



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 02:31 PM UTC

PDB ID : 7A0G / pdb_00007a0g
Title : Structure of the SmhB pore of the tripartite alpha-pore forming toxin, Smh, from *Serratia marcescens*.
Authors : Churchill-Angus, A.M.; Baker, P.J.
Deposited on : 2020-08-08
Resolution : 6.98 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

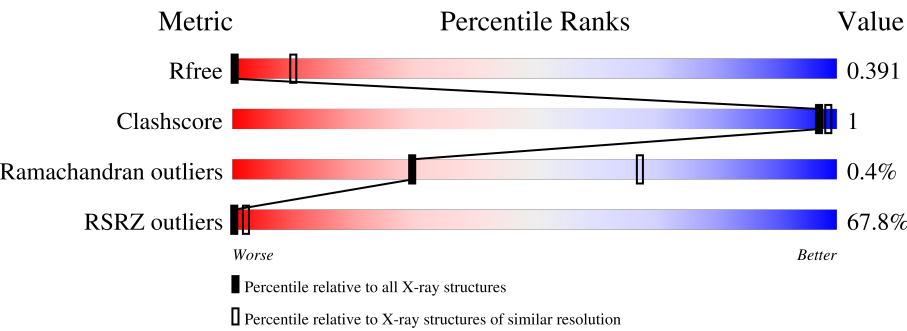
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 6.98 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	1166 (9.70-4.00)
Clashscore	190562	1007 (9.70-4.04)
Ramachandran outliers	187476	1053 (9.70-4.00)
RSRZ outliers	180081	1159 (9.70-4.00)

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	AAA	366	63% 87% 10%
1	BBB	366	59% 86% 13%
1	CCC	366	64% 87% 10%
1	DDD	366	61% 85% 13%
1	EEE	366	61% 88% 10%
1	FFF	366	57% 83% 14%
1	GGG	366	56% 88% 10%

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Mol	Chain	Length	Quality of chain
1	HHH	366	60% 87% 10%
1	III	366	55% 84% 14%
1	JJJ	366	62% 85% 13%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 27767 atoms, of which 11987 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 SmhB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	329	Total	C	H	N	O	261	0	0
			2830	950	1222	329	329			
1	BBB	320	Total	C	H	N	O	254	0	0
			2751	924	1187	320	320			
1	CCC	329	Total	C	H	N	O	262	0	0
			2829	950	1221	329	329			
1	DDD	318	Total	C	H	N	O	254	0	0
			2735	919	1180	318	318			
1	EEE	329	Total	C	H	N	O	259	1	0
			2834	951	1225	329	329			
1	FFF	313	Total	C	H	N	O	249	0	0
			2691	904	1161	313	313			
1	GGG	329	Total	C	H	N	O	261	0	0
			2830	950	1222	329	329			
1	HHH	328	Total	C	H	N	O	260	0	0
			2822	947	1219	328	328			
1	III	313	Total	C	H	N	O	250	0	0
			2694	905	1163	313	313			
1	JJJ	320	Total	C	H	N	O	254	0	0
			2751	924	1187	320	320			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	368	LEU	-	expression tag	UNP A0A1Q4NVM7
AAA	369	GLU	-	expression tag	UNP A0A1Q4NVM7
AAA	370	HIS	-	expression tag	UNP A0A1Q4NVM7
AAA	371	HIS	-	expression tag	UNP A0A1Q4NVM7
AAA	372	HIS	-	expression tag	UNP A0A1Q4NVM7
AAA	373	HIS	-	expression tag	UNP A0A1Q4NVM7
AAA	374	HIS	-	expression tag	UNP A0A1Q4NVM7
AAA	375	HIS	-	expression tag	UNP A0A1Q4NVM7
BBB	368	LEU	-	expression tag	UNP A0A1Q4NVM7

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Chain	Residue	Modelled	Actual	Comment	Reference
BBB	369	GLU	-	expression tag	UNP A0A1Q4NVM7
BBB	370	HIS	-	expression tag	UNP A0A1Q4NVM7
BBB	371	HIS	-	expression tag	UNP A0A1Q4NVM7
BBB	372	HIS	-	expression tag	UNP A0A1Q4NVM7
BBB	373	HIS	-	expression tag	UNP A0A1Q4NVM7
BBB	374	HIS	-	expression tag	UNP A0A1Q4NVM7
BBB	375	HIS	-	expression tag	UNP A0A1Q4NVM7
CCC	368	LEU	-	expression tag	UNP A0A1Q4NVM7
CCC	369	GLU	-	expression tag	UNP A0A1Q4NVM7
CCC	370	HIS	-	expression tag	UNP A0A1Q4NVM7
CCC	371	HIS	-	expression tag	UNP A0A1Q4NVM7
CCC	372	HIS	-	expression tag	UNP A0A1Q4NVM7
CCC	373	HIS	-	expression tag	UNP A0A1Q4NVM7
CCC	374	HIS	-	expression tag	UNP A0A1Q4NVM7
CCC	375	HIS	-	expression tag	UNP A0A1Q4NVM7
DDD	368	LEU	-	expression tag	UNP A0A1Q4NVM7
DDD	369	GLU	-	expression tag	UNP A0A1Q4NVM7
DDD	370	HIS	-	expression tag	UNP A0A1Q4NVM7
DDD	371	HIS	-	expression tag	UNP A0A1Q4NVM7
DDD	372	HIS	-	expression tag	UNP A0A1Q4NVM7
DDD	373	HIS	-	expression tag	UNP A0A1Q4NVM7
DDD	374	HIS	-	expression tag	UNP A0A1Q4NVM7
DDD	375	HIS	-	expression tag	UNP A0A1Q4NVM7
EEE	368	LEU	-	expression tag	UNP A0A1Q4NVM7
EEE	369	GLU	-	expression tag	UNP A0A1Q4NVM7
EEE	370	HIS	-	expression tag	UNP A0A1Q4NVM7
EEE	371	HIS	-	expression tag	UNP A0A1Q4NVM7
EEE	372	HIS	-	expression tag	UNP A0A1Q4NVM7
EEE	373	HIS	-	expression tag	UNP A0A1Q4NVM7
EEE	374	HIS	-	expression tag	UNP A0A1Q4NVM7
EEE	375	HIS	-	expression tag	UNP A0A1Q4NVM7
FFF	368	LEU	-	expression tag	UNP A0A1Q4NVM7
FFF	369	GLU	-	expression tag	UNP A0A1Q4NVM7
FFF	370	HIS	-	expression tag	UNP A0A1Q4NVM7
FFF	371	HIS	-	expression tag	UNP A0A1Q4NVM7
FFF	372	HIS	-	expression tag	UNP A0A1Q4NVM7
FFF	373	HIS	-	expression tag	UNP A0A1Q4NVM7
FFF	374	HIS	-	expression tag	UNP A0A1Q4NVM7
FFF	375	HIS	-	expression tag	UNP A0A1Q4NVM7
GGG	368	LEU	-	expression tag	UNP A0A1Q4NVM7
GGG	369	GLU	-	expression tag	UNP A0A1Q4NVM7
GGG	370	HIS	-	expression tag	UNP A0A1Q4NVM7

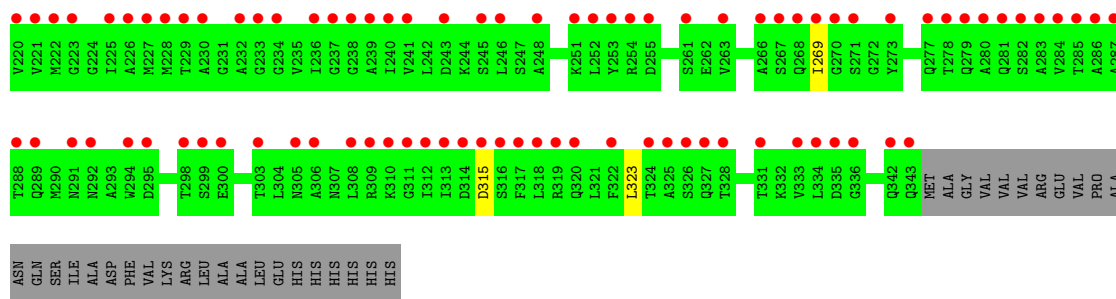
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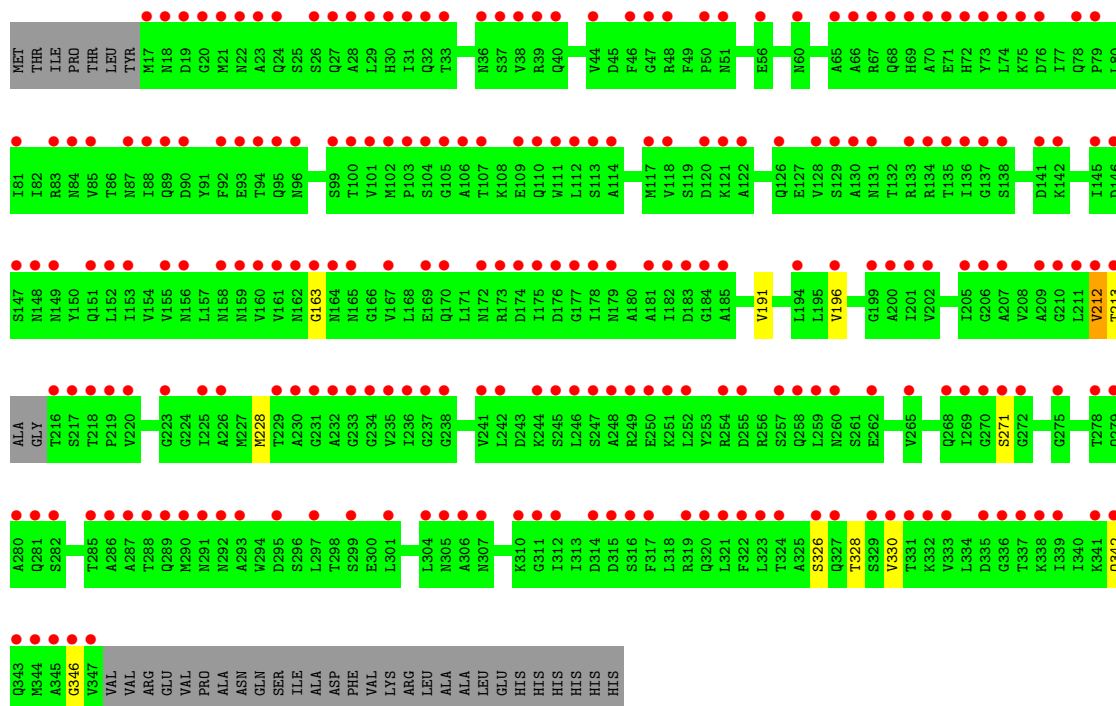
Chain	Residue	Modelled	Actual	Comment	Reference
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GGG	372	HIS	-	expression tag	UNP A0A1Q4NVM7
GGG	373	HIS	-	expression tag	UNP A0A1Q4NVM7
GGG	374	HIS	-	expression tag	UNP A0A1Q4NVM7
GGG	375	HIS	-	expression tag	UNP A0A1Q4NVM7
HHH	368	LEU	-	expression tag	UNP A0A1Q4NVM7
HHH	369	GLU	-	expression tag	UNP A0A1Q4NVM7
HHH	370	HIS	-	expression tag	UNP A0A1Q4NVM7
HHH	371	HIS	-	expression tag	UNP A0A1Q4NVM7
HHH	372	HIS	-	expression tag	UNP A0A1Q4NVM7
HHH	373	HIS	-	expression tag	UNP A0A1Q4NVM7
HHH	374	HIS	-	expression tag	UNP A0A1Q4NVM7
HHH	375	HIS	-	expression tag	UNP A0A1Q4NVM7
III	368	LEU	-	expression tag	UNP A0A1Q4NVM7
III	369	GLU	-	expression tag	UNP A0A1Q4NVM7
III	370	HIS	-	expression tag	UNP A0A1Q4NVM7
III	371	HIS	-	expression tag	UNP A0A1Q4NVM7
III	372	HIS	-	expression tag	UNP A0A1Q4NVM7
III	373	HIS	-	expression tag	UNP A0A1Q4NVM7
III	374	HIS	-	expression tag	UNP A0A1Q4NVM7
III	375	HIS	-	expression tag	UNP A0A1Q4NVM7
JJJ	368	LEU	-	expression tag	UNP A0A1Q4NVM7
JJJ	369	GLU	-	expression tag	UNP A0A1Q4NVM7
JJJ	370	HIS	-	expression tag	UNP A0A1Q4NVM7
JJJ	371	HIS	-	expression tag	UNP A0A1Q4NVM7
JJJ	372	HIS	-	expression tag	UNP A0A1Q4NVM7
JJJ	373	HIS	-	expression tag	UNP A0A1Q4NVM7
JJJ	374	HIS	-	expression tag	UNP A0A1Q4NVM7
JJJ	375	HIS	-	expression tag	UNP A0A1Q4NVM7

