



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 22, 2023 – 02:33 PM JST

PDB ID : 7YIC
Title : Crystal structure of reductase LSADH
Authors : Tang, J.; Liuqing, C.
Deposited on : 2022-07-15
Resolution : 2.16 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 : 2.36
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) : 2.36

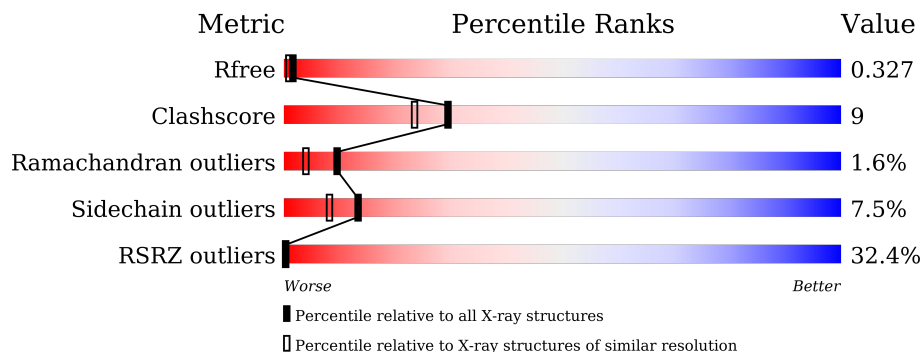
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.16 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	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

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	250	
1	B	250	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3518 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 Short chain alcohol dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	250	1752	1101	300	348	3	0	0	0
1	B	250	1752	1101	300	348	3	0	0	0

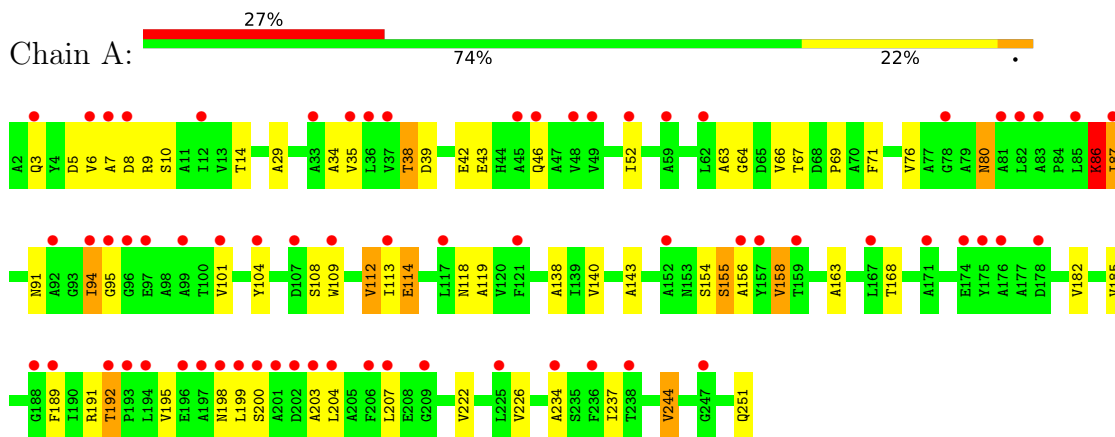
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	7	Total	O	0	0
			7	7		
2	B	7	Total	O	0	0
			7	7		

