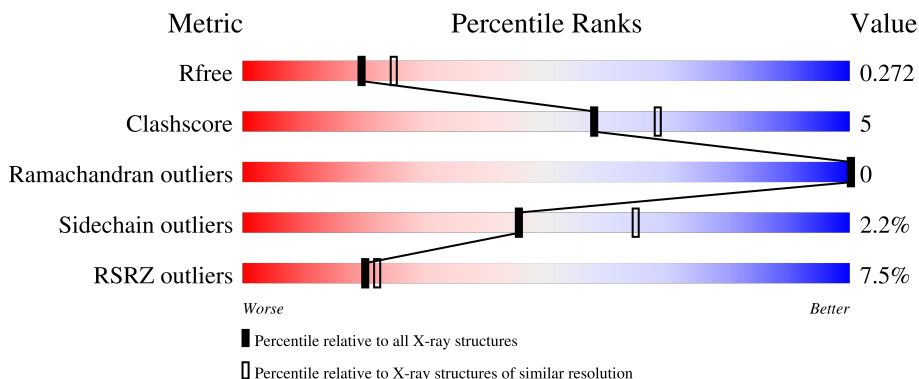
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	330	3% 86% 10% •
1	B	330	9% 80% 14% 5%
1	C	330	13% 78% 12% • 8%
1	D	330	2% 84% 10% 6%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10117 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 Tagatose-6-phosphate kinase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	318	Total	C	N	O	S	Se	0	3	0
			2459	1560	416	478	3	2			
1	B	312	Total	C	N	O	S	Se	0	2	0
			2413	1531	406	471	3	2			
1	C	303	Total	C	N	O	S	Se	0	3	0
			2350	1494	395	456	3	2			
1	D	310	Total	C	N	O	S	Se	0	2	0
			2396	1519	404	467	3	3			

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MSE	-	cloning artifact	UNP Q5HE12
A	-18	GLY	-	cloning artifact	UNP Q5HE12
A	-17	SER	-	cloning artifact	UNP Q5HE12
A	-16	SER	-	cloning artifact	UNP Q5HE12
A	-15	HIS	-	cloning artifact	UNP Q5HE12
A	-14	HIS	-	cloning artifact	UNP Q5HE12
A	-13	HIS	-	cloning artifact	UNP Q5HE12
A	-12	HIS	-	cloning artifact	UNP Q5HE12
A	-11	HIS	-	cloning artifact	UNP Q5HE12
A	-10	HIS	-	cloning artifact	UNP Q5HE12
A	-9	SER	-	cloning artifact	UNP Q5HE12
A	-8	SER	-	cloning artifact	UNP Q5HE12
A	-7	GLY	-	cloning artifact	UNP Q5HE12
A	-6	LEU	-	cloning artifact	UNP Q5HE12
A	-5	VAL	-	cloning artifact	UNP Q5HE12
A	-4	PRO	-	cloning artifact	UNP Q5HE12
A	-3	ARG	-	cloning artifact	UNP Q5HE12
A	-2	GLY	-	cloning artifact	UNP Q5HE12
A	-1	SER	-	cloning artifact	UNP Q5HE12
A	0	HIS	-	cloning artifact	UNP Q5HE12
A	1	MSE	MET	modified residue	UNP Q5HE12

