



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 10:15 PM UTC

PDB ID : 6IRV / pdb_00006irv
Title : Crystal structure of the human cap-specific adenosine methyltransferase
Authors : Hirano, S.; Nishimasu, H.; Ishitani, R.; Nureki, O.
Deposited on : 2018-11-14
Resolution : 2.70 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

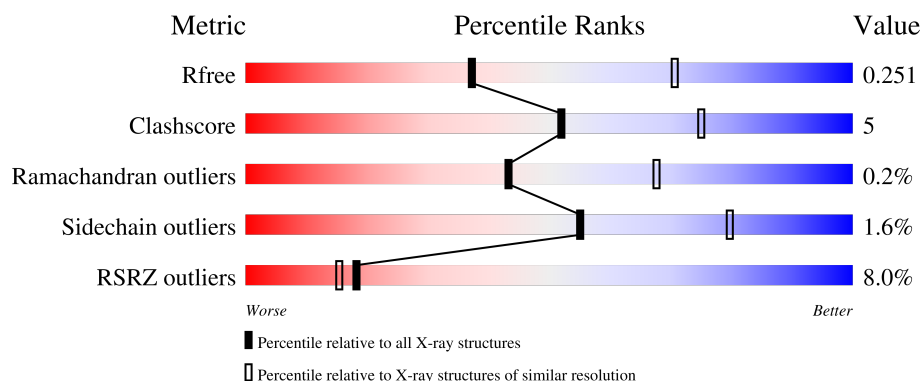
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	508	9% 83% 14% .
1	B	508	6% 83% 14% ..

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8079 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 Phosphorylated CTD-interacting factor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	494	Total	C	N	O	S	0	0	0
			4009	2566	707	708	28			
1	B	494	Total	C	N	O	S	0	0	0
			4006	2563	708	707	28			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	165	GLU	-	expression tag	UNP Q9H4Z3
A	166	ASN	-	expression tag	UNP Q9H4Z3
A	167	LEU	-	expression tag	UNP Q9H4Z3
A	168	TYR	-	expression tag	UNP Q9H4Z3
A	169	PHE	-	expression tag	UNP Q9H4Z3
A	170	GLN	-	expression tag	UNP Q9H4Z3
A	171	GLY	-	expression tag	UNP Q9H4Z3
A	172	SER	-	expression tag	UNP Q9H4Z3
A	173	HIS	-	expression tag	UNP Q9H4Z3
B	165	GLU	-	expression tag	UNP Q9H4Z3
B	166	ASN	-	expression tag	UNP Q9H4Z3
B	167	LEU	-	expression tag	UNP Q9H4Z3
B	168	TYR	-	expression tag	UNP Q9H4Z3
B	169	PHE	-	expression tag	UNP Q9H4Z3
B	170	GLN	-	expression tag	UNP Q9H4Z3
B	171	GLY	-	expression tag	UNP Q9H4Z3
B	172	SER	-	expression tag	UNP Q9H4Z3
B	173	HIS	-	expression tag	UNP Q9H4Z3

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	30	Total	O	0	0
			30	30		

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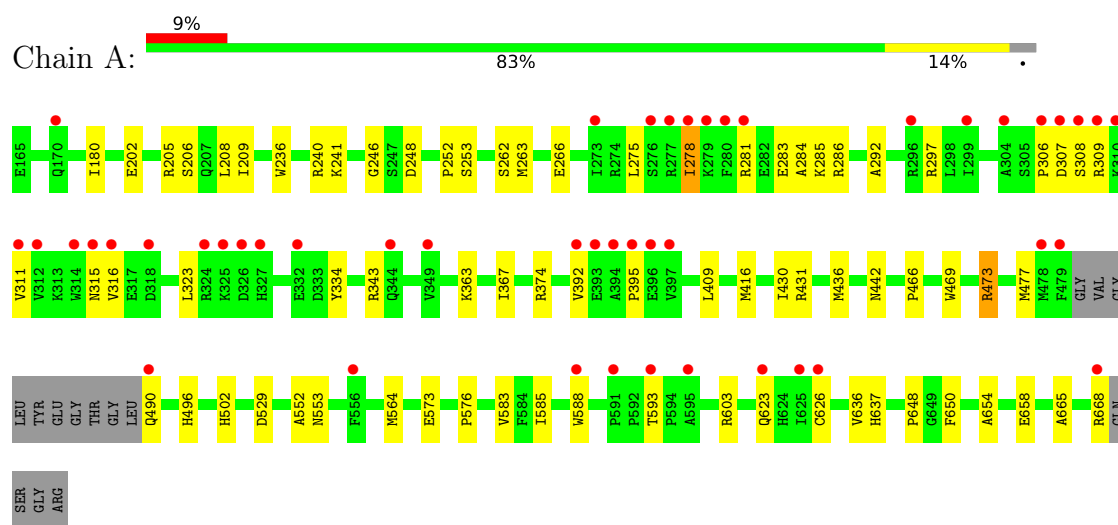
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	34	Total	O	0	0
			34	34		

