



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 12:31 AM UTC

PDB ID : 5IUU / pdb_00005iuu
Title : Crystal Structure of Indole-3-acetaldehyde Dehydrogenase in Apo form
Authors : Lee, S.G.; McClerklin, S.; Kunkel, B.; Jez, J.M.
Deposited on : 2016-03-18
Resolution : 2.09 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

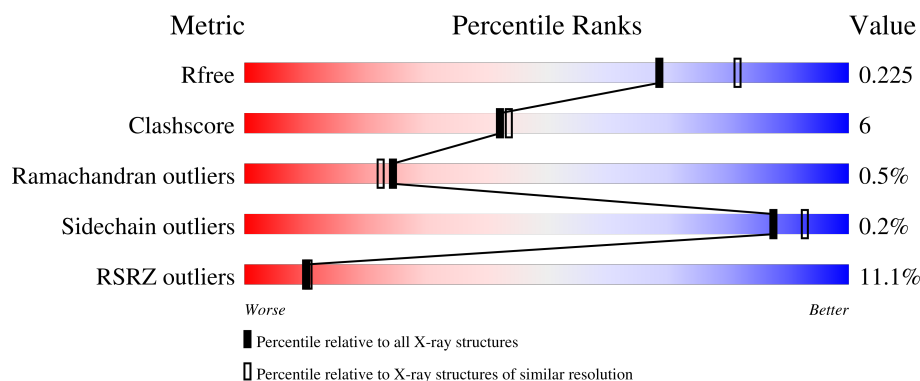
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.09 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	497	11% 76% 11% 12%
1	B	497	8% 76% 8% 15%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6787 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 Aldehyde dehydrogenase family protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	436	Total	C	N	O	S	0	0	0
			3263	2070	561	620	12			
1	B	423	Total	C	N	O	S	0	0	0
			3162	2004	547	599	12			

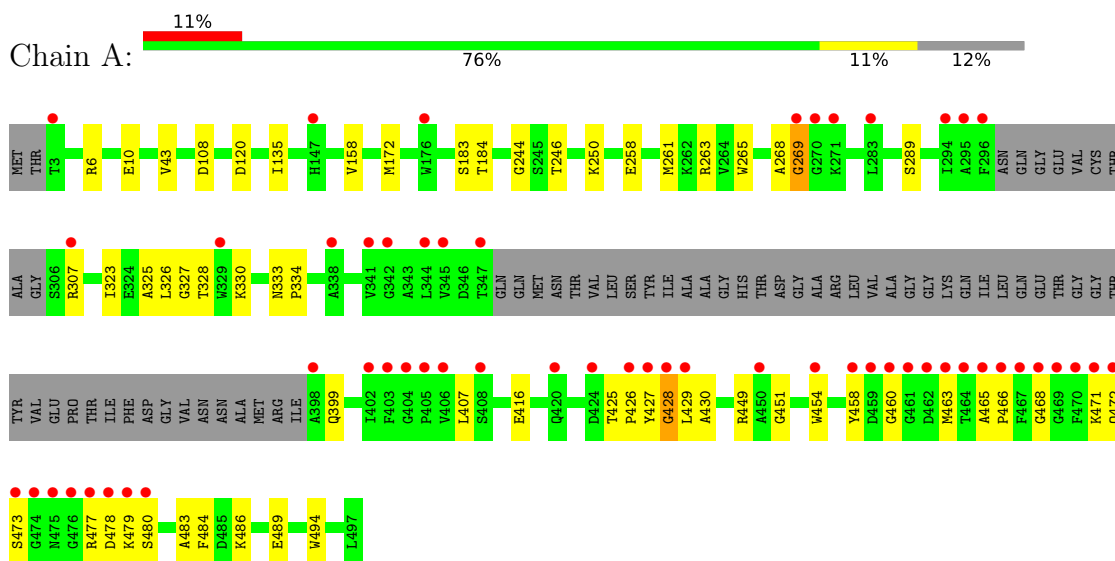
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	177	Total	O	0	0
			177	177		
2	B	185	Total	O	0	0
			185	185		

