



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 02:24 AM GMT

PDB ID : 3LX6
Title : Crystal structure of putative dna cytosine methylase from shigella flexneri 2a str. 2457T
Authors : Ramagopal, U.A.; Toro, R.; Burley, S.K.; Almo, S.C.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on : 2010-02-24
Resolution : 2.29 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

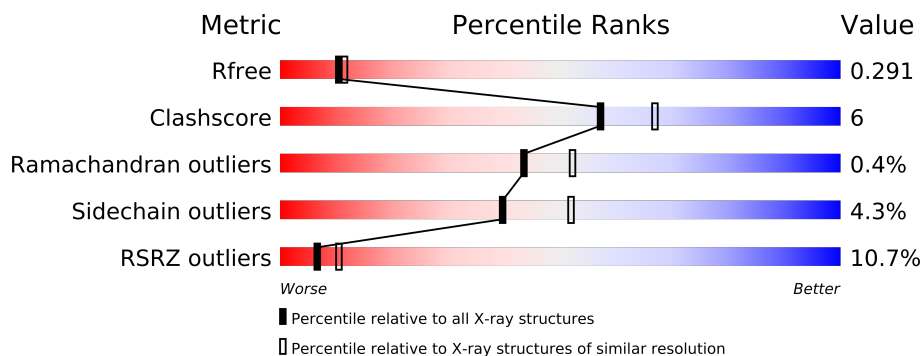
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance



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}	66092	2929 (2.30-2.30)
Clashscore	79885	3679 (2.30-2.30)
Ramachandran outliers	78287	3642 (2.30-2.30)
Sidechain outliers	78261	3641 (2.30-2.30)
RSRZ outliers	66119	2930 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	410	
1	B	410	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5835 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Cytosine-specific methyltransferase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	368	Total	C	N	O	S	Se	0	0	0
			2964	1889	531	532	6	6			
1	B	362	Total	C	N	O	S	Se	0	0	0
			2842	1800	514	516	6	6			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	61	MSE	-	EXPRESSION TAG	UNP E3Y0J2
A	62	SER	-	EXPRESSION TAG	UNP E3Y0J2
A	463	GLU	-	EXPRESSION TAG	UNP E3Y0J2
A	464	GLY	-	EXPRESSION TAG	UNP E3Y0J2
A	465	HIS	-	EXPRESSION TAG	UNP E3Y0J2
A	466	HIS	-	EXPRESSION TAG	UNP E3Y0J2
A	467	HIS	-	EXPRESSION TAG	UNP E3Y0J2
A	468	HIS	-	EXPRESSION TAG	UNP E3Y0J2
A	469	HIS	-	EXPRESSION TAG	UNP E3Y0J2
A	470	HIS	-	EXPRESSION TAG	UNP E3Y0J2
B	61	MSE	-	EXPRESSION TAG	UNP E3Y0J2
B	62	SER	-	EXPRESSION TAG	UNP E3Y0J2
B	463	GLU	-	EXPRESSION TAG	UNP E3Y0J2
B	464	GLY	-	EXPRESSION TAG	UNP E3Y0J2
B	465	HIS	-	EXPRESSION TAG	UNP E3Y0J2
B	466	HIS	-	EXPRESSION TAG	UNP E3Y0J2
B	467	HIS	-	EXPRESSION TAG	UNP E3Y0J2
B	468	HIS	-	EXPRESSION TAG	UNP E3Y0J2
B	469	HIS	-	EXPRESSION TAG	UNP E3Y0J2
B	470	HIS	-	EXPRESSION TAG	UNP E3Y0J2

- Molecule 2 is water.

