



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 10:07 AM UTC

PDB ID : 7R9G / pdb_00007r9g
Title : Catalytically inactive yeast Pseudouridine Synthase, PUS1, bound to RNA
Authors : Doyle, L.A.; Stoddard, B.L.
Deposited on : 2021-06-29
Resolution : 2.40 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 Phenix2.0
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

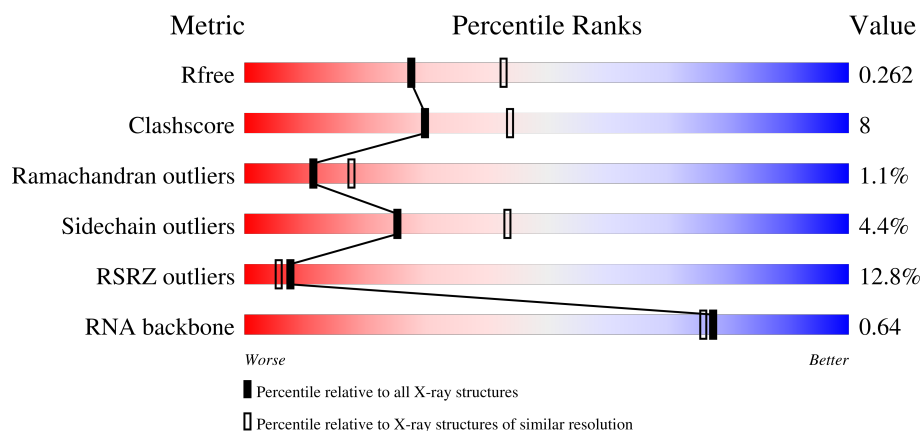
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)
RNA backbone	3983	1155 (2.70-2.10)

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	544	9% 55% 13% 29%
2	B	18	6% 50% 17% 33%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 3241 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 tRNA pseudouridine synthase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	386	2931	1887	481	548	15	0	1	0

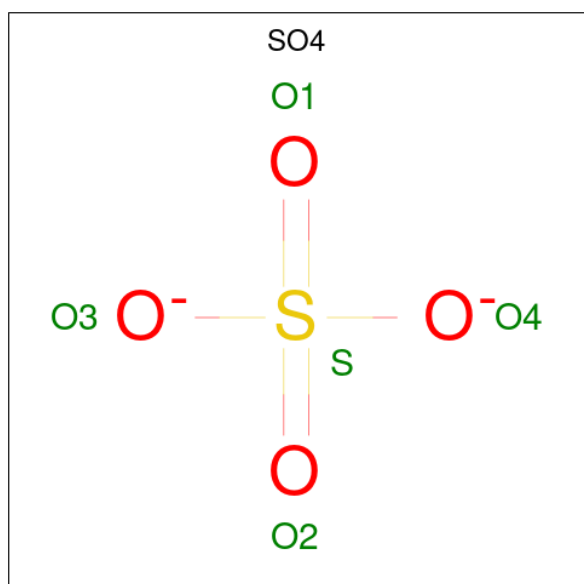
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	134	ALA	ASP	engineered mutation	UNP Q12211

- Molecule 2 is a RNA chain called RNA (5'-R(*AP*AP*AP*UP*CP*GP*GP*GP*AP*UP*UP*CP*CP*GP*GP*AP*UP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	B	12	254	115	47	81	11	0	0	0

