



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:05 AM UTC

PDB ID : 6R9I / pdb_00006r9i
Title : Structure of Saccharomyces cerevisiae apo Pan2 pseudoubiquitin hydrolase-RNA exonuclease (UCH-Exo) module
Authors : Tang, T.T.L.; Stowell, J.A.W.; Hill, C.H.; Passmore, L.A.
Deposited on : 2019-04-03
Resolution : 3.00 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
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

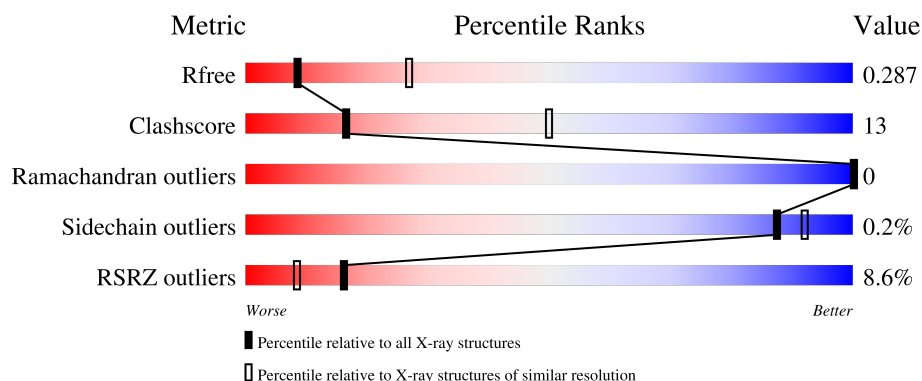
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	672	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 4542 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 PAN2-PAN3 deadenylation complex catalytic subunit PAN2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	605	4542	2901	749	874	18	0	0	0

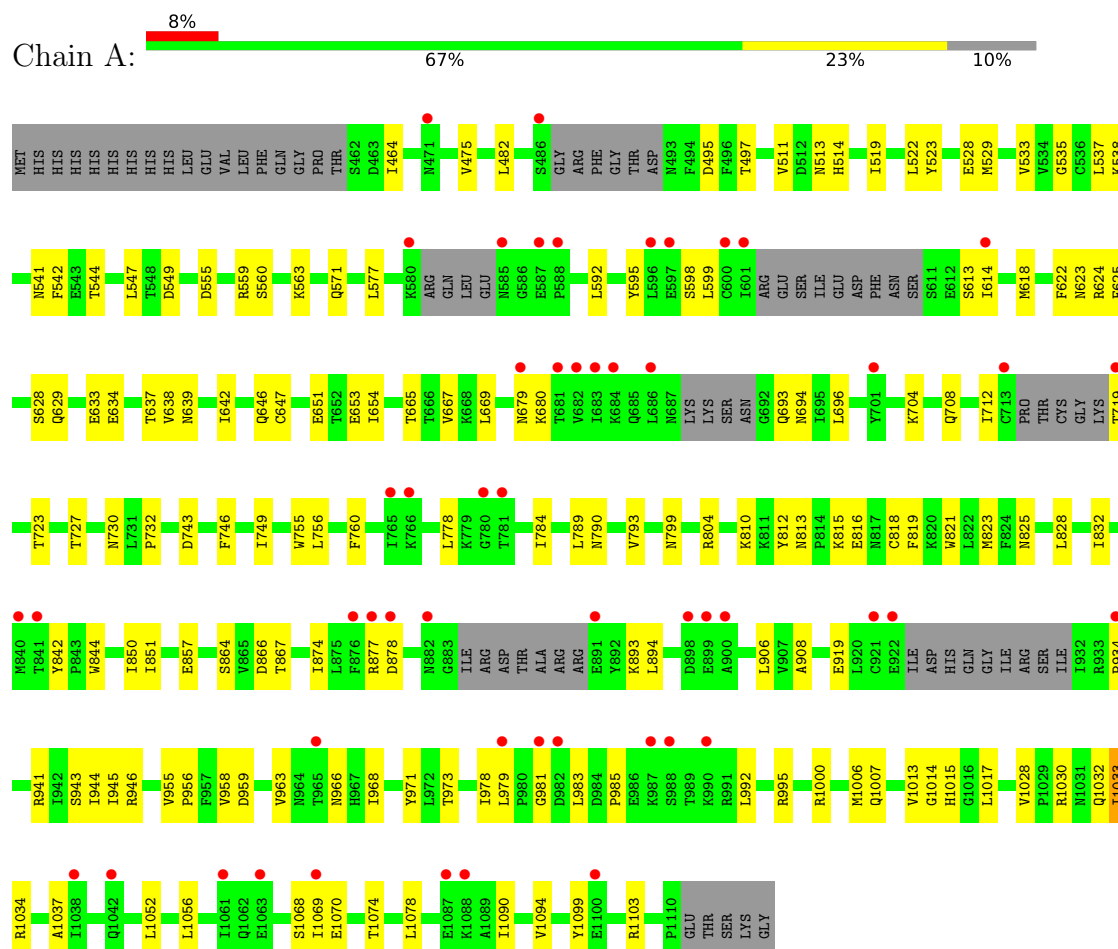
There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	444	MET	-	initiating methionine	UNP P53010
A	445	HIS	-	expression tag	UNP P53010
A	446	HIS	-	expression tag	UNP P53010
A	447	HIS	-	expression tag	UNP P53010
A	448	HIS	-	expression tag	UNP P53010
A	449	HIS	-	expression tag	UNP P53010
A	450	HIS	-	expression tag	UNP P53010
A	451	HIS	-	expression tag	UNP P53010
A	452	HIS	-	expression tag	UNP P53010
A	453	LEU	-	expression tag	UNP P53010
A	454	GLU	-	expression tag	UNP P53010
A	455	VAL	-	expression tag	UNP P53010
A	456	LEU	-	expression tag	UNP P53010
A	457	PHE	-	expression tag	UNP P53010
A	458	GLN	-	expression tag	UNP P53010
A	459	GLY	-	expression tag	UNP P53010
A	460	PRO	-	expression tag	UNP P53010
A	912	ALA	GLU	engineered mutation	UNP P53010