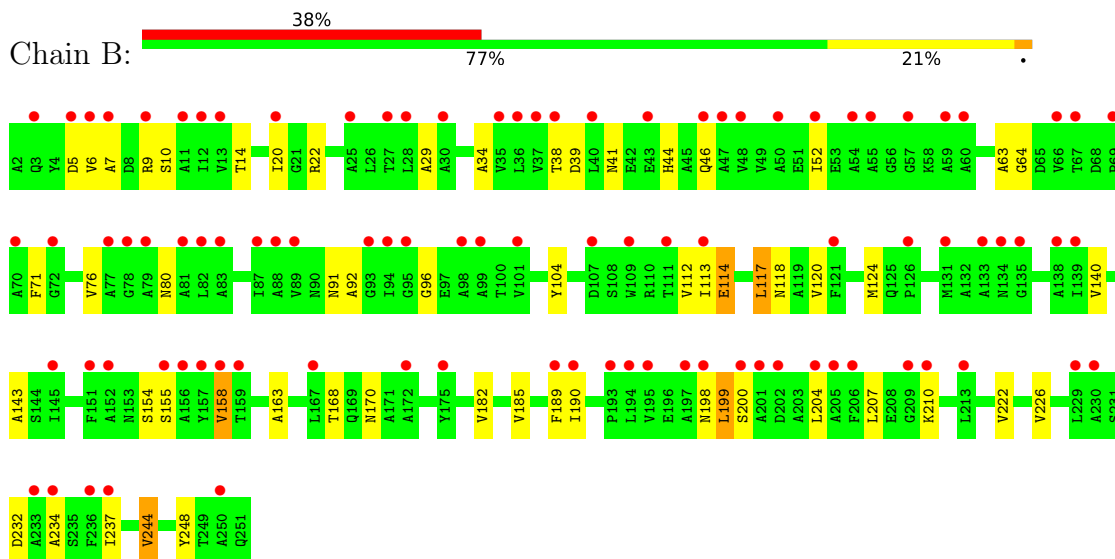
3 Residue-property plots [i](#)

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: Short chain alcohol dehydrogenase



- Molecule 1: Short chain alcohol dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	69.28Å 109.93Å 120.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.81 – 2.16 19.80 – 2.16	Depositor EDS
% Data completeness (in resolution range)	97.9 (19.81-2.16) 98.1 (19.80-2.16)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.20 (at 2.17Å)	Xtrriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.296 , 0.324 0.299 , 0.327	Depositor DCC
R_{free} test set	1213 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	37.1	Xtrriage
Anisotropy	1.610	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 15.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	3518	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.23% 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	0.57	2/1777 (0.1%)	0.70	1/2422 (0.0%)
1	B	0.48	1/1777 (0.1%)	0.65	0/2422
All	All	0.53	3/3554 (0.1%)	0.67	1/4844 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	114	GLU	CD-OE2	-8.47	1.16	1.25
1	A	114	GLU	CG-CD	6.51	1.61	1.51
1	B	114	GLU	CG-CD	5.31	1.59	1.51

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	86	LYS	N-CA-C	-5.71	95.59	111.00

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	1752	0	1735	38	0
1	B	1752	0	1735	32	0
2	A	7	0	0	0	0
2	B	7	0	0	0	0
All	All	3518	0	3470	66	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 9.

