



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 06:27 pm GMT

PDB ID : 3B5X
Title : Crystal Structure of MsbA from *Vibrio cholerae*
Authors : Ward, A.; Reyes, C.L.; Yu, J.; Roth, C.B.; Chang, G.
Deposited on : 2007-10-26
Resolution : 5.50 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

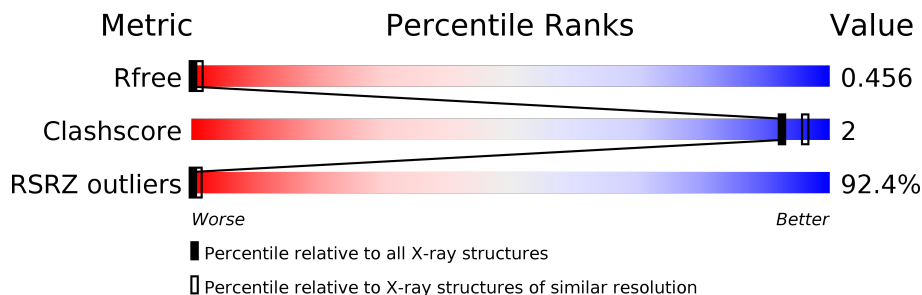
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 5.50 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}	100719	1052 (7.20-3.70)
Clashscore	112137	1021 (7.20-3.76)
RSRZ outliers	101464	1061 (7.20-3.70)

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. 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	582	
1	B	582	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1144 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.

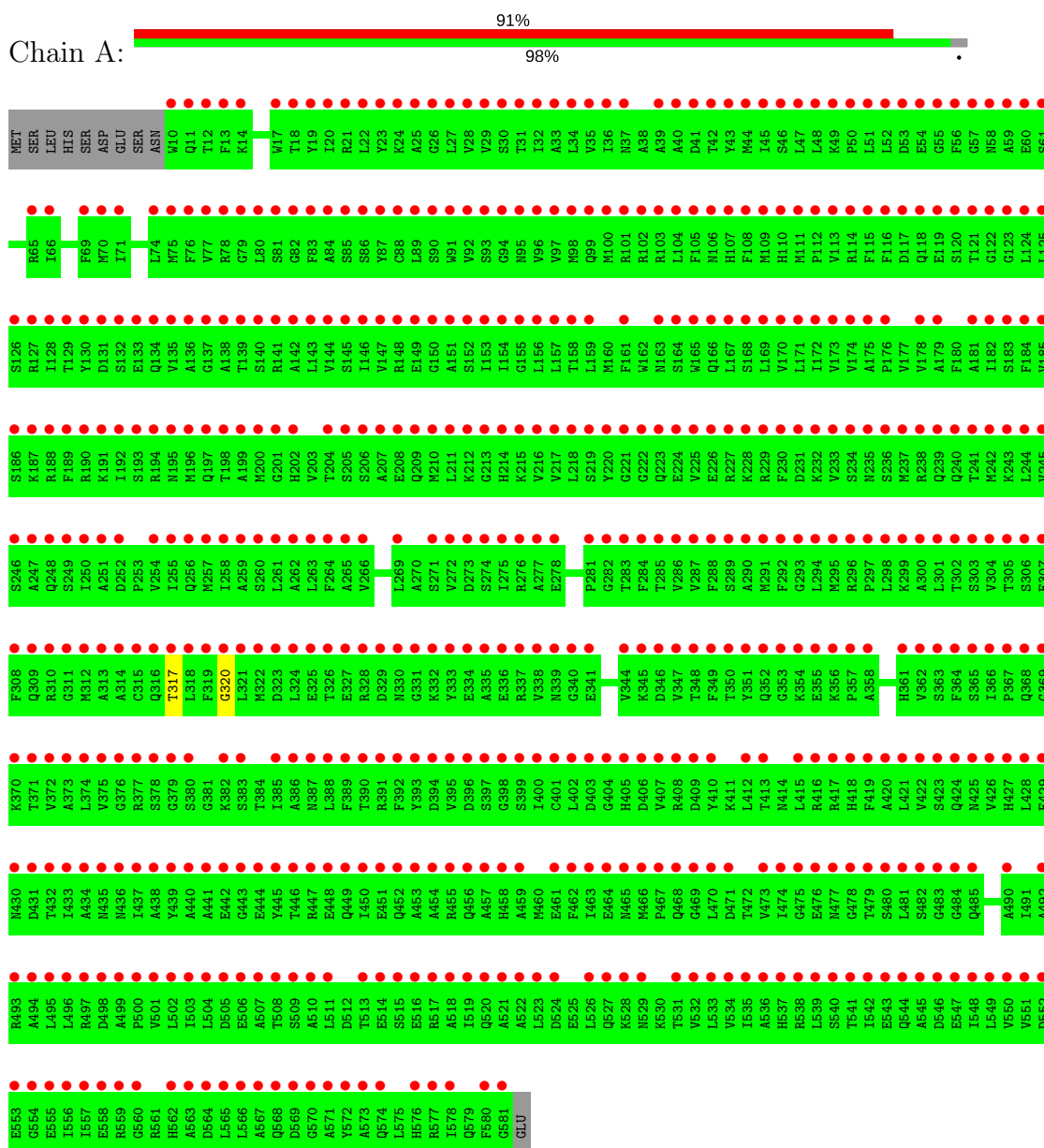
- Molecule 1 is a protein called Lipid A export ATP-binding/permease protein msbA.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
1	A	572	Total	C	0	0	572
			572	572			
1	B	572	Total	C	0	0	572
			572	572			

