



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:32 PM UTC

PDB ID : 4CKK / pdb_00004ckk
Title : Apo structure of 55 kDa N-terminal domain of E. coli DNA gyrase A subunit
Authors : Hearnshaw, S.J.; Edwards, M.J.; Stevenson, C.E.M.; Lawson, D.M.; Maxwell, A.
Deposited on : 2014-01-07
Resolution : 1.90 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

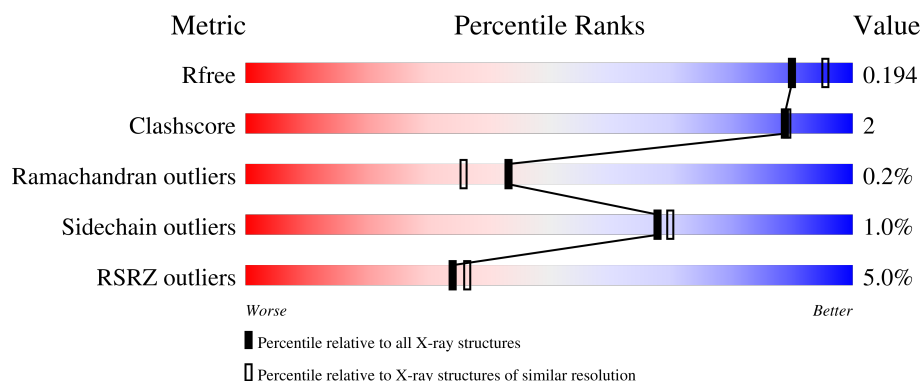
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	493	4% 94% 5% ..
1	B	493	4% 94% 5% ..
1	C	493	6% 93% 5% ..
1	D	493	6% 92% 5% ..

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 16106 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 DNA GYRASE SUBUNIT A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	485	Total	C	N	O	S	0	2	0
			3788	2389	681	705	13			
1	B	484	Total	C	N	O	S	0	3	0
			3783	2391	676	703	13			
1	C	484	Total	C	N	O	S	0	0	0
			3710	2350	656	691	13			
1	D	484	Total	C	N	O	S	0	0	0
			3769	2378	666	712	13			

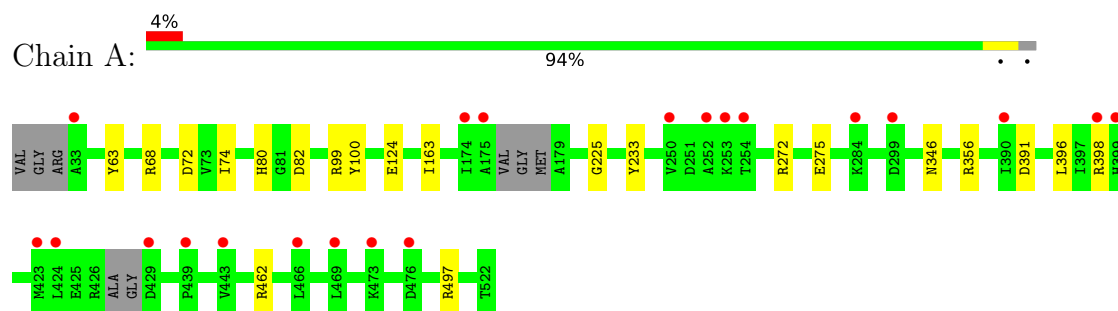
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	279	Total	O	0	0
			279	279		
2	B	257	Total	O	0	0
			257	257		
2	C	281	Total	O	0	0
			281	281		
2	D	239	Total	O	0	0
			239	239		