- Molecule 1: SmhB

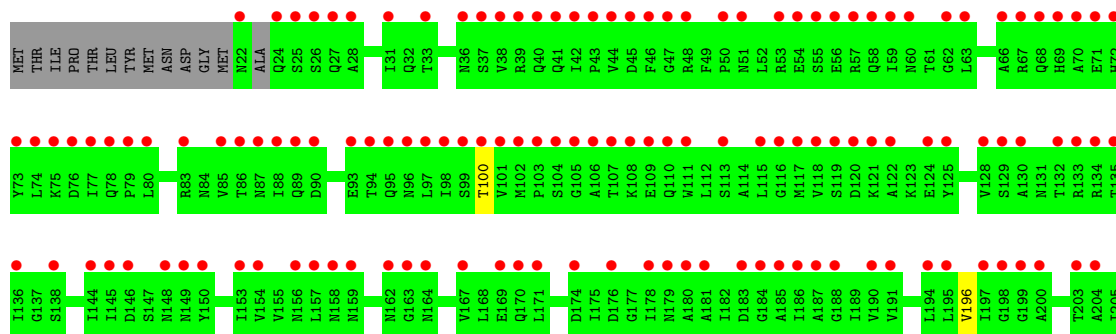


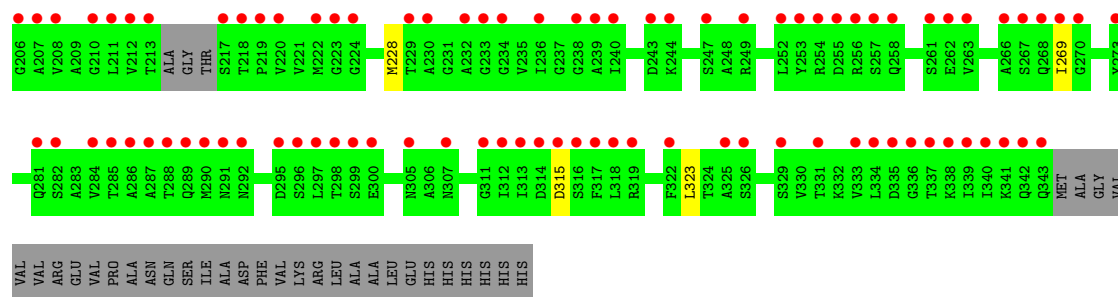


• Molecule 1: SmhB

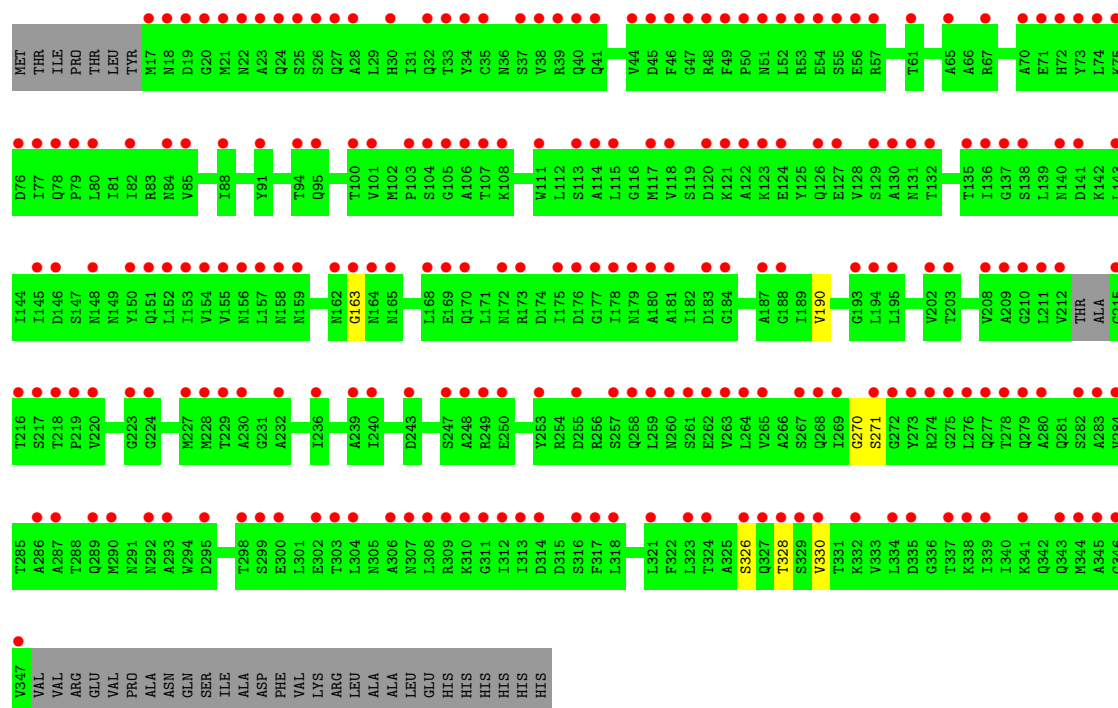


• Molecule 1: SmhB

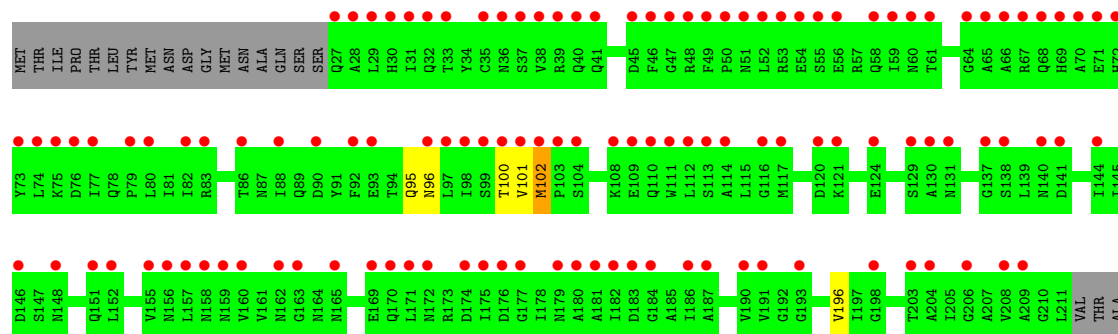
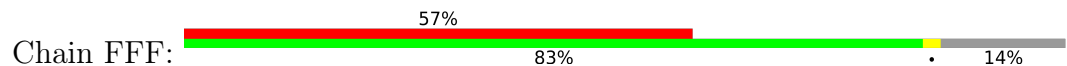


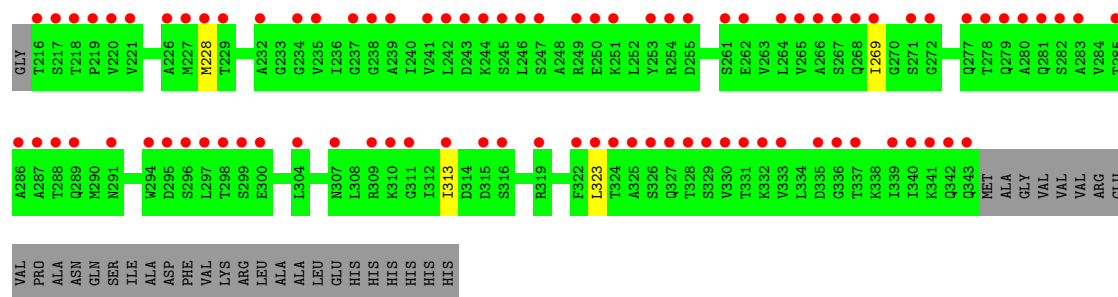


• Molecule 1: SmhB

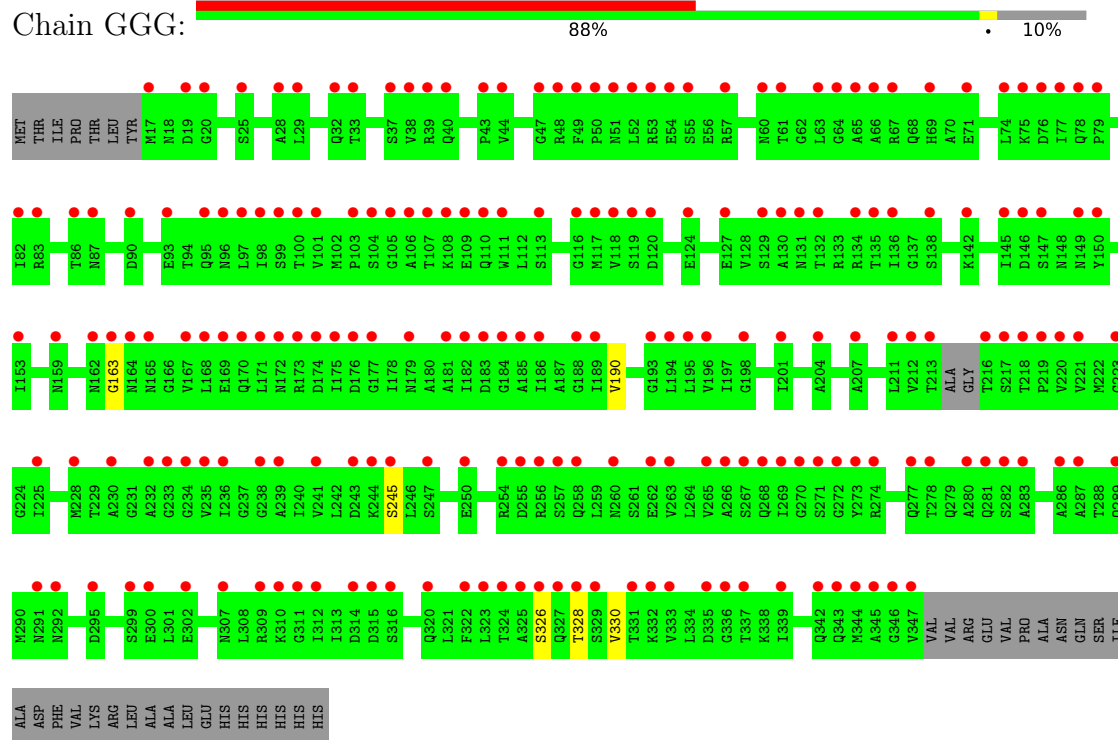


• Molecule 1: SmhB

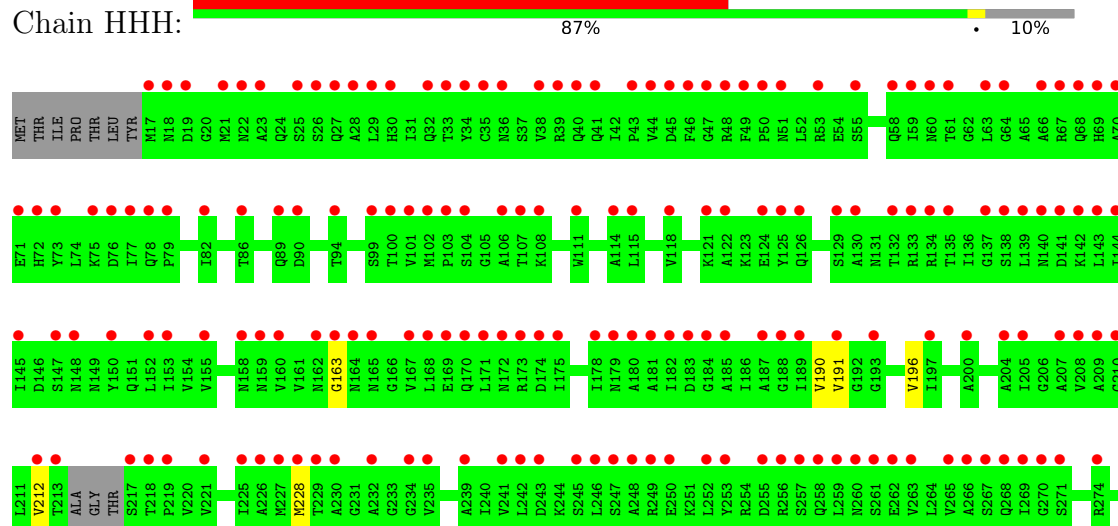
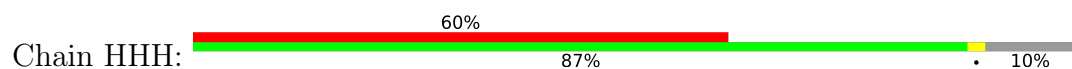


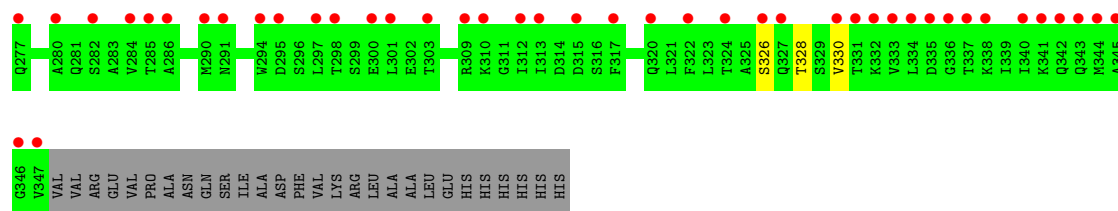


• Molecule 1: SmhB

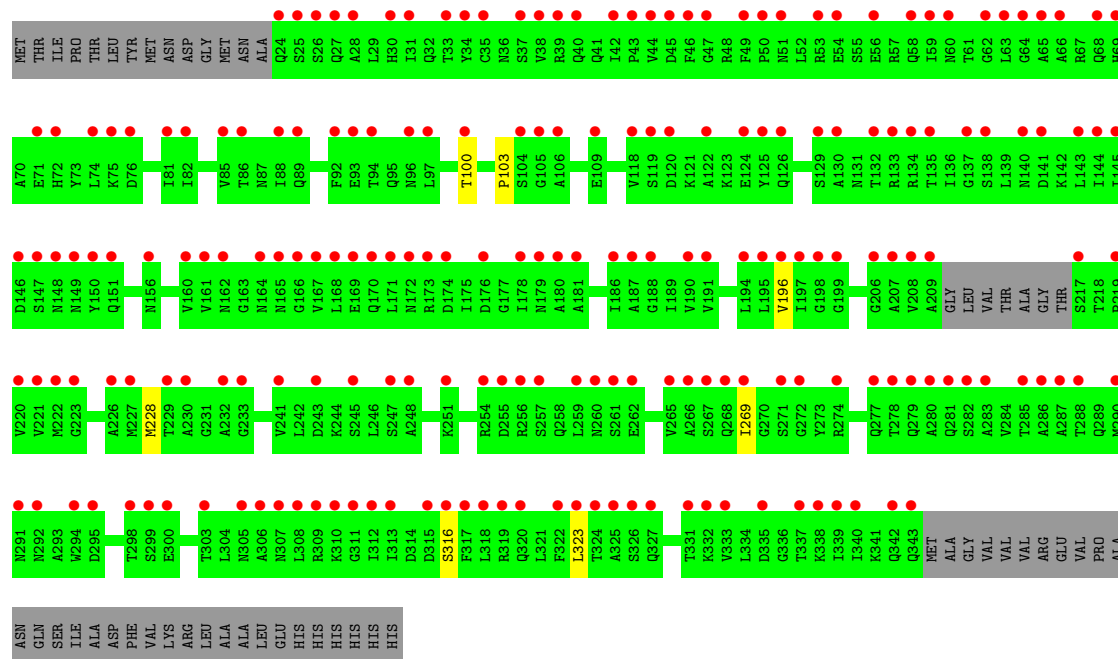
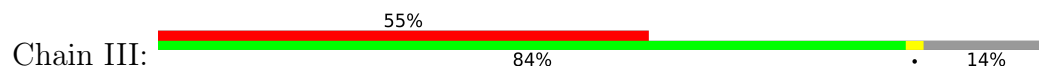


• Molecule 1: SmhB

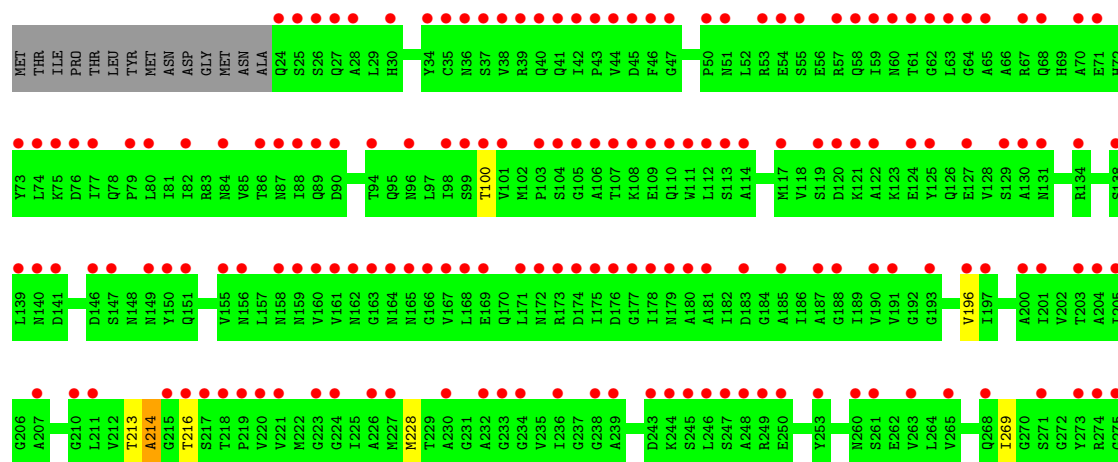
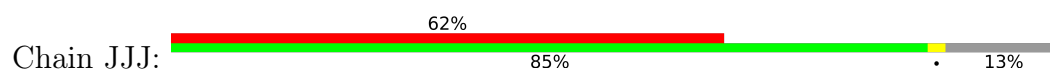