All (66) 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:109:TRP:HZ3	1:B:118:ASN:OD1	1.51	0.90
1:B:114:GLU:HA	1:B:118:ASN:HD22	1.48	0.78
1:B:14:THR:HG22	1:B:92:ALA:H	1.60	0.67
1:A:114:GLU:HA	1:A:118:ASN:HD22	1.60	0.66
1:A:108:SER:O	1:A:112:VAL:HG13	1.98	0.63
1:A:109:TRP:CZ3	1:B:118:ASN:OD1	2.43	0.61
1:A:168:THR:HG23	1:A:182:VAL:HG12	1.84	0.59
1:B:168:THR:HG23	1:B:182:VAL:HG12	1.85	0.58
1:B:120:VAL:HG12	1:B:124:MET:HE3	1.87	0.56
1:B:189:PHE:CE2	1:B:207:LEU:HD22	2.40	0.56
1:A:154:SER:O	1:A:158:VAL:HG13	2.08	0.54
1:B:120:VAL:HG12	1:B:124:MET:CE	2.40	0.52
1:B:154:SER:O	1:B:158:VAL:HG13	2.11	0.51
1:A:189:PHE:CE2	1:A:207:LEU:HD12	2.46	0.50
1:A:64:GLY:HA3	1:A:71:PHE:CE1	2.46	0.50
1:A:14:THR:O	1:A:91:ASN:HB3	2.12	0.49
1:B:29:ALA:HB1	1:B:52:ILE:HG23	1.94	0.49
1:B:185:VAL:HG21	1:B:226:VAL:HG22	1.94	0.49
1:B:14:THR:O	1:B:91:ASN:HB3	2.12	0.49
1:B:41:ASN:ND2	1:B:44:HIS:CD2	2.81	0.48
1:A:10:SER:HA	1:A:34:ALA:O	2.13	0.48
1:B:10:SER:HA	1:B:34:ALA:O	2.14	0.48
1:A:29:ALA:HB1	1:A:52:ILE:HG23	1.96	0.48
1:B:64:GLY:HA3	1:B:71:PHE:CE1	2.48	0.48
1:B:113:ILE:HG22	1:B:118:ASN:HD21	1.77	0.48
1:A:109:TRP:HH2	1:B:117:LEU:HD13	1.78	0.47
1:A:39:ASP:O	1:A:63:ALA:HA	2.14	0.47
1:A:42:GLU:HG3	1:A:43:GLU:N	2.30	0.47
1:A:5:ASP:O	1:A:7:ALA:N	2.47	0.47
1:A:109:TRP:CD1	1:A:156:ALA:HB2	2.50	0.47
1:A:14:THR:HG22	1:A:38:THR:HG21	1.96	0.47
1:B:140:VAL:HG11	1:B:226:VAL:HG13	1.96	0.46
1:B:39:ASP:O	1:B:63:ALA:HA	2.15	0.46
1:B:5:ASP:O	1:B:7:ALA:N	2.49	0.46
1:A:86:LYS:O	1:A:87:ILE:O	2.34	0.46
1:A:113:ILE:HG22	1:A:118:ASN:HD21	1.81	0.46
1:A:140:VAL:HG11	1:A:226:VAL:HG13	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:VAL:CG1	1:A:52:ILE:HD13	2.46	0.45
1:A:87:ILE:HA	1:A:138:ALA:O	2.16	0.45
1:A:191:ARG:HH12	1:A:204:LEU:HD21	1.80	0.45
1:A:199:LEU:HD21	1:A:204:LEU:N	2.31	0.45
1:B:222:VAL:O	1:B:226:VAL:HG23	2.16	0.45
1:A:185:VAL:HG21	1:A:226:VAL:HG22	1.97	0.45
1:A:112:VAL:CG2	1:A:156:ALA:HB1	2.47	0.44
1:A:163:ALA:HB2	1:B:163:ALA:HB2	1.99	0.44
1:A:192:THR:HG22	1:A:195:VAL:HG23	2.00	0.44
1:A:42:GLU:O	1:A:46:GLN:HB2	2.18	0.44
1:B:76:VAL:O	1:B:80:ASN:HB2	2.18	0.43
1:A:222:VAL:O	1:A:226:VAL:HG23	2.18	0.43
1:B:234:ALA:HB1	1:B:237:ILE:HD12	1.99	0.43
1:A:112:VAL:HG22	1:A:156:ALA:HB1	2.01	0.43
1:A:234:ALA:HB1	1:A:237:ILE:HD12	2.01	0.43
1:B:210:LYS:HG3	1:B:248:TYR:CE2	2.54	0.43
1:B:9:ARG:NH2	1:B:232:ASP:OD2	2.51	0.42
1:B:198:ASN:O	1:B:199:LEU:HB2	2.19	0.42
1:B:200:SER:O	1:B:204:LEU:HG	2.19	0.42
1:A:66:VAL:HB	1:A:119:ALA:HB1	2.02	0.41
1:A:203:ALA:O	1:A:207:LEU:HD22	2.20	0.41
1:A:67:THR:O	1:A:69:PRO:HD3	2.21	0.41
1:B:198:ASN:O	1:B:199:LEU:CB	2.69	0.41
1:A:76:VAL:O	1:A:80:ASN:HB2	2.21	0.41
1:A:101:VAL:HG22	1:A:155:SER:HB3	2.03	0.41
1:B:20:ILE:HD11	1:B:190:ILE:HG13	2.02	0.41
1:A:94:ILE:HD12	1:A:95:GLY:H	1.86	0.41
1:B:96:GLY:HA3	1:B:112:VAL:HG21	2.03	0.41
1:B:210:LYS:CG	1:B:248:TYR:CE2	3.03	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	248/250 (99%)	233 (94%)	11 (4%)	4 (2%)	9	4
1	B	248/250 (99%)	234 (94%)	10 (4%)	4 (2%)	9	4
All	All	496/500 (99%)	467 (94%)	21 (4%)	8 (2%)	9	4