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Chain	Residue	Modelled	Actual	Comment	Reference
A	282	MSE	MET	modified residue	UNP Q5HE12
B	-19	MSE	-	cloning artifact	UNP Q5HE12
B	-18	GLY	-	cloning artifact	UNP Q5HE12
B	-17	SER	-	cloning artifact	UNP Q5HE12
B	-16	SER	-	cloning artifact	UNP Q5HE12
B	-15	HIS	-	cloning artifact	UNP Q5HE12
B	-14	HIS	-	cloning artifact	UNP Q5HE12
B	-13	HIS	-	cloning artifact	UNP Q5HE12
B	-12	HIS	-	cloning artifact	UNP Q5HE12
B	-11	HIS	-	cloning artifact	UNP Q5HE12
B	-10	HIS	-	cloning artifact	UNP Q5HE12
B	-9	SER	-	cloning artifact	UNP Q5HE12
B	-8	SER	-	cloning artifact	UNP Q5HE12
B	-7	GLY	-	cloning artifact	UNP Q5HE12
B	-6	LEU	-	cloning artifact	UNP Q5HE12
B	-5	VAL	-	cloning artifact	UNP Q5HE12
B	-4	PRO	-	cloning artifact	UNP Q5HE12
B	-3	ARG	-	cloning artifact	UNP Q5HE12
B	-2	GLY	-	cloning artifact	UNP Q5HE12
B	-1	SER	-	cloning artifact	UNP Q5HE12
B	0	HIS	-	cloning artifact	UNP Q5HE12
B	1	MSE	MET	modified residue	UNP Q5HE12
B	282	MSE	MET	modified residue	UNP Q5HE12
C	-19	MSE	-	cloning artifact	UNP Q5HE12
C	-18	GLY	-	cloning artifact	UNP Q5HE12
C	-17	SER	-	cloning artifact	UNP Q5HE12
C	-16	SER	-	cloning artifact	UNP Q5HE12
C	-15	HIS	-	cloning artifact	UNP Q5HE12
C	-14	HIS	-	cloning artifact	UNP Q5HE12
C	-13	HIS	-	cloning artifact	UNP Q5HE12
C	-12	HIS	-	cloning artifact	UNP Q5HE12
C	-11	HIS	-	cloning artifact	UNP Q5HE12
C	-10	HIS	-	cloning artifact	UNP Q5HE12
C	-9	SER	-	cloning artifact	UNP Q5HE12
C	-8	SER	-	cloning artifact	UNP Q5HE12
C	-7	GLY	-	cloning artifact	UNP Q5HE12
C	-6	LEU	-	cloning artifact	UNP Q5HE12
C	-5	VAL	-	cloning artifact	UNP Q5HE12
C	-4	PRO	-	cloning artifact	UNP Q5HE12
C	-3	ARG	-	cloning artifact	UNP Q5HE12
C	-2	GLY	-	cloning artifact	UNP Q5HE12
C	-1	SER	-	cloning artifact	UNP Q5HE12

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Chain	Residue	Modelled	Actual	Comment	Reference
C	0	HIS	-	cloning artifact	UNP Q5HE12
C	1	MSE	MET	modified residue	UNP Q5HE12
C	282	MSE	MET	modified residue	UNP Q5HE12
D	-19	MSE	-	cloning artifact	UNP Q5HE12
D	-18	GLY	-	cloning artifact	UNP Q5HE12
D	-17	SER	-	cloning artifact	UNP Q5HE12
D	-16	SER	-	cloning artifact	UNP Q5HE12
D	-15	HIS	-	cloning artifact	UNP Q5HE12
D	-14	HIS	-	cloning artifact	UNP Q5HE12
D	-13	HIS	-	cloning artifact	UNP Q5HE12
D	-12	HIS	-	cloning artifact	UNP Q5HE12
D	-11	HIS	-	cloning artifact	UNP Q5HE12
D	-10	HIS	-	cloning artifact	UNP Q5HE12
D	-9	SER	-	cloning artifact	UNP Q5HE12
D	-8	SER	-	cloning artifact	UNP Q5HE12
D	-7	GLY	-	cloning artifact	UNP Q5HE12
D	-6	LEU	-	cloning artifact	UNP Q5HE12
D	-5	VAL	-	cloning artifact	UNP Q5HE12
D	-4	PRO	-	cloning artifact	UNP Q5HE12
D	-3	ARG	-	cloning artifact	UNP Q5HE12
D	-2	GLY	-	cloning artifact	UNP Q5HE12
D	-1	SER	-	cloning artifact	UNP Q5HE12
D	0	HIS	-	cloning artifact	UNP Q5HE12
D	1	MSE	MET	modified residue	UNP Q5HE12
D	282	MSE	MET	modified residue	UNP Q5HE12