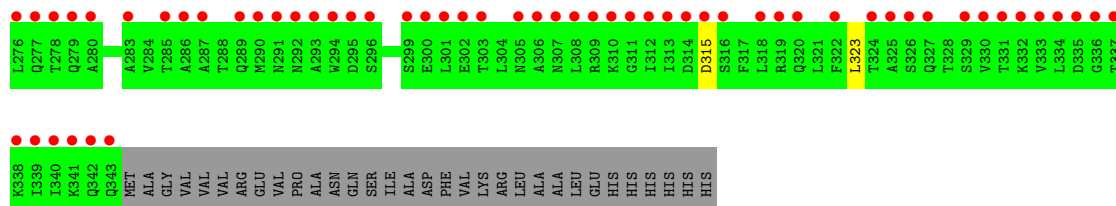


- Molecule 1: SmhB



- Molecule 1: SmhB





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	224.48Å 118.06Å 209.53Å 90.00° 109.44° 90.00°	Depositor
Resolution (Å)	66.77 – 6.98 66.77 – 6.98	Depositor EDS
% Data completeness (in resolution range)	98.7 (66.77-6.98) 80.4 (66.77-6.98)	Depositor EDS
R_{merge}	2.29	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.33 (at 6.71Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.334 , 0.335 0.350 , 0.391	Depositor DCC
R_{free} test set	380 reflections (4.57%)	wwPDB-VP
Wilson B-factor (Å ²)	-102.2	Xtriage
Anisotropy	-2.359	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.17 , 76.1	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	0.66	EDS
Total number of atoms	27767	wwPDB-VP
Average B, all atoms (Å ²)	0.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.53% 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	AAA	1.34	0/1606	2.39	10/2223 (0.4%)
1	BBB	1.36	0/1563	2.34	2/2165 (0.1%)
1	CCC	1.34	0/1606	2.39	7/2223 (0.3%)
1	DDD	1.34	0/1552	2.35	2/2147 (0.1%)
1	EEE	1.36	2/1610 (0.1%)	2.37	5/2228 (0.2%)
1	FFF	1.35	0/1528	2.35	2/2115 (0.1%)
1	GGG	1.35	1/1606 (0.1%)	2.38	4/2223 (0.2%)
1	HHH	1.35	1/1601 (0.1%)	2.38	5/2216 (0.2%)
1	III	1.36	0/1529	2.35	4/2117 (0.2%)
1	JJJ	1.35	0/1563	2.35	2/2165 (0.1%)
All	All	1.35	4/15764 (0.0%)	2.37	43/21822 (0.2%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	HHH	190	VAL	C-O	5.87	1.30	1.24
1	EEE	190	VAL	C-O	5.38	1.29	1.24
1	EEE	270	GLY	C-O	5.25	1.30	1.23
1	GGG	190	VAL	C-O	5.03	1.29	1.24

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	GGG	163	GLY	CA-C-O	-6.08	118.03	122.23
1	HHH	163	GLY	CA-C-O	-6.01	118.08	122.23
1	III	316	SER	CA-C-O	-5.98	116.36	119.77
1	GGG	328	THR	O-C-N	5.95	125.23	120.83
1	EEE	328	THR	O-C-N	5.89	125.19	120.83
1	HHH	328	THR	O-C-N	5.87	125.17	120.83
1	DDD	269	ILE	CA-C-N	5.85	126.43	119.94
1	DDD	269	ILE	C-N-CA	5.85	126.43	119.94
1	AAA	328	THR	O-C-N	5.81	125.13	120.83
1	CCC	163	GLY	CA-C-O	-5.81	118.22	122.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	CCC	328	THR	O-C-N	5.79	125.11	120.83
1	AAA	163	GLY	CA-C-O	-5.72	118.28	122.23
1	JJJ	269	ILE	CA-C-N	5.67	126.23	119.94
1	JJJ	269	ILE	C-N-CA	5.67	126.23	119.94
1	III	269	ILE	CA-C-N	5.64	126.20	119.94
1	III	269	ILE	C-N-CA	5.64	126.20	119.94
1	FFF	269	ILE	CA-C-N	5.63	126.19	119.94
1	FFF	269	ILE	C-N-CA	5.63	126.19	119.94
1	BBB	269	ILE	CA-C-N	5.62	126.18	119.94
1	BBB	269	ILE	C-N-CA	5.62	126.18	119.94
1	GGG	328	THR	CB-CA-C	-5.52	104.23	115.27
1	CCC	328	THR	CB-CA-C	-5.44	104.39	115.27
1	AAA	328	THR	CB-CA-C	-5.43	104.41	115.27
1	HHH	328	THR	CB-CA-C	-5.42	104.43	115.27
1	EEE	328	THR	CB-CA-C	-5.40	104.47	115.27
1	EEE	163	GLY	CA-C-O	-5.36	118.53	122.23
1	GGG	245	SER	CA-C-O	-5.28	115.26	120.70
1	CCC	271	SER	CA-C-N	5.17	125.68	119.94
1	CCC	271	SER	C-N-CA	5.17	125.68	119.94
1	EEE	271	SER	CA-C-N	5.17	125.68	119.94
1	EEE	271	SER	C-N-CA	5.17	125.68	119.94
1	CCC	191	VAL	CA-C-N	5.17	125.67	119.94
1	CCC	191	VAL	C-N-CA	5.17	125.67	119.94
1	AAA	271	SER	CA-C-N	5.15	125.66	119.94
1	AAA	271	SER	C-N-CA	5.15	125.66	119.94
1	HHH	191	VAL	CA-C-N	5.10	125.61	119.94
1	HHH	191	VAL	C-N-CA	5.10	125.61	119.94
1	AAA	191	VAL	CA-C-N	5.05	125.55	119.94
1	AAA	191	VAL	C-N-CA	5.05	125.55	119.94
1	III	316	SER	O-C-N	5.04	124.56	120.83
1	AAA	245	SER	CA-C-O	-5.04	115.51	120.70
1	AAA	183	ASP	CA-C-N	5.02	125.55	119.98
1	AAA	183	ASP	C-N-CA	5.02	125.55	119.98

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	AAA	1608	1222	769	2	0
1	BBB	1564	1187	748	2	0
1	CCC	1608	1221	766	4	0
1	DDD	1555	1180	738	2	0
1	EEE	1609	1225	772	1	0
1	FFF	1530	1161	729	3	0
1	GGG	1608	1222	769	1	0
1	HHH	1603	1219	767	2	0
1	III	1531	1163	728	2	0
1	JJJ	1564	1187	748	3	0
All	All	15780	11987	7534	22	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 1.

All (22) 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:III:100:THR:CB	1:III:323:LEU:CB	2.67	0.72
1:FFF:101:VAL:O	1:FFF:102:MET:CB	2.41	0.68
1:BBB:100:THR:HA	1:BBB:323:LEU:CB	2.26	0.64
1:DDD:100:THR:HA	1:DDD:323:LEU:CB	2.28	0.63
1:JJJ:100:THR:HA	1:JJJ:323:LEU:CB	2.29	0.62
1:FFF:100:THR:HA	1:FFF:323:LEU:CB	2.41	0.51
1:GGG:326:SER:HA	1:GGG:330:VAL:CB	2.44	0.47
1:HHH:326:SER:HA	1:HHH:330:VAL:CB	2.45	0.47
1:CCC:326:SER:HA	1:CCC:330:VAL:CB	2.45	0.46
1:AAA:326:SER:HA	1:AAA:330:VAL:CB	2.46	0.45
1:BBB:213:THR:O	1:BBB:214:ALA:C	2.59	0.45
1:EEE:326:SER:HA	1:EEE:330:VAL:CB	2.46	0.45
1:CCC:342:GLN:O	1:CCC:346:GLY:N	2.50	0.42
1:FFF:196:VAL:HA	1:FFF:228:MET:HA	2.02	0.42
1:HHH:196:VAL:HA	1:HHH:228:MET:HA	2.02	0.42
1:JJJ:196:VAL:HA	1:JJJ:228:MET:HA	2.03	0.41
1:DDD:196:VAL:HA	1:DDD:228:MET:HA	2.02	0.41
1:AAA:212:VAL:O	1:AAA:213:THR:C	2.63	0.41
1:CCC:196:VAL:HA	1:CCC:228:MET:HA	2.03	0.41
1:III:196:VAL:HA	1:III:228:MET:HA	2.03	0.41
1:JJJ:213:THR:O	1:JJJ:214:ALA:C	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CCC:212:VAL:O	1:CCC:213:THR:C	2.64	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	AAA	325/366 (89%)	313 (96%)	12 (4%)	0	100	100
1	BBB	318/366 (87%)	303 (95%)	12 (4%)	3 (1%)	14	51
1	CCC	325/366 (89%)	314 (97%)	10 (3%)	1 (0%)	36	72
1	DDD	313/366 (86%)	302 (96%)	10 (3%)	1 (0%)	36	72
1	EEE	326/366 (89%)	315 (97%)	11 (3%)	0	100	100
1	FFF	309/366 (84%)	297 (96%)	8 (3%)	4 (1%)	9	42
1	GGG	325/366 (89%)	313 (96%)	12 (4%)	0	100	100
1	HHH	324/366 (88%)	313 (97%)	10 (3%)	1 (0%)	36	72
1	III	309/366 (84%)	297 (96%)	11 (4%)	1 (0%)	36	72
1	JJJ	318/366 (87%)	304 (96%)	11 (4%)	3 (1%)	14	51
All	All	3192/3660 (87%)	3071 (96%)	107 (3%)	14 (0%)	30	67

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	BBB	214	ALA
1	BBB	216	THR
1	BBB	315	ASP
1	DDD	315	ASP
1	FFF	95	GLN
1	FFF	102	MET

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Mol	Chain	Res	Type
1	JJJ	315	ASP
1	JJJ	216	THR
1	FFF	96	ASN
1	JJJ	214	ALA
1	CCC	212	VAL
1	III	103	PRO
1	HHH	212	VAL
1	FFF	313	ILE

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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	AAA	329/366 (89%)	3.22	229 (69%) 0 2	0, 0, 0, 0	0
1	BBB	320/366 (87%)	2.91	217 (67%) 0 2	0, 0, 0, 0	0
1	CCC	329/366 (89%)	3.31	234 (71%) 0 2	0, 0, 0, 0	0
1	DDD	318/366 (86%)	3.30	222 (69%) 0 2	0, 0, 0, 0	0
1	EEE	329/366 (89%)	3.25	225 (68%) 0 2	0, 0, 0, 0	1 (0%)
1	FFF	313/366 (85%)	2.93	208 (66%) 0 2	0, 0, 0, 0	0
1	GGG	329/366 (89%)	2.86	206 (62%) 0 2	0, 0, 0, 0	0
1	HHH	328/366 (89%)	2.98	219 (66%) 0 2	0, 0, 0, 0	0
1	III	313/366 (85%)	2.91	203 (64%) 0 2	0, 0, 0, 0	0
1	JJJ	320/366 (87%)	3.16	226 (70%) 0 2	0, 0, 0, 0	0
All	All	3228/3660 (88%)	3.09	2189 (67%) 0 2	0, 0, 0, 0	1 (0%)

All (2189) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	BBB	25	SER	23.2
1	AAA	50	PRO	13.9
1	III	105	GLY	13.8
1	AAA	312	ILE	13.4
1	GGG	165	ASN	13.1
1	AAA	314	ASP	13.0
1	DDD	211	LEU	12.9
1	HHH	229	THR	12.8
1	EEE	169	GLU	12.8
1	JJJ	104	SER	12.2
1	AAA	53	ARG	12.1
1	AAA	104	SER	12.0
1	JJJ	74	LEU	11.9

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Mol	Chain	Res	Type	RSRZ
1	JJJ	75	LYS	11.7
1	GGG	54	GLU	11.7
1	AAA	109	GLU	11.6
1	DDD	22	ASN	11.5
1	III	25	SER	11.4
1	EEE	346	GLY	11.1
1	III	325	ALA	11.1
1	EEE	307	ASN	11.0
1	AAA	311	GLY	10.9
1	AAA	56	GLU	10.9
1	DDD	208	VAL	10.9
1	EEE	176	ASP	10.8
1	CCC	324	THR	10.8
1	EEE	170	GLN	10.7
1	JJJ	98	ILE	10.6
1	HHH	210	GLY	10.5
1	III	47	GLY	10.5
1	CCC	216	THR	10.4
1	AAA	51	ASN	10.4
1	JJJ	108	LYS	10.4
1	JJJ	315	ASP	10.3
1	AAA	100	THR	10.2
1	CCC	317	PHE	10.1
1	HHH	164	ASN	10.0
1	CCC	251	LYS	10.0
1	HHH	71	GLU	9.9
1	HHH	40	GLN	9.9
1	DDD	37	SER	9.9
1	JJJ	109	GLU	9.7
1	DDD	25	SER	9.7
1	AAA	322	PHE	9.6
1	FFF	296	SER	9.6
1	DDD	106	ALA	9.5
1	AAA	160	VAL	9.5
1	HHH	255	ASP	9.5
1	GGG	204	ALA	9.3
1	FFF	35	CYS	9.1
1	CCC	249	ARG	9.1
1	HHH	122	ALA	9.1
1	CCC	255	ASP	9.1
1	III	316	SER	9.1
1	CCC	213	THR	9.0

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Mol	Chain	Res	Type	RSRZ
1	DDD	230	ALA	9.0
1	AAA	170	GLN	8.9
1	DDD	89	GLN	8.8
1	DDD	342	GLN	8.8
1	FFF	110	GLN	8.8
1	BBB	219	PRO	8.8
1	HHH	312	ILE	8.7
1	HHH	343	GLN	8.7
1	DDD	95	GLN	8.6
1	EEE	155	VAL	8.6
1	GGG	335	ASP	8.5
1	GGG	234	GLY	8.5
1	DDD	285	THR	8.5
1	CCC	149	ASN	8.4
1	CCC	250	GLU	8.4
1	JJJ	216	THR	8.4
1	CCC	70	ALA	8.4
1	CCC	176	ASP	8.4
1	EEE	314	ASP	8.4
1	III	97	LEU	8.4
1	JJJ	205	ILE	8.3
1	III	324	THR	8.3
1	EEE	209	ALA	8.3
1	CCC	345	ALA	8.3
1	JJJ	279	GLN	8.2
1	GGG	347	VAL	8.2
1	CCC	211	LEU	8.2
1	FFF	208	VAL	8.2
1	FFF	37	SER	8.0
1	III	68	GLN	8.0
1	AAA	327	GLN	7.9
1	AAA	213	THR	7.9
1	DDD	338	LYS	7.9
1	AAA	52	LEU	7.9
1	CCC	105	GLY	7.9
1	JJJ	131	ASN	7.9
1	DDD	217	SER	7.9
1	JJJ	247	SER	7.9
1	DDD	329	SER	7.8
1	DDD	339	ILE	7.8
1	DDD	170	GLN	7.8
1	EEE	306	ALA	7.8

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Mol	Chain	Res	Type	RSRZ
1	EEE	272	GLY	7.8
1	AAA	310	LYS	7.8
1	JJJ	311	GLY	7.8
1	HHH	17	MET	7.7
1	CCC	342	GLN	7.7
1	FFF	159	ASN	7.7
1	CCC	84	ASN	7.7
1	GGG	216	THR	7.6
1	III	96	ASN	7.6
1	AAA	110	GLN	7.5
1	DDD	24	GLN	7.5
1	EEE	259	LEU	7.5
1	DDD	314	ASP	7.5
1	JJJ	223	GLY	7.5
1	AAA	108	LYS	7.5
1	HHH	313	ILE	7.5
1	JJJ	25	SER	7.4
1	III	280	ALA	7.4
1	HHH	267	SER	7.4
1	GGG	238	GLY	7.4
1	DDD	319	ARG	7.4
1	JJJ	162	ASN	7.4
1	EEE	335	ASP	7.4
1	AAA	320	GLN	7.3
1	AAA	169	GLU	7.3
1	AAA	107	THR	7.3
1	BBB	106	ALA	7.3
1	FFF	113	SER	7.3
1	DDD	220	VAL	7.2
1	EEE	347	VAL	7.2
1	FFF	111	TRP	7.2
1	CCC	72	HIS	7.2
1	JJJ	71	GLU	7.2
1	JJJ	293	ALA	7.2
1	BBB	54	GLU	7.2
1	EEE	308	LEU	7.2
1	AAA	101	VAL	7.1
1	CCC	310	LYS	7.1
1	CCC	103	PRO	7.1
1	CCC	138	SER	7.1
1	EEE	262	GLU	7.1
1	EEE	111	TRP	7.1

