



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 2, 2024 – 08:29 PM JST

PDB ID : 8HYR
Title : Crystal structure of human KARS apo
Authors : Zhang, X.; Wang, Y.
Deposited on : 2023-01-07
Resolution : 2.55 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 : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.37.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.37.1

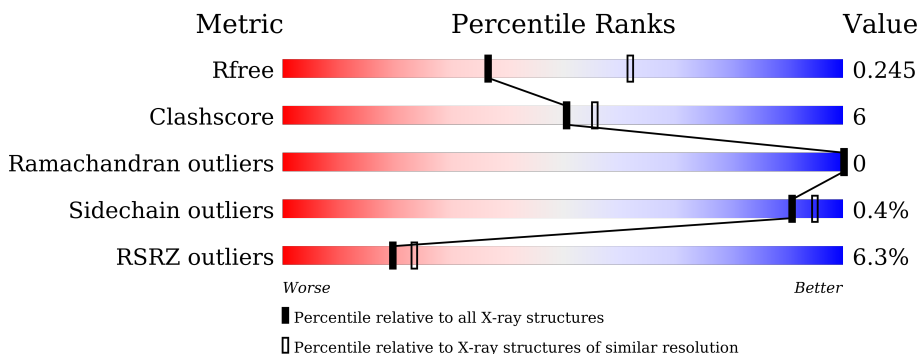
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.55 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}	130704	1284 (2.56-2.52)
Clashscore	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)

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	520	
1	B	520	

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 16395 atoms, of which 8101 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 Lysine-tRNA ligase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	499	8101	2598	4048	689	739	27	0	0	0
1	B	500	8111	2601	4053	690	740	27	0	0	0

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	69	MET	-	initiating methionine	UNP Q15046
A	581	LEU	-	expression tag	UNP Q15046
A	582	GLU	-	expression tag	UNP Q15046
A	583	HIS	-	expression tag	UNP Q15046
A	584	HIS	-	expression tag	UNP Q15046
A	585	HIS	-	expression tag	UNP Q15046
A	586	HIS	-	expression tag	UNP Q15046
A	587	HIS	-	expression tag	UNP Q15046
A	588	HIS	-	expression tag	UNP Q15046
B	69	MET	-	initiating methionine	UNP Q15046
B	581	LEU	-	expression tag	UNP Q15046
B	582	GLU	-	expression tag	UNP Q15046
B	583	HIS	-	expression tag	UNP Q15046
B	584	HIS	-	expression tag	UNP Q15046
B	585	HIS	-	expression tag	UNP Q15046
B	586	HIS	-	expression tag	UNP Q15046
B	587	HIS	-	expression tag	UNP Q15046
B	588	HIS	-	expression tag	UNP Q15046

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	102	Total	O	0	0
			102	102		

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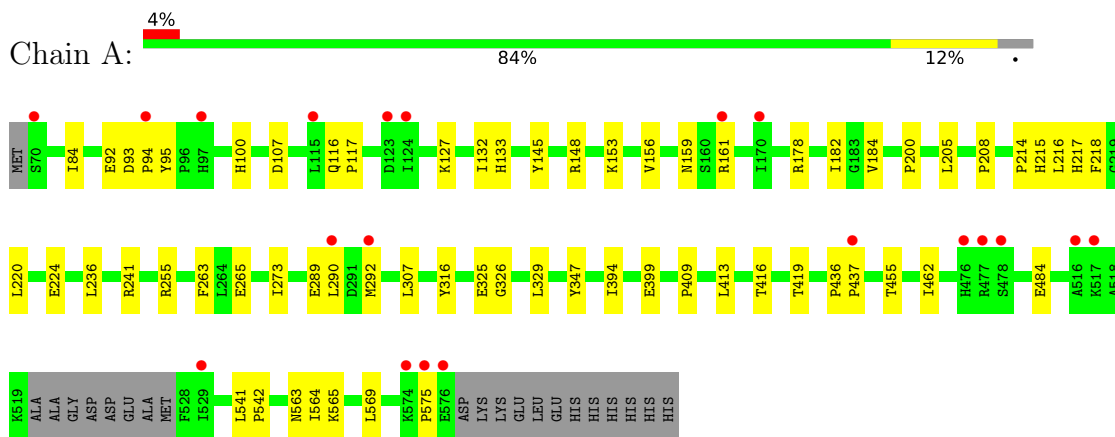
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	81	Total	O	0	0
			81	81		

