



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:31 AM UTC

PDB ID : 6IZZ / pdb_00006izz
Title : The RNA-dependent RNA polymerase domain of dengue 3 NS5, bound with RK-0404678
Authors : Shimizu, H.; Sekine, S.
Deposited on : 2018-12-20
Resolution : 1.97 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

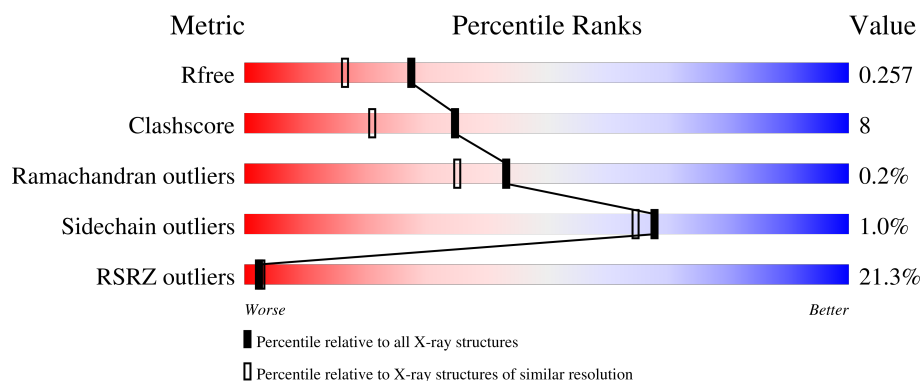
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.97 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	1506 (1.98-1.98)
Clashscore	190562	1534 (1.98-1.98)
Ramachandran outliers	187476	1518 (1.98-1.98)
Sidechain outliers	187428	1518 (1.98-1.98)
RSRZ outliers	180081	1506 (1.98-1.98)

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	647	19% 74% 14% 12%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 4960 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.

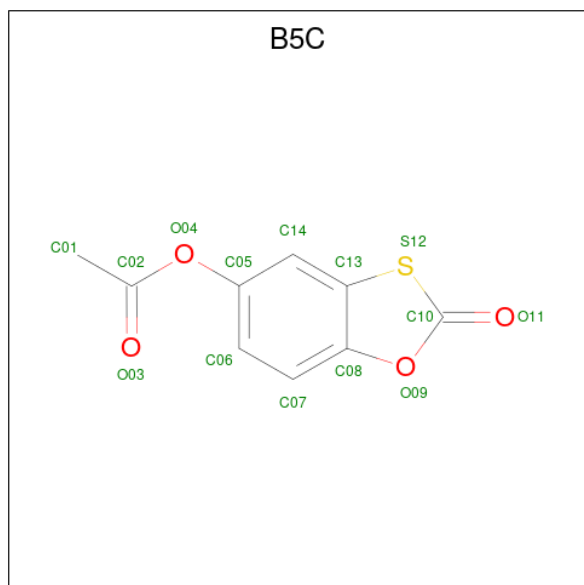
- Molecule 1 is a protein called Genome polyprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	568	Total	C	N	O	S	0	0	0
			4615	2909	825	850	31			

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Zn	0	0
			2	2		

- Molecule 3 is 2-oxo-2H-1,3-benzoxathiol-5-yl acetate (CCD ID: B5C) (formula: C₉H₆O₄S).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	S	0	0
			14	9	4	1		