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Cl	0	0
			1	1		

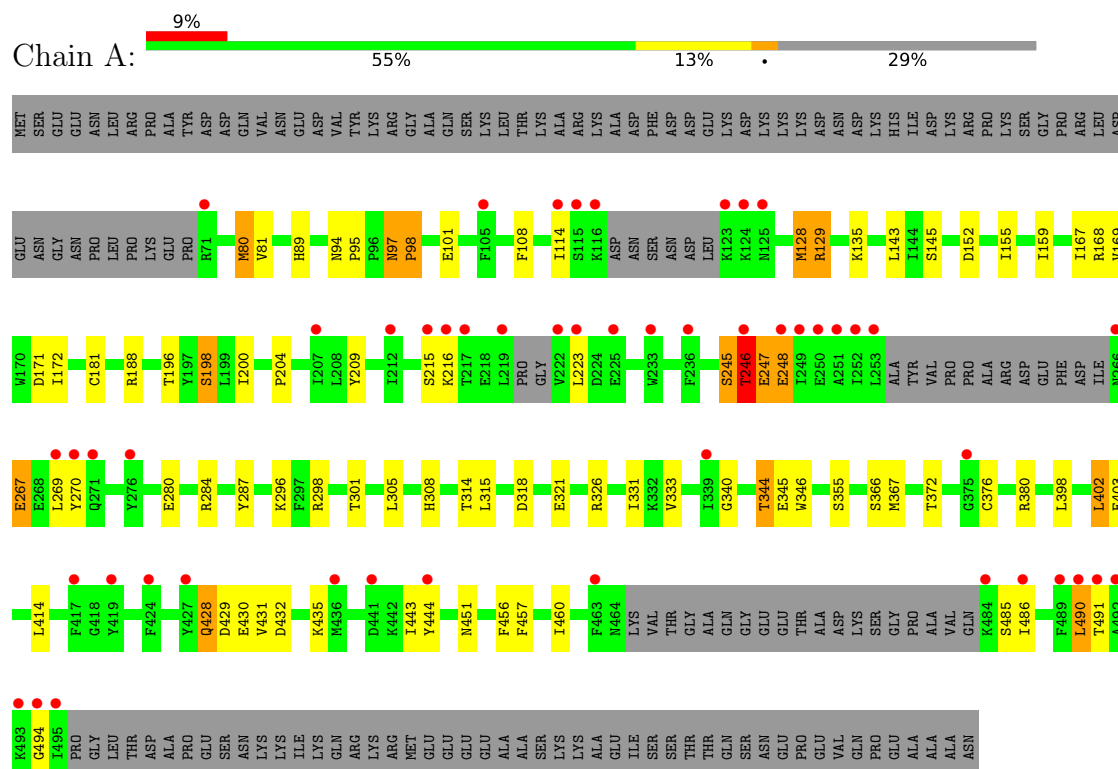
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	47	Total	O	0	0
			47	47		
5	B	3	Total	O	0	0
			3	3		

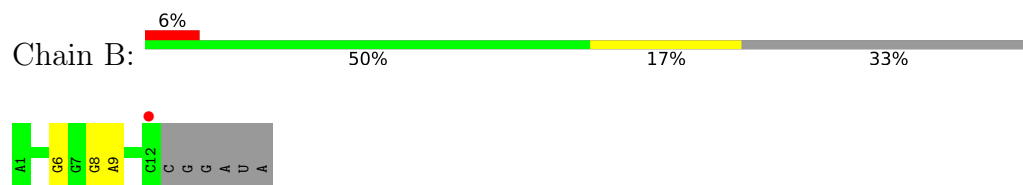
3 Residue-property plots [i](#)

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: tRNA pseudouridine synthase 1



- Molecule 2: RNA (5'-R(*AP*AP*AP*UP*CP*GP*GP*GP*AP*UP*UP*CP*CP*GP*GP*AP*UP*A)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	104.19Å 98.34Å 72.24Å 90.00° 102.80° 90.00°	Depositor
Resolution (Å)	49.17 – 2.40 49.17 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.5 (49.17-2.40) 94.2 (49.17-2.40)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.98 (at 2.39Å)	Xtriage
Refinement program	PHENIX 1.18	Depositor
R, R_{free}	0.222 , 0.264 0.227 , 0.262	Depositor DCC
R_{free} test set	1993 reflections (7.21%)	wwPDB-VP
Wilson B-factor (Å ²)	50.2	Xtriage
Anisotropy	0.465	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 53.2	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	0.94	EDS
Total number of atoms	3241	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.39% 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: SO4, CL

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	0.87	12/2995 (0.4%)	0.68	9/4053 (0.2%)
2	B	0.12	0/284	0.24	0/441
All	All	0.83	12/3279 (0.4%)	0.65	9/4494 (0.2%)

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	367	MET	C-O	-6.11	1.17	1.24
1	A	167	ILE	C-O	-5.91	1.18	1.24
1	A	486	ILE	C-O	-5.86	1.17	1.24
1	A	129	ARG	C-O	-5.59	1.16	1.23
1	A	169	VAL	C-O	-5.58	1.18	1.24
1	A	168	ARG	C-O	-5.51	1.17	1.23
1	A	98	PRO	C-O	-5.49	1.17	1.23
1	A	95	PRO	C-O	-5.38	1.18	1.24
1	A	80	MET	C-O	-5.36	1.17	1.24
1	A	81	VAL	C-O	-5.34	1.17	1.23
1	A	402	LEU	C-O	-5.12	1.17	1.24
1	A	94	ASN	C-O	-5.03	1.18	1.24