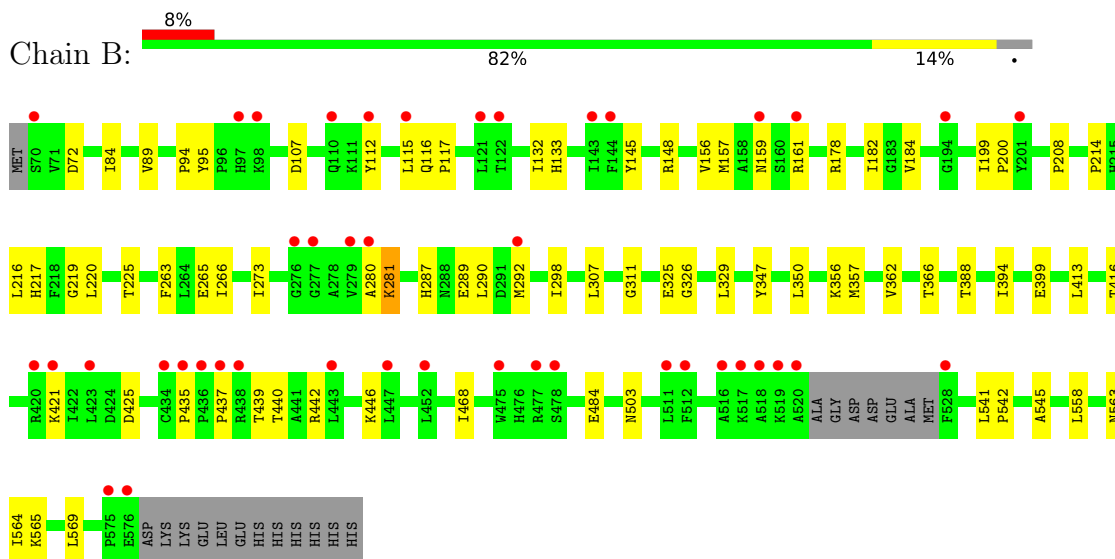
3 Residue-property plots [i](#)

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: Lysine-tRNA ligase



- Molecule 1: Lysine-tRNA ligase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	90.33Å 107.66Å 130.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.24 – 2.55 46.24 – 2.55	Depositor EDS
% Data completeness (in resolution range)	99.7 (46.24-2.55) 99.9 (46.24-2.55)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.04 (at 2.54Å)	Xtrriage
Refinement program	PHENIX 1.19_4092	Depositor
R, R_{free}	0.215 , 0.245 0.214 , 0.245	Depositor DCC
R_{free} test set	2000 reflections (4.74%)	wwPDB-VP
Wilson B-factor (Å ²)	39.4	Xtrriage
Anisotropy	0.622	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 43.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	16395	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 47.41 % 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 9.9650e-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	0.29	0/4149	0.54	0/5603
1	B	0.30	0/4154	0.53	0/5610
All	All	0.30	0/8303	0.53	0/11213

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	4053	4048	4048	42	0
1	B	4058	4053	4053	58	0
2	A	102	0	0	5	0
2	B	81	0	0	9	0
All	All	8294	8101	8101	92	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 6.