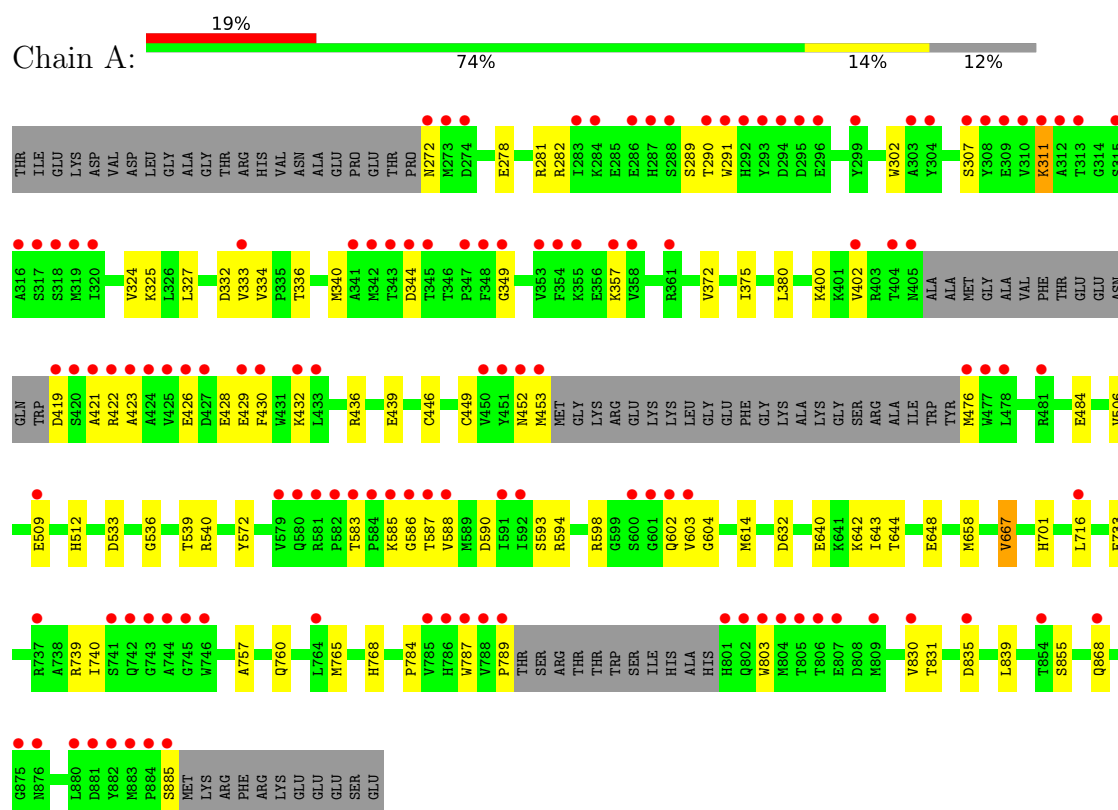
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	329	Total 329	O 329	0	0

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: Genome polypeptide



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	164.04Å 179.29Å 58.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	56.15 – 1.97 56.15 – 1.97	Depositor EDS
% Data completeness (in resolution range)	99.2 (56.15-1.97) 99.2 (56.15-1.97)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.18 (at 1.97Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.223 , 0.255 0.226 , 0.257	Depositor DCC
R_{free} test set	3059 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	35.3	Xtriage
Anisotropy	0.348	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 38.5	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	0.95	EDS
Total number of atoms	4960	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.02% 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: ZN, B5C

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	0.25	0/4727	0.45	0/6395

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	311	LYS	Peptide

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	4615	0	4519	68	0
2	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	14	0	0	1	0
4	A	329	0	0	15	1
All	All	4960	0	4519	69	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 8.