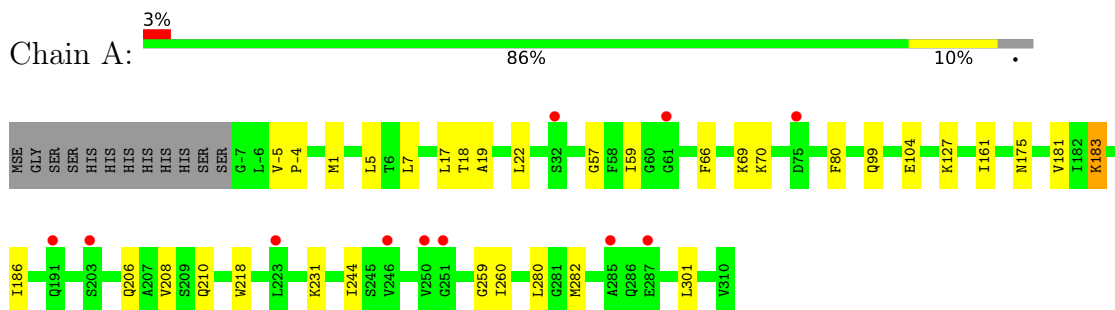
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	122	Total O 122 122	0	0
2	B	136	Total O 136 136	0	0
2	C	99	Total O 99 99	0	0
2	D	142	Total O 142 142	0	0

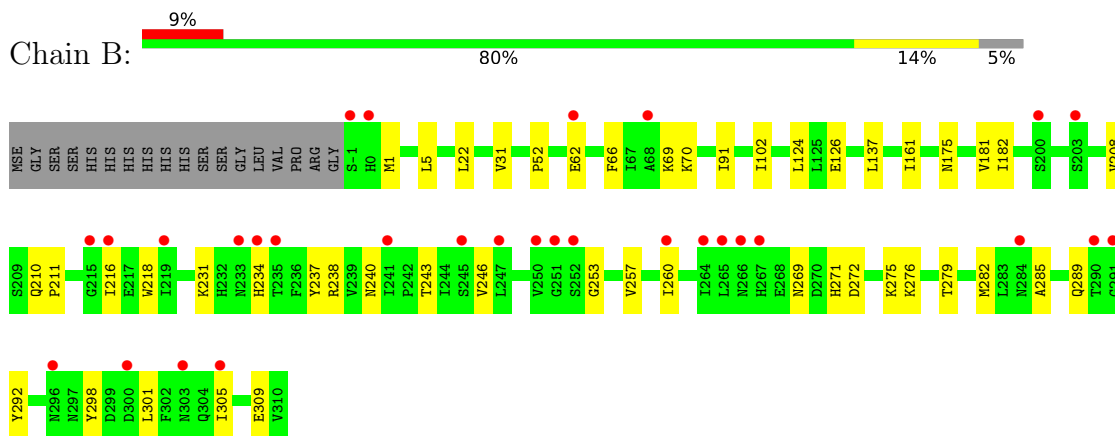
3 Residue-property plots [i](#)

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.

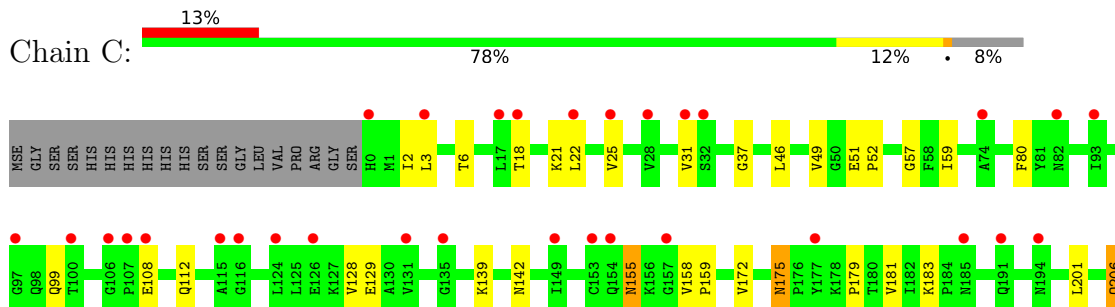
- Molecule 1: Tagatose-6-phosphate kinase

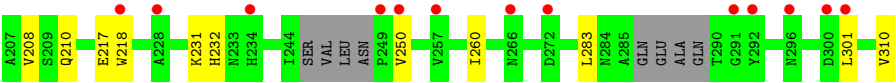


- Molecule 1: Tagatose-6-phosphate kinase

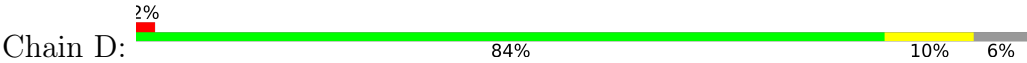


- Molecule 1: Tagatose-6-phosphate kinase





● Molecule 1: Tagatose-6-phosphate kinase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	76.95Å 96.94Å 94.48Å 90.00° 94.42° 90.00°	Depositor
Resolution (Å)	14.99 – 2.30 14.99 – 2.30	Depositor EDS
% Data completeness (in resolution range)	90.1 (14.99-2.30) 89.7 (14.99-2.30)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.85 (at 2.29Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.215 , 0.283 0.209 , 0.272	Depositor DCC
R_{free} test set	2729 reflections (4.45%)	wwPDB-VP
Wilson B-factor (Å ²)	39.9	Xtriage
Anisotropy	0.053	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 42.4	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	0.91	EDS
Total number of atoms	10117	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.63% 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](#)