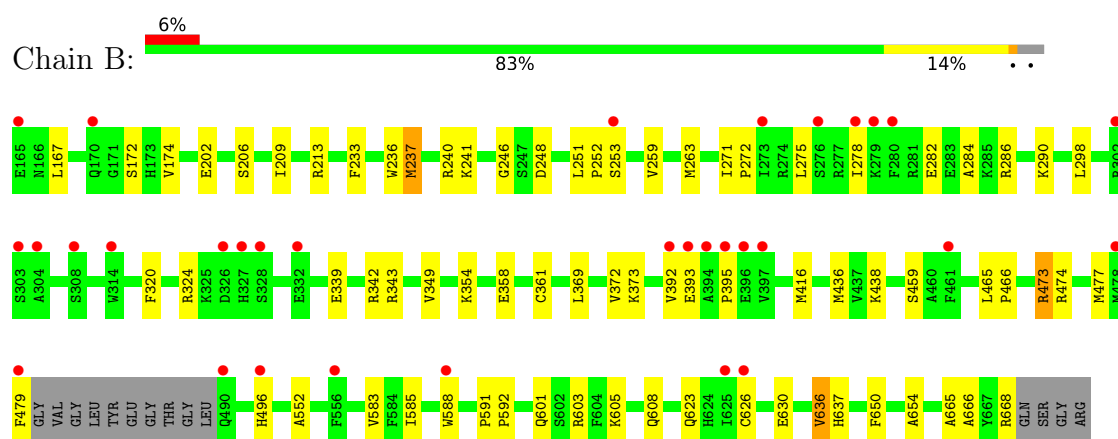
3 Residue-property plots [i](#)

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: Phosphorylated CTD-interacting factor 1



• Molecule 1: Phosphorylated CTD-interacting factor 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	70.70Å 120.31Å 156.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.12 – 2.70 48.12 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.12-2.70) 99.9 (48.12-2.70)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.65 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.214 , 0.252 0.212 , 0.251	Depositor DCC
R_{free} test set	1883 reflections (3.88%)	wwPDB-VP
Wilson B-factor (Å ²)	51.2	Xtriage
Anisotropy	0.381	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 44.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8079	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 48.59 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 8.4136e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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	0.12	0/4123	0.33	0/5587
1	B	0.12	0/4121	0.31	0/5587
All	All	0.12	0/8244	0.32	0/11174

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	4009	0	3907	44	1
1	B	4006	0	3892	40	0
2	A	30	0	0	0	0
2	B	34	0	0	0	0
All	All	8079	0	7799	81	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 5.