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	247	GLU	N-CA-C	-8.53	101.94	111.07
1	A	216	LYS	N-CA-C	-7.38	103.41	113.30
1	A	248	GLU	N-CA-C	6.19	123.98	110.80
1	A	402	LEU	N-CA-C	-5.77	99.79	108.96
1	A	97	ASN	CA-C-N	5.63	125.91	119.83
1	A	97	ASN	C-N-CA	5.63	125.91	119.83
1	A	344	THR	CB-CA-C	5.51	119.46	109.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	94	ASN	CA-C-N	5.37	125.91	120.38
1	A	94	ASN	C-N-CA	5.37	125.91	120.38

There are no chirality outliers.

There are no planarity outliers.

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	2931	0	2677	50	0
2	B	254	0	131	1	0
3	A	5	0	0	1	0
4	A	1	0	0	0	0
5	A	47	0	0	1	0
5	B	3	0	0	0	0
All	All	3241	0	2808	51	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 8.

All (51) 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:428:GLN:NE2	1:A:432:ASP:OD2	1.72	1.22
1:A:223:LEU:HD13	1:A:491:THR:HG22	1.36	1.04
1:A:380:ARG:NH1	1:A:490:LEU:O	1.91	1.03
1:A:101:GLU:OE2	1:A:129:ARG:HD3	1.59	1.01
1:A:80:MET:CE	1:A:171:ASP:HB3	2.10	0.82
1:A:80:MET:HE3	1:A:171:ASP:HB3	1.65	0.77
1:A:101:GLU:OE2	1:A:129:ARG:CD	2.32	0.75
1:A:246:THR:HA	1:A:248:GLU:HG2	1.74	0.69
1:A:344:THR:HG23	1:A:346:TRP:HE1	1.64	0.62
1:A:280:GLU:OE1	1:A:284:ARG:NH2	2.32	0.62
1:A:223:LEU:CD1	1:A:491:THR:HG22	2.23	0.60
1:A:101:GLU:OE2	1:A:129:ARG:CG	2.50	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:196:THR:OG1	1:A:345:GLU:HB3	2.06	0.56
1:A:248:GLU:OE2	1:A:248:GLU:HA	2.06	0.55
1:A:267:GLU:HG3	1:A:270:TYR:H	1.72	0.53
1:A:128:MET:HE2	1:A:145:SER:HB3	1.90	0.53
1:A:89:HIS:HA	1:A:135:LYS:HG3	1.91	0.52
1:A:296:LYS:NZ	1:A:376:CYS:O	2.33	0.52
1:A:326:ARG:NH1	1:A:355:SER:OG	2.43	0.52
1:A:128:MET:HE3	1:A:181:CYS:H	1.75	0.52
1:A:171:ASP:OD1	1:A:172:ILE:N	2.42	0.51
2:B:8:G:H2'	2:B:9:A:C8	2.46	0.51
1:A:215:SER:HB3	1:A:491:THR:HG23	1.94	0.50
1:A:198:SER:HB3	1:A:457:PHE:CE2	2.47	0.50
1:A:215:SER:HB3	1:A:491:THR:CG2	2.41	0.50
1:A:298:ARG:HG2	1:A:333:VAL:HB	1.95	0.49
1:A:318:ASP:HB3	1:A:321:GLU:HG3	1.94	0.49
1:A:128:MET:HE2	1:A:128:MET:HB2	1.70	0.48
1:A:305:LEU:O	1:A:308:HIS:NE2	2.42	0.47
1:A:456:PHE:CZ	1:A:460:ILE:HD11	2.49	0.47
1:A:143:LEU:HD23	1:A:181:CYS:SG	2.56	0.46
1:A:108:PHE:HB3	1:A:114:ILE:HG12	1.97	0.46
1:A:296:LYS:HG2	1:A:372:THR:HG23	1.97	0.46
1:A:398:LEU:HD11	1:A:443:ILE:HA	1.97	0.46
1:A:340:GLY:HA3	1:A:444[A]:TYR:CE1	2.51	0.45
1:A:269:LEU:HD12	1:A:269:LEU:HA	1.50	0.45
1:A:97:ASN:HA	1:A:98:PRO:HD3	1.82	0.45
1:A:155:ILE:O	1:A:159:ILE:HG13	2.17	0.45
1:A:429:ASP:OD1	1:A:430:GLU:N	2.50	0.45
1:A:431:VAL:HG12	1:A:435:LYS:HG3	1.98	0.44
1:A:451:ASN:ND2	5:A:709:HOH:O	2.44	0.44
1:A:490:LEU:HA	1:A:490:LEU:HD12	1.58	0.44
1:A:152:ASP:HB3	1:A:155:ILE:HB	1.99	0.43
1:A:80:MET:HE2	1:A:171:ASP:C	2.44	0.43
1:A:200:ILE:HD11	1:A:287:TYR:CG	2.53	0.43
1:A:129:ARG:HE	1:A:129:ARG:HB2	1.75	0.43
1:A:301:THR:HB	1:A:331:ILE:HG21	2.01	0.43
1:A:314:THR:OG1	1:A:315:LEU:N	2.52	0.42
1:A:204:PRO:HA	1:A:209:TYR:CD2	2.54	0.42
1:A:246:THR:CA	1:A:248:GLU:HG2	2.45	0.41
1:A:188:ARG:NH2	3:A:601:SO4:O4	2.53	0.40