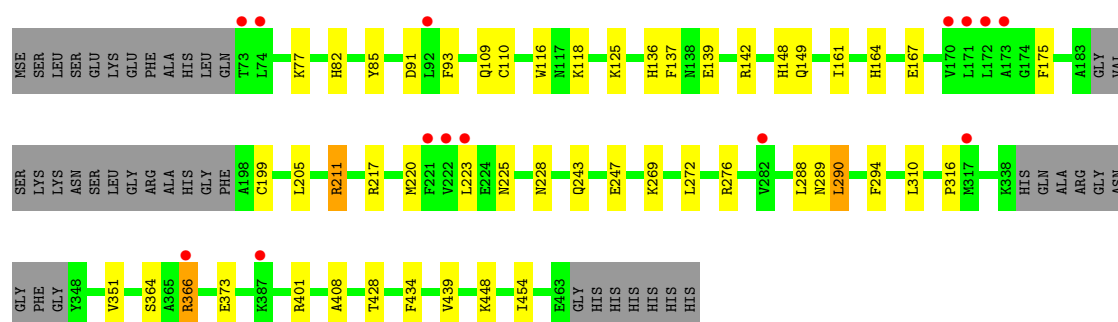
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	24	Total 24	O 24	0	0
2	B	5	Total 5	O 5	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

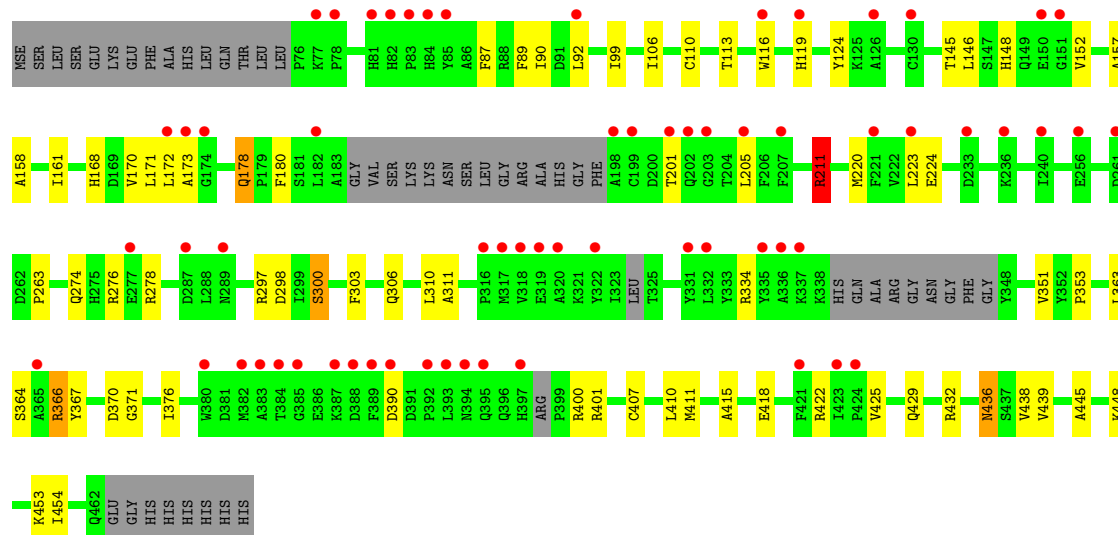
• Molecule 1: Cytosine-specific methyltransferase

Chain A:



• Molecule 1: Cytosine-specific methyltransferase

Chain B:



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	122.96Å 83.81Å 113.24Å 90.00° 118.51° 90.00°	Depositor
Resolution (Å)	31.26 – 2.29 31.26 – 2.29	Depositor EDS
% Data completeness (in resolution range)	96.5 (31.26-2.29) 96.5 (31.26-2.29)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.24 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.243 , 0.288 0.248 , 0.291	Depositor DCC
R_{free} test set	2214 reflections (5.31%)	DCC
Wilson B-factor (Å ²)	43.5	Xtriage
Anisotropy	0.355	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 36.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 43908 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	5835	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.40% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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	0.76	1/3034 (0.0%)	0.77	1/4100 (0.0%)
1	B	0.62	0/2903	0.68	1/3919 (0.0%)
All	All	0.70	1/5937 (0.0%)	0.73	2/8019 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	110	CYS	CB-SG	-5.04	1.73	1.81

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	91	ASP	CB-CG-OD1	-5.14	113.67	118.30
1	B	211	ARG	NE-CZ-NH1	5.01	122.80	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2964	0	2911	26	0
1	B	2842	0	2733	50	0
2	A	24	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	5	0	0	0	0
All	All	5835	0	5644	73	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 6.

