



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 24, 2025 – 03:06 pm GMT

PDB ID : 8S3G
Title : Atomic structure of truncated worm GdH
Authors : Mourao, A.; Sattler, M.; Geerlof, A.
Deposited on : 2024-02-20
Resolution : 2.29 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	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41

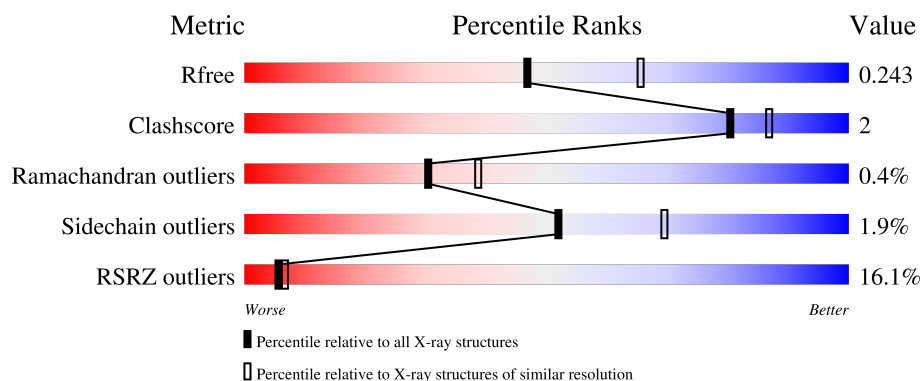
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.29 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}	164625	5963 (2.30-2.30)
Clashscore	180529	6698 (2.30-2.30)
Ramachandran outliers	177936	6640 (2.30-2.30)
Sidechain outliers	177891	6640 (2.30-2.30)
RSRZ outliers	164620	5963 (2.30-2.30)

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	537	<div> <div>5%</div> <div>88%</div> <div>6%</div> <div>6%</div> </div>
1	B	537	<div> <div>26%</div> <div>85%</div> <div>8%</div> <div>6%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7920 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 Glutamate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	504	Total	C	N	O	S	0	2	0
			3882	2470	667	722	23			
1	B	504	Total	C	N	O	S	0	0	0
			3864	2458	662	722	22			

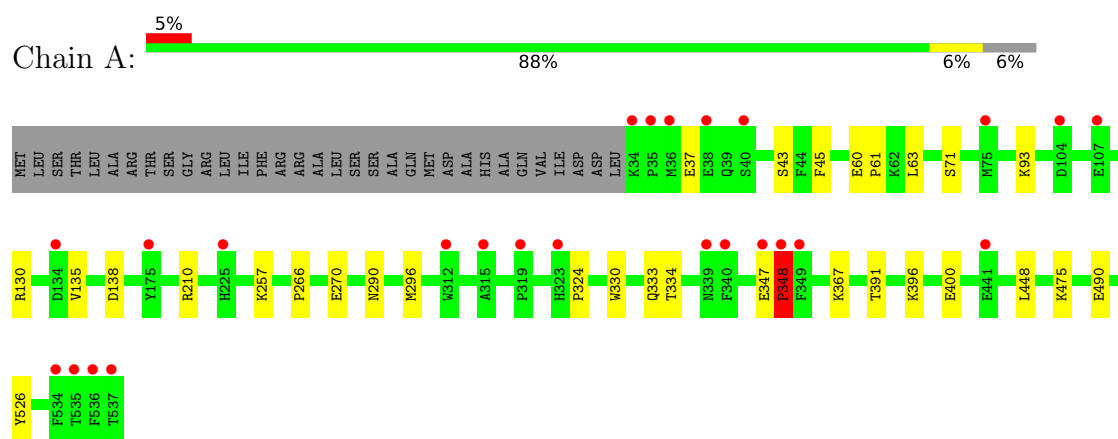
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	95	Total	O	0	0
			95	95		
2	B	79	Total	O	0	0
			79	79		