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Mol	Chain	Res	Type	RSRZ
1	JJJ	24	GLN	7.1
1	III	50	PRO	7.1
1	BBB	53	ARG	7.0
1	CCC	96	ASN	7.0
1	DDD	96	ASN	7.0
1	FFF	50	PRO	7.0
1	FFF	169	GLU	7.0
1	DDD	108	LYS	7.0
1	EEE	344	MET	7.0
1	GGG	75	LYS	7.0
1	CCC	141	ASP	7.0
1	III	245	SER	7.0
1	BBB	103	PRO	7.0
1	FFF	120	ASP	7.0
1	CCC	174	ASP	7.0
1	FFF	28	ALA	6.9
1	III	45	ASP	6.9
1	BBB	328	THR	6.9
1	AAA	315	ASP	6.9
1	EEE	258	GLN	6.8
1	GGG	169	GLU	6.8
1	GGG	213	THR	6.8
1	EEE	159	ASN	6.8
1	III	106	ALA	6.8
1	HHH	147	SER	6.8
1	JJJ	292	ASN	6.8
1	BBB	220	VAL	6.8
1	FFF	239	ALA	6.8
1	AAA	94	THR	6.7
1	HHH	218	THR	6.7
1	CCC	344	MET	6.7
1	FFF	33	THR	6.7
1	DDD	101	VAL	6.7
1	EEE	25	SER	6.7
1	DDD	100	THR	6.7
1	JJJ	193	GLY	6.7
1	III	151	GLN	6.7
1	FFF	98	ILE	6.7
1	HHH	67	ARG	6.7
1	III	75	LYS	6.7
1	CCC	93	GLU	6.7
1	BBB	102	MET	6.7

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Mol	Chain	Res	Type	RSRZ
1	BBB	229	THR	6.6
1	GGG	212	VAL	6.6
1	EEE	267	SER	6.6
1	JJJ	326	SER	6.6
1	HHH	159	ASN	6.6
1	BBB	55	SER	6.6
1	III	220	VAL	6.6
1	GGG	343	GLN	6.5
1	III	167	VAL	6.5
1	BBB	218	THR	6.5
1	EEE	52	LEU	6.5
1	HHH	345	ALA	6.5
1	III	217	SER	6.5
1	JJJ	174	ASP	6.5
1	CCC	182	ILE	6.4
1	GGG	218	THR	6.4
1	CCC	245	SER	6.4
1	GGG	346	GLY	6.4
1	HHH	346	GLY	6.4
1	DDD	207	ALA	6.4
1	III	170	GLN	6.4
1	HHH	243	ASP	6.4
1	DDD	97	LEU	6.4
1	HHH	100	THR	6.4
1	FFF	172	ASN	6.4
1	DDD	102	MET	6.4
1	AAA	93	GLU	6.4
1	III	147	SER	6.4
1	DDD	311	GLY	6.4
1	BBB	191	VAL	6.3
1	BBB	324	THR	6.3
1	III	260	ASN	6.3
1	AAA	345	ALA	6.3
1	JJJ	343	GLN	6.3
1	JJJ	113	SER	6.3
1	FFF	124	GLU	6.3
1	DDD	104	SER	6.3
1	JJJ	313	ILE	6.3
1	DDD	43	PRO	6.3
1	GGG	47	GLY	6.3
1	JJJ	289	GLN	6.3
1	FFF	280	ALA	6.2

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Mol	Chain	Res	Type	RSRZ
1	EEE	24	GLN	6.2
1	CCC	238	GLY	6.2
1	CCC	113	SER	6.2
1	GGG	323	LEU	6.2
1	EEE	250	GLU	6.2
1	DDD	125	TYR	6.2
1	III	331	THR	6.2
1	FFF	243	ASP	6.2
1	III	230	ALA	6.2
1	HHH	228	MET	6.2
1	III	337	THR	6.2
1	FFF	40	GLN	6.1
1	EEE	55	SER	6.1
1	BBB	24	GLN	6.1
1	III	227	MET	6.1
1	AAA	304	LEU	6.1
1	III	323	LEU	6.1
1	CCC	271	SER	6.1
1	CCC	281	GLN	6.1
1	HHH	162	ASN	6.1
1	DDD	315	ASP	6.1
1	AAA	338	LYS	6.1
1	HHH	78	GLN	6.1
1	JJJ	220	VAL	6.1
1	III	283	ALA	6.1
1	CCC	248	ALA	6.0
1	EEE	292	ASN	6.0
1	DDD	162	ASN	6.0
1	FFF	330	VAL	6.0
1	CCC	312	ILE	6.0
1	AAA	300	GLU	6.0
1	EEE	56	GLU	6.0
1	JJJ	47	GLY	6.0
1	JJJ	276	LEU	6.0
1	CCC	347	VAL	6.0
1	BBB	243	ASP	6.0
1	EEE	299	SER	6.0
1	JJJ	342	GLN	6.0
1	DDD	38	VAL	6.0
1	CCC	258	GLN	5.9
1	HHH	89	GLN	5.9
1	AAA	344	MET	5.9

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Mol	Chain	Res	Type	RSRZ
1	EEE	50	PRO	5.9
1	EEE	172	ASN	5.9
1	HHH	172	ASN	5.9
1	AAA	299	SER	5.9
1	III	271	SER	5.9
1	AAA	45	ASP	5.9
1	DDD	239	ALA	5.9
1	CCC	260	ASN	5.9
1	FFF	99	SER	5.9
1	BBB	233	GLY	5.9
1	DDD	75	LYS	5.9
1	FFF	339	ILE	5.9
1	BBB	223	GLY	5.9
1	GGG	106	ALA	5.9
1	DDD	107	THR	5.9
1	EEE	53	ARG	5.9
1	EEE	143	LEU	5.9
1	CCC	135	THR	5.8
1	AAA	57	ARG	5.8
1	GGG	225	ILE	5.8
1	GGG	164	ASN	5.8
1	HHH	163	GLY	5.8
1	JJJ	190	VAL	5.8
1	JJJ	299	SER	5.8
1	JJJ	280	ALA	5.8
1	CCC	262	GLU	5.8
1	BBB	96	ASN	5.8
1	DDD	60	ASN	5.8
1	DDD	33	THR	5.8
1	DDD	223	GLY	5.8
1	HHH	226	ALA	5.8
1	DDD	36	ASN	5.8
1	DDD	292	ASN	5.8
1	III	104	SER	5.8
1	DDD	326	SER	5.8
1	DDD	44	VAL	5.8
1	AAA	216	THR	5.8
1	EEE	165	ASN	5.8
1	EEE	215	GLY	5.7
1	DDD	181	ALA	5.7
1	HHH	25	SER	5.7
1	BBB	287	ALA	5.7

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Mol	Chain	Res	Type	RSRZ
1	CCC	74	LEU	5.7
1	AAA	335	ASP	5.7
1	GGG	17	MET	5.7
1	DDD	129	SER	5.7
1	CCC	146	ASP	5.7
1	FFF	27	GLN	5.7
1	FFF	204	ALA	5.7
1	JJJ	248	ALA	5.7
1	III	100	THR	5.7
1	BBB	254	ARG	5.7
1	JJJ	239	ALA	5.7
1	GGG	87	ASN	5.7
1	AAA	35	CYS	5.7
1	JJJ	327	GLN	5.7
1	EEE	17	MET	5.6
1	III	148	ASN	5.6
1	FFF	47	GLY	5.6
1	DDD	183	ASP	5.6
1	CCC	148	ASN	5.6
1	EEE	303	THR	5.6
1	FFF	216	THR	5.6
1	HHH	170	GLN	5.6
1	FFF	217	SER	5.6
1	CCC	167	VAL	5.6
1	EEE	33	THR	5.6
1	AAA	90	ASP	5.6
1	AAA	156	ASN	5.6
1	FFF	160	VAL	5.6
1	BBB	225	ILE	5.6
1	HHH	104	SER	5.6
1	AAA	157	LEU	5.6
1	HHH	47	GLY	5.6
1	FFF	65	ALA	5.6
1	BBB	97	LEU	5.6
1	EEE	311	GLY	5.5
1	AAA	211	LEU	5.5
1	HHH	68	GLN	5.5
1	JJJ	150	TYR	5.5
1	DDD	191	VAL	5.5
1	JJJ	306	ALA	5.5
1	EEE	156	ASN	5.5
1	BBB	132	THR	5.5

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Mol	Chain	Res	Type	RSRZ
1	III	54	GLU	5.5
1	CCC	320	GLN	5.5
1	JJJ	39	ARG	5.5
1	AAA	91	TYR	5.5
1	DDD	122	ALA	5.5
1	EEE	187	ALA	5.5
1	FFF	343	GLN	5.5
1	HHH	347	VAL	5.5
1	EEE	337	THR	5.5
1	III	40	GLN	5.5
1	CCC	156	ASN	5.5
1	III	180	ALA	5.5
1	AAA	179	ASN	5.4
1	EEE	131	ASN	5.4
1	FFF	75	LYS	5.4
1	EEE	103	PRO	5.4
1	BBB	75	LYS	5.4
1	BBB	209	ALA	5.4
1	CCC	165	ASN	5.4
1	CCC	48	ARG	5.4
1	EEE	253	TYR	5.4
1	HHH	246	LEU	5.4
1	III	66	ALA	5.4
1	JJJ	99	SER	5.4
1	HHH	69	HIS	5.4
1	HHH	250	GLU	5.4
1	DDD	47	GLY	5.4
1	HHH	208	VAL	5.4
1	JJJ	322	PHE	5.4
1	EEE	20	GLY	5.4
1	JJJ	319	ARG	5.3
1	FFF	117	MET	5.3
1	FFF	158	ASN	5.3
1	FFF	246	LEU	5.3
1	BBB	285	THR	5.3
1	FFF	333	VAL	5.3
1	AAA	17	MET	5.3
1	CCC	21	MET	5.3
1	CCC	183	ASP	5.3
1	GGG	147	SER	5.3
1	HHH	108	LYS	5.3
1	EEE	104	SER	5.3

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Mol	Chain	Res	Type	RSRZ
1	GGG	55	SER	5.3
1	HHH	342	GLN	5.3
1	EEE	317	PHE	5.3
1	AAA	159	ASN	5.3
1	AAA	347	VAL	5.3
1	III	27	GLN	5.3
1	BBB	104	SER	5.3
1	EEE	57	ARG	5.3
1	HHH	34	TYR	5.3
1	CCC	202	VAL	5.3
1	JJJ	112	LEU	5.3
1	BBB	143	LEU	5.2
1	DDD	67	ARG	5.2
1	CCC	346	GLY	5.2
1	III	226	ALA	5.2
1	EEE	82	ILE	5.2
1	GGG	185	ALA	5.2
1	HHH	232	ALA	5.2
1	HHH	50	PRO	5.2
1	JJJ	100	THR	5.2
1	FFF	226	ALA	5.2
1	GGG	344	MET	5.2
1	FFF	93	GLU	5.2
1	DDD	243	ASP	5.2
1	GGG	117	MET	5.2
1	JJJ	129	SER	5.2
1	CCC	177	GLY	5.2
1	GGG	332	LYS	5.2
1	CCC	307	ASN	5.1
1	III	332	LYS	5.1
1	DDD	210	GLY	5.1
1	GGG	170	GLN	5.1
1	EEE	140	ASN	5.1
1	DDD	28	ALA	5.1
1	CCC	175	ILE	5.1
1	DDD	213	THR	5.1
1	DDD	232	ALA	5.1
1	HHH	205	ILE	5.1
1	III	169	GLU	5.1
1	CCC	341	LYS	5.1
1	DDD	343	GLN	5.1
1	DDD	331	THR	5.1

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Mol	Chain	Res	Type	RSRZ
1	JJJ	310	LYS	5.1
1	AAA	67	ARG	5.1
1	FFF	342	GLN	5.1
1	AAA	96	ASN	5.1
1	CCC	106	ALA	5.1
1	CCC	71	GLU	5.1
1	GGG	263	VAL	5.1
1	AAA	258	GLN	5.1
1	DDD	174	ASP	5.1
1	FFF	49	PHE	5.0
1	BBB	226	ALA	5.0
1	CCC	181	ALA	5.0
1	AAA	279	GLN	5.0
1	BBB	66	ALA	5.0
1	JJJ	243	ASP	5.0
1	BBB	193	GLY	5.0
1	EEE	21	MET	5.0
1	DDD	233	GLY	5.0
1	EEE	76	ASP	5.0
1	III	311	GLY	5.0
1	JJJ	134	ARG	5.0
1	FFF	310	LYS	5.0
1	DDD	258	GLN	5.0
1	JJJ	40	GLN	5.0
1	EEE	220	VAL	5.0
1	CCC	142	LYS	5.0
1	CCC	134	ARG	5.0
1	CCC	287	ALA	5.0
1	GGG	53	ARG	5.0
1	EEE	263	VAL	5.0
1	GGG	82	ILE	5.0
1	FFF	184	GLY	5.0
1	EEE	91	TYR	5.0
1	AAA	43	PRO	5.0
1	FFF	51	ASN	5.0
1	AAA	331	THR	5.0
1	CCC	226	ALA	5.0
1	EEE	249	ARG	5.0
1	EEE	283	ALA	5.0
1	FFF	329	SER	4.9
1	CCC	67	ARG	4.9
1	CCC	339	ILE	4.9

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Mol	Chain	Res	Type	RSRZ
1	EEE	46	PHE	4.9
1	BBB	48	ARG	4.9
1	GGG	130	ALA	4.9
1	GGG	270	GLY	4.9
1	HHH	324	THR	4.9
1	JJJ	303	THR	4.9
1	DDD	27	GLN	4.9
1	GGG	100	THR	4.9
1	CCC	83	ARG	4.9
1	JJJ	314	ASP	4.9
1	FFF	74	LEU	4.9
1	JJJ	103	PRO	4.9
1	DDD	180	ALA	4.9
1	JJJ	187	ALA	4.9
1	CCC	36	ASN	4.9
1	DDD	291	ASN	4.9
1	FFF	156	ASN	4.9
1	JJJ	41	GLN	4.9
1	AAA	79	PRO	4.9
1	GGG	109	GLU	4.9
1	DDD	163	GLY	4.9
1	BBB	255	ASP	4.9
1	III	126	GLN	4.9
1	CCC	131	ASN	4.9
1	DDD	179	ASN	4.9
1	III	179	ASN	4.9
1	HHH	217	SER	4.8
1	GGG	324	THR	4.8
1	III	229	THR	4.8
1	HHH	225	ILE	4.8
1	CCC	272	GLY	4.8
1	GGG	198	GLY	4.8
1	EEE	327	GLN	4.8
1	BBB	238	GLY	4.8
1	FFF	69	HIS	4.8
1	CCC	220	VAL	4.8
1	DDD	295	ASP	4.8
1	EEE	71	GLU	4.8
1	AAA	97	LEU	4.8
1	CCC	104	SER	4.8
1	BBB	342	GLN	4.8
1	HHH	82	ILE	4.8

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Mol	Chain	Res	Type	RSRZ
1	DDD	187	ALA	4.8
1	HHH	70	ALA	4.8
1	DDD	111	TRP	4.8
1	AAA	71	GLU	4.8
1	CCC	327	GLN	4.8
1	JJJ	45	ASP	4.8
1	CCC	87	ASN	4.8
1	EEE	74	LEU	4.8
1	EEE	164	ASN	4.8
1	GGG	69	HIS	4.8
1	EEE	255	ASP	4.8
1	AAA	124	GLU	4.7
1	III	241	VAL	4.8
1	AAA	106	ALA	4.7
1	DDD	57	ARG	4.7
1	HHH	48	ARG	4.7
1	III	174	ASP	4.7
1	III	309	ARG	4.7
1	III	118	VAL	4.7
1	III	278	THR	4.7
1	DDD	240	ILE	4.7
1	HHH	169	GLU	4.7
1	CCC	233	GLY	4.7
1	FFF	279	GLN	4.7
1	GGG	184	GLY	4.7
1	BBB	241	VAL	4.7
1	AAA	75	LYS	4.7
1	DDD	286	ALA	4.7
1	JJJ	330	VAL	4.7
1	HHH	86	THR	4.7
1	CCC	164	ASN	4.7
1	GGG	131	ASN	4.7
1	BBB	210	GLY	4.7
1	DDD	290	MET	4.7
1	FFF	112	LEU	4.7
1	DDD	66	ALA	4.7
1	FFF	36	ASN	4.7
1	GGG	336	GLY	4.7
1	FFF	261	SER	4.7
1	GGG	19	ASP	4.7
1	JJJ	335	ASP	4.7
1	HHH	298	THR	4.7