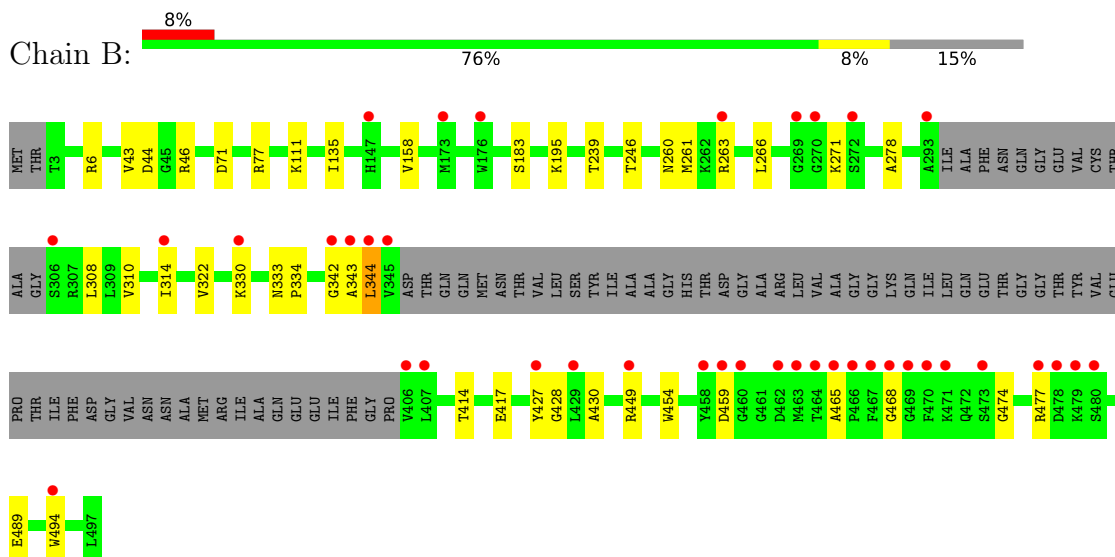
3 Residue-property plots [i](#)

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: Aldehyde dehydrogenase family protein



• Molecule 1: Aldehyde dehydrogenase family protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2 ₁	Depositor
Cell constants a, b, c, α , β , γ	80.89Å 109.07Å 143.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.45 – 2.09 40.45 – 2.09	Depositor EDS
% Data completeness (in resolution range)	99.8 (40.45-2.09) 91.9 (40.45-2.09)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.48 (at 2.08Å)	Xtriage
Refinement program	PHENIX (1.10.1 _2155: ???)	Depositor
R, R_{free}	0.197 , 0.222 0.199 , 0.225	Depositor DCC
R_{free} test set	2000 reflections (2.63%)	wwPDB-VP
Wilson B-factor (Å ²)	38.0	Xtriage
Anisotropy	0.543	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 42.6	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	0.96	EDS
Total number of atoms	6787	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.94% 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	0.34	0/3328	0.51	0/4525
1	B	0.35	0/3224	0.51	0/4383
All	All	0.34	0/6552	0.51	0/8908

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

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	3263	0	3268	59	0
1	B	3162	0	3177	30	0
2	A	177	0	0	6	1
2	B	185	0	0	2	1
All	All	6787	0	6445	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 6.