All (81) 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:278:ILE:HD13	1:B:284:ALA:HA	1.62	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:573:GLU:HG2	1:A:603:ARG:HH22	1.50	0.76
1:B:206:SER:HB3	1:B:477:MET:HE2	1.73	0.70
1:A:241:LYS:NZ	1:A:248:ASP:O	2.23	0.69
1:A:278:ILE:HG21	1:A:284:ALA:HB2	1.74	0.68
1:B:259:VAL:HG21	1:B:358:GLU:HG2	1.78	0.66
1:B:241:LYS:NZ	1:B:248:ASP:O	2.25	0.66
1:A:206:SER:HB3	1:A:477:MET:HE2	1.76	0.66
1:A:286:ARG:HG3	1:B:636:VAL:HG11	1.80	0.64
1:B:339:GLU:HB3	1:B:343:ARG:NH2	2.13	0.63
1:A:431:ARG:HE	1:A:436:MET:HE2	1.65	0.62
1:A:636:VAL:HG21	1:B:290:LYS:HE3	1.81	0.61
1:B:167:LEU:HD22	1:B:172:SER:HB3	1.82	0.61
1:A:306:PRO:HA	1:A:309:ARG:HB3	1.84	0.59
1:B:665:ALA:HA	1:B:668:ARG:HD2	1.85	0.59
1:A:246:GLY:HA3	1:A:253:SER:HB3	1.86	0.56
1:A:416:MET:HE3	1:A:466:PRO:HB2	1.87	0.56
1:B:416:MET:HE3	1:B:466:PRO:HB2	1.87	0.56
1:A:573:GLU:HG2	1:A:603:ARG:NH2	2.19	0.54
1:A:363:LYS:HE3	1:A:367:ILE:HD11	1.89	0.53
1:A:205:ARG:O	1:A:209:ILE:HG12	2.09	0.52
1:A:278:ILE:HD12	1:A:283:GLU:HG2	1.92	0.52
1:B:552:ALA:HB3	1:B:583:VAL:HG22	1.92	0.52
1:A:430:ILE:HG22	1:A:469:TRP:HD1	1.76	0.51
1:B:282:GLU:O	1:B:286:ARG:HG3	2.11	0.51
1:A:307:ASP:O	1:A:311:VAL:N	2.44	0.49
1:A:623:GLN:HA	1:A:626:CYS:SG	2.54	0.48
1:B:605:LYS:HE2	1:B:608:GLN:HB2	1.96	0.48
1:B:233:PHE:CZ	1:B:237:MET:HE3	2.49	0.48
1:A:473:ARG:O	1:A:477:MET:HG3	2.14	0.47
1:A:202:GLU:OE2	1:A:205:ARG:NH2	2.46	0.47
1:A:311:VAL:O	1:A:315:ASN:ND2	2.47	0.47
1:A:392:VAL:HG12	1:A:395:PRO:HD3	1.96	0.47
1:B:320:PHE:O	1:B:324:ARG:HG3	2.15	0.47
1:B:213:ARG:NH2	1:B:477:MET:O	2.46	0.47
1:A:496:HIS:CD2	1:A:496:HIS:H	2.33	0.46
1:B:392:VAL:HG12	1:B:395:PRO:HD3	1.97	0.46
1:A:240:ARG:HB3	1:A:252:PRO:HB3	1.98	0.45
1:A:285:LYS:HG3	1:A:323:LEU:HD22	1.98	0.45
1:B:240:ARG:HB3	1:B:252:PRO:HB3	1.98	0.45
1:A:262:SER:O	1:A:266:GLU:HG3	2.18	0.44
1:A:650:PHE:O	1:A:654:ALA:HB2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:658:GLU:H	1:A:658:GLU:CD	2.26	0.44
1:B:259:VAL:HG13	1:B:361:CYS:HB2	2.00	0.44
1:B:473:ARG:O	1:B:477:MET:HG3	2.17	0.44
1:A:442:ASN:OD1	1:A:442:ASN:N	2.51	0.44
1:B:623:GLN:HA	1:B:626:CYS:SG	2.58	0.44
1:B:236:TRP:CG	1:B:263:MET:HE3	2.52	0.44
1:B:496:HIS:ND1	1:B:666:ALA:O	2.51	0.43
1:A:665:ALA:O	1:A:668:ARG:HG2	2.18	0.43
1:A:180:ILE:HD12	1:A:502:HIS:CE1	2.53	0.43
1:A:236:TRP:CG	1:A:263:MET:HE3	2.53	0.43
1:B:202:GLU:OE2	1:B:474:ARG:NH2	2.39	0.43
1:B:354:LYS:O	1:B:358:GLU:HB2	2.19	0.43
1:A:409:LEU:HD11	1:A:529:ASP:HA	1.99	0.43
1:B:650:PHE:O	1:B:654:ALA:HB2	2.19	0.43
1:A:275:LEU:HD23	1:A:275:LEU:HA	1.87	0.43
1:A:588:TRP:HD1	1:A:637:HIS:CG	2.37	0.43
1:B:246:GLY:HA3	1:B:253:SER:HB3	2.01	0.43
1:B:465:LEU:HD23	1:B:465:LEU:HA	1.90	0.43
1:A:292:ALA:HB1	1:A:316:VAL:HG13	2.01	0.42
1:B:436:MET:HE3	1:B:438:LYS:HE3	2.00	0.42
1:B:473:ARG:HD2	1:B:473:ARG:HA	1.62	0.42
1:A:285:LYS:HB2	1:A:334:TYR:CE2	2.54	0.42
1:B:588:TRP:HD1	1:B:637:HIS:CD2	2.38	0.42
1:A:490:GLN:NE2	1:A:553:ASN:OD1	2.52	0.42
1:B:271:ILE:HA	1:B:272:PRO:C	2.45	0.42
1:B:298:LEU:HD22	1:B:349:VAL:HG23	2.01	0.42
1:B:373:LYS:HA	1:B:373:LYS:HD3	1.77	0.42
1:B:591:PRO:HA	1:B:592:PRO:HD2	1.96	0.41
1:A:576:PRO:O	1:A:648:PRO:HG3	2.20	0.41
1:B:237:MET:HE1	1:B:251:LEU:HD23	2.03	0.41
1:B:253:SER:O	1:B:369:LEU:HD13	2.20	0.41
1:A:308:SER:HA	1:A:311:VAL:HB	2.03	0.41
1:A:552:ALA:HB3	1:A:583:VAL:HG22	2.02	0.41
1:A:564:MET:HE2	1:A:564:MET:HB3	1.98	0.41
1:B:248:ASP:HB2	1:B:372:VAL:HG13	2.02	0.41
1:A:278:ILE:HG13	1:A:284:ALA:HA	2.04	0.40
1:B:275:LEU:HD11	1:B:342:ARG:HD2	2.03	0.40
1:A:208:LEU:HD21	1:A:374:ARG:HH21	1.85	0.40
1:A:297:ARG:HH21	1:B:630:GLU:HA	1.85	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)
1:A:281:ARG:NH2	1:A:307:ASP:OD2[4_455]	2.16	0.04