All (73) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:178:GLN:HE22	1:B:205:LEU:H	0.96	0.91
1:A:205:LEU:HD21	1:B:306:GLN:NE2	1.91	0.86
1:B:415:ALA:HB3	1:B:418:GLU:HG3	1.59	0.84
1:B:90:ILE:HD11	1:B:171:LEU:HD12	1.65	0.77
1:B:274:GLN:HB2	1:B:410:LEU:HD11	1.68	0.75
1:B:180:PHE:CD1	1:B:201:THR:HA	2.22	0.74
1:B:178:GLN:HE22	1:B:205:LEU:N	1.80	0.74
1:A:310:LEU:CD2	1:A:351:VAL:HG11	2.22	0.70
1:B:178:GLN:NE2	1:B:205:LEU:H	1.82	0.67
1:A:243:GLN:O	1:A:247:GLU:HG3	1.99	0.62
1:A:310:LEU:HD22	1:A:351:VAL:HG11	1.79	0.62
1:A:82:HIS:HD2	1:A:85:TYR:OH	1.82	0.61
1:B:300:SER:O	1:B:303:PHE:HB2	2.01	0.61
1:A:428:THR:HG21	1:B:298:ASP:OD2	2.00	0.61
1:B:371:GLY:HA3	1:B:401:ARG:HD3	1.83	0.60
1:B:276:ARG:HD3	1:B:439:VAL:CG2	2.32	0.60
1:B:310:LEU:CD2	1:B:351:VAL:HG11	2.32	0.60
1:A:220:MSE:HE1	1:A:454:ILE:HA	1.85	0.58
1:B:146:LEU:CD1	1:B:152:VAL:HG11	2.34	0.58
1:B:445:ALA:HA	1:B:448:LYS:HE2	1.86	0.57
1:B:263:PRO:HB3	1:B:297:ARG:HG3	1.87	0.57
1:B:311:ALA:HB2	1:B:353:PRO:O	2.05	0.56
1:B:220:MSE:HE1	1:B:454:ILE:HA	1.87	0.56
1:B:90:ILE:HD11	1:B:171:LEU:CD1	2.35	0.55
1:A:408:ALA:HB2	1:A:434:PHE:CZ	2.42	0.54
1:B:376:ILE:HB	1:B:400:ARG:HG2	1.90	0.54
1:B:99:ILE:HG22	1:B:172:LEU:HD13	1.90	0.54
1:A:276:ARG:HD3	1:A:439:VAL:HG23	1.91	0.53
1:B:363:LEU:HD11	1:B:407:CYS:SG	2.48	0.53
1:B:276:ARG:HD3	1:B:439:VAL:HG23	1.91	0.53
1:B:276:ARG:NE	1:B:411:MSE:HE1	2.25	0.52
1:A:93:PHE:CD1	1:A:116:TRP:HZ3	2.29	0.51
1:A:93:PHE:CZ	1:A:205:LEU:HD22	2.46	0.50
1:A:136:HIS:NE2	1:A:164:HIS:O	2.38	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:146:LEU:HD13	1:B:152:VAL:HG11	1.94	0.49
1:A:161:ILE:HD11	1:A:211:ARG:HG2	1.94	0.49
1:B:87:PHE:HE2	1:B:106:ILE:HG13	1.77	0.49
1:B:367:TYR:OH	1:B:401:ARG:HG2	2.13	0.48