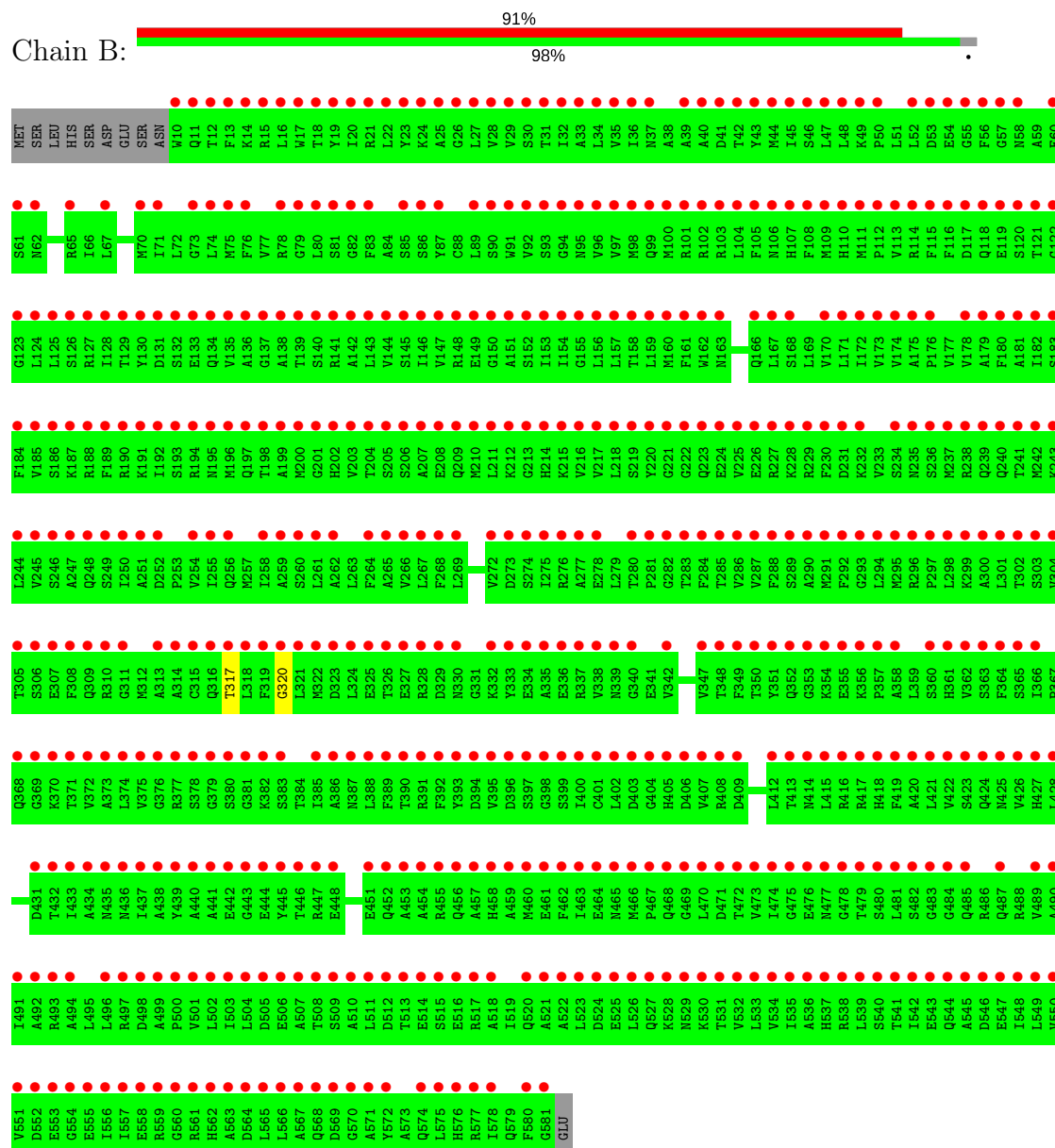
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: Lipid A export ATP-binding/permease protein msbA