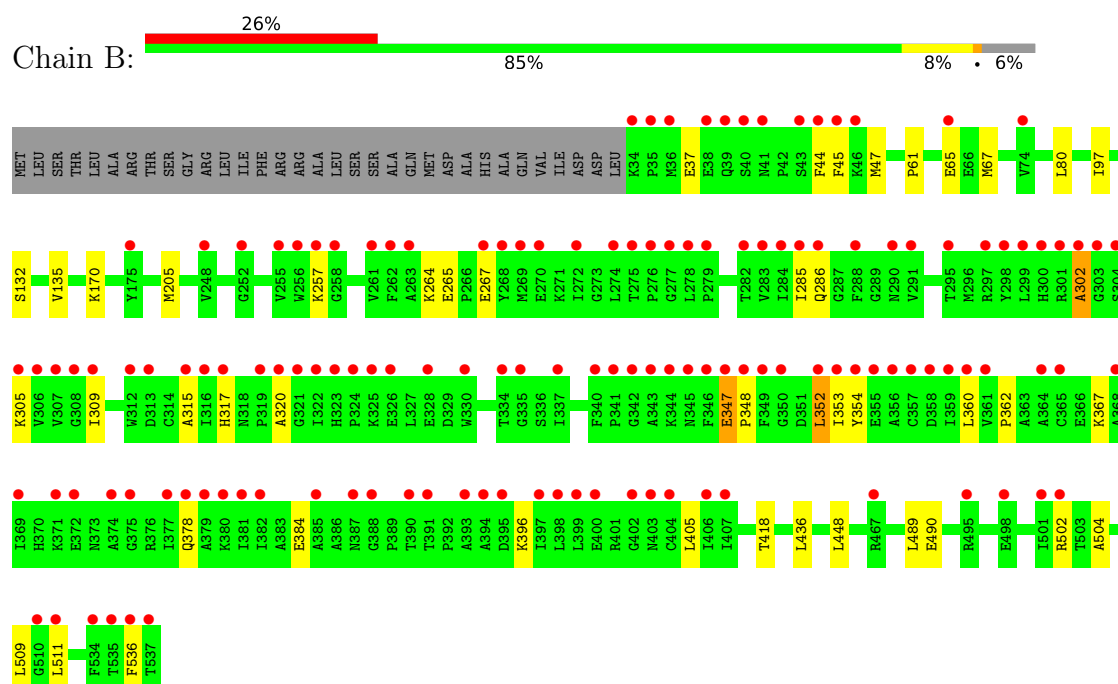
3 Residue-property plots [i](#)

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: Glutamate dehydrogenase



- Molecule 1: Glutamate dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants a, b, c, α , β , γ	151.25Å 151.25Å 146.04Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	97.51 – 2.29 97.51 – 2.29	Depositor EDS
% Data completeness (in resolution range)	99.3 (97.51-2.29) 99.4 (97.51-2.29)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.71 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.21_5207	Depositor
R, R_{free}	0.224 , 0.248 0.221 , 0.243	Depositor DCC
R_{free} test set	4236 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	39.2	Xtriage
Anisotropy	0.476	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 30.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.010 for -h,-k,l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7920	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.58% 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](#)

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	0.43	0/3974	0.59	0/5376
1	B	0.43	0/3949	0.57	0/5343
All	All	0.43	0/7923	0.58	0/10719