1:A:93:PHE:HD1	1:A:116:TRP:HZ3	1.61	0.48
1:B:119:HIS:N	1:B:119:HIS:CD2	2.82	0.48
1:A:93:PHE:CE1	1:A:205:LEU:HD22	2.49	0.48
1:B:180:PHE:HD1	1:B:201:THR:HA	1.74	0.48
1:B:145:THR:O	1:B:211:ARG:NH2	2.39	0.47
1:B:90:ILE:HD13	1:B:168:HIS:CE1	2.50	0.47
1:B:89:PHE:CZ	1:B:110:CYS:HB2	2.50	0.46
1:A:364:SER:CB	1:A:366:ARG:HE	2.28	0.46
1:B:92:LEU:HB2	1:B:173:ALA:HB2	1.98	0.46
1:B:310:LEU:HD22	1:B:351:VAL:HG11	1.98	0.46
1:A:175:PHE:HE1	1:A:223:LEU:HB3	1.83	0.44
1:B:173:ALA:O	1:B:223:LEU:HA	2.17	0.44
1:B:425:VAL:HB	1:B:429:GLN:HB2	1.99	0.44
1:B:432:ARG:O	1:B:436:ASN:HB2	2.17	0.44
1:A:142:ARG:HD3	1:B:306:GLN:OE1	2.18	0.44
1:A:85:TYR:CG	1:A:109:GLN:HB2	2.54	0.43
1:B:146:LEU:HD12	1:B:152:VAL:HG11	1.99	0.43
1:B:367:TYR:CD1	1:B:371:GLY:HA2	2.54	0.43
1:B:170:VAL:HA	1:B:220:MSE:O	2.19	0.43
1:B:113:THR:HG21	1:B:124:TYR:CZ	2.54	0.42
1:B:274:GLN:HB2	1:B:410:LEU:CD1	2.44	0.42
1:B:158:ALA:HA	1:B:161:ILE:HD12	2.02	0.42
1:A:118:LYS:HE3	1:A:139:GLU:OE2	2.20	0.41
1:A:276:ARG:HD3	1:A:439:VAL:CG2	2.49	0.41
1:A:294:PHE:C	1:A:294:PHE:CD2	2.93	0.41
1:B:310:LEU:HD23	1:B:351:VAL:HG11	2.02	0.41
1:B:92:LEU:HB2	1:B:173:ALA:CB	2.50	0.41
1:A:125:LYS:HE2	1:A:137:PHE:CE2	2.56	0.41
1:A:269:LYS:HA	1:A:272:LEU:O	2.21	0.41
1:B:274:GLN:HB3	1:B:274:GLN:HE21	1.67	0.40
1:B:364:SER:HB2	1:B:366:ARG:HH21	1.86	0.40
1:B:99:ILE:HG13	1:B:438:VAL:HG21	2.03	0.40
1:B:146:LEU:HD12	1:B:157:ALA:HA	2.03	0.40
1:A:288:LEU:HB3	1:A:290:LEU:HD12	2.03	0.40
1:A:401:ARG:HH21	1:A:401:ARG:HD3	1.75	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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	362/410 (88%)	353 (98%)	8 (2%)	1 (0%)	50	60
1	B	352/410 (86%)	334 (95%)	16 (4%)	2 (1%)	33	39
All	All	714/820 (87%)	687 (96%)	24 (3%)	3 (0%)	43	52