All (92) 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:219:GLY:O	2:B:601:HOH:O	1.87	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:357:MET:SD	2:B:678:HOH:O	2.26	0.92
1:B:72:ASP:OD1	2:B:602:HOH:O	1.94	0.85
1:A:84:ILE:HG23	1:A:94:PRO:HG2	1.65	0.79
1:B:107:ASP:OD2	2:B:603:HOH:O	2.01	0.79
1:B:84:ILE:HG23	1:B:94:PRO:HG2	1.67	0.77
1:B:356:LYS:NZ	2:B:607:HOH:O	2.18	0.77
1:A:455:THR:OG1	2:A:601:HOH:O	2.02	0.77
1:B:289:GLU:OE1	2:B:604:HOH:O	2.08	0.71
1:B:263:PHE:O	2:B:605:HOH:O	2.09	0.70
1:B:503:ASN:O	2:B:606:HOH:O	2.10	0.70
1:A:409:PRO:O	2:A:602:HOH:O	2.11	0.69
1:A:178:ARG:NH1	1:A:214:PRO:O	2.27	0.68
1:B:394:ILE:HB	1:B:399:GLU:HG3	1.76	0.68
1:A:394:ILE:HB	1:A:399:GLU:HG3	1.75	0.67
1:B:290:LEU:HD13	1:B:292:MET:HE2	1.78	0.65
1:B:329:LEU:HD22	1:B:563:ASN:HD21	1.62	0.65
1:A:329:LEU:HD22	1:A:563:ASN:HD21	1.63	0.64
1:A:413:LEU:O	1:A:416:THR:HG22	1.98	0.64
1:A:255:ARG:NH2	1:B:265:GLU:OE1	2.31	0.64
1:B:281:LYS:HD3	1:B:325:GLU:HB3	1.81	0.62
1:A:325:GLU:OE2	2:A:603:HOH:O	2.16	0.60
1:B:178:ARG:NH1	1:B:214:PRO:O	2.33	0.59
1:A:273:ILE:HD13	1:A:292:MET:HE3	1.84	0.58
1:B:145:TYR:HB2	1:B:156:VAL:HB	1.85	0.58
1:A:569:LEU:HD13	1:B:307:LEU:HD11	1.86	0.58
1:B:157:MET:HB3	1:B:199:ILE:HD13	1.85	0.58
1:B:413:LEU:O	1:B:416:THR:HG22	2.04	0.57
1:A:416:THR:HG23	1:A:419:THR:H	1.71	0.55
1:B:157:MET:HB3	1:B:199:ILE:CD1	2.37	0.55
1:B:116:GLN:HG3	1:B:117:PRO:HD2	1.90	0.54
1:B:273:ILE:HD13	1:B:292:MET:HE3	1.89	0.54
1:A:93:ASP:HB3	2:A:615:HOH:O	2.08	0.53
1:A:107:ASP:OD2	2:A:604:HOH:O	2.18	0.53
1:A:575:PRO:HD3	1:B:290:LEU:HD22	1.91	0.53
1:B:347:TYR:CD1	1:B:484:GLU:HB3	2.44	0.53
1:A:290:LEU:HD13	1:A:292:MET:HE2	1.91	0.53
1:A:307:LEU:HD11	1:B:569:LEU:HD13	1.90	0.53
1:B:112:TYR:O	1:B:115:LEU:HD13	2.09	0.53
1:B:541:LEU:HD12	1:B:542:PRO:HD2	1.91	0.52
1:A:541:LEU:HD12	1:A:542:PRO:HD2	1.92	0.52
1:B:281:LYS:H	1:B:281:LYS:CE	2.23	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:287:HIS:CE1	1:B:289:GLU:HB3	2.46	0.50
1:B:281:LYS:H	1:B:281:LYS:CD	2.24	0.50
1:A:347:TYR:CD1	1:A:484:GLU:HB3	2.47	0.49
1:A:329:LEU:O	1:A:564:ILE:HG22	2.12	0.49
1:B:435:PRO:HD2	1:B:446:LYS:HE3	1.95	0.49
1:B:133:HIS:CG	1:B:148:ARG:HG3	2.48	0.48
1:A:326:GLY:HA2	1:B:289:GLU:HG2	1.93	0.48
1:B:132:ILE:HD11	1:B:182:ILE:HD13	1.95	0.48
1:B:388:THR:O	2:B:609:HOH:O	2.20	0.48
1:B:437:PRO:O	1:B:442:ARG:NE	2.46	0.47
1:A:148:ARG:HD3	1:A:153:LYS:HB2	1.96	0.47
1:A:132:ILE:HD11	1:A:182:ILE:HD13	1.96	0.47
1:B:440:THR:OG1	1:B:468:ILE:HD13	2.14	0.47
1:B:287:HIS:HE1	1:B:289:GLU:HB3	1.80	0.46
1:A:255:ARG:HD3	1:A:265:GLU:OE2	2.14	0.46
1:A:159:ASN:OD1	1:A:161:ARG:HG2	2.14	0.46
1:B:435:PRO:O	1:B:442:ARG:NH2	2.43	0.46
1:A:94:PRO:HB3	1:A:205:LEU:HD23	1.98	0.46
1:A:394:ILE:HD11	1:A:462:ILE:HG12	1.98	0.46
1:A:289:GLU:HG2	1:B:326:GLY:HA2	1.96	0.45
1:A:216:LEU:O	1:A:217:HIS:HB2	2.16	0.45
1:B:362:VAL:O	1:B:366:THR:HB	2.17	0.45
1:B:350:LEU:HD22	1:B:545:ALA:HB1	1.99	0.45
1:B:159:ASN:OD1	1:B:161:ARG:HG2	2.16	0.45
1:B:563:ASN:OD1	1:B:565:LYS:N	2.49	0.45
1:B:421:LYS:HD3	1:B:425:ASP:OD2	2.17	0.44
1:B:184:VAL:HG13	1:B:200:PRO:HB3	1.99	0.43
1:B:329:LEU:O	1:B:564:ILE:HG22	2.18	0.43
1:A:116:GLN:HG3	1:A:117:PRO:HD2	2.00	0.43
1:B:421:LYS:HE2	1:B:425:ASP:OD1	2.18	0.43
1:A:563:ASN:OD1	1:A:565:LYS:N	2.52	0.43
1:A:145:TYR:HB2	1:A:156:VAL:HB	2.02	0.42
1:B:220:LEU:HD21	1:B:225:THR:HG22	2.01	0.42
1:B:266:ILE:HD13	1:B:307:LEU:HD12	2.02	0.42
1:B:437:PRO:HB2	1:B:439:THR:HG23	2.01	0.42
1:B:329:LEU:HD22	1:B:563:ASN:ND2	2.30	0.42
1:A:133:HIS:CG	1:A:148:ARG:HG3	2.54	0.42
1:A:575:PRO:HD3	1:B:290:LEU:CD2	2.50	0.42
1:A:215:HIS:HB3	1:A:218:PHE:CD1	2.55	0.42
1:A:263:PHE:HB3	1:A:316:TYR:HD1	1.85	0.42
1:A:241:ARG:NH2	1:B:311:GLY:O	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:95:TYR:CE1	1:B:208:PRO:HD2	2.55	0.41
1:A:184:VAL:HG13	1:A:200:PRO:HB3	2.02	0.41
1:A:100:HIS:O	1:A:127:LYS:HE2	2.20	0.41
1:B:362:VAL:HG22	1:B:558:LEU:HD21	2.02	0.41
1:B:216:LEU:O	1:B:217:HIS:HB2	2.20	0.41
1:A:436:PRO:HA	1:A:437:PRO:C	2.41	0.41
1:B:280:ALA:CB	1:B:298:ILE:HD12	2.51	0.41
1:A:95:TYR:CE1	1:A:208:PRO:HD2	2.56	0.40
1:A:220:LEU:HB2	1:A:236:LEU:HD12	2.04	0.40