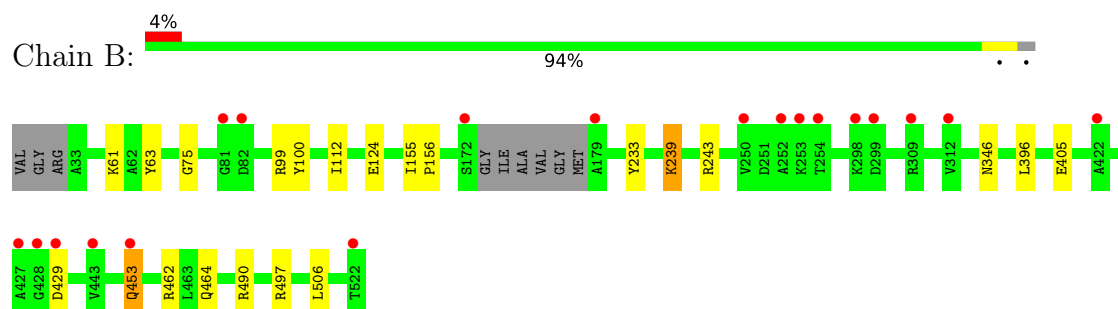
3 Residue-property plots

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.

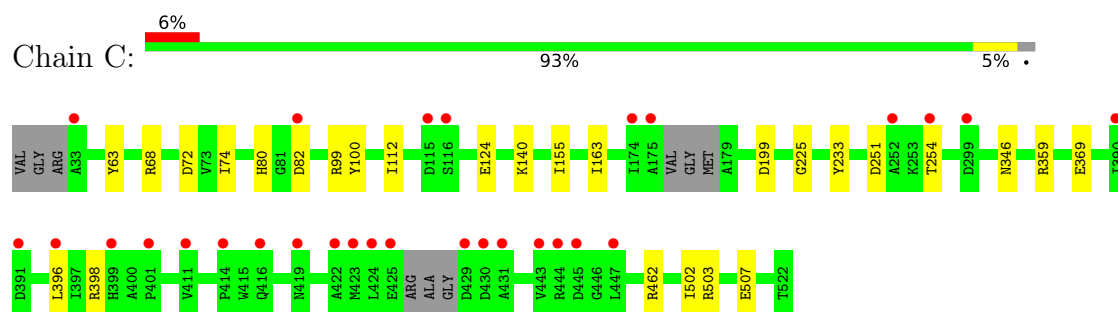
• Molecule 1: DNA GYRASE SUBUNIT A



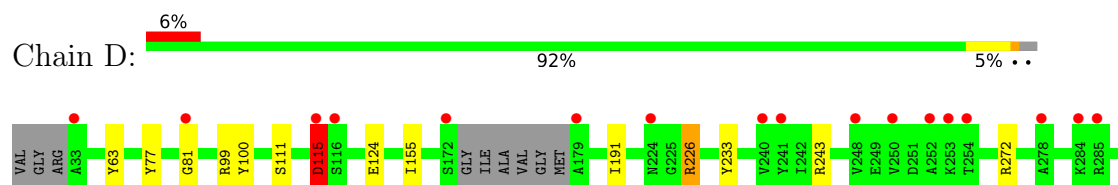
• Molecule 1: DNA GYRASE SUBUNIT A

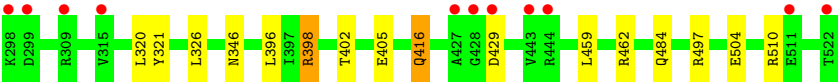


• Molecule 1: DNA GYRASE SUBUNIT A



• Molecule 1: DNA GYRASE SUBUNIT A





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	93.57Å 95.53Å 95.89Å 105.16° 118.81° 103.42°	Depositor
Resolution (Å)	81.51 – 1.90 81.51 – 1.90	Depositor EDS
% Data completeness (in resolution range)	97.0 (81.51-1.90) 97.0 (81.51-1.90)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.40 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.169 , 0.189 0.176 , 0.194	Depositor DCC
R_{free} test set	9799 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	26.0	Xtriage
Anisotropy	0.062	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 35.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.024 for h+k+l,-h,-k 0.024 for -k,-l,h+k+l 0.024 for k,h,-h-k-l 0.047 for l,-h-k-l,h 0.025 for -l,-k,-h 0.024 for -h-k-l,l,k 0.024 for -h,h+k+l,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	16106	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.70% 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