- Molecule 1: Lipid A export ATP-binding/permease protein msbA



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	120.59Å 150.42Å 148.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.97 – 5.50 19.97 – 5.50	Depositor EDS
% Data completeness (in resolution range)	84.0 (19.97-5.50) 84.0 (19.97-5.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.71 (at 5.55Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.348 , 0.360 0.427 , 0.456	Depositor DCC
R_{free} test set	740 reflections (9.86%)	DCC
Wilson B-factor (Å ²)	215.7	Xtriage
Anisotropy	0.730	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 82.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.030 for -h,l,k	Xtriage
F_o, F_c correlation	0.81	EDS
Total number of atoms	1144	wwPDB-VP
Average B, all atoms (Å ²)	309.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 30.55 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.2845e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical 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).

There are no protein, RNA or DNA chains available to summarize Z scores of covalent bonds and angles.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [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	572	0	0	1	0
1	B	572	0	0	1	0
All	All	1144	0	0	2	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (2) 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:317:THR:CA	1:A:320:GLY:CA	2.91	0.48
1:B:317:THR:CA	1:B:320:GLY:CA	2.92	0.48

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

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 carbohydrates 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	572/582 (98%)	8.84	530 (92%)  	309, 309, 309, 309	0
1	B	572/582 (98%)	8.15	527 (92%)  	309, 309, 309, 309	0
All	All	1144/1164 (98%)	8.49	1057 (92%)  	309, 309, 309, 309	0

All (1057) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	246	SER	35.3
1	A	31	THR	34.1
1	A	117	ASP	33.3
1	A	296	ARG	32.9
1	A	147	VAL	32.7
1	A	198	THR	31.3
1	A	230	PHE	30.4
1	B	92	VAL	28.8
1	B	243	LYS	28.5
1	A	235	ASN	28.2
1	A	227	ARG	27.9
1	A	231	ASP	27.9
1	A	299	LYS	27.0
1	B	198	THR	26.8
1	A	21	ARG	26.7
1	B	242	MET	26.3
1	B	93	SER	25.8
1	B	505	ASP	25.6
1	A	204	THR	25.6
1	A	137	GLY	25.2
1	A	289	SER	25.2
1	A	568	GLN	25.0
1	B	235	ASN	24.8
1	A	236	SER	24.6