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	0.58	0/2508	0.87	1/3403 (0.0%)
1	B	0.76	4/2458 (0.2%)	0.87	1/3335 (0.0%)
1	C	0.77	2/2397 (0.1%)	0.90	3/3250 (0.1%)
1	D	0.62	0/2440	0.89	0/3306
All	All	0.69	6/9803 (0.1%)	0.88	5/13294 (0.0%)

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	155	ASN	CG-OD1	18.12	1.57	1.23
1	C	155	ASN	CG-ND2	17.37	1.69	1.33
1	B	240	ASN	C-N	11.29	1.46	1.33
1	B	234	HIS	CE1-NE2	6.89	1.39	1.32
1	B	238	ARG	C-N	6.26	1.41	1.33

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	155	ASN	OD1-CG-ND2	9.38	131.98	122.60
1	C	37	GLY	N-CA-C	-8.39	102.33	112.48
1	A	186	ILE	N-CA-C	5.87	116.61	110.62
1	C	155	ASN	CB-CG-ND2	-5.57	108.05	116.40
1	B	240	ASN	O-C-N	5.23	129.21	122.93

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	2459	0	2482	25	0
1	B	2413	0	2430	24	0
1	C	2350	0	2365	28	0
1	D	2396	0	2404	16	0
2	A	122	0	0	1	0
2	B	136	0	0	0	0
2	C	99	0	0	3	0
2	D	142	0	0	2	0
All	All	10117	0	9681	87	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 5.

The worst 5 of 87 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:155:ASN:ND2	1:C:155:ASN:CG	1.69	1.51
1:C:129:GLU:O	1:C:159:PRO:HD2	1.70	0.91
1:A:183:LYS:O	1:A:183:LYS:HG2	1.77	0.83
1:A:244:ILE:HD13	1:A:282:MSE:HG2	1.67	0.75
1:A:244:ILE:HG21	1:A:282:MSE:HE3	1.74	0.70

There are no symmetry-related clashes.

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	319/330 (97%)	313 (98%)	6 (2%)	0	100	100
1	B	312/330 (94%)	305 (98%)	7 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	300/330 (91%)	293 (98%)	7 (2%)	0	100	100
1	D	306/330 (93%)	302 (99%)	4 (1%)	0	100	100
All	All	1237/1320 (94%)	1213 (98%)	24 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	272/277 (98%)	268 (98%)	4 (2%)	57	75
1	B	267/277 (96%)	259 (97%)	8 (3%)	36	53
1	C	260/277 (94%)	254 (98%)	6 (2%)	44	63
1	D	264/277 (95%)	258 (98%)	6 (2%)	44	63
All	All	1063/1108 (96%)	1039 (98%)	24 (2%)	45	63

5 of 24 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	22	LEU
1	C	206	GLN
1	C	183	LYS
1	D	5	LEU
1	B	126	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	195	GLN
1	D	304	GLN
1	B	286	GLN
1	B	294	ASN
1	B	304	GLN

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	316/330 (95%)	0.46	11 (3%) 47 49	24, 42, 49, 53	3 (0%)
1	B	310/330 (93%)	0.87	30 (9%) 13 15	24, 43, 51, 55	2 (0%)
1	C	301/330 (91%)	1.09	44 (14%) 6 6	23, 43, 49, 55	3 (0%)
1	D	308/330 (93%)	0.38	8 (2%) 57 59	27, 42, 49, 54	1 (0%)
All	All	1235/1320 (93%)	0.70	93 (7%) 20 22	23, 42, 50, 55	9 (0%)

The worst 5 of 93 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	290	THR	4.5
1	C	0	HIS	4.3
1	C	22	LEU	4.3
1	D	250	VAL	4.3
1	B	200	SER	4.2

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.