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	B	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	B	302	ALA	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	3882	0	3853	13	0
1	B	3864	0	3826	26	0
2	A	95	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	79	0	0	4	0
All	All	7920	0	7679	38	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 (38) 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:315:ALA:HB1	1:B:352:LEU:HD12	1.48	0.96
1:B:257:LYS:HE3	1:B:490:GLU:HG2	1.62	0.81
1:B:37:GLU:OE2	1:B:37:GLU:N	2.25	0.66
1:B:37:GLU:HB2	1:B:396:LYS:HD2	1.82	0.60
1:B:285:ILE:HB	1:B:309:ILE:HD13	1.87	0.55
1:B:353:ILE:HG22	1:B:360:LEU:HD11	1.89	0.54
1:A:93:LYS:HG2	1:B:97:ILE:HG22	1.88	0.54
1:B:286:GLN:HB3	1:B:362:PRO:HA	1.89	0.53
1:A:347:GLU:O	1:A:348:PRO:C	2.46	0.52
1:B:302:ALA:HB1	2:B:660:HOH:O	2.11	0.50
1:A:266:PRO:O	1:A:270:GLU:HG2	2.12	0.50
1:B:61:PRO:O	1:B:65:GLU:HG2	2.12	0.48
1:B:44:PHE:HA	1:B:47:MET:HE2	1.96	0.48
1:B:418:THR:HG21	1:B:489:LEU:HA	1.95	0.48
1:B:347:GLU:CB	1:B:348:PRO:HD3	2.44	0.48
1:A:37:GLU:HB2	1:A:396:LYS:HD3	1.96	0.47
1:B:265:GLU:HG3	1:B:267:GLU:OE2	2.14	0.47
1:A:396:LYS:HE3	1:A:400:GLU:OE2	2.15	0.47
1:B:502:ARG:HB3	2:B:625:HOH:O	2.13	0.46
1:B:205:MET:HE3	2:B:643:HOH:O	2.14	0.46
1:B:354:TYR:O	1:B:378:GLN:NE2	2.50	0.45
1:B:504:ALA:HA	1:B:509:LEU:HD12	1.99	0.45
1:A:290:ASN:ND2	2:A:602:HOH:O	2.50	0.45
1:A:330:TRP:CE2	1:A:334:THR:HG21	2.52	0.44
1:B:47:MET:HE1	1:B:367:LYS:HD3	2.00	0.43
1:A:63:LEU:HD22	1:A:526:TYR:CD2	2.53	0.43
1:B:405:LEU:HD13	1:B:511:LEU:HD22	2.00	0.43
1:B:44:PHE:HD1	1:B:47:MET:HE3	1.84	0.43
1:A:130:ARG:HD2	1:A:135:VAL:HG12	2.01	0.43
1:A:60:GLU:HB3	1:A:61:PRO:HD3	2.01	0.42
1:A:257:LYS:HE2	1:A:490:GLU:HG2	2.02	0.42
1:B:132:SER:O	1:B:135:VAL:HG13	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:405:LEU:HB2	1:B:511:LEU:HD22	2.02	0.42
1:A:367:LYS:HG2	1:A:391:THR:HG22	2.02	0.41
1:A:296:MET:HE3	1:A:324:PRO:HB3	2.02	0.41
1:B:67:MET:SD	1:B:80:LEU:HD23	2.61	0.41
1:B:305:LYS:HE3	1:B:320:ALA:O	2.21	0.40
1:B:264:LYS:HD2	2:B:636:HOH:O	2.21	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	504/537 (94%)	489 (97%)	14 (3%)	1 (0%)	44	55
1	B	502/537 (94%)	474 (94%)	25 (5%)	3 (1%)	22	27
All	All	1006/1074 (94%)	963 (96%)	39 (4%)	4 (0%)	30	39

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	348	PRO
1	B	536	PHE
1	B	384	GLU
1	B	347	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	402/435 (92%)	393 (98%)	9 (2%)	47	65
1	B	399/435 (92%)	393 (98%)	6 (2%)	60	76
All	All	801/870 (92%)	786 (98%)	15 (2%)	52	69

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

Mol	Chain	Res	Type
1	A	43	SER
1	A	45	PHE
1	A	71	SER
1	A	138	ASP
1	A	210	ARG
1	A	333	GLN
1	A	348	PRO
1	A	448	LEU
1	A	475	LYS
1	B	45	PHE
1	B	170	LYS
1	B	317	HIS
1	B	352	LEU
1	B	436	LEU
1	B	448	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	413	ASN
1	B	445	ASN

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 [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	504/537 (93%)	0.40	25 (4%) 35 36	25, 40, 64, 85	2 (0%)
1	B	504/537 (93%)	1.17	137 (27%) 2 2	25, 46, 87, 105	0
All	All	1008/1074 (93%)	0.78	162 (16%) 5 7	25, 42, 80, 105	2 (0%)

All (162) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	536	PHE	8.1
1	B	536	PHE	7.9
1	B	321	GLY	6.3
1	B	320	ALA	6.3
1	B	306	VAL	6.3
1	B	35	PRO	6.1
1	A	34	LYS	6.0
1	B	348	PRO	5.9
1	B	353	ILE	5.5
1	A	323[A]	HIS	5.4
1	B	40	SER	5.3
1	B	38	GLU	5.2
1	B	34	LYS	5.1
1	B	537	THR	4.9
1	B	356	ALA	4.8
1	B	382	ILE	4.8
1	B	352	LEU	4.8
1	A	537	THR	4.8
1	B	263	ALA	4.7
1	B	175	TYR	4.7
1	B	302	ALA	4.7
1	B	36	MET	4.5
1	B	256	TRP	4.4
1	B	304	SER	4.4