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Mol	Chain	Res	Type	RSRZ
1	CCC	196	VAL	4.7
1	III	343	GLN	4.7
1	CCC	111	TRP	4.7
1	CCC	69	HIS	4.7
1	DDD	56	GLU	4.7
1	EEE	298	THR	4.7
1	GGG	39	ARG	4.7
1	JJJ	188	GLY	4.6
1	BBB	162	ASN	4.6
1	EEE	268	GLN	4.6
1	JJJ	119	SER	4.6
1	GGG	280	ALA	4.6
1	GGG	174	ASP	4.6
1	EEE	229	THR	4.6
1	CCC	242	LEU	4.6
1	CCC	259	LEU	4.6
1	III	24	GLN	4.6
1	EEE	280	ALA	4.6
1	III	53	ARG	4.6
1	III	282	SER	4.6
1	BBB	50	PRO	4.6
1	HHH	19	ASP	4.6
1	DDD	287	ALA	4.6
1	GGG	65	ALA	4.6
1	EEE	47	GLY	4.6
1	CCC	170	GLN	4.6
1	EEE	287	ALA	4.6
1	EEE	313	ILE	4.6
1	III	161	VAL	4.6
1	BBB	26	SER	4.6
1	FFF	97	LEU	4.6
1	GGG	104	SER	4.6
1	EEE	120	ASP	4.6
1	HHH	309	ARG	4.6
1	AAA	243	ASP	4.6
1	III	146	ASP	4.6
1	BBB	213	THR	4.6
1	AAA	84	ASN	4.6
1	CCC	178	ILE	4.5
1	CCC	201	ILE	4.5
1	III	198	GLY	4.5
1	GGG	127	GLU	4.5

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Mol	Chain	Res	Type	RSRZ
1	FFF	340	ILE	4.5
1	JJJ	28	ALA	4.5
1	AAA	166	GLY	4.5
1	EEE	122	ALA	4.5
1	JJJ	290	MET	4.5
1	EEE	49	PHE	4.5
1	AAA	184	GLY	4.5
1	CCC	305	ASN	4.5
1	JJJ	173	ARG	4.5
1	HHH	29	LEU	4.5
1	AAA	70	ALA	4.5
1	FFF	157	LEU	4.5
1	AAA	346	GLY	4.5
1	III	255	ASP	4.5
1	FFF	241	VAL	4.5
1	AAA	250	GLU	4.5
1	EEE	228	MET	4.5
1	JJJ	114	ALA	4.5
1	AAA	267	SER	4.5
1	CCC	289	GLN	4.5
1	GGG	43	PRO	4.5
1	III	342	GLN	4.5
1	AAA	321	LEU	4.5
1	CCC	321	LEU	4.5
1	DDD	86	THR	4.5
1	GGG	183	ASP	4.5
1	BBB	144	ILE	4.5
1	CCC	316	SER	4.5
1	HHH	242	LEU	4.4
1	HHH	165	ASN	4.4
1	EEE	332	LYS	4.4
1	BBB	327	GLN	4.4
1	GGG	67	ARG	4.4
1	DDD	335	ASP	4.4
1	BBB	185	ALA	4.4
1	JJJ	181	ALA	4.4
1	HHH	336	GLY	4.4
1	AAA	55	SER	4.4
1	CCC	160	VAL	4.4
1	EEE	217	SER	4.4
1	EEE	94	THR	4.4
1	EEE	135	THR	4.4

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Mol	Chain	Res	Type	RSRZ
1	FFF	80	LEU	4.4
1	BBB	51	ASN	4.4
1	DDD	159	ASN	4.4
1	HHH	75	LYS	4.4
1	EEE	37	SER	4.4
1	EEE	248	ALA	4.4
1	HHH	193	GLY	4.4
1	EEE	179	ASN	4.4
1	AAA	32	GLN	4.4
1	AAA	89	GLN	4.4
1	EEE	279	GLN	4.4
1	III	46	PHE	4.4
1	EEE	152	LEU	4.4
1	BBB	288	THR	4.4
1	BBB	295	ASP	4.4
1	EEE	216	THR	4.4
1	EEE	302	GLU	4.4
1	JJJ	55	SER	4.4
1	AAA	309	ARG	4.4
1	EEE	39	ARG	4.4
1	JJJ	275	GLY	4.4
1	CCC	17	MET	4.4
1	HHH	327	GLN	4.4
1	III	277	GLN	4.4
1	EEE	129	SER	4.3
1	BBB	31	ILE	4.3
1	HHH	35	CYS	4.3
1	AAA	44	VAL	4.3
1	III	320	GLN	4.3
1	BBB	325	ALA	4.3
1	AAA	339	ILE	4.3
1	GGG	189	ILE	4.3
1	III	274	ARG	4.3
1	BBB	208	VAL	4.3
1	JJJ	43	PRO	4.3
1	CCC	279	GLN	4.3
1	HHH	277	GLN	4.3
1	JJJ	27	GLN	4.3
1	BBB	82	ILE	4.3
1	JJJ	340	ILE	4.3
1	CCC	247	SER	4.3
1	FFF	234	GLY	4.3

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Mol	Chain	Res	Type	RSRZ
1	FFF	245	SER	4.3
1	AAA	54	GLU	4.3
1	GGG	217	SER	4.3
1	BBB	43	PRO	4.3
1	CCC	172	ASN	4.3
1	GGG	228	MET	4.3
1	HHH	60	ASN	4.3
1	AAA	20	GLY	4.3
1	BBB	217	SER	4.3
1	CCC	23	ALA	4.3
1	CCC	314	ASP	4.3
1	JJJ	312	ILE	4.3
1	EEE	202	VAL	4.3
1	BBB	108	LYS	4.3
1	DDD	158	ASN	4.3
1	HHH	332	LYS	4.3
1	EEE	316	SER	4.3
1	DDD	236	ILE	4.3
1	BBB	266	ALA	4.3
1	FFF	286	ALA	4.3
1	BBB	277	GLN	4.3
1	JJJ	246	LEU	4.3
1	JJJ	175	ILE	4.2
1	EEE	132	THR	4.2
1	FFF	324	THR	4.2
1	HHH	310	LYS	4.2
1	JJJ	273	TYR	4.2
1	HHH	315	ASP	4.2
1	BBB	131	ASN	4.2
1	HHH	260	ASN	4.2
1	AAA	326	SER	4.2
1	AAA	329	SER	4.2
1	CCC	99	SER	4.2
1	EEE	329	SER	4.2
1	HHH	207	ALA	4.2
1	HHH	248	ALA	4.2
1	CCC	102	MET	4.2
1	EEE	100	THR	4.2
1	EEE	328	THR	4.2
1	AAA	342	GLN	4.2
1	FFF	60	ASN	4.2
1	FFF	70	ALA	4.2

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Mol	Chain	Res	Type	RSRZ
1	GGG	111	TRP	4.2
1	III	92	PHE	4.2
1	AAA	151	GLN	4.2
1	CCC	89	GLN	4.2
1	III	219	PRO	4.2
1	BBB	333	VAL	4.2
1	EEE	22	ASN	4.2
1	EEE	158	ASN	4.2
1	GGG	287	ALA	4.2
1	HHH	171	LEU	4.2
1	EEE	75	LYS	4.2
1	EEE	260	ASN	4.2
1	HHH	188	GLY	4.2
1	GGG	236	ILE	4.2
1	III	81	ILE	4.2
1	HHH	39	ARG	4.2
1	AAA	129	SER	4.2
1	DDD	288	THR	4.2
1	BBB	149	ASN	4.1
1	CCC	47	GLY	4.1
1	GGG	105	GLY	4.1
1	BBB	299	SER	4.1
1	HHH	247	SER	4.1
1	EEE	126	GLN	4.1
1	FFF	151	GLN	4.1
1	JJJ	70	ALA	4.1
1	FFF	146	ASP	4.1
1	BBB	237	GLY	4.1
1	EEE	136	ILE	4.1
1	EEE	168	LEU	4.1
1	GGG	326	SER	4.1
1	HHH	258	GLN	4.1
1	HHH	320	GLN	4.1
1	AAA	29	LEU	4.1
1	AAA	48	ARG	4.1
1	GGG	159	ASN	4.1
1	FFF	79	PRO	4.1
1	FFF	129	SER	4.1
1	GGG	337	THR	4.1
1	JJJ	331	THR	4.1
1	FFF	163	GLY	4.1
1	GGG	74	LEU	4.1

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Mol	Chain	Res	Type	RSRZ
1	HHH	141	ASP	4.1
1	BBB	310	LYS	4.1
1	AAA	30	HIS	4.1
1	FFF	155	VAL	4.1
1	AAA	165	ASN	4.1
1	EEE	290	MET	4.1
1	GGG	60	ASN	4.1
1	AAA	126	GLN	4.1
1	BBB	207	ALA	4.1
1	GGG	345	ALA	4.1
1	III	63	LEU	4.1
1	BBB	81	ILE	4.1
1	BBB	311	GLY	4.1
1	GGG	98	ILE	4.1
1	CCC	219	PRO	4.1
1	DDD	282	SER	4.1
1	FFF	100	THR	4.1
1	GGG	223	GLY	4.1
1	JJJ	300	GLU	4.1
1	AAA	291	ASN	4.1
1	FFF	325	ALA	4.1
1	GGG	232	ALA	4.1
1	CCC	270	GLY	4.1
1	III	65	ALA	4.0
1	AAA	131	ASN	4.0
1	CCC	60	ASN	4.0
1	EEE	309	ARG	4.0
1	EEE	282	SER	4.0
1	HHH	138	SER	4.0
1	DDD	74	LEU	4.0
1	AAA	114	ALA	4.0
1	GGG	124	GLU	4.0
1	HHH	204	ALA	4.0
1	GGG	163	GLY	4.0
1	BBB	227	MET	4.0
1	EEE	106	ALA	4.0
1	CCC	68	GLN	4.0
1	BBB	140	ASN	4.0
1	III	51	ASN	4.0
1	JJJ	34	TYR	4.0
1	AAA	80	LEU	4.0
1	BBB	239	ALA	4.0

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Mol	Chain	Res	Type	RSRZ
1	HHH	66	ALA	4.0
1	III	122	ALA	4.0
1	HHH	76	ASP	4.0
1	BBB	58	GLN	4.0
1	EEE	51	ASN	4.0
1	GGG	51	ASN	4.0
1	GGG	267	SER	4.0
1	III	326	SER	4.0
1	EEE	23	ALA	4.0
1	CCC	199	GLY	4.0
1	CCC	343	GLN	4.0
1	III	281	GLN	4.0
1	FFF	96	ASN	4.0
1	EEE	230	ALA	4.0
1	EEE	293	ALA	4.0
1	HHH	107	THR	4.0
1	BBB	300	GLU	4.0
1	FFF	102	MET	4.0
1	EEE	115	LEU	4.0
1	GGG	176	ASP	4.0
1	BBB	89	GLN	4.0
1	DDD	281	GLN	4.0
1	JJJ	307	ASN	4.0
1	GGG	207	ALA	4.0
1	GGG	230	ALA	4.0
1	AAA	167	VAL	4.0
1	BBB	71	GLU	3.9
1	GGG	311	GLY	3.9
1	CCC	315	ASP	3.9
1	EEE	45	ASP	3.9
1	FFF	295	ASP	3.9
1	BBB	232	ALA	3.9
1	EEE	84	ASN	3.9
1	JJJ	160	VAL	3.9
1	AAA	227	MET	3.9
1	DDD	252	LEU	3.9
1	FFF	30	HIS	3.9
1	AAA	262	GLU	3.9
1	DDD	110	GLN	3.9
1	HHH	230	ALA	3.9
1	III	187	ALA	3.9
1	FFF	140	ASN	3.9

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Mol	Chain	Res	Type	RSRZ
1	EEE	121	LYS	3.9
1	GGG	20	GLY	3.9
1	AAA	88	ILE	3.9
1	CCC	145	ILE	3.9
1	GGG	320	GLN	3.9
1	JJJ	68	GLN	3.9
1	FFF	45	ASP	3.9
1	JJJ	295	ASP	3.9
1	JJJ	185	ALA	3.9
1	EEE	323	LEU	3.9
1	EEE	32	GLN	3.9
1	EEE	78	GLN	3.9
1	CCC	28	ALA	3.9
1	EEE	157	LEU	3.9
1	HHH	22	ASN	3.9
1	JJJ	165	ASN	3.9
1	BBB	267	SER	3.9
1	DDD	318	LEU	3.9
1	DDD	103	PRO	3.9
1	FFF	272	GLY	3.9
1	FFF	182	ILE	3.9
1	EEE	261	SER	3.9
1	EEE	28	ALA	3.9
1	JJJ	58	GLN	3.9
1	DDD	120	ASP	3.9
1	III	76	ASP	3.9
1	DDD	206	GLY	3.9
1	BBB	156	ASN	3.9
1	EEE	118	VAL	3.9
1	GGG	71	GLU	3.9
1	FFF	322	PHE	3.8
1	GGG	278	THR	3.8
1	HHH	344	MET	3.8
1	GGG	116	GLY	3.8
1	III	72	HIS	3.8
1	III	319	ARG	3.8
1	JJJ	53	ARG	3.8
1	JJJ	191	VAL	3.8
1	FFF	56	GLU	3.8
1	JJJ	169	GLU	3.8
1	JJJ	329	SER	3.8
1	AAA	40	GLN	3.8

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Mol	Chain	Res	Type	RSRZ
1	AAA	298	THR	3.8
1	BBB	320	GLN	3.8
1	III	43	PRO	3.8
1	FFF	336	GLY	3.8
1	HHH	290	MET	3.8
1	AAA	87	ASN	3.8
1	EEE	180	ALA	3.8
1	III	93	GLU	3.8
1	DDD	249	ARG	3.8
1	JJJ	309	ARG	3.8
1	BBB	45	ASP	3.8
1	CCC	76	ASP	3.8
1	III	176	ASP	3.8
1	JJJ	54	GLU	3.8
1	JJJ	236	ILE	3.8
1	DDD	94	THR	3.8
1	EEE	194	LEU	3.8
1	FFF	64	GLY	3.8
1	AAA	154	VAL	3.8
1	JJJ	333	VAL	3.8
1	GGG	300	GLU	3.8
1	JJJ	63	LEU	3.8
1	BBB	319	ARG	3.8
1	III	33	THR	3.8
1	CCC	330	VAL	3.8
1	DDD	212	VAL	3.8
1	EEE	310	LYS	3.8
1	DDD	253	TYR	3.8
1	BBB	28	ALA	3.8
1	FFF	266	ALA	3.8
1	DDD	224	GLY	3.8
1	CCC	331	THR	3.8
1	DDD	118	VAL	3.8
1	GGG	44	VAL	3.8
1	AAA	180	ALA	3.8
1	BBB	315	ASP	3.8
1	DDD	98	ILE	3.8
1	HHH	72	HIS	3.8
1	EEE	264	LEU	3.8
1	CCC	179	ASN	3.7
1	GGG	244	LYS	3.7
1	BBB	147	SER	3.7