There are no symmetry-related clashes.

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	495/520 (95%)	485 (98%)	10 (2%)	0	100	100
1	B	496/520 (95%)	487 (98%)	9 (2%)	0	100	100
All	All	991/1040 (95%)	972 (98%)	19 (2%)	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	445/462 (96%)	443 (100%)	2 (0%)	91	95
1	B	445/462 (96%)	443 (100%)	2 (0%)	91	95
All	All	890/924 (96%)	886 (100%)	4 (0%)	91	95

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	92	GLU
1	A	224	GLU
1	B	89	VAL
1	B	281	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	100	HIS

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 monosaccharides 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

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	499/520 (95%)	0.41	20 (4%) 38 45	26, 48, 75, 105	0
1	B	500/520 (96%)	0.57	43 (8%) 10 12	29, 51, 84, 104	0
All	All	999/1040 (96%)	0.49	63 (6%) 20 23	26, 49, 81, 105	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	97	HIS	5.9
1	B	478	SER	5.8
1	A	477	ARG	5.7
1	A	575	PRO	5.1
1	B	477	ARG	5.0
1	A	478	SER	4.1
1	B	576	GLU	4.0
1	B	115	LEU	3.9
1	B	575	PRO	3.9
1	B	512	PHE	3.8
1	B	519	LYS	3.8
1	A	97	HIS	3.8
1	A	161	ARG	3.7
1	A	123	ASP	3.6
1	B	110	GLN	3.6
1	B	520	ALA	3.5
1	B	121	LEU	3.4
1	A	124	ILE	3.4
1	B	161	ARG	3.4
1	B	437	PRO	3.3
1	A	576	GLU	3.3
1	B	438	ARG	3.3
1	B	423	LEU	3.2
1	B	516	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	518	ALA	3.1
1	B	98	LYS	3.0
1	B	443	LEU	2.9
1	B	528	PHE	2.9
1	A	170	ILE	2.8
1	B	436	PRO	2.8
1	B	201	TYR	2.7
1	B	434	CYS	2.7
1	B	70	SER	2.6
1	B	122	THR	2.6
1	A	290	LEU	2.6
1	A	529	ILE	2.6
1	B	511	LEU	2.6
1	B	447	LEU	2.6
1	A	70	SER	2.6
1	B	194	GLY	2.5
1	A	437	PRO	2.5
1	B	517	LYS	2.5
1	A	94	PRO	2.5
1	A	517	LYS	2.5
1	B	277	GLY	2.5
1	A	516	ALA	2.5
1	B	112	TYR	2.4
1	B	276	GLY	2.4
1	B	435	PRO	2.4
1	B	475	TRP	2.4
1	A	574	LYS	2.3
1	B	159	ASN	2.3
1	B	292	MET	2.3
1	A	115	LEU	2.3
1	B	279	VAL	2.2
1	A	292	MET	2.2
1	B	420	ARG	2.1
1	B	280	ALA	2.1
1	B	143	ILE	2.1
1	B	144	PHE	2.1
1	B	452	LEU	2.1
1	B	421	LYS	2.1
1	A	476	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 monosaccharides 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.