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	0.88	0/3854	0.90	2/5220 (0.0%)
1	B	0.93	0/3853	0.90	2/5217 (0.0%)
1	C	0.93	0/3770	0.90	3/5114 (0.1%)
1	D	0.88	0/3830	0.93	6/5192 (0.1%)
All	All	0.90	0/15307	0.91	13/20743 (0.1%)

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	226	ARG	N-CA-CB	6.50	121.48	110.49
1	D	398	ARG	CA-CB-CG	5.87	125.83	114.10
1	B	239	LYS	N-CA-CB	-5.78	101.49	110.57
1	D	398	ARG	CB-CA-C	-5.70	100.09	110.63
1	A	80	HIS	N-CA-C	5.45	119.01	111.71
1	D	398	ARG	CB-CG-CD	-5.45	98.78	111.30
1	D	115	ASP	N-CA-CB	5.41	117.96	110.17
1	C	80	HIS	CB-CA-C	-5.35	102.15	111.35
1	C	163	ILE	CB-CA-C	-5.26	104.95	110.53
1	B	243	ARG	CB-CG-CD	-5.14	99.47	111.30
1	D	81	GLY	N-CA-C	5.13	123.89	115.73
1	A	163	ILE	CB-CA-C	-5.12	104.89	110.37
1	C	80	HIS	N-CA-C	5.07	116.94	110.61

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	3788	0	3787	13	0
1	B	3783	0	3801	15	0
1	C	3710	0	3673	18	0
1	D	3769	0	3757	19	0
2	A	279	0	0	2	0
2	B	257	0	0	5	0
2	C	281	0	0	3	0
2	D	239	0	0	4	0
All	All	16106	0	15018	56	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 2.