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: PAN2-PAN3 deadenylation complex catalytic subunit PAN2



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	91.37Å 117.08Å 255.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	86.03 – 3.00 86.03 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.8 (86.03-3.00) 99.8 (86.03-3.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.60 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.243 , 0.289 0.243 , 0.287	Depositor DCC
R_{free} test set	1332 reflections (4.77%)	wwPDB-VP
Wilson B-factor (Å ²)	98.2	Xtriage
Anisotropy	0.460	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 105.3	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	0.93	EDS
Total number of atoms	4542	wwPDB-VP
Average B, all atoms (Å ²)	113.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.42% 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	0.14	0/4634	0.38	0/6330

There are no bond length outliers.

There are no bond angle outliers.

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	4542	0	4141	112	0
All	All	4542	0	4141	112	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 13.

All (112) 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:908:ALA:HB3	1:A:945:ILE:HB	1.59	0.83
1:A:956:PRO:HG3	1:A:1069:ILE:HD11	1.65	0.79
1:A:789:LEU:O	1:A:810:LYS:CE	2.34	0.76
1:A:825:ASN:HB3	1:A:828:LEU:HB3	1.67	0.74
1:A:642:ILE:HD13	1:A:646:GLN:HG3	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:523:TYR:OH	1:A:623:ASN:OD1	2.08	0.69
1:A:642:ILE:HD12	1:A:642:ILE:C	2.18	0.69
1:A:944:ILE:HG12	1:A:958:VAL:HG22	1.75	0.68
1:A:519:ILE:HD13	1:A:622:PHE:HD2	1.59	0.67
1:A:789:LEU:O	1:A:810:LYS:HE3	1.95	0.65
1:A:789:LEU:O	1:A:810:LYS:HE2	1.97	0.63
1:A:464:ILE:HD11	1:A:482:LEU:HD22	1.80	0.62
1:A:1028:VAL:HB	1:A:1033:ILE:HD11	1.82	0.60
1:A:874:ILE:HD12	1:A:874:ILE:H	1.65	0.60
1:A:549:ASP:OD2	1:A:995:ARG:NH2	2.33	0.60
1:A:971:TYR:HB3	1:A:973:THR:HG23	1.83	0.60
1:A:529:MET:O	1:A:533:VAL:HG12	2.02	0.59
1:A:577:LEU:HD21	1:A:629:GLN:HG2	1.82	0.59
1:A:522:LEU:HD22	1:A:793:VAL:HG23	1.84	0.59
1:A:749:ILE:HD11	1:A:755:TRP:NE1	2.18	0.59
1:A:944:ILE:HG12	1:A:958:VAL:CG2	2.34	0.57
1:A:513:ASN:OD1	1:A:571:GLN:HG3	2.04	0.56
1:A:749:ILE:HD11	1:A:755:TRP:CD1	2.41	0.56
1:A:642:ILE:C	1:A:642:ILE:CD1	2.78	0.56
1:A:653:GLU:HB2	1:A:727:THR:HG23	1.86	0.56
1:A:1030:ARG:HD2	1:A:1030:ARG:H	1.71	0.56
1:A:653:GLU:HG2	1:A:667:VAL:HG22	1.88	0.55
1:A:541:ASN:HB3	1:A:544:THR:CG2	2.37	0.55
1:A:749:ILE:HD11	1:A:755:TRP:CE2	2.40	0.55
1:A:825:ASN:O	1:A:828:LEU:N	2.39	0.55
1:A:537:LEU:O	1:A:1000:ARG:NH1	2.41	0.54
1:A:522:LEU:HD21	1:A:851:ILE:HG12	1.89	0.54
1:A:704:LYS:HG3	1:A:727:THR:HB	1.88	0.54
1:A:864:SER:O	1:A:867:THR:HG22	2.07	0.54
1:A:535:GLY:O	1:A:538:LYS:HG3	2.07	0.54
1:A:708:GLN:HA	1:A:723:THR:HA	1.89	0.53
1:A:946:ARG:HD2	1:A:955:VAL:HG13	1.90	0.53
1:A:1070:GLU:O	1:A:1074:THR:HG23	2.10	0.52
1:A:983:LEU:HG	1:A:985:PRO:HD2	1.92	0.52
1:A:693:GLN:O	1:A:755:TRP:HD1	1.92	0.52
1:A:945:ILE:HA	1:A:956:PRO:HA	1.93	0.51
1:A:712:ILE:O	1:A:719:THR:N	2.44	0.51
1:A:647:CYS:O	1:A:732:PRO:HB2	2.10	0.51