All (69) 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)
3:A:903:B5C:O09	3:A:903:B5C:C08	1.65	1.27
1:A:593:SER:OG	4:A:1001:HOH:O	1.90	0.90
1:A:340:MET:HE1	1:A:733:GLU:HA	1.53	0.89
1:A:716:LEU:HD21	1:A:839:LEU:HD23	1.59	0.84
1:A:272:ASN:N	4:A:1005:HOH:O	2.13	0.81
1:A:332:ASP:O	4:A:1003:HOH:O	2.02	0.76
1:A:357:LYS:HG3	1:A:539:THR:HG21	1.73	0.71
1:A:533:ASP:OD1	4:A:1004:HOH:O	2.12	0.67
1:A:855:SER:HB3	4:A:1241:HOH:O	1.93	0.67
1:A:426:GLU:OE1	1:A:426:GLU:N	2.22	0.66
1:A:311:LYS:HA	1:A:587:THR:HB	1.78	0.64
1:A:344:ASP:HB3	1:A:349:GLY:HA3	1.80	0.63
1:A:583:THR:HG23	1:A:585:LYS:H	1.65	0.61
1:A:426:GLU:H	1:A:426:GLU:CD	2.08	0.61
1:A:290:THR:N	4:A:1021:HOH:O	2.33	0.59
1:A:311:LYS:HE2	1:A:586:GLY:HA3	1.84	0.59
1:A:757:ALA:HB2	1:A:789:PRO:HB3	1.85	0.59
1:A:476:MET:SD	4:A:1079:HOH:O	2.57	0.58
1:A:701:HIS:ND1	4:A:1022:HOH:O	2.32	0.57
1:A:311:LYS:HD3	1:A:587:THR:H	1.70	0.57
1:A:333:VAL:HG12	1:A:333:VAL:O	2.05	0.57
1:A:436:ARG:HG3	4:A:1060:HOH:O	2.05	0.56
1:A:421:ALA:O	1:A:422:ARG:HD2	2.05	0.56
1:A:439:GLU:OE1	4:A:1007:HOH:O	2.18	0.55
1:A:402:VAL:HG11	1:A:426:GLU:OE2	2.05	0.55
1:A:419:ASP:N	4:A:1030:HOH:O	2.40	0.54
1:A:484:GLU:OE2	1:A:572:TYR:OH	2.17	0.54
1:A:760:GLN:NE2	1:A:803:TRP:O	2.40	0.53
1:A:340:MET:HB3	1:A:740:ILE:HD11	1.90	0.53
1:A:604:GLY:HA2	4:A:1017:HOH:O	2.09	0.52
1:A:423:ALA:HA	1:A:426:GLU:OE2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:291:TRP:N	4:A:1021:HOH:O	2.32	0.51
1:A:506:VAL:C	1:A:509:GLU:HG2	2.36	0.51
1:A:658:MET:HG2	1:A:667:VAL:HB	1.93	0.51
1:A:278:GLU:OE1	1:A:282:ARG:HD2	2.13	0.49
1:A:830:VAL:HG13	1:A:835:ASP:HB2	1.94	0.48
1:A:432:LYS:HD3	1:A:432:LYS:HA	1.75	0.48
1:A:512:HIS:CD2	1:A:512:HIS:H	2.31	0.48
1:A:334:VAL:N	4:A:1038:HOH:O	2.47	0.48
1:A:380:LEU:HD11	1:A:614:MET:HE2	1.96	0.47
1:A:632:ASP:OD2	1:A:642:LYS:NZ	2.48	0.46
1:A:598:ARG:HG3	1:A:598:ARG:HH11	1.80	0.46
1:A:446:CYS:SG	1:A:449:CYS:HB2	2.56	0.46
1:A:281:ARG:HH21	1:A:281:ARG:HG2	1.80	0.45
1:A:325:LYS:HA	1:A:739:ARG:HH11	1.82	0.44
1:A:400:LYS:HE3	1:A:400:LYS:HB2	1.63	0.44
1:A:452:ASN:OD1	1:A:453:MET:N	2.50	0.44
1:A:644:THR:O	1:A:648:GLU:HG3	2.17	0.44
1:A:484:GLU:OE2	1:A:602:GLN:HB3	2.18	0.44
1:A:868:GLN:O	1:A:868:GLN:NE2	2.51	0.44
1:A:784:PRO:HG2	1:A:787:TRP:CE2	2.53	0.43
1:A:506:VAL:O	1:A:509:GLU:HG2	2.18	0.43
1:A:642:LYS:HG3	1:A:643:ILE:N	2.33	0.43
1:A:307:SER:HB3	1:A:588:VAL:HG13	2.01	0.43
1:A:333:VAL:O	1:A:333:VAL:CG1	2.67	0.43
1:A:512:HIS:HB3	1:A:765:MET:HE1	2.00	0.43
1:A:332:ASP:HA	1:A:739:ARG:HH22	1.84	0.42
1:A:375:ILE:HD11	1:A:640:GLU:HG2	2.01	0.42
1:A:307:SER:OG	1:A:590:ASP:OD1	2.33	0.42
1:A:311:LYS:CD	1:A:587:THR:H	2.30	0.42
1:A:428:GLU:C	1:A:430:PHE:H	2.27	0.42
1:A:484:GLU:CD	1:A:603:VAL:HG12	2.45	0.42
1:A:289:SER:O	1:A:290:THR:OG1	2.35	0.41
1:A:336:THR:HG22	1:A:340:MET:HE3	2.01	0.41
1:A:302:TRP:CE2	1:A:594:ARG:HD2	2.56	0.41
1:A:536:GLY:O	1:A:540:ARG:HG2	2.21	0.40
1:A:768:HIS:CD2	1:A:768:HIS:H	2.39	0.40
1:A:307:SER:HB3	1:A:588:VAL:CG1	2.52	0.40
1:A:831:THR:OG1	4:A:1002:HOH:O	2.21	0.40