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Mol	Chain	Res	Type	RSRZ
1	A	145	SER	24.2
1	A	32	ILE	24.0
1	B	133	GLU	23.3
1	A	34	LEU	23.3
1	B	134	GLN	23.0
1	B	25	ALA	22.7
1	A	133	GLU	22.6
1	A	577	ARG	22.4
1	B	183	SER	22.3
1	A	224	GLU	22.3
1	A	75	MET	22.3
1	A	78	ARG	22.2
1	A	431	ASP	21.9
1	B	75	MET	21.7
1	B	152	SER	21.6
1	A	150	GLY	21.6
1	B	245	VAL	21.6
1	B	112	PRO	21.3
1	B	456	GLN	21.2
1	A	132	SER	21.2
1	A	477	ASN	21.0
1	A	363	SER	20.9
1	B	137	GLY	20.8
1	B	248	GLN	20.7
1	B	363	SER	20.5
1	A	421	LEU	20.5
1	B	355	GLU	20.2
1	B	227	ARG	20.2
1	A	300	ALA	20.1
1	A	259	ALA	20.0
1	B	265	ALA	20.0
1	B	157	LEU	19.9
1	A	243	LYS	19.8
1	B	422	VAL	19.8
1	A	245	VAL	19.8
1	A	423	SER	19.7
1	A	258	ILE	19.7
1	B	262	ALA	19.7
1	A	116	PHE	19.6
1	A	425	ASN	19.5
1	A	527	GLN	19.2
1	A	250	ILE	19.2

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Mol	Chain	Res	Type	RSRZ
1	A	265	ALA	19.2
1	B	53	ASP	19.1
1	A	547	GLU	19.1
1	A	222	GLY	19.1
1	A	422	VAL	19.0
1	B	423	SER	19.0
1	B	542	ILE	18.8
1	B	258	ILE	18.8
1	A	470	LEU	18.7
1	B	425	ASN	18.7
1	B	577	ARG	18.6
1	A	557	ILE	18.4
1	B	231	ASP	18.4
1	B	122	GLY	18.3
1	A	106	ASN	18.3
1	B	21	ARG	18.3
1	A	438	ALA	18.2
1	B	473	VAL	18.2
1	B	158	THR	18.2
1	A	18	THR	18.1
1	A	221	GLY	17.9
1	A	408	ARG	17.7
1	A	284	PHE	17.7
1	A	134	GLN	17.6
1	B	195	ASN	17.6
1	A	424	GLN	17.5
1	A	112	PRO	17.5
1	B	228	LYS	17.5
1	B	140	SER	17.5
1	A	549	LEU	17.5
1	B	354	LYS	17.4
1	B	276	ARG	17.4
1	A	239	GLN	17.3
1	A	202	HIS	17.3
1	A	514	GLU	17.2
1	B	26	GLY	17.2
1	B	418	HIS	17.1
1	A	505	ASP	17.0
1	B	307	GLU	17.0
1	B	454	ALA	17.0
1	B	457	ALA	17.0
1	B	91	TRP	16.9

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Mol	Chain	Res	Type	RSRZ
1	B	18	THR	16.9
1	A	37	ASN	16.9
1	A	448	GLU	16.9
1	A	25	ALA	16.8
1	B	251	ALA	16.8
1	A	215	LYS	16.7
1	B	502	LEU	16.7
1	A	330	ASN	16.7
1	A	223	GLN	16.6
1	A	418	HIS	16.5
1	A	129	THR	16.5
1	A	504	LEU	16.5
1	A	159	LEU	16.4
1	A	307	GLU	16.0
1	B	578	ILE	16.0
1	B	11	GLN	16.0
1	A	22	LEU	15.7
1	A	550	VAL	15.7
1	B	506	GLU	15.6
1	A	435	ASN	15.6
1	A	329	ASP	15.6
1	B	558	GLU	15.6
1	B	244	LEU	15.5
1	B	239	GLN	15.4
1	B	31	THR	15.4
1	A	238	ARG	15.3
1	A	285	THR	15.3
1	A	483	GLY	15.3
1	B	22	LEU	15.2
1	B	461	GLU	15.2
1	B	14	LYS	15.2
1	B	30	SER	15.2
1	A	409	ASP	15.1
1	A	182	ILE	15.1
1	A	403	ASP	15.1
1	A	283	THR	15.0
1	A	301	LEU	15.0
1	A	556	ILE	15.0
1	A	131	ASP	14.9
1	A	506	GLU	14.9
1	A	58	ASN	14.9
1	A	96	VAL	14.8