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Mol	Chain	Res	Type	RSRZ
1	DDD	119	SER	3.7
1	HHH	26	SER	3.7
1	JJJ	117	MET	3.7
1	FFF	176	ASP	3.7
1	GGG	262	GLU	3.7
1	AAA	164	ASN	3.7
1	FFF	229	THR	3.7
1	III	303	THR	3.7
1	EEE	334	LEU	3.7
1	DDD	46	PHE	3.7
1	DDD	124	GLU	3.7
1	HHH	249	ARG	3.7
1	HHH	103	PRO	3.7
1	GGG	37	SER	3.7
1	DDD	178	ILE	3.7
1	EEE	239	ALA	3.7
1	HHH	23	ALA	3.7
1	DDD	270	GLY	3.7
1	AAA	119	SER	3.7
1	BBB	70	ALA	3.7
1	FFF	283	ALA	3.7
1	III	28	ALA	3.7
1	BBB	94	THR	3.7
1	BBB	100	THR	3.7
1	EEE	154	VAL	3.7
1	CCC	137	GLY	3.7
1	EEE	77	ILE	3.7
1	JJJ	277	GLN	3.7
1	JJJ	285	THR	3.7
1	BBB	317	PHE	3.7
1	BBB	195	LEU	3.7
1	AAA	268	GLN	3.7
1	AAA	25	SER	3.7
1	BBB	322	PHE	3.7
1	DDD	48	ARG	3.7
1	DDD	53	ARG	3.7
1	JJJ	101	VAL	3.7
1	AAA	195	LEU	3.7
1	CCC	109	GLU	3.7
1	GGG	302	GLU	3.7
1	JJJ	250	GLU	3.7
1	AAA	251	LYS	3.7

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Mol	Chain	Res	Type	RSRZ
1	CCC	332	LYS	3.7
1	FFF	183	ASP	3.7
1	FFF	55	SER	3.6
1	BBB	112	LEU	3.6
1	EEE	219	PRO	3.6
1	FFF	103	PRO	3.6
1	DDD	71	GLU	3.6
1	GGG	93	GLU	3.6
1	EEE	345	ALA	3.6
1	HHH	28	ALA	3.6
1	III	89	GLN	3.6
1	JJJ	111	TRP	3.6
1	JJJ	325	ALA	3.6
1	CCC	85	VAL	3.6
1	GGG	38	VAL	3.6
1	AAA	22	ASN	3.6
1	CCC	112	LEU	3.6
1	CCC	152	LEU	3.6
1	CCC	20	GLY	3.6
1	FFF	82	ILE	3.6
1	JJJ	278	THR	3.6
1	FFF	262	GLU	3.6
1	AAA	306	ALA	3.6
1	FFF	232	ALA	3.6
1	FFF	38	VAL	3.6
1	EEE	184	GLY	3.6
1	AAA	162	ASN	3.6
1	AAA	260	ASN	3.6
1	CCC	51	ASN	3.6
1	CCC	299	SER	3.6
1	DDD	51	ASN	3.6
1	JJJ	341	LYS	3.6
1	HHH	150	TYR	3.6
1	CCC	101	VAL	3.6
1	GGG	101	VAL	3.6
1	AAA	26	SER	3.6
1	CCC	282	SER	3.6
1	AAA	127	GLU	3.6
1	DDD	39	ARG	3.6
1	DDD	185	ALA	3.6
1	III	322	PHE	3.6
1	BBB	234	GLY	3.6

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Mol	Chain	Res	Type	RSRZ
1	CCC	90	ASP	3.6
1	HHH	270	GLY	3.6
1	JJJ	183	ASP	3.6
1	DDD	50	PRO	3.6
1	GGG	299	SER	3.6
1	HHH	179	ASN	3.6
1	JJJ	260	ASN	3.6
1	JJJ	305	ASN	3.6
1	CCC	306	ALA	3.6
1	JJJ	218	THR	3.6
1	DDD	340	ILE	3.6
1	III	64	GLY	3.6
1	JJJ	234	GLY	3.6
1	AAA	317	PHE	3.6
1	FFF	307	ASN	3.6
1	HHH	180	ALA	3.6
1	III	69	HIS	3.6
1	DDD	93	GLU	3.6
1	FFF	54	GLU	3.6
1	BBB	313	ILE	3.6
1	CCC	246	LEU	3.5
1	GGG	257	SER	3.5
1	GGG	271	SER	3.5
1	AAA	278	THR	3.5
1	CCC	100	THR	3.5
1	BBB	240	ILE	3.5
1	DDD	341	LYS	3.5
1	AAA	116	GLY	3.5
1	CCC	234	GLY	3.5
1	AAA	323	LEU	3.5
1	FFF	190	VAL	3.5
1	GGG	134	ARG	3.5
1	EEE	19	ASP	3.5
1	JJJ	90	ASP	3.5
1	GGG	110	GLN	3.5
1	HHH	118	VAL	3.5
1	FFF	141	ASP	3.5
1	FFF	174	ASP	3.5
1	GGG	315	ASP	3.5
1	DDD	99	SER	3.5
1	JJJ	124	GLU	3.5
1	AAA	234	GLY	3.5

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Mol	Chain	Res	Type	RSRZ
1	BBB	198	GLY	3.5
1	GGG	194	LEU	3.5
1	AAA	92	PHE	3.5
1	GGG	50	PRO	3.5
1	DDD	186	ILE	3.5
1	EEE	178	ILE	3.5
1	BBB	261	SER	3.5
1	FFF	247	SER	3.5
1	HHH	234	GLY	3.5
1	JJJ	336	GLY	3.5
1	EEE	38	VAL	3.5
1	JJJ	46	PHE	3.5
1	CCC	338	LYS	3.5
1	III	209	ALA	3.5
1	AAA	125	TYR	3.5
1	GGG	273	TYR	3.5
1	FFF	335	ASP	3.5
1	EEE	105	GLY	3.5
1	III	308	LEU	3.5
1	HHH	55	SER	3.5
1	BBB	172	ASN	3.5
1	FFF	86	THR	3.5
1	JJJ	268	GLN	3.5
1	EEE	341	LYS	3.5
1	JJJ	244	LYS	3.5
1	BBB	252	LEU	3.5
1	BBB	137	GLY	3.5
1	EEE	224	GLY	3.5
1	GGG	64	GLY	3.5
1	HHH	212	VAL	3.5
1	CCC	329	SER	3.5
1	CCC	32	GLN	3.5
1	JJJ	51	ASN	3.5
1	JJJ	94	THR	3.5
1	EEE	181	ALA	3.5
1	GGG	181	ALA	3.5
1	AAA	47	GLY	3.4
1	AAA	198	GLY	3.4
1	III	256	ARG	3.4
1	JJJ	57	ARG	3.4
1	JJJ	166	GLY	3.4
1	DDD	190	VAL	3.4

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Mol	Chain	Res	Type	RSRZ
1	GGG	76	ASP	3.4
1	EEE	124	GLU	3.4
1	BBB	187	ALA	3.4
1	DDD	313	ILE	3.4
1	HHH	340	ILE	3.4
1	EEE	35	CYS	3.4
1	BBB	67	ARG	3.4
1	DDD	188	GLY	3.4
1	EEE	212	VAL	3.4
1	FFF	319	ARG	3.4
1	III	30	HIS	3.4
1	JJJ	64	GLY	3.4
1	AAA	240	ILE	3.4
1	CCC	269	ILE	3.4
1	EEE	312	ILE	3.4
1	CCC	95	GLN	3.4
1	DDD	113	SER	3.4
1	FFF	66	ALA	3.4
1	FFF	209	ALA	3.4
1	GGG	32	GLN	3.4
1	GGG	268	GLN	3.4
1	DDD	148	ASN	3.4
1	JJJ	318	LEU	3.4
1	AAA	105	GLY	3.4
1	CCC	210	GLY	3.4
1	EEE	240	ILE	3.4
1	III	109	GLU	3.4
1	GGG	97	LEU	3.4
1	AAA	245	SER	3.4
1	III	208	VAL	3.4
1	BBB	47	GLY	3.4
1	EEE	72	HIS	3.4
1	HHH	197	ILE	3.4
1	JJJ	82	ILE	3.4
1	HHH	262	GLU	3.4
1	BBB	202	VAL	3.4
1	HHH	333	VAL	3.4
1	III	333	VAL	3.4
1	BBB	175	ILE	3.4
1	EEE	195	LEU	3.4
1	FFF	250	GLU	3.4
1	AAA	176	ASP	3.4

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Mol	Chain	Res	Type	RSRZ
1	GGG	95	GLN	3.4
1	III	315	ASP	3.4
1	DDD	85	VAL	3.4
1	GGG	99	SER	3.4
1	GGG	220	VAL	3.4
1	HHH	263	VAL	3.4
1	CCC	33	THR	3.4
1	DDD	116	GLY	3.4
1	III	162	ASN	3.4
1	DDD	63	LEU	3.4
1	EEE	232	ALA	3.4
1	BBB	142	LYS	3.4
1	FFF	90	ASP	3.4
1	GGG	196	VAL	3.4
1	AAA	36	ASN	3.4
1	DDD	218	THR	3.4
1	EEE	177	GLY	3.4
1	III	261	SER	3.4
1	GGG	86	THR	3.4
1	JJJ	61	THR	3.4
1	JJJ	215	GLY	3.4
1	DDD	54	GLU	3.3
1	CCC	241	VAL	3.3
1	DDD	41	GLN	3.3
1	DDD	263	VAL	3.3
1	AAA	141	ASP	3.3
1	BBB	105	GLY	3.3
1	HHH	297	LEU	3.3
1	III	144	ILE	3.3
1	FFF	131	ASN	3.3
1	GGG	179	ASN	3.3
1	GGG	283	ALA	3.3
1	HHH	106	ALA	3.3
1	AAA	46	PHE	3.3
1	BBB	169	GLU	3.3
1	BBB	228	MET	3.3
1	EEE	40	GLN	3.3
1	FFF	165	ASN	3.3
1	BBB	221	VAL	3.3
1	GGG	219	PRO	3.3
1	III	265	VAL	3.3
1	JJJ	197	ILE	3.3

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Mol	Chain	Res	Type	RSRZ
1	BBB	146	ASP	3.3
1	DDD	138	SER	3.3
1	AAA	207	ALA	3.3
1	FFF	130	ALA	3.3
1	FFF	181	ALA	3.3
1	BBB	111	TRP	3.3
1	EEE	208	VAL	3.3
1	III	44	VAL	3.3
1	HHH	253	TYR	3.3
1	AAA	78	GLN	3.3
1	DDD	105	GLY	3.3
1	BBB	174	ASP	3.3
1	GGG	25	SER	3.3
1	GGG	138	SER	3.3
1	AAA	39	ARG	3.3
1	GGG	57	ARG	3.3
1	HHH	256	ARG	3.3
1	AAA	60	ASN	3.3
1	III	156	ASN	3.3
1	AAA	253	TYR	3.3
1	EEE	88	ILE	3.3
1	III	178	ILE	3.3
1	CCC	121	LYS	3.3
1	GGG	142	LYS	3.3
1	BBB	120	ASP	3.3
1	BBB	335	ASP	3.3
1	DDD	204	ALA	3.3
1	DDD	322	PHE	3.3
1	III	295	ASP	3.3
1	JJJ	146	ASP	3.3
1	CCC	288	THR	3.3
1	FFF	104	SER	3.3
1	GGG	329	SER	3.3
1	HHH	94	THR	3.3
1	FFF	175	ILE	3.3
1	HHH	189	ILE	3.3
1	BBB	40	GLN	3.3
1	CCC	130	ALA	3.3
1	FFF	249	ARG	3.3
1	JJJ	106	ALA	3.3
1	AAA	290	MET	3.3
1	BBB	314	ASP	3.3

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Mol	Chain	Res	Type	RSRZ
1	BBB	326	SER	3.3
1	AAA	34	TYR	3.3
1	AAA	135	THR	3.3
1	FFF	337	THR	3.3
1	GGG	331	THR	3.3
1	III	26	SER	3.3
1	BBB	69	HIS	3.2
1	HHH	73	TYR	3.3
1	HHH	291	ASN	3.2
1	BBB	251	LYS	3.2
1	HHH	64	GLY	3.2
1	III	251	LYS	3.2
1	HHH	49	PHE	3.2
1	AAA	319	ARG	3.2
1	GGG	48	ARG	3.2
1	EEE	243	ASP	3.2
1	FFF	31	ILE	3.2
1	AAA	121	LYS	3.2
1	CCC	229	THR	3.2
1	DDD	55	SER	3.2
1	DDD	135	THR	3.2
1	HHH	331	THR	3.2
1	III	94	THR	3.2
1	CCC	184	GLY	3.2
1	CCC	311	GLY	3.2
1	FFF	327	GLN	3.2
1	GGG	289	GLN	3.2
1	AAA	293	ALA	3.2
1	CCC	118	VAL	3.2
1	CCC	333	VAL	3.2
1	JJJ	286	ALA	3.2
1	FFF	219	PRO	3.2
1	CCC	75	LYS	3.2
1	DDD	150	TYR	3.2
1	FFF	331	THR	3.2
1	BBB	284	VAL	3.2
1	CCC	66	ALA	3.2
1	CCC	151	GLN	3.2
1	III	58	GLN	3.2
1	III	171	LEU	3.2
1	CCC	185	ALA	3.2
1	EEE	70	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
1	CCC	88	ILE	3.2
1	EEE	175	ILE	3.2
1	AAA	86	THR	3.2
1	CCC	217	SER	3.2
1	FFF	203	THR	3.2
1	III	119	SER	3.2
1	BBB	334	LEU	3.2
1	CCC	252	LEU	3.2
1	GGG	292	ASN	3.2
1	BBB	32	GLN	3.2
1	CCC	230	ALA	3.2
1	III	130	ALA	3.2
1	AAA	210	GLY	3.2
1	JJJ	120	ASP	3.2
1	CCC	285	THR	3.2
1	GGG	113	SER	3.2
1	HHH	155	VAL	3.2
1	HHH	330	VAL	3.2
1	JJJ	263	VAL	3.2
1	BBB	98	ILE	3.2
1	CCC	162	ASN	3.2
1	FFF	268	GLN	3.2
1	GGG	342	GLN	3.2
1	JJJ	88	ILE	3.2
1	JJJ	320	GLN	3.2
1	III	35	CYS	3.2
1	III	143	LEU	3.2
1	CCC	161	VAL	3.2
1	HHH	241	VAL	3.2
1	CCC	205	ILE	3.2
1	FFF	61	THR	3.2
1	FFF	326	SER	3.2
1	GGG	28	ALA	3.2
1	III	207	ALA	3.2
1	III	247	SER	3.2
1	DDD	164	ASN	3.2
1	EEE	27	GLN	3.2
1	HHH	268	GLN	3.2
1	HHH	252	LEU	3.2
1	JJJ	171	LEU	3.2
1	BBB	212	VAL	3.2
1	FFF	235	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
1	DDD	229	THR	3.1
1	JJJ	245	SER	3.1
1	JJJ	96	ASN	3.1
1	AAA	274	ARG	3.1
1	DDD	254	ARG	3.1
1	FFF	313	ILE	3.1
1	HHH	338	LYS	3.1
1	III	286	ALA	3.1
1	III	287	ALA	3.1
1	AAA	295	ASP	3.1
1	BBB	76	ASP	3.1
1	AAA	324	THR	3.1
1	EEE	218	THR	3.1
1	HHH	271	SER	3.1
1	DDD	194	LEU	3.1
1	EEE	304	LEU	3.1
1	GGG	162	ASN	3.1
1	AAA	208	VAL	3.1
1	CCC	212	VAL	3.1
1	GGG	241	VAL	3.1
1	AAA	31	ILE	3.1
1	GGG	153	ILE	3.1
1	AAA	296	SER	3.1
1	EEE	107	THR	3.1
1	FFF	267	SER	3.1
1	GGG	33	THR	3.1
1	JJJ	301	LEU	3.1
1	EEE	289	GLN	3.1
1	CCC	254	ARG	3.1
1	HHH	167	VAL	3.1
1	DDD	312	ILE	3.1
1	HHH	269	ILE	3.1
1	JJJ	339	ILE	3.1
1	CCC	110	GLN	3.1
1	CCC	268	GLN	3.1
1	JJJ	196	VAL	3.1
1	BBB	116	GLY	3.1
1	DDD	136	ILE	3.1
1	GGG	182	ILE	3.1
1	III	88	ILE	3.1
1	AAA	281	GLN	3.1
1	HHH	58	GLN	3.1