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	377/544 (69%)	352 (93%)	21 (6%)	4 (1%)	11	18

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	245	SER
1	A	246	THR
1	A	428	GLN
1	A	494	GLY

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	273/470 (58%)	261 (96%)	12 (4%)	25	43

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	128	MET
1	A	198	SER
1	A	245	SER
1	A	246	THR
1	A	247	GLU
1	A	267	GLU
1	A	366	SER

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Mol	Chain	Res	Type
1	A	402	LEU
1	A	403	GLU
1	A	414	LEU
1	A	485	SER
1	A	490	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	11/18 (61%)	1 (9%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	6	G

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

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	SO4	A	601	-	4,4,4	0.24	0	6,6,6	0.07	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	601	SO4	1	0

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	386/544 (70%)	0.89	50 (12%) 7 5	30, 63, 96, 116	1 (0%)
2	B	12/18 (66%)	0.81	1 (8%) 17 14	53, 78, 94, 111	0
All	All	398/562 (70%)	0.89	51 (12%) 7 6	30, 63, 96, 116	1 (0%)

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	444[A]	TYR	5.8
1	A	125	ASN	5.6
1	A	270	TYR	3.9
1	A	124	LYS	3.9
1	A	253	LEU	3.8
1	A	495	ILE	3.8
1	A	123	LYS	3.7
1	A	217	THR	3.6
1	A	116	LYS	3.6
1	A	266	ASN	3.4
1	A	492	ALA	3.4
1	A	252	ILE	3.1
1	A	269	LEU	3.1
1	A	248	GLU	3.1
1	A	222	VAL	3.1
1	A	249	ILE	3.1
1	A	436	MET	3.0
1	A	115	SER	3.0
1	A	493	LYS	2.9
1	A	271	GLN	2.9
1	A	276	TYR	2.9
1	A	486	ILE	2.8
1	A	71	ARG	2.8
1	A	251	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	491	THR	2.8
1	A	417	PHE	2.8
1	A	215	SER	2.7
1	A	463	PHE	2.6
1	A	419	TYR	2.6
1	A	339	ILE	2.6
1	A	207	ILE	2.5
1	A	494	GLY	2.4
1	A	484	LYS	2.4
1	A	216	LYS	2.4
1	A	246	THR	2.3
1	A	441	ASP	2.3
2	B	12	C	2.3
1	A	489	PHE	2.3
1	A	236	PHE	2.3
1	A	424	PHE	2.3
1	A	250	GLU	2.2
1	A	219	LEU	2.2
1	A	114	ILE	2.1
1	A	105	PHE	2.1
1	A	212	ILE	2.1
1	A	233	TRP	2.1
1	A	490	LEU	2.1
1	A	225	GLU	2.1
1	A	375	GLY	2.0
1	A	427	TYR	2.0
1	A	223	LEU	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 oligosaccharides 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($\text{\AA}^2$)	Q<0.9
3	SO4	A	601	5/5	0.96	0.07	60,62,67,69	0
4	CL	A	602	1/1	0.98	0.06	52,52,52,52	0

6.5 Other polymers [i](#)

There are no such residues in this entry.