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:A:258:GLU:OE2	2:A:501:HOH:O	1.82	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:GLU:OE2	2:A:503:HOH:O	1.91	0.86
1:A:427:TYR:HD2	1:A:471:LYS:HB3	1.43	0.83
1:A:454:TRP:NE1	1:A:460:GLY:O	2.12	0.81
1:A:425:THR:HG22	1:A:427:TYR:H	1.45	0.79
1:A:120:ASP:HA	1:A:172:MET:HE2	1.69	0.74
1:A:430:ALA:HB1	1:A:454:TRP:HZ3	1.53	0.73
1:A:463:MET:SD	1:A:479:LYS:HD2	2.30	0.72
1:A:468:GLY:HA3	1:A:477:ARG:HD3	1.73	0.71
1:A:449:ARG:NH1	2:A:507:HOH:O	2.24	0.69
1:A:399:GLN:NE2	2:A:508:HOH:O	2.25	0.68
1:A:325:ALA:O	1:A:328:THR:OG1	2.12	0.67
1:B:158:VAL:HG12	1:B:489:GLU:HG2	1.76	0.66
1:A:427:TYR:HB3	1:A:428:GLY:HA3	1.80	0.63
1:A:289:SER:HB2	1:A:458:TYR:CD2	2.34	0.62
1:A:265:TRP:CD2	1:A:486:LYS:HG2	2.37	0.60
1:A:307:ARG:NH2	1:A:425:THR:OG1	2.35	0.60
1:A:263:ARG:NE	1:A:489:GLU:OE1	2.32	0.59
1:A:463:MET:HA	1:A:479:LYS:HE2	1.84	0.59
1:B:71:ASP:O	1:B:77:ARG:NH2	2.36	0.58
1:A:6:ARG:NH1	1:A:333:ASN:HD22	2.01	0.58
1:A:454:TRP:HE1	1:A:460:GLY:C	2.10	0.56
1:A:471:LYS:NZ	2:A:510:HOH:O	2.40	0.54
1:B:343:ALA:O	1:B:344:LEU:HB2	2.07	0.53
1:A:451:GLY:HA3	1:A:468:GLY:O	2.09	0.53
1:A:465:ALA:HB2	1:B:494:TRP:CZ2	2.43	0.53
1:B:278:ALA:HA	1:B:314:ILE:HG12	1.89	0.53
1:A:425:THR:HG22	1:A:427:TYR:N	2.21	0.52
1:B:414:THR:OG1	1:B:417:GLU:HG3	2.09	0.52
1:A:269:GLY:O	1:A:429:LEU:HB2	2.10	0.51
1:B:43:VAL:HG22	1:B:334:PRO:HG2	1.92	0.51
1:A:108:ASP:O	2:A:505:HOH:O	2.20	0.51
1:A:184:THR:HG23	1:A:484:PHE:HD2	1.77	0.50
1:A:416:GLU:CD	1:A:416:GLU:H	2.19	0.50
1:A:463:MET:SD	1:A:479:LYS:CD	3.00	0.50
1:A:135:ILE:HG12	1:A:183:SER:HB3	1.93	0.49
1:B:449:ARG:NH1	2:B:508:HOH:O	2.45	0.49
1:A:479:LYS:O	1:A:483:ALA:HB2	2.13	0.49
1:A:268:ALA:O	1:A:473:SER:HA	2.13	0.48
1:B:430:ALA:HB1	1:B:454:TRP:CZ3	2.47	0.48
1:A:43:VAL:HG22	1:A:334:PRO:HG2	1.96	0.48
1:A:6:ARG:HD3	1:A:10:GLU:OE2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:326:LEU:HD23	1:A:326:LEU:O	2.14	0.47
1:B:44:ASP:OD2	1:B:46:ARG:NH2	2.47	0.47
1:A:465:ALA:O	1:A:479:LYS:HB2	2.15	0.47
1:A:471:LYS:HG3	1:A:472:GLN:H	1.79	0.47
1:B:468:GLY:HA3	1:B:477:ARG:HD3	1.96	0.46
1:A:246:THR:HG23	1:B:261:MET:CE	2.46	0.46
1:A:323:ILE:HD11	1:A:407:LEU:HD22	1.98	0.45
1:A:428:GLY:N	1:A:473:SER:OG	2.49	0.45
1:A:430:ALA:HB1	1:A:454:TRP:CZ3	2.41	0.45
1:A:425:THR:CG2	1:A:427:TYR:H	2.23	0.45
1:A:494:TRP:CZ2	1:B:465:ALA:HB2	2.51	0.45
1:A:261:MET:CE	1:B:246:THR:HG23	2.47	0.45
1:A:158:VAL:HG12	1:A:489:GLU:HG2	2.00	0.44
1:B:195:LYS:O	2:B:501:HOH:O	2.21	0.44
1:A:466:PRO:HD3	1:A:480:SER:OG	2.19	0.43
1:B:271:LYS:HD3	1:B:427:TYR:HD1	1.82	0.43
1:A:427:TYR:CD2	1:A:471:LYS:HB3	2.35	0.43
1:A:244:GLY:O	1:A:268:ALA:HA	2.19	0.43
1:B:342:GLY:C	1:B:344:LEU:HD13	2.44	0.42
1:A:250:LYS:HG3	1:B:261:MET:HE2	2.01	0.42
1:B:6:ARG:HE	1:B:333:ASN:HD22	1.67	0.42
1:A:466:PRO:HA	1:A:478:ASP:O	2.18	0.42
1:B:271:LYS:HD3	1:B:427:TYR:CD1	2.54	0.42
1:A:327:GLY:O	1:A:330:LYS:HE3	2.19	0.42
1:B:459:ASP:CG	1:B:459:ASP:O	2.62	0.42
1:A:425:THR:C	1:A:427:TYR:N	2.78	0.42
1:B:330:LYS:O	1:B:330:LYS:HG3	2.20	0.41
1:B:266:LEU:O	1:B:474:GLY:HA3	2.21	0.41
1:A:425:THR:C	1:A:427:TYR:H	2.28	0.41
1:B:239:THR:OG1	1:B:263:ARG:NH1	2.49	0.41
1:A:426:PRO:O	1:A:427:TYR:HB2	2.20	0.41
1:A:465:ALA:HA	1:B:494:TRP:HZ2	1.84	0.41
1:A:427:TYR:CB	1:A:428:GLY:HA3	2.48	0.41
1:A:471:LYS:HE3	1:B:260:ASN:ND2	2.36	0.40
1:B:308:LEU:HG	1:B:310:VAL:CG2	2.50	0.40
1:A:265:TRP:HB3	1:A:486:LYS:HD3	2.03	0.40
1:A:465:ALA:CB	1:B:494:TRP:CZ2	3.04	0.40
1:B:135:ILE:HG12	1:B:183:SER:HB3	2.03	0.40
1:B:111:LYS:HB2	1:B:111:LYS:HE2	1.69	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)
2:A:669:HOH:O	2:B:659:HOH:O[2_597]	2.17	0.03