All (56) 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:B:453:GLN:NE2	2:B:2224:HOH:O	2.29	0.65
1:D:484:GLN:OE1	2:D:2216:HOH:O	2.14	0.65
1:D:416:GLN:HG2	2:D:2091:HOH:O	2.02	0.59
1:B:462:ARG:HH12	1:D:462:ARG:CZ	2.15	0.59
1:D:416:GLN:NE2	2:D:2190:HOH:O	2.35	0.59
1:B:462:ARG:HH12	1:D:462:ARG:NH2	2.02	0.57
1:A:74:ILE:HD11	1:A:82:ASP:HA	1.87	0.56
1:C:74:ILE:HD11	1:C:82:ASP:HA	1.86	0.56
1:B:462:ARG:NH1	1:D:462:ARG:CZ	2.69	0.56
1:D:402:THR:OG1	1:D:405:GLU:OE1	2.10	0.56
1:A:462:ARG:CZ	1:C:462:ARG:HH12	2.18	0.55
1:C:68:ARG:NH1	1:C:72:ASP:OD1	2.40	0.55
1:C:155:ILE:HD12	2:C:2018:HOH:O	2.10	0.50
1:C:63:TYR:HB3	1:C:124:GLU:HB3	1.94	0.50
1:A:356:ARG:HD3	2:A:2225:HOH:O	2.11	0.50
1:A:462:ARG:CZ	1:C:462:ARG:NH1	2.74	0.50
1:A:68[A]:ARG:NH1	1:A:72:ASP:OD1	2.44	0.49
1:B:63:TYR:HB3	1:B:124:GLU:HB3	1.94	0.49
1:A:63:TYR:HB3	1:A:124:GLU:HB3	1.95	0.49
1:A:462:ARG:NH2	1:C:462:ARG:HH12	2.11	0.48
1:B:506:LEU:HD23	2:B:2100:HOH:O	2.13	0.48
1:B:155:ILE:HG13	1:B:156:PRO:HD2	1.95	0.48
1:B:464:GLN:HB3	1:D:459:LEU:HB3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:199:ASP:OD1	1:C:503:ARG:NH1	2.48	0.46
1:A:275:GLU:OE1	2:A:2191:HOH:O	2.20	0.46
1:D:63:TYR:HB3	1:D:124:GLU:HB3	1.96	0.46
1:C:140:LYS:HE2	1:C:369:GLU:OE2	2.16	0.45
1:B:396:LEU:C	1:B:396:LEU:HD23	2.41	0.45
1:C:99:ARG:HG3	1:C:100:TYR:CE2	2.52	0.44
1:C:199:ASP:OD1	1:C:503:ARG:NH2	2.47	0.44
1:B:75:GLY:HA3	2:B:2038:HOH:O	2.18	0.44
1:B:99:ARG:HG3	1:B:100:TYR:CE2	2.53	0.44
1:C:507:GLU:HG3	2:C:2269:HOH:O	2.17	0.44
1:D:243:ARG:HG3	1:D:321:TYR:CE1	2.53	0.44
1:D:233:TYR:O	1:D:346:ASN:HB2	2.18	0.43
1:B:462:ARG:NH1	1:D:462:ARG:NH2	2.67	0.43
1:C:233:TYR:O	1:C:346:ASN:HB2	2.19	0.43
1:B:233:TYR:O	1:B:346:ASN:HB2	2.19	0.43
1:D:504:GLU:HG3	2:D:2222:HOH:O	2.19	0.43
1:C:359:ARG:HA	1:C:502:ILE:HD11	2.01	0.43
1:C:251:ASP:CG	1:C:254:THR:HG22	2.44	0.43
1:C:396:LEU:C	1:C:396:LEU:HD23	2.43	0.43
1:D:99:ARG:HG3	1:D:100:TYR:CE2	2.54	0.43
1:C:112:ILE:HD11	2:C:2189:HOH:O	2.19	0.42
1:D:396:LEU:C	1:D:396:LEU:HD23	2.44	0.42
1:A:396:LEU:C	1:A:396:LEU:HD23	2.44	0.42
1:B:61:LYS:HD3	2:B:2024:HOH:O	2.18	0.42
1:D:111:SER:OG	1:D:115:ASP:OD2	2.37	0.42
1:D:191:ILE:HG21	1:D:510:ARG:HB2	2.02	0.42
1:A:391:ASP:OD1	1:C:398:ARG:NH2	2.53	0.42
1:D:77:TYR:CE1	1:D:155:ILE:HG12	2.54	0.42
1:B:112:ILE:HD11	2:B:2157:HOH:O	2.19	0.42
1:A:74:ILE:HD11	1:A:82:ASP:CA	2.51	0.41
1:A:99:ARG:HG3	1:A:100:TYR:CE2	2.56	0.41
1:D:320:LEU:HB3	1:D:326:LEU:HD12	2.03	0.41
1:A:233:TYR:O	1:A:346:ASN:HB2	2.22	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	481/493 (98%)	474 (98%)	6 (1%)	1 (0%)	43	36
1	B	483/493 (98%)	476 (99%)	7 (1%)	0	100	100
1	C	478/493 (97%)	470 (98%)	7 (2%)	1 (0%)	43	36
1	D	480/493 (97%)	472 (98%)	7 (2%)	1 (0%)	43	36
All	All	1922/1972 (98%)	1892 (98%)	27 (1%)	3 (0%)	43	36

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	226	ARG
1	A	225	GLY
1	C	225	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	389/411 (95%)	386 (99%)	3 (1%)	73	75
1	B	390/411 (95%)	384 (98%)	6 (2%)	57	56
1	C	373/411 (91%)	373 (100%)	0	100	100
1	D	390/411 (95%)	384 (98%)	6 (2%)	57	56
All	All	1542/1644 (94%)	1527 (99%)	15 (1%)	68	70

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	272	ARG
1	A	398	ARG
1	A	497	ARG
1	B	239	LYS
1	B	405	GLU
1	B	429	ASP
1	B	453	GLN
1	B	490	ARG
1	B	497	ARG
1	D	115	ASP
1	D	272	ARG
1	D	398	ARG
1	D	416	GLN
1	D	429	ASP
1	D	497	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	ASN
1	A	224	ASN
1	A	267	GLN
1	A	339	HIS
1	A	453	GLN
1	B	57	ASN
1	B	325	GLN
1	B	456	GLN
1	B	464	GLN
1	B	484	GLN
1	C	57	ASN
1	C	325	GLN
1	C	339	HIS
1	D	57	ASN
1	D	80	HIS
1	D	338	HIS
1	D	416	GLN
1	D	453	GLN
1	D	464	GLN