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	6	VAL
1	B	6	VAL
1	B	199	LEU
1	A	87	ILE
1	A	143	ALA
1	B	143	ALA
1	A	244	VAL
1	B	244	VAL

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	166/166 (100%)	150 (90%)	16 (10%)	8	4
1	B	166/166 (100%)	157 (95%)	9 (5%)	22	18
All	All	332/332 (100%)	307 (92%)	25 (8%)	13	8

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	8	ASP
1	A	9	ARG
1	A	38	THR
1	A	80	ASN
1	A	86	LYS
1	A	94	ILE
1	A	104	TYR

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Mol	Chain	Res	Type
1	A	112	VAL
1	A	155	SER
1	A	158	VAL
1	A	192	THR
1	A	198	ASN
1	A	200	SER
1	A	244	VAL
1	A	251	GLN
1	B	22	ARG
1	B	38	THR
1	B	46	GLN
1	B	104	TYR
1	B	117	LEU
1	B	155	SER
1	B	158	VAL
1	B	170	ASN
1	B	244	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	118	ASN
1	A	198	ASN
1	B	44	HIS
1	B	118	ASN
1	B	153	ASN

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 [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	250/250 (100%)	1.57	67 (26%) 0 0	49, 55, 72, 85	0
1	B	250/250 (100%)	1.78	95 (38%) 0 0	50, 58, 67, 75	0
All	All	500/500 (100%)	1.68	162 (32%) 0 0	49, 56, 68, 85	0

All (162) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	95	GLY	7.9
1	A	200	SER	6.5
1	B	197	ALA	6.3
1	A	209	GLY	6.3
1	A	199	LEU	5.8
1	A	201	ALA	5.8
1	A	193	PRO	5.6
1	B	94	ILE	5.5
1	A	81	ALA	5.3
1	A	95	GLY	5.3
1	B	201	ALA	5.2
1	A	194	LEU	5.1
1	A	198	ASN	5.0
1	B	198	ASN	4.9
1	B	107	ASP	4.8
1	B	57	GLY	4.8
1	B	194	LEU	4.8
1	B	193	PRO	4.6
1	B	60	ALA	4.4
1	B	59	ALA	4.4
1	B	9	ARG	4.4
1	B	190	ILE	4.3
1	B	40	LEU	4.2
1	B	35	VAL	4.2