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Mol	Chain	Res	Type	RSRZ
1	B	404	CYS	4.4
1	B	535	THR	4.3
1	A	348	PRO	4.3
1	B	534	PHE	4.3
1	B	369	ILE	4.3
1	B	347	GLU	4.3
1	B	349	PHE	4.2
1	B	379	ALA	4.2
1	B	343	ALA	4.2
1	B	340	PHE	4.2
1	B	262	PHE	4.1
1	B	377	ILE	4.1
1	B	277	GLY	4.1
1	A	35	PRO	4.1
1	A	40	SER	4.1
1	B	357	CYS	4.1
1	B	39	GLN	4.1
1	A	535	THR	4.0
1	B	309	ILE	3.9
1	A	347	GLU	3.9
1	B	312	TRP	3.8
1	B	399	LEU	3.8
1	B	270	GLU	3.7
1	B	381	ILE	3.7
1	B	298	TYR	3.7
1	B	380	LYS	3.7
1	B	360	LEU	3.7
1	B	313	ASP	3.7
1	B	346	PHE	3.6
1	B	368	ALA	3.5
1	B	325	LYS	3.5
1	B	322	ILE	3.5
1	B	278	LEU	3.4
1	B	395	ASP	3.4
1	B	288	PHE	3.3
1	B	365	CYS	3.3
1	B	74	VAL	3.3
1	A	38	GLU	3.3
1	A	175	TYR	3.3
1	B	398	LEU	3.3
1	B	308	GLY	3.3
1	B	344	LYS	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	276	PRO	3.2
1	B	388	GLY	3.2
1	B	324	PRO	3.2
1	B	406	ILE	3.2
1	B	364	ALA	3.2
1	B	319	PRO	3.1
1	B	337	ILE	3.1
1	B	269	MET	3.1
1	B	397	ILE	3.1
1	B	350	GLY	3.1
1	B	359	ILE	3.1
1	B	291	VAL	3.1
1	B	390	THR	3.0
1	B	402	GLY	3.0
1	B	307	VAL	2.9
1	B	316	ILE	2.9
1	B	511	LEU	2.9
1	B	295	THR	2.8
1	B	326	GLU	2.8
1	B	282	THR	2.8
1	B	248	VAL	2.8
1	B	361	VAL	2.8
1	B	301	ARG	2.8
1	B	323	HIS	2.8
1	B	495	ARG	2.8
1	B	299	LEU	2.8
1	B	341	PRO	2.7
1	B	317	HIS	2.7
1	B	394	ALA	2.7
1	B	391	THR	2.7
1	A	75[A]	MET	2.7
1	A	107	GLU	2.7
1	B	257	LYS	2.7
1	B	510	GLY	2.7
1	B	267	GLU	2.7
1	A	534	PHE	2.7
1	B	330	TRP	2.6
1	B	261	VAL	2.6
1	B	45	PHE	2.6
1	B	375	GLY	2.6
1	B	41	ASN	2.6
1	B	284	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	349	PHE	2.6
1	B	305	LYS	2.6
1	B	345	ASN	2.5
1	B	342	GLY	2.5
1	B	315	ALA	2.5
1	B	378	GLN	2.5
1	A	441	GLU	2.5
1	B	283	VAL	2.5
1	B	393	ALA	2.5
1	B	403	ASN	2.5
1	B	358	ASP	2.4
1	A	315	ALA	2.4
1	B	44	PHE	2.4
1	B	354	TYR	2.4
1	B	334	THR	2.4
1	B	43	SER	2.4
1	B	286	GLN	2.4
1	B	268	TYR	2.4
1	B	335	GLY	2.4
1	B	290	ASN	2.4
1	A	134	ASP	2.3
1	B	400	GLU	2.3
1	B	371	LYS	2.3
1	B	272	ILE	2.3
1	B	498	GLU	2.3
1	B	255	VAL	2.3
1	B	502	ARG	2.3
1	B	300	HIS	2.3
1	B	467	ARG	2.3
1	B	65	GLU	2.2
1	A	340	PHE	2.2
1	A	312	TRP	2.2
1	B	407	ILE	2.2
1	B	328	GLU	2.2
1	B	501	ILE	2.2
1	B	303	GLY	2.2
1	B	279	PRO	2.2
1	B	297	ARG	2.1
1	A	339	ASN	2.1
1	A	319	PRO	2.1
1	A	36	MET	2.1
1	B	285	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	274	LEU	2.1
1	B	387	ASN	2.1
1	B	275	THR	2.1
1	B	385	ALA	2.1
1	B	46	LYS	2.1
1	A	225	HIS	2.1
1	B	374	ALA	2.1
1	B	355	GLU	2.0
1	B	372	GLU	2.0
1	A	104	ASP	2.0
1	B	252	GLY	2.0
1	B	258	GLY	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.