1:A:544:THR:OG1	1:A:547:LEU:HB3	2.11	0.50
1:A:812:TYR:HB2	1:A:819:PHE:HE2	1.77	0.50
1:A:894:LEU:HD12	1:A:894:LEU:H	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:973:THR:HG22	1:A:978:ILE:H	1.75	0.50
1:A:973:THR:HG22	1:A:978:ILE:N	2.27	0.50
1:A:696:LEU:HD21	1:A:760:PHE:CG	2.46	0.49
1:A:1099:TYR:O	1:A:1103:ARG:NE	2.39	0.49
1:A:1006:MET:HG3	1:A:1028:VAL:HG13	1.94	0.49
1:A:624:ARG:O	1:A:628:SER:OG	2.23	0.48
1:A:1014:GLY:HA3	1:A:1017:LEU:HD21	1.95	0.48
1:A:823:MET:HB2	1:A:832:ILE:HD13	1.95	0.48
1:A:528:GLU:OE1	1:A:857:GLU:HG2	2.13	0.48
1:A:614:ILE:HD11	1:A:618:MET:HB3	1.95	0.48
1:A:813:ASN:HD21	1:A:815:LYS:HB2	1.79	0.47
1:A:850:ILE:O	1:A:851:ILE:HD13	2.14	0.47
1:A:874:ILE:HD13	1:A:1000:ARG:HH21	1.79	0.47
1:A:555:ASP:O	1:A:559:ARG:HG2	2.14	0.47
1:A:679:ASN:OD1	1:A:680:LYS:N	2.34	0.47
1:A:893:LYS:O	1:A:946:ARG:NH2	2.33	0.47
1:A:514:HIS:ND1	1:A:613:SER:O	2.46	0.47
1:A:592:LEU:HD12	1:A:592:LEU:H	1.80	0.47
1:A:482:LEU:HD11	1:A:828:LEU:HB2	1.95	0.47
1:A:1090:ILE:HG22	1:A:1094:VAL:HG23	1.97	0.46
1:A:1013:VAL:HG12	1:A:1034:ARG:HB2	1.97	0.46
1:A:519:ILE:HD13	1:A:622:PHE:CD2	2.47	0.46
1:A:877:ARG:HG2	1:A:878:ASP:N	2.29	0.46
1:A:810:LYS:HG3	1:A:821:TRP:CZ2	2.51	0.46
1:A:634:GLU:O	1:A:637:THR:HG22	2.15	0.46
1:A:743:ASP:HA	1:A:746:PHE:HB2	1.98	0.46
1:A:919:GLU:HA	1:A:934:PRO:HB3	1.98	0.46
1:A:595:TYR:O	1:A:598:SER:N	2.48	0.46
1:A:651:GLU:HG3	1:A:730:ASN:HB2	1.98	0.46
1:A:945:ILE:HD13	1:A:956:PRO:HB3	1.98	0.45
1:A:694:ASN:HA	1:A:755:TRP:HA	1.98	0.45
1:A:495:ASP:OD1	1:A:497:THR:HG22	2.17	0.45
1:A:639:ASN:O	1:A:639:ASN:ND2	2.43	0.44
1:A:979:LEU:O	1:A:981:GLY:N	2.41	0.44
1:A:595:TYR:HE1	1:A:625:PHE:CG	2.36	0.44
1:A:629:GLN:O	1:A:633:GLU:HG3	2.17	0.44
1:A:968:ILE:HD11	1:A:971:TYR:CE2	2.53	0.44
1:A:746:PHE:O	1:A:749:ILE:HG22	2.17	0.44
1:A:866:ASP:OD2	1:A:1007:GLN:NE2	2.47	0.44
1:A:804:ARG:HB3	1:A:804:ARG:NH2	2.32	0.44
1:A:966:ASN:OD1	1:A:966:ASN:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:789:LEU:HD23	1:A:790:ASN:N	2.33	0.43
1:A:669:LEU:HD12	1:A:669:LEU:HA	1.89	0.43
1:A:941:ARG:HH21	1:A:959:ASP:CG	2.26	0.43
1:A:542:PHE:HE1	1:A:1000:ARG:HD2	1.84	0.43
1:A:1015:HIS:HE1	1:A:1037:ALA:HA	1.84	0.43
1:A:637:THR:OG1	1:A:638:VAL:N	2.51	0.43
1:A:906:LEU:HD23	1:A:906:LEU:HA	1.76	0.43
1:A:756:LEU:HD21	1:A:789:LEU:HD11	2.01	0.43
1:A:560:SER:HB3	1:A:563:LYS:HB3	2.00	0.43
1:A:654:ILE:O	1:A:665:THR:HA	2.18	0.43
1:A:874:ILE:HD13	1:A:1000:ARG:HD3	2.01	0.43
1:A:595:TYR:O	1:A:599:LEU:HD13	2.19	0.42
1:A:511:VAL:HG12	1:A:571:GLN:NE2	2.33	0.42
1:A:968:ILE:HD11	1:A:971:TYR:CZ	2.55	0.42
1:A:475:VAL:HG12	1:A:799:ASN:OD1	2.20	0.42
1:A:908:ALA:O	1:A:944:ILE:HA	2.20	0.42
1:A:1028:VAL:HG12	1:A:1032:GLN:HB2	2.01	0.42
1:A:963:VAL:HG12	1:A:992:LEU:HD23	2.02	0.41
1:A:1052:LEU:O	1:A:1056:LEU:HB2	2.20	0.41
1:A:778:LEU:HD13	1:A:784:ILE:HD12	2.02	0.41
1:A:816:GLU:HB3	1:A:818:CYS:SG	2.61	0.41
1:A:1052:LEU:HB3	1:A:1078:LEU:HD11	2.02	0.41
1:A:694:ASN:HD21	1:A:696:LEU:HD12	1.86	0.40
1:A:943:SER:OG	1:A:1068:SER:OG	2.39	0.40
1:A:842:TYR:HB3	1:A:844:TRP:CE2	2.56	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	589/672 (88%)	544 (92%)	45 (8%)	0	100	100