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Mol	Chain	Res	Type	RSRZ
1	HHH	133	ARG	3.1
1	AAA	206	GLY	3.1
1	BBB	123	LYS	3.1
1	BBB	215	GLY	3.1
1	CCC	218	THR	3.1
1	DDD	337	THR	3.1
1	FFF	121	LYS	3.1
1	HHH	303	THR	3.1
1	FFF	179	ASN	3.1
1	DDD	317	PHE	3.1
1	HHH	173	ARG	3.1
1	DDD	59	ILE	3.1
1	FFF	68	GLN	3.1
1	FFF	186	ILE	3.1
1	BBB	216	THR	3.1
1	HHH	335	ASP	3.1
1	III	62	GLY	3.1
1	JJJ	271	SER	3.1
1	BBB	65	ALA	3.1
1	DDD	130	ALA	3.1
1	GGG	172	ASN	3.1
1	III	149	ASN	3.1
1	III	248	ALA	3.1
1	HHH	322	PHE	3.1
1	JJJ	30	HIS	3.1
1	DDD	117	MET	3.1
1	GGG	108	LYS	3.1
1	HHH	145	ILE	3.1
1	III	42	ILE	3.1
1	BBB	139	LEU	3.0
1	DDD	26	SER	3.0
1	DDD	45	ASP	3.0
1	DDD	146	ASP	3.0
1	DDD	176	ASP	3.0
1	GGG	282	SER	3.0
1	CCC	280	ALA	3.0
1	CCC	293	ALA	3.0
1	DDD	273	TYR	3.0
1	JJJ	308	LEU	3.0
1	BBB	316	SER	3.0
1	HHH	286	ALA	3.0
1	III	132	THR	3.0

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Mol	Chain	Res	Type	RSRZ
1	BBB	101	VAL	3.0
1	JJJ	172	ASN	3.0
1	EEE	210	GLY	3.0
1	FFF	323	LEU	3.0
1	GGG	250	GLU	3.0
1	DDD	115	LEU	3.0
1	HHH	300	GLU	3.0
1	AAA	28	ALA	3.0
1	BBB	138	SER	3.0
1	CCC	326	SER	3.0
1	FFF	285	THR	3.0
1	JJJ	332	LYS	3.0
1	DDD	133	ARG	3.0
1	AAA	178	ILE	3.0
1	FFF	242	LEU	3.0
1	JJJ	105	GLY	3.0
1	DDD	169	GLU	3.0
1	HHH	124	GLU	3.0
1	HHH	317	PHE	3.0
1	JJJ	207	ALA	3.0
1	CCC	155	VAL	3.0
1	AAA	174	ASP	3.0
1	BBB	205	ILE	3.0
1	CCC	236	ILE	3.0
1	HHH	183	ASP	3.0
1	DDD	171	LEU	3.0
1	FFF	311	GLY	3.0
1	JJJ	127	GLU	3.0
1	DDD	289	GLN	3.0
1	EEE	44	VAL	3.0
1	FFF	221	VAL	3.0
1	JJJ	227	MET	3.0
1	EEE	324	THR	3.0
1	GGG	245	SER	3.0
1	GGG	316	SER	3.0
1	HHH	261	SER	3.0
1	HHH	79	PRO	3.0
1	JJJ	177	GLY	3.0
1	BBB	165	ASN	3.0
1	JJJ	140	ASN	3.0
1	GGG	66	ALA	3.0
1	JJJ	130	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
1	FFF	170	GLN	3.0
1	GGG	256	ARG	3.0
1	JJJ	167	VAL	3.0
1	EEE	80	LEU	2.9
1	BBB	99	SER	2.9
1	AAA	273	TYR	2.9
1	CCC	50	PRO	2.9
1	JJJ	338	LYS	2.9
1	III	292	ASN	2.9
1	JJJ	180	ALA	2.9
1	AAA	38	VAL	2.9
1	BBB	263	VAL	2.9
1	AAA	289	GLN	2.9
1	BBB	289	GLN	2.9
1	DDD	145	ILE	2.9
1	HHH	53	ARG	2.9
1	HHH	59	ILE	2.9
1	AAA	303	THR	2.9
1	FFF	271	SER	2.9
1	GGG	107	THR	2.9
1	AAA	266	ALA	2.9
1	AAA	18	ASN	2.9
1	BBB	158	ASN	2.9
1	CCC	323	LEU	2.9
1	EEE	330	VAL	2.9
1	FFF	227	MET	2.9
1	GGG	77	ILE	2.9
1	HHH	77	ILE	2.9
1	FFF	294	TRP	2.9
1	EEE	34	TYR	2.9
1	HHH	257	SER	2.9
1	JJJ	37	SER	2.9
1	BBB	190	VAL	2.9
1	FFF	77	ILE	2.9
1	GGG	274	ARG	2.9
1	GGG	309	ARG	2.9
1	GGG	333	VAL	2.9
1	HHH	266	ALA	2.9
1	III	294	TRP	2.9
1	BBB	273	TYR	2.9
1	BBB	122	ALA	2.9
1	JJJ	203	THR	2.9

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Mol	Chain	Res	Type	RSRZ
1	BBB	30	HIS	2.9
1	BBB	90	ASP	2.9
1	III	120	ASP	2.9
1	JJJ	217	SER	2.9
1	FFF	109	GLU	2.9
1	III	327	GLN	2.9
1	FFF	171	LEU	2.9
1	JJJ	211	LEU	2.9
1	HHH	38	VAL	2.9
1	III	82	ILE	2.9
1	JJJ	201	ILE	2.9
1	AAA	113	SER	2.9
1	CCC	257	SER	2.9
1	EEE	113	SER	2.9
1	CCC	19	ASP	2.9
1	BBB	294	TRP	2.9
1	BBB	171	LEU	2.9
1	GGG	235	VAL	2.9
1	HHH	125	TYR	2.9
1	JJJ	50	PRO	2.9
1	JJJ	219	PRO	2.9
1	III	298	THR	2.9
1	HHH	45	ASP	2.9
1	EEE	127	GLU	2.9
1	AAA	68	GLN	2.9
1	CCC	27	GLN	2.9
1	FFF	29	LEU	2.9
1	BBB	57	ARG	2.8
1	III	340	ILE	2.8
1	CCC	107	THR	2.8
1	JJJ	35	CYS	2.8
1	JJJ	147	SER	2.8
1	EEE	54	GLU	2.8
1	BBB	279	GLN	2.8
1	III	233	GLY	2.8
1	CCC	158	ASN	2.8
1	EEE	48	ARG	2.8
1	EEE	274	ARG	2.8
1	III	306	ALA	2.8
1	FFF	341	LYS	2.8
1	AAA	285	THR	2.8
1	CCC	37	SER	2.8

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Mol	Chain	Res	Type	RSRZ
1	III	318	LEU	2.8
1	JJJ	107	THR	2.8
1	AAA	136	ILE	2.8
1	AAA	294	TRP	2.8
1	BBB	151	GLN	2.8
1	BBB	192	GLY	2.8
1	HHH	294	TRP	2.8
1	DDD	256	ARG	2.8
1	III	223	GLY	2.8
1	JJJ	224	GLY	2.8
1	BBB	291	ASN	2.8
1	DDD	149	ASN	2.8
1	HHH	142	LYS	2.8
1	BBB	278	THR	2.8
1	CCC	56	GLU	2.8
1	EEE	247	SER	2.8
1	EEE	300	GLU	2.8
1	GGG	243	ASP	2.8
1	III	268	GLN	2.8
1	JJJ	89	GLN	2.8
1	JJJ	110	GLN	2.8
1	JJJ	156	ASN	2.8
1	HHH	259	LEU	2.8
1	BBB	203	THR	2.8
1	DDD	284	VAL	2.8
1	GGG	254	ARG	2.8
1	EEE	193	GLY	2.8
1	HHH	326	SER	2.8
1	III	285	THR	2.8
1	HHH	90	ASP	2.8
1	DDD	266	ALA	2.8
1	CCC	18	ASN	2.8
1	EEE	18	ASN	2.8
1	FFF	291	ASN	2.8
1	JJJ	168	LEU	2.8
1	AAA	191	VAL	2.8
1	FFF	116	GLY	2.8
1	GGG	272	GLY	2.8
1	AAA	203	THR	2.8
1	AAA	229	THR	2.8
1	FFF	277	GLN	2.8
1	FFF	255	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
1	GGG	90	ASP	2.8
1	HHH	295	ASP	2.8
1	JJJ	122	ALA	2.8
1	JJJ	283	ALA	2.8
1	EEE	211	LEU	2.8
1	AAA	220	VAL	2.8
1	EEE	117	MET	2.8
1	BBB	170	GLN	2.8
1	DDD	78	GLN	2.8
1	FFF	32	GLN	2.8
1	FFF	41	GLN	2.8
1	III	124	GLU	2.8
1	DDD	76	ASP	2.8
1	CCC	38	VAL	2.7
1	DDD	144	ILE	2.7
1	GGG	307	ASN	2.7
1	GGG	312	ILE	2.7
1	HHH	284	VAL	2.7
1	III	197	ILE	2.7
1	CCC	231	GLY	2.7
1	FFF	108	LYS	2.7
1	HHH	137	GLY	2.7
1	III	272	GLY	2.7
1	HHH	209	ALA	2.7
1	JJJ	139	LEU	2.7
1	DDD	203	THR	2.7
1	III	49	PHE	2.7
1	GGG	175	ILE	2.7
1	DDD	134	ARG	2.7
1	JJJ	38	VAL	2.7
1	CCC	275	GLY	2.7
1	DDD	198	GLY	2.7
1	FFF	238	GLY	2.7
1	EEE	276	LEU	2.7
1	III	195	LEU	2.7
1	EEE	286	ALA	2.7
1	CCC	78	GLN	2.7
1	DDD	296	SER	2.7
1	EEE	138	SER	2.7
1	III	135	THR	2.7
1	FFF	144	ILE	2.7
1	CCC	173	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
1	DDD	83	ARG	2.7
1	HHH	274	ARG	2.7
1	JJJ	141	ASP	2.7
1	BBB	157	LEU	2.7
1	JJJ	125	TYR	2.7
1	CCC	92	PHE	2.7
1	CCC	337	THR	2.7
1	BBB	271	SER	2.7
1	CCC	44	VAL	2.7
1	EEE	26	SER	2.7
1	JJJ	221	VAL	2.7
1	CCC	290	MET	2.7
1	BBB	52	LEU	2.7
1	III	164	ASN	2.7
1	JJJ	87	ASN	2.7
1	JJJ	291	ASN	2.7
1	HHH	30	HIS	2.7
1	HHH	280	ALA	2.7
1	EEE	150	TYR	2.7
1	BBB	136	ILE	2.7
1	AAA	341	LYS	2.7
1	EEE	278	THR	2.7
1	DDD	297	LEU	2.7
1	DDD	234	GLY	2.7
1	DDD	238	GLY	2.7
1	FFF	92	PHE	2.7
1	FFF	187	ALA	2.7
1	JJJ	232	ALA	2.7
1	HHH	18	ASN	2.7
1	III	165	ASN	2.7
1	CCC	225	ILE	2.7
1	EEE	79	PRO	2.7
1	EEE	85	VAL	2.7
1	JJJ	249	ARG	2.7
1	FFF	298	THR	2.7
1	DDD	62	GLY	2.7
1	AAA	19	ASP	2.7
1	FFF	76	ASP	2.7
1	AAA	239	ALA	2.7
1	BBB	230	ALA	2.7
1	CCC	114	ALA	2.7
1	CCC	200	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	CCC	209	ALA	2.7
1	EEE	30	HIS	2.7
1	GGG	136	ILE	2.7
1	III	307	ASN	2.7
1	CCC	133	ARG	2.7
1	EEE	173	ARG	2.7
1	EEE	227	MET	2.7
1	III	194	LEU	2.7
1	EEE	257	SER	2.7
1	EEE	65	ALA	2.6
1	GGG	266	ALA	2.6
1	AAA	73	TYR	2.6
1	BBB	281	GLN	2.6
1	GGG	78	GLN	2.6
1	HHH	213	THR	2.6
1	CCC	129	SER	2.6
1	DDD	257	SER	2.6
1	FFF	138	SER	2.6
1	HHH	187	ALA	2.6
1	DDD	197	ILE	2.6
1	DDD	222	MET	2.6
1	HHH	115	LEU	2.6
1	AAA	158	ASN	2.6
1	DDD	307	ASN	2.6
1	III	291	ASN	2.6
1	EEE	41	GLN	2.6
1	III	71	GLU	2.6
1	FFF	177	GLY	2.6
1	BBB	280	ALA	2.6
1	CCC	278	THR	2.6
1	III	339	ILE	2.6
1	JJJ	67	ARG	2.6
1	JJJ	161	VAL	2.6
1	CCC	194	LEU	2.6
1	CCC	295	ASP	2.6
1	AAA	307	ASN	2.6
1	FFF	162	ASN	2.6
1	CCC	206	GLY	2.6
1	CCC	286	ALA	2.6
1	EEE	339	ILE	2.6
1	JJJ	42	ILE	2.6
1	DDD	132	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	AAA	217	SER	2.6
1	EEE	67	ARG	2.6
1	III	173	ARG	2.6
1	JJJ	324	THR	2.6
1	GGG	63	LEU	2.6
1	HHH	219	PRO	2.6
1	GGG	40	GLN	2.6
1	HHH	32	GLN	2.6
1	BBB	62	GLY	2.6
1	GGG	339	ILE	2.6
1	HHH	144	ILE	2.6
1	HHH	130	ALA	2.6
1	AAA	115	LEU	2.6
1	HHH	265	VAL	2.6
1	III	222	MET	2.6
1	III	37	SER	2.6
1	JJJ	76	ASP	2.6
1	BBB	145	ILE	2.6
1	DDD	153	ILE	2.6
1	DDD	269	ILE	2.6
1	CCC	65	ALA	2.6
1	DDD	128	VAL	2.6
1	GGG	167	VAL	2.6
1	AAA	247	SER	2.6
1	DDD	267	SER	2.6
1	DDD	299	SER	2.6
1	JJJ	296	SER	2.6
1	DDD	69	HIS	2.6
1	BBB	124	GLU	2.6
1	GGG	258	GLN	2.6
1	GGG	281	GLN	2.6
1	JJJ	151	GLN	2.6
1	BBB	148	ASN	2.6
1	CCC	265	VAL	2.6
1	EEE	284	VAL	2.6
1	GGG	291	ASN	2.6
1	JJJ	159	ASN	2.6
1	DDD	79	PRO	2.6
1	CCC	46	PHE	2.5
1	EEE	271	SER	2.5
1	BBB	312	ILE	2.5
1	BBB	184	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	DDD	334	LEU	2.5
1	FFF	52	LEU	2.5
1	GGG	146	ASP	2.5
1	GGG	295	ASP	2.5
1	HHH	63	LEU	2.5
1	III	269	ILE	2.5
1	JJJ	210	GLY	2.5
1	DDD	167	VAL	2.5
1	III	181	ALA	2.5
1	III	290	MET	2.5
1	GGG	61	THR	2.5
1	HHH	33	THR	2.5
1	JJJ	86	THR	2.5
1	FFF	297	LEU	2.5
1	GGG	195	LEU	2.5
1	III	186	ILE	2.5
1	FFF	191	VAL	2.5
1	GGG	193	GLY	2.5
1	AAA	343	GLN	2.5
1	DDD	68	GLN	2.5
1	JJJ	164	ASN	2.5
1	HHH	285	THR	2.5
1	JJJ	59	ILE	2.5
1	BBB	167	VAL	2.5
1	GGG	83	ARG	2.5
1	GGG	118	VAL	2.5
1	GGG	233	GLY	2.5
1	BBB	181	ALA	2.5
1	BBB	343	GLN	2.5
1	DDD	262	GLU	2.5
1	HHH	126	GLN	2.5
1	CCC	291	ASN	2.5
1	GGG	322	PHE	2.5
1	JJJ	79	PRO	2.5
1	HHH	178	ILE	2.5
1	BBB	270	GLY	2.5
1	FFF	237	GLY	2.5
1	FFF	288	THR	2.5
1	GGG	221	VAL	2.5
1	HHH	191	VAL	2.5
1	DDD	316	SER	2.5
1	BBB	73	TYR	2.5