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	430/497 (86%)	410 (95%)	18 (4%)	2 (0%)	24	22
1	B	417/497 (84%)	402 (96%)	13 (3%)	2 (0%)	24	22
All	All	847/994 (85%)	812 (96%)	31 (4%)	4 (0%)	24	22

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	269	GLY
1	A	428	GLY
1	B	344	LEU
1	B	428	GLY

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	334/380 (88%)	334 (100%)	0	100	100
1	B	324/380 (85%)	323 (100%)	1 (0%)	86	91
All	All	658/760 (87%)	657 (100%)	1 (0%)	87	93

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

Mol	Chain	Res	Type
1	B	322	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	96	GLN
1	A	251	GLN
1	B	147	HIS
1	B	251	GLN
1	B	472	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](#)

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	436/497 (87%)	0.64	56 (12%) 7 8	34, 45, 73, 87	0
1	B	423/497 (85%)	0.43	39 (9%) 14 15	32, 44, 65, 81	0
All	All	859/994 (86%)	0.54	95 (11%) 10 10	32, 45, 70, 87	0

All (95) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	465	ALA	6.9
1	A	465	ALA	6.6
1	A	468	GLY	6.6
1	A	470	PHE	6.5
1	A	473	SER	6.4
1	A	479	LYS	6.3
1	A	427	TYR	6.0
1	A	464	THR	6.0
1	B	345	VAL	5.3
1	A	471	LYS	5.2
1	B	470	PHE	5.1
1	B	468	GLY	5.1
1	A	467	PHE	4.9
1	A	469	GLY	4.9
1	A	466	PRO	4.9
1	A	269	GLY	4.9
1	B	469	GLY	4.9
1	B	466	PRO	4.8
1	B	406	VAL	4.7
1	A	406	VAL	4.7
1	B	467	PHE	4.7
1	A	476	GLY	4.7
1	A	428	GLY	4.5
1	A	404	GLY	4.3

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Mol	Chain	Res	Type	RSRZ
1	B	427	TYR	4.3
1	A	403	PHE	4.2
1	A	405	PRO	4.2
1	A	480	SER	4.2
1	B	464	THR	4.1
1	A	347	THR	4.1
1	B	343	ALA	4.1
1	A	296	PHE	3.9
1	A	460	GLY	3.9
1	A	474	GLY	3.9
1	A	478	ASP	3.8
1	B	460	GLY	3.7
1	B	147	HIS	3.6
1	A	176	TRP	3.5
1	A	398	ALA	3.5
1	B	269	GLY	3.5
1	A	462	ASP	3.4
1	B	344	LEU	3.4
1	A	472	GLN	3.3
1	B	479	LYS	3.3
1	B	270	GLY	3.2
1	A	270	GLY	3.2
1	A	344	LEU	3.2
1	A	463	MET	3.2
1	B	471	LYS	3.1
1	A	424	ASP	3.0
1	B	429	LEU	3.0
1	B	463	MET	3.0
1	A	307	ARG	2.9
1	B	473	SER	2.9
1	B	458	TYR	2.8
1	B	263	ARG	2.8
1	B	407	LEU	2.8
1	A	408	SER	2.8
1	A	295	ALA	2.8
1	A	429	LEU	2.7
1	A	294	ILE	2.7
1	B	462	ASP	2.6
1	B	293	ALA	2.6
1	B	459	ASP	2.6
1	A	475	ASN	2.5
1	A	420	GLN	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	494	TRP	2.5
1	A	461	GLY	2.5
1	A	345	VAL	2.5
1	A	458	TYR	2.4
1	A	342	GLY	2.4
1	B	480	SER	2.4
1	A	341	VAL	2.4
1	A	426	PRO	2.4
1	A	271	LYS	2.3
1	A	3	THR	2.3
1	B	342	GLY	2.3
1	B	478	ASP	2.3
1	A	454	TRP	2.3
1	A	459	ASP	2.2
1	B	272	SER	2.2
1	B	330	LYS	2.2
1	A	450	ALA	2.2
1	A	147	HIS	2.2
1	B	477	ARG	2.2
1	A	283	LEU	2.1
1	B	306	SER	2.1
1	A	402	ILE	2.1
1	A	477	ARG	2.1
1	B	314	ILE	2.1
1	A	329	TRP	2.1
1	B	173	MET	2.1
1	B	176	TRP	2.1
1	B	449	ARG	2.0
1	A	338	ALA	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 ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.