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)
4:A:1160:HOH:O	4:A:1270:HOH:O[3_555]	2.09	0.11

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	560/647 (87%)	539 (96%)	20 (4%)	1 (0%)	43 35

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	429	GLU

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	497/561 (89%)	492 (99%)	5 (1%)	68 65

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

Mol	Chain	Res	Type
1	A	324	VAL
1	A	327	LEU
1	A	372	VAL
1	A	667	VAL
1	A	885	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	405	ASN
1	A	492	ASN
1	A	562	GLN
1	A	580	GLN
1	A	617	GLN
1	A	701	HIS
1	A	760	GLN
1	A	868	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](#)

Of 3 ligands modelled in this entry, 2 are 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	B5C	A	903	-	14,15,15	5.10	5 (35%)	18,21,21	3.73	5 (27%)

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	B5C	A	903	-	-	4/4/4/4	0/2/2/2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	903	B5C	O09-C08	16.28	1.65	1.38
3	A	903	B5C	C13-S12	-5.49	1.63	1.74
3	A	903	B5C	O09-C10	5.15	1.48	1.38
3	A	903	B5C	C08-C13	4.62	1.48	1.40
3	A	903	B5C	C06-C05	3.08	1.44	1.38

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	903	B5C	C13-S12-C10	14.40	106.16	91.66
3	A	903	B5C	O04-C02-C01	3.57	118.72	110.97
3	A	903	B5C	O09-C10-O11	3.46	126.01	121.68
3	A	903	B5C	O09-C08-C07	2.39	131.52	126.49
3	A	903	B5C	C14-C13-S12	2.29	131.78	126.07

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	903	B5C	C14-C05-O04-C02
3	A	903	B5C	C01-C02-O04-C05
3	A	903	B5C	O03-C02-O04-C05
3	A	903	B5C	C06-C05-O04-C02

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	903	B5C	1	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	568/647 (87%)	1.11	121 (21%) 2 3	27, 45, 95, 114	0