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Mol	Chain	Res	Type	RSRZ
1	BBB	141	ASP	2.5
1	CCC	292	ASN	2.5
1	DDD	305	ASN	2.5
1	BBB	222	MET	2.5
1	CCC	336	GLY	2.5
1	DDD	184	GLY	2.5
1	FFF	53	ARG	2.5
1	III	137	GLY	2.5
1	BBB	135	THR	2.5
1	DDD	200	ALA	2.5
1	JJJ	226	ALA	2.5
1	FFF	264	LEU	2.5
1	GGG	211	LEU	2.5
1	GGG	314	ASP	2.5
1	III	312	ILE	2.5
1	III	313	ILE	2.5
1	HHH	44	VAL	2.5
1	CCC	163	GLY	2.5
1	BBB	86	THR	2.5
1	EEE	108	LYS	2.5
1	GGG	135	THR	2.5
1	CCC	126	GLN	2.5
1	III	262	GLU	2.5
1	EEE	236	ILE	2.5
1	III	31	ILE	2.5
1	CCC	79	PRO	2.5
1	DDD	90	ASP	2.5
1	FFF	315	ASP	2.5
1	CCC	235	VAL	2.5
1	FFF	83	ARG	2.5
1	BBB	336	GLY	2.5
1	FFF	198	GLY	2.5
1	HHH	51	ASN	2.5
1	AAA	65	ALA	2.5
1	BBB	298	THR	2.4
1	JJJ	80	LEU	2.4
1	AAA	316	SER	2.4
1	DDD	40	GLN	2.4
1	FFF	59	ILE	2.4
1	FFF	71	GLU	2.4
1	AAA	155	VAL	2.4
1	EEE	163	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	III	166	GLY	2.4
1	AAA	292	ASN	2.4
1	HHH	36	ASN	2.4
1	HHH	181	ALA	2.4
1	HHH	152	LEU	2.4
1	III	86	THR	2.4
1	AAA	37	SER	2.4
1	BBB	78	GLN	2.4
1	FFF	316	SER	2.4
1	III	300	GLU	2.4
1	HHH	235	VAL	2.4
1	JJJ	155	VAL	2.4
1	AAA	21	MET	2.4
1	GGG	149	ASN	2.4
1	JJJ	84	ASN	2.4
1	DDD	42	ILE	2.4
1	JJJ	253	TYR	2.4
1	AAA	117	MET	2.4
1	BBB	119	SER	2.4
1	HHH	134	ARG	2.4
1	III	38	VAL	2.4
1	III	196	VAL	2.4
1	AAA	64	GLY	2.4
1	DDD	199	GLY	2.4
1	EEE	338	LYS	2.4
1	GGG	310	LYS	2.4
1	III	243	ASP	2.4
1	JJJ	233	GLY	2.4
1	AAA	122	ALA	2.4
1	CCC	122	ALA	2.4
1	CCC	232	ALA	2.4
1	GGG	171	LEU	2.4
1	JJJ	230	ALA	2.4
1	DDD	88	ILE	2.4
1	EEE	148	ASN	2.4
1	FFF	148	ASN	2.4
1	AAA	218	THR	2.4
1	CCC	319	ARG	2.4
1	FFF	289	GLN	2.4
1	HHH	135	THR	2.4
1	AAA	271	SER	2.4
1	AAA	318	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	BBB	163	GLY	2.4
1	EEE	318	LEU	2.4
1	III	259	LEU	2.4
1	AAA	232	ALA	2.4
1	HHH	185	ALA	2.4
1	CCC	120	ASP	2.4
1	DDD	255	ASP	2.4
1	JJJ	176	ASP	2.4
1	III	145	ILE	2.4
1	JJJ	178	ILE	2.4
1	HHH	160	VAL	2.4
1	III	39	ARG	2.4
1	III	160	VAL	2.4
1	JJJ	36	ASN	2.4
1	JJJ	73	TYR	2.4
1	CCC	117	MET	2.4
1	AAA	277	GLN	2.4
1	BBB	268	GLN	2.4
1	EEE	151	GLN	2.4
1	GGG	132	THR	2.4
1	EEE	223	GLY	2.4
1	AAA	248	ALA	2.4
1	BBB	204	ALA	2.4
1	GGG	239	ALA	2.4
1	BBB	269	ILE	2.4
1	CCC	81	ILE	2.4
1	EEE	73	TYR	2.4
1	DDD	121	LYS	2.4
1	DDD	244	LYS	2.4
1	AAA	95	GLN	2.4
1	AAA	246	LEU	2.4
1	BBB	303	THR	2.4
1	BBB	214	ALA	2.4
1	EEE	130	ALA	2.4
1	FFF	282	SER	2.4
1	BBB	201	ILE	2.4
1	AAA	128	VAL	2.4
1	BBB	160	VAL	2.4
1	BBB	176	ASP	2.4
1	FFF	101	VAL	2.4
1	FFF	309	ARG	2.4
1	CCC	244	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	AAA	74	LEU	2.4
1	BBB	164	ASN	2.4
1	CCC	22	ASN	2.4
1	GGG	103	PRO	2.3
1	III	172	ASN	2.4
1	CCC	223	GLY	2.3
1	DDD	336	GLY	2.3
1	EEE	343	GLN	2.3
1	GGG	188	GLY	2.3
1	DDD	325	ALA	2.3
1	EEE	203	THR	2.3
1	HHH	200	ALA	2.3
1	III	288	THR	2.3
1	GGG	119	SER	2.3
1	III	138	SER	2.3
1	EEE	101	VAL	2.3
1	FFF	304	LEU	2.3
1	GGG	79	PRO	2.3
1	GGG	260	ASN	2.3
1	AAA	313	ILE	2.3
1	CCC	94	THR	2.3
1	BBB	282	SER	2.3
1	HHH	129	SER	2.3
1	III	190	VAL	2.3
1	III	191	VAL	2.3
1	JJJ	261	SER	2.3
1	GGG	150	TYR	2.3
1	GGG	255	ASP	2.3
1	III	141	ASP	2.3
1	BBB	64	GLY	2.3
1	DDD	298	THR	2.3
1	BBB	39	ARG	2.3
1	FFF	39	ARG	2.3
1	III	133	ARG	2.3
1	DDD	195	LEU	2.3
1	GGG	168	LEU	2.3
1	HHH	334	LEU	2.3
1	III	299	SER	2.3
1	AAA	49	PHE	2.3
1	GGG	120	ASP	2.3
1	HHH	43	PRO	2.3
1	AAA	205	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	BBB	177	GLY	2.3
1	EEE	137	GLY	2.3
1	GGG	186	ILE	2.3
1	III	59	ILE	2.3
1	CCC	40	GLN	2.3
1	CCC	159	ASN	2.3
1	EEE	162	ASN	2.3
1	BBB	44	VAL	2.3
1	EEE	321	LEU	2.3
1	EEE	273	TYR	2.3
1	HHH	282	SER	2.3
1	AAA	175	ILE	2.3
1	FFF	88	ILE	2.3
1	FFF	180	ALA	2.3
1	III	310	LYS	2.3
1	BBB	292	ASN	2.3
1	FFF	152	LEU	2.3
1	GGG	29	LEU	2.3
1	GGG	96	ASN	2.3
1	HHH	140	ASN	2.3
1	III	254	ARG	2.3
1	AAA	99	SER	2.3
1	DDD	219	PRO	2.3
1	HHH	239	ALA	2.3
1	III	338	LYS	2.3
1	DDD	333	VAL	2.3
1	EEE	277	GLN	2.3
1	GGG	327	GLN	2.3
1	HHH	168	LEU	2.3
1	JJJ	158	ASN	2.3
1	DDD	31	ILE	2.3
1	HHH	99	SER	2.3
1	III	257	SER	2.3
1	EEE	275	GLY	2.3
1	FFF	206	GLY	2.3
1	BBB	180	ALA	2.3
1	HHH	121	LYS	2.3
1	BBB	246	LEU	2.3
1	CCC	301	LEU	2.3
1	CCC	304	LEU	2.3
1	EEE	265	VAL	2.3
1	HHH	301	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	EEE	95	GLN	2.3
1	JJJ	60	ASN	2.2
1	HHH	46	PHE	2.2
1	III	150	TYR	2.2
1	EEE	153	ILE	2.2
1	EEE	269	ILE	2.2
1	HHH	153	ILE	2.2
1	AAA	332	LYS	2.2
1	GGG	129	SER	2.2
1	JJJ	316	SER	2.2
1	AAA	280	ALA	2.2
1	BBB	248	ALA	2.2
1	GGG	286	ALA	2.2
1	III	221	VAL	2.2
1	AAA	254	ARG	2.2
1	FFF	48	ARG	2.2
1	FFF	300	GLU	2.2
1	CCC	31	ILE	2.2
1	HHH	182	ILE	2.2
1	JJJ	179	ASN	2.2
1	AAA	194	LEU	2.2
1	DDD	80	LEU	2.2
1	AAA	23	ALA	2.2
1	AAA	261	SER	2.2
1	CCC	147	SER	2.2
1	EEE	114	ALA	2.2
1	JJJ	44	VAL	2.2
1	HHH	27	GLN	2.2
1	BBB	74	LEU	2.2
1	BBB	159	ASN	2.2
1	HHH	148	ASN	2.2
1	CCC	128	VAL	2.2
1	FFF	265	VAL	2.2
1	FFF	114	ALA	2.2
1	JJJ	62	GLY	2.2
1	AAA	249	ARG	2.2
1	BBB	117	MET	2.2
1	JJJ	204	ALA	2.2
1	III	129	SER	2.2
1	JJJ	26	SER	2.2
1	JJJ	138	SER	2.2
1	GGG	201	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	III	279	GLN	2.2
1	AAA	120	ASP	2.2
1	JJJ	302	GLU	2.2
1	CCC	297	LEU	2.2
1	DDD	157	LEU	2.2
1	III	34	TYR	2.2
1	DDD	87	ASN	2.2
1	III	305	ASN	2.2
1	JJJ	65	ALA	2.2
1	JJJ	200	ALA	2.2
1	JJJ	337	THR	2.2
1	AAA	257	SER	2.2
1	BBB	95	GLN	2.2
1	DDD	58	GLN	2.2
1	III	125	TYR	2.2
1	III	335	ASP	2.2
1	GGG	177	GLY	2.2
1	GGG	325	ALA	2.2
1	III	140	ASN	2.2
1	GGG	328	THR	2.2
1	AAA	98	ILE	2.2
1	CCC	322	PHE	2.2
1	DDD	247	SER	2.2
1	EEE	145	ILE	2.2
1	FFF	72	HIS	2.2
1	GGG	247	SER	2.2
1	JJJ	77	ILE	2.2
1	DDD	300	GLU	2.2
1	AAA	241	VAL	2.2
1	HHH	221	VAL	2.2
1	BBB	309	ARG	2.2
1	FFF	67	ARG	2.2
1	HHH	102	MET	2.2
1	III	134	ARG	2.2
1	CCC	237	GLY	2.2
1	FFF	328	THR	2.2
1	HHH	337	THR	2.2
1	CCC	30	HIS	2.2
1	CCC	24	GLN	2.2
1	FFF	281	GLN	2.2
1	GGG	265	VAL	2.2
1	AAA	134	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	CCC	335	ASP	2.1
1	EEE	146	ASP	2.1
1	EEE	295	ASP	2.1
1	HHH	184	GLY	2.1
1	FFF	332	LYS	2.1
1	HHH	158	ASN	2.1
1	AAA	328	THR	2.1
1	HHH	61	THR	2.1
1	HHH	245	SER	2.1
1	III	85	VAL	2.1
1	III	267	SER	2.1
1	FFF	58	GLN	2.1
1	FFF	73	TYR	2.1
1	AAA	187	ALA	2.1
1	BBB	286	ALA	2.1
1	III	232	ALA	2.1
1	III	266	ALA	2.1
1	EEE	183	ASP	2.1
1	BBB	308	LEU	2.1
1	DDD	77	ILE	2.1
1	GGG	49	PHE	2.1
1	HHH	139	LEU	2.1
1	JJJ	121	LYS	2.1
1	DDD	156	ASN	2.1
1	FFF	278	THR	2.1
1	DDD	154	VAL	2.1
1	BBB	245	SER	2.1
1	BBB	253	TYR	2.1
1	DDD	268	GLN	2.1
1	BBB	306	ALA	2.1
1	JJJ	294	TRP	2.1
1	BBB	211	LEU	2.1
1	CCC	153	ILE	2.1
1	HHH	175	ILE	2.1
1	III	168	LEU	2.1
1	III	317	PHE	2.1
1	III	60	ASN	2.1
1	CCC	73	TYR	2.1
1	DDD	73	TYR	2.1
1	AAA	177	GLY	2.1
1	CCC	169	GLU	2.1
1	CCC	207	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	JJJ	238	GLY	2.1
1	HHH	227	MET	2.1
1	BBB	107	THR	2.1
1	AAA	130	ALA	2.1
1	AAA	153	ILE	2.1
1	BBB	236	ILE	2.1
1	CCC	26	SER	2.1
1	FFF	299	SER	2.1
1	HHH	114	ALA	2.1
1	HHH	111	TRP	2.1
1	III	56	GLU	2.1
1	EEE	141	ASP	2.1
1	AAA	69	HIS	2.1
1	FFF	46	PHE	2.1
1	FFF	193	GLY	2.1
1	FFF	251	LYS	2.1
1	GGG	52	LEU	2.1
1	JJJ	149	ASN	2.1
1	AAA	272	GLY	2.1
1	III	206	GLY	2.1
1	HHH	101	VAL	2.1
1	BBB	173	ARG	2.1
1	CCC	39	ARG	2.1
1	HHH	143	LEU	2.1
1	AAA	77	ILE	2.1
1	AAA	226	ALA	2.1
1	AAA	238	GLY	2.1
1	CCC	136	ILE	2.1
1	DDD	70	ALA	2.1
1	III	199	GLY	2.1
1	AAA	33	THR	2.1
1	EEE	61	THR	2.1
1	HHH	41	GLN	2.1
1	DDD	109	GLU	2.1
1	DDD	261	SER	2.1
1	JJJ	265	VAL	2.1
1	HHH	21	MET	2.0
1	JJJ	274	ARG	2.0
1	AAA	112	LEU	2.0
1	HHH	341	LYS	2.0
1	III	74	LEU	2.0
1	AAA	150	TYR	2.0

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Mol	Chain	Res	Type	RSRZ
1	FFF	287	ALA	2.0
1	GGG	145	ILE	2.0
1	GGG	277	GLN	2.0
1	EEE	326	SER	2.0
1	FFF	254	ARG	2.0
1	GGG	173	ARG	2.0
1	AAA	276	LEU	2.0
1	CCC	29	LEU	2.0
1	EEE	123	LYS	2.0
1	FFF	269	ILE	2.0
1	GGG	269	ILE	2.0
1	EEE	188	GLY	2.0
1	FFF	137	GLY	2.0
1	III	188	GLY	2.0
1	JJJ	163	GLY	2.0
1	BBB	305	ASN	2.0
1	HHH	132	THR	2.0
1	BBB	318	LEU	2.0
1	JJJ	334	LEU	2.0
1	FFF	253	TYR	2.0
1	BBB	283	ALA	2.0
1	JJJ	287	ALA	2.0
1	DDD	72	HIS	2.0
1	HHH	174	ASP	2.0
1	BBB	110	GLN	2.0
1	FFF	220	VAL	2.0
1	AAA	61	THR	2.0
1	AAA	152	LEU	2.0
1	AAA	301	LEU	2.0
1	AAA	337	THR	2.0
1	BBB	331	THR	2.0
1	FFF	218	THR	2.0
1	FFF	228	MET	2.0
1	FFF	244	LYS	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 [i](#)

There are no oligosaccharides 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.