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	490/508 (96%)	473 (96%)	17 (4%)	0	100	100
1	B	490/508 (96%)	480 (98%)	8 (2%)	2 (0%)	30	54
All	All	980/1016 (96%)	953 (97%)	25 (3%)	2 (0%)	43	68

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	393	GLU
1	B	459	SER

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	434/459 (95%)	429 (99%)	5 (1%)	63	84
1	B	433/459 (94%)	424 (98%)	9 (2%)	47	75
All	All	867/918 (94%)	853 (98%)	14 (2%)	55	80

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	278	ILE
1	A	343	ARG
1	A	473	ARG
1	A	585	ILE
1	A	593	THR
1	B	174	VAL
1	B	209	ILE
1	B	237	MET
1	B	473	ARG
1	B	479	PHE
1	B	585	ILE
1	B	601	GLN
1	B	603	ARG
1	B	636	VAL

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	215	HIS
1	A	315	ASN
1	A	490	GLN
1	A	502	HIS
1	A	623	GLN
1	B	188	HIS
1	B	422	HIS
1	B	476	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no ligands in this entry.

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	494/508 (97%)	0.36	47 (9%)	14 11	29, 55, 125, 171	0
1	B	494/508 (97%)	0.24	32 (6%)	25 22	31, 57, 108, 164	0
All	All	988/1016 (97%)	0.30	79 (7%)	18 15	29, 57, 117, 171	0

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	479	PHE	5.3
1	B	479	PHE	5.0
1	B	327	HIS	4.9
1	A	392	VAL	4.7
1	A	308	SER	4.6
1	A	394	ALA	4.3
1	B	392	VAL	4.2
1	A	278	ILE	4.2
1	B	625	ILE	4.2
1	A	311	VAL	4.0
1	B	326	ASP	3.9
1	B	394	ALA	3.9
1	B	478	MET	3.9
1	B	588	TRP	3.8
1	B	395	PRO	3.8
1	A	395	PRO	3.7
1	A	326	ASP	3.7
1	A	314	TRP	3.7
1	A	276	SER	3.7
1	B	397	VAL	3.6
1	A	306	PRO	3.6
1	A	397	VAL	3.6
1	A	625	ILE	3.6
1	A	393	GLU	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	490	GLN	3.6
1	B	278	ILE	3.5
1	A	327	HIS	3.5
1	B	304	ALA	3.4
1	A	277	ARG	3.3
1	A	307	ASP	3.3
1	A	304	ALA	3.2
1	A	280	PHE	3.0
1	A	312	VAL	3.0
1	A	310	LYS	3.0
1	A	593	THR	3.0
1	A	396	GLU	2.9
1	A	309	ARG	2.9
1	A	588	TRP	2.9
1	A	478	MET	2.8
1	A	316	VAL	2.8
1	A	591	PRO	2.8
1	A	595	ALA	2.8
1	B	308	SER	2.7
1	A	170	GLN	2.6
1	A	315	ASN	2.6
1	A	344	GLN	2.6
1	B	393	GLU	2.6
1	A	332	GLU	2.6
1	B	490	GLN	2.6
1	A	299	ILE	2.5
1	B	170	GLN	2.5
1	B	273	ILE	2.5
1	B	314	TRP	2.5
1	B	461	PHE	2.5
1	A	668	ARG	2.5
1	A	623	GLN	2.5
1	B	165	GLU	2.4
1	B	276	SER	2.4
1	B	328	SER	2.4
1	A	318	ASP	2.4
1	B	253	SER	2.4
1	B	396	GLU	2.4
1	A	325	LYS	2.3
1	B	280	PHE	2.3
1	A	279	LYS	2.3
1	B	279	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	556	PHE	2.3
1	A	349	VAL	2.2
1	A	324	ARG	2.2
1	B	556	PHE	2.2
1	A	281	ARG	2.1
1	A	273	ILE	2.1
1	B	302	ARG	2.1
1	A	626	CYS	2.0
1	B	626	CYS	2.0
1	A	296	ARG	2.0
1	B	332	GLU	2.0
1	B	303	SER	2.0
1	B	496	HIS	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.