All (121) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	421	ALA	7.9
1	A	803	TRP	7.2
1	A	884	PRO	7.1
1	A	353	VAL	6.8
1	A	312	ALA	6.3
1	A	425	VAL	6.2
1	A	333	VAL	5.7
1	A	430	PHE	5.7
1	A	343	THR	5.3
1	A	423	ALA	5.2
1	A	341	ALA	5.1
1	A	310	VAL	5.1
1	A	804	MET	5.0
1	A	588	VAL	4.9
1	A	348	PHE	4.9
1	A	805	THR	4.6
1	A	603	VAL	4.6
1	A	885	SER	4.6
1	A	316	ALA	4.6
1	A	579	VAL	4.4
1	A	744	ALA	4.4
1	A	342	MET	4.2
1	A	789	PRO	4.2
1	A	451	TYR	4.2
1	A	601	GLY	4.1
1	A	801	HIS	4.1
1	A	426	GLU	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	587	THR	3.9
1	A	357	LYS	3.9
1	A	318	SER	3.8
1	A	311	LYS	3.8
1	A	584	PRO	3.8
1	A	883	MET	3.8
1	A	746	TRP	3.8
1	A	453	MET	3.7
1	A	345	THR	3.5
1	A	424	ALA	3.5
1	A	450	VAL	3.5
1	A	313	THR	3.4
1	A	354	PHE	3.4
1	A	745	GLY	3.4
1	A	452	ASN	3.4
1	A	788	VAL	3.4
1	A	422	ARG	3.3
1	A	405	ASN	3.3
1	A	476	MET	3.3
1	A	882	TYR	3.3
1	A	293	TYR	3.2
1	A	582	PRO	3.2
1	A	347	PRO	3.2
1	A	477	TRP	3.1
1	A	602	GLN	3.1
1	A	317	SER	3.1
1	A	358	VAL	3.1
1	A	404	THR	3.1
1	A	402	VAL	3.1
1	A	854	THR	3.1
1	A	309	GLU	3.0
1	A	290	THR	3.0
1	A	420	SER	3.0
1	A	292	HIS	2.9
1	A	583	THR	2.9
1	A	591	ILE	2.9
1	A	600	SER	2.9
1	A	291	TRP	2.9
1	A	478	LEU	2.9
1	A	592	ILE	2.9
1	A	806	THR	2.8
1	A	787	TRP	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	742	GLN	2.8
1	A	743	GLY	2.8
1	A	737	ARG	2.8
1	A	786	HIS	2.7
1	A	581	ARG	2.7
1	A	287	HIS	2.7
1	A	741	SER	2.6
1	A	272	ASN	2.6
1	A	315	SER	2.5
1	A	586	GLY	2.4
1	A	419	ASP	2.4
1	A	308	TYR	2.4
1	A	344	ASP	2.4
1	A	509	GLU	2.4
1	A	876	ASN	2.4
1	A	433	LEU	2.3
1	A	304	TYR	2.3
1	A	830	VAL	2.3
1	A	881	ASP	2.3
1	A	296	GLU	2.3
1	A	868	GLN	2.3
1	A	355	LYS	2.3
1	A	320	ILE	2.3
1	A	427	ASP	2.3
1	A	807	GLU	2.3
1	A	429	GLU	2.2
1	A	785	VAL	2.2
1	A	361	ARG	2.2
1	A	880	LEU	2.2
1	A	295	ASP	2.2
1	A	284	LYS	2.2
1	A	299	TYR	2.1
1	A	294	ASP	2.1
1	A	835	ASP	2.1
1	A	875	GLY	2.1
1	A	481	ARG	2.1
1	A	764	LEU	2.1
1	A	802	GLN	2.1
1	A	288	SER	2.1
1	A	319	MET	2.1
1	A	716	LEU	2.1
1	A	585	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	349	GLY	2.1
1	A	580	GLN	2.1
1	A	283	ILE	2.0
1	A	286	GLU	2.0
1	A	432	LYS	2.0
1	A	273	MET	2.0
1	A	809	MET	2.0
1	A	303	ALA	2.0
1	A	274	ASP	2.0
1	A	307	SER	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(Å ²)	Q<0.9
3	B5C	A	903	14/14	0.64	0.20	62,73,82,99	0
2	ZN	A	901	1/1	0.99	0.04	50,50,50,50	0
2	ZN	A	902	1/1	1.00	0.02	35,35,35,35	0

6.5 Other polymers [i](#)

There are no such residues in this entry.