5.3.3 RNA ⓘ

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	485/493 (98%)	0.25	21 (4%)	40 42	13, 29, 56, 84	2 (0%)
1	B	484/493 (98%)	0.17	19 (3%)	43 46	16, 27, 54, 85	3 (0%)
1	C	484/493 (98%)	0.20	29 (5%)	27 29	15, 28, 59, 89	0
1	D	484/493 (98%)	0.32	28 (5%)	29 30	16, 31, 55, 77	0
All	All	1937/1972 (98%)	0.24	97 (5%)	34 36	13, 29, 56, 89	5 (0%)

All (97) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	429	ASP	6.1
1	A	175	ALA	6.0
1	C	445	ASP	5.8
1	D	81	GLY	4.5
1	C	444	ARG	4.2
1	B	427	ALA	4.1
1	B	254	THR	4.0
1	C	429	ASP	4.0
1	A	252	ALA	4.0
1	C	175	ALA	4.0
1	A	254	THR	3.9
1	A	469	LEU	3.8
1	D	427	ALA	3.8
1	D	522	THR	3.8
1	C	174	ILE	3.8
1	D	428	GLY	3.7
1	A	174	ILE	3.5
1	B	252	ALA	3.4
1	D	179	ALA	3.4
1	D	298	LYS	3.4
1	D	253	LYS	3.4

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Mol	Chain	Res	Type	RSRZ
1	D	33	ALA	3.3
1	B	179	ALA	3.1
1	C	299	ASP	3.1
1	A	253	LYS	3.1
1	A	33	ALA	3.1
1	B	172	SER	3.1
1	D	299	ASP	3.0
1	D	252	ALA	3.0
1	C	419	ASN	2.9
1	C	252	ALA	2.9
1	C	447	LEU	2.9
1	B	250	VAL	2.9
1	A	399	HIS	2.9
1	D	511	GLU	2.8
1	C	416	GLN	2.8
1	C	401	PRO	2.8
1	C	422	ALA	2.7
1	B	253	LYS	2.7
1	D	443	VAL	2.7
1	A	390	ILE	2.7
1	C	443	VAL	2.7
1	C	431	ALA	2.7
1	D	429	ASP	2.7
1	D	284	LYS	2.7
1	D	115	ASP	2.6
1	D	241	TYR	2.6
1	A	398	ARG	2.6
1	B	299	ASP	2.6
1	B	428	GLY	2.6
1	C	254	THR	2.6
1	B	453	GLN	2.5
1	B	522	THR	2.5
1	D	172	SER	2.5
1	D	278	ALA	2.5
1	B	81	GLY	2.4
1	B	443	VAL	2.4
1	C	424	LEU	2.4
1	D	285	ARG	2.4
1	C	423	MET	2.4
1	C	82	ASP	2.4
1	D	224	ASN	2.4
1	B	312	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	116	SER	2.3
1	D	250	VAL	2.3
1	B	429	ASP	2.3
1	C	414	PRO	2.3
1	C	390	ILE	2.3
1	D	309	ARG	2.3
1	C	425	GLU	2.3
1	C	396	LEU	2.3
1	B	82[A]	ASP	2.2
1	C	115	ASP	2.2
1	C	430	ASP	2.2
1	A	443	VAL	2.2
1	D	315	VAL	2.2
1	B	422	ALA	2.2
1	A	299	ASP	2.1
1	D	240	VAL	2.1
1	A	466	LEU	2.1
1	D	254	THR	2.1
1	A	473	LYS	2.1
1	C	33	ALA	2.1
1	B	309	ARG	2.1
1	D	116	SER	2.1
1	D	444	ARG	2.1
1	C	411	VAL	2.1
1	B	298	LYS	2.0
1	A	423	MET	2.0
1	D	248	VAL	2.0
1	A	424	LEU	2.0
1	A	476	ASP	2.0
1	C	391	ASP	2.0
1	A	284	LYS	2.0
1	C	399	HIS	2.0
1	A	439	PRO	2.0
1	A	250	VAL	2.0

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 [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.