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	300	SER
1	B	370	ASP
1	A	316	PRO

5.3.2 Protein sidechains ⓘ

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	313/340 (92%)	299 (96%)	14 (4%)	38	50
1	B	290/340 (85%)	278 (96%)	12 (4%)	41	55
All	All	603/680 (89%)	577 (96%)	26 (4%)	40	52

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	77	LYS
1	A	148	HIS
1	A	149	GLN
1	A	167	GLU
1	A	199	CYS
1	A	211	ARG

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Mol	Chain	Res	Type
1	A	217	ARG
1	A	225	ASN
1	A	228	ASN
1	A	289	ASN
1	A	290	LEU
1	A	366	ARG
1	A	373	GLU
1	A	448	LYS
1	B	116	TRP
1	B	148	HIS
1	B	178	GLN
1	B	211	ARG
1	B	224	GLU
1	B	278	ARG
1	B	334	ARG
1	B	366	ARG
1	B	390	ASP
1	B	422	ARG
1	B	436	ASN
1	B	453	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	82	HIS
1	A	228	ASN
1	A	258	ASN
1	A	354	ASN
1	A	436	ASN
1	B	82	HIS
1	B	178	GLN
1	B	228	ASN
1	B	258	ASN
1	B	357	GLN
1	B	433	GLN
1	B	456	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates 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	368/410 (89%)	0.17	14 (3%)	38 49	19, 30, 43, 77	0
1	B	362/410 (88%)	0.91	64 (17%)	2 4	19, 33, 48, 80	0
All	All	730/820 (89%)	0.54	78 (10%)	6 10	19, 32, 47, 80	0

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	383	ALA	6.6
1	B	182	LEU	6.3
1	B	199	CYS	6.2
1	B	316	PRO	5.9
1	B	331	TYR	5.7
1	B	336	ALA	4.9
1	B	317	MSE	4.9
1	B	335	TYR	4.8
1	B	319	GLU	4.7
1	B	318	VAL	4.6
1	B	203	GLY	4.5
1	B	390	ASP	4.2
1	B	77	LYS	3.9
1	B	421	PHE	3.9
1	B	83	PRO	3.8
1	B	150	GLU	3.6
1	A	73	THR	3.6
1	A	74	LEU	3.3
1	B	151	GLY	3.3
1	B	202	GLN	3.2
1	A	317	MSE	3.2
1	B	395	GLN	3.1
1	B	126	ALA	3.1
1	B	320	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	256	GLU	3.0
1	B	81	HIS	3.0
1	A	222	VAL	3.0
1	A	221	PHE	3.0
1	B	78	PRO	3.0
1	B	119	HIS	3.0
1	B	332	LEU	2.9
1	B	240	ILE	2.9
1	A	387	LYS	2.9
1	B	84	HIS	2.9
1	B	198	ALA	2.8
1	B	382	MSE	2.8
1	B	261	ASP	2.8
1	B	389	PHE	2.8
1	B	384	THR	2.7
1	A	172	LEU	2.6
1	B	423	ILE	2.6
1	B	394	ASN	2.6
1	B	82	HIS	2.6
1	B	173	ALA	2.5
1	B	172	LEU	2.5
1	B	287	ASP	2.5
1	B	393	LEU	2.5
1	A	171	LEU	2.5
1	A	170	VAL	2.5
1	B	322	TYR	2.5
1	B	223	LEU	2.5
1	B	174	GLY	2.4
1	B	207	PHE	2.4
1	A	282	VAL	2.4
1	A	223	LEU	2.4
1	B	397	HIS	2.4
1	B	233	ASP	2.4
1	B	289	ASN	2.3
1	B	392	PRO	2.3
1	B	337	LYS	2.3
1	B	365	ALA	2.3
1	B	424	PRO	2.3
1	B	85	TYR	2.3
1	B	130	CYS	2.3
1	A	366	ARG	2.3
1	B	236	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	92	LEU	2.2
1	B	92	LEU	2.2
1	B	385	GLY	2.2
1	B	387	LYS	2.2
1	B	116	TRP	2.2
1	B	221	PHE	2.2
1	B	205	LEU	2.1
1	A	173	ALA	2.1
1	B	201	THR	2.1
1	B	277	GLU	2.1
1	B	388	ASP	2.0
1	B	380	TRP	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 carbohydrates 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.