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Mol	Chain	Res	Type	RSRZ
1	B	135	GLY	4.2
1	B	175	TYR	4.1
1	B	20	ILE	4.0
1	A	104	TYR	4.0
1	B	99	ALA	3.9
1	A	192	THR	3.8
1	A	107	ASP	3.7
1	B	87	ILE	3.7
1	B	234	ALA	3.7
1	A	94	ILE	3.7
1	A	97	GLU	3.6
1	A	197	ALA	3.6
1	A	202	ASP	3.6
1	A	101	VAL	3.5
1	B	37	VAL	3.5
1	B	66	VAL	3.5
1	B	12	ILE	3.5
1	B	55	ALA	3.5
1	B	50	ALA	3.5
1	B	11	ALA	3.4
1	B	157	TYR	3.4
1	A	152	ALA	3.4
1	B	204	LEU	3.4
1	B	109	TRP	3.4
1	A	178	ASP	3.4
1	B	195	VAL	3.4
1	B	230	ALA	3.3
1	B	36	LEU	3.3
1	A	157	TYR	3.3
1	A	45	ALA	3.3
1	A	8	ASP	3.3
1	B	156	ALA	3.2
1	A	234	ALA	3.2
1	B	77	ALA	3.2
1	A	36	LEU	3.2
1	B	7	ALA	3.2
1	A	159	THR	3.2
1	B	237	ILE	3.2
1	A	7	ALA	3.1
1	B	159	THR	3.1
1	A	206	PHE	3.1
1	A	203	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	175	TYR	3.0
1	B	88	ALA	3.0
1	B	67	THR	3.0
1	A	37	VAL	3.0
1	B	52	ILE	3.0
1	B	236	PHE	3.0
1	B	5	ASP	3.0
1	A	196	GLU	3.0
1	B	3	GLN	3.0
1	B	89	VAL	2.9
1	B	93	GLY	2.9
1	B	206	PHE	2.9
1	B	6	VAL	2.9
1	B	158	VAL	2.9
1	A	189	PHE	2.9
1	B	189	PHE	2.9
1	A	78	GLY	2.9
1	A	207	LEU	2.9
1	B	200	SER	2.9
1	A	49	VAL	2.8
1	B	210	LYS	2.8
1	B	83	ALA	2.8
1	A	204	LEU	2.8
1	B	43	GLU	2.7
1	A	225	LEU	2.7
1	B	30	ALA	2.7
1	B	70	ALA	2.7
1	B	126	PRO	2.7
1	B	81	ALA	2.7
1	B	145	ILE	2.7
1	A	96	GLY	2.7
1	A	109	TRP	2.7
1	B	98	ALA	2.7
1	B	202	ASP	2.7
1	A	35	VAL	2.6
1	B	229	LEU	2.6
1	A	85	LEU	2.6
1	B	209	GLY	2.6
1	B	113	ILE	2.6
1	A	167	LEU	2.6
1	B	101	VAL	2.5
1	B	25	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	3	GLN	2.5
1	B	111	THR	2.5
1	A	52	ILE	2.5
1	A	247	GLY	2.5
1	B	79	ALA	2.5
1	B	139	ILE	2.5
1	A	156	ALA	2.5
1	B	250	ALA	2.4
1	A	6	VAL	2.4
1	B	172	ALA	2.4
1	A	99	ALA	2.4
1	A	121	PHE	2.4
1	A	46	GLN	2.4
1	B	213	LEU	2.3
1	B	13	VAL	2.3
1	B	152	ALA	2.3
1	B	233	ALA	2.3
1	A	12	ILE	2.3
1	A	117	LEU	2.3
1	A	236	PHE	2.3
1	B	54	ALA	2.3
1	B	48	VAL	2.3
1	A	92	ALA	2.3
1	B	167	LEU	2.3
1	B	121	PHE	2.3
1	B	205	ALA	2.3
1	A	176	ALA	2.3
1	B	27	THR	2.3
1	A	188	GLY	2.3
1	B	72	GLY	2.3
1	A	171	ALA	2.2
1	A	33	ALA	2.2
1	A	59	ALA	2.2
1	A	62	LEU	2.2
1	B	78	GLY	2.2
1	A	113	ILE	2.2
1	B	133	ALA	2.2
1	A	82	LEU	2.2
1	B	69	PRO	2.2
1	A	174	GLU	2.1
1	A	238	THR	2.1
1	B	46	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	47	ALA	2.1
1	B	151	PHE	2.1
1	B	38	THR	2.1
1	A	87	ILE	2.1
1	B	155	SER	2.1
1	B	131	MET	2.1
1	B	134	ASN	2.1
1	A	83	ALA	2.1
1	B	28	LEU	2.0
1	B	138	ALA	2.0
1	A	48	VAL	2.0
1	B	82	LEU	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.