There are no Ramachandran outliers to report.

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	457/617 (74%)	456 (100%)	1 (0%)	87 92

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1033	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	591	HIS
1	A	801	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 ⓘ

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	605/672 (90%)	0.60	52 (8%) 16 8	59, 110, 182, 230	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	713	CYS	4.6
1	A	683	ILE	4.4
1	A	601	ILE	3.9
1	A	891	GLU	3.8
1	A	981	GLY	3.6
1	A	988	SER	3.5
1	A	682	VAL	3.4
1	A	686	LEU	3.3
1	A	922	GLU	3.3
1	A	979	LEU	3.2
1	A	1063	GLU	3.1
1	A	471	ASN	3.1
1	A	987	LYS	3.0
1	A	1061	ILE	3.0
1	A	900	ALA	2.9
1	A	600	CYS	2.9
1	A	921	CYS	2.8
1	A	876	PHE	2.8
1	A	580	LYS	2.7
1	A	780	GLY	2.7
1	A	878	ASP	2.6
1	A	597	GLU	2.6
1	A	588	PRO	2.6
1	A	719	THR	2.6
1	A	990	LYS	2.5
1	A	1038	ILE	2.5
1	A	1069	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	587	GLU	2.4
1	A	684	LYS	2.4
1	A	766	LYS	2.4
1	A	614	ILE	2.4
1	A	765	ILE	2.4
1	A	1100	GLU	2.4
1	A	1087	GLU	2.4
1	A	486	SER	2.4
1	A	965	THR	2.3
1	A	781	THR	2.3
1	A	899	GLU	2.3
1	A	934	PRO	2.3
1	A	898	ASP	2.3
1	A	982	ASP	2.2
1	A	1088	LYS	2.2
1	A	877	ARG	2.2
1	A	585	ASN	2.1
1	A	596	LEU	2.1
1	A	1042	GLN	2.1
1	A	882	ASN	2.1
1	A	841	THR	2.1
1	A	679	ASN	2.1
1	A	840	MET	2.1
1	A	701	TYR	2.1
1	A	681	THR	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.