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Mol	Chain	Res	Type	RSRZ
1	B	191	LYS	14.8
1	A	558	GLU	14.8
1	B	232	LYS	14.8
1	A	456	GLN	14.8
1	A	546	ASP	14.7
1	A	232	LYS	14.7
1	A	30	SER	14.7
1	B	462	PHE	14.7
1	B	325	GLU	14.6
1	B	29	VAL	14.6
1	B	230	PHE	14.5
1	B	188	ARG	14.5
1	A	436	ASN	14.4
1	B	413	THR	14.4
1	A	479	THR	14.4
1	A	559	ARG	14.4
1	A	27	LEU	14.4
1	A	387	ASN	14.3
1	A	511	LEU	14.3
1	A	515	SER	14.3
1	B	466	MET	14.3
1	A	386	ALA	14.2
1	A	454	ALA	14.2
1	B	527	GLN	14.2
1	B	146	ILE	14.1
1	B	131	ASP	14.1
1	A	398	GLY	14.0
1	A	48	LEU	14.0
1	A	71	ILE	14.0
1	A	156	LEU	14.0
1	B	96	VAL	14.0
1	B	23	TYR	14.0
1	B	446	THR	14.0
1	A	128	ILE	13.9
1	B	482	SER	13.9
1	A	19	TYR	13.9
1	A	264	PHE	13.9
1	B	404	GLY	13.9
1	A	354	LYS	13.9
1	A	70	MET	13.8
1	B	426	VAL	13.8
1	B	202	HIS	13.8

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Mol	Chain	Res	Type	RSRZ
1	A	473	VAL	13.8
1	B	447	ARG	13.7
1	B	339	ASN	13.7
1	A	463	ILE	13.7
1	A	407	VAL	13.7
1	B	371	THR	13.7
1	B	468	GLN	13.7
1	A	148	ARG	13.6
1	B	41	ASP	13.6
1	B	483	GLY	13.6
1	A	502	LEU	13.6
1	B	421	LEU	13.6
1	A	439	TYR	13.5
1	B	174	VAL	13.5
1	A	293	GLY	13.4
1	B	435	ASN	13.4
1	B	127	ARG	13.3
1	B	224	GLU	13.3
1	B	432	THR	13.2
1	B	229	ARG	13.2
1	A	97	VAL	13.2
1	B	424	GLN	13.2
1	B	118	GLN	13.0
1	A	542	ILE	12.9
1	A	214	HIS	12.9
1	A	40	ALA	12.9
1	B	327	GLU	12.9
1	B	557	ILE	12.9
1	B	369	GLY	12.8
1	A	337	ARG	12.8
1	B	138	ALA	12.8
1	A	122	GLY	12.8
1	A	29	VAL	12.7
1	A	406	ASP	12.7
1	B	246	SER	12.7
1	A	309	GLN	12.7
1	A	432	THR	12.7
1	B	159	LEU	12.6
1	A	334	GLU	12.6
1	B	221	GLY	12.6
1	B	401	CYS	12.6
1	A	462	PHE	12.6

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Mol	Chain	Res	Type	RSRZ
1	B	113	VAL	12.6
1	A	364	PHE	12.5
1	A	201	GLY	12.5
1	B	391	ARG	12.5
1	B	153	ILE	12.5
1	B	218	LEU	12.5
1	A	339	ASN	12.4
1	B	293	GLY	12.4
1	A	304	VAL	12.4
1	A	102	ARG	12.3
1	B	194	ARG	12.3
1	B	206	SER	12.3
1	A	157	LEU	12.3
1	A	35	VAL	12.3
1	A	103	ARG	12.3
1	B	136	ALA	12.3
1	B	298	LEU	12.2
1	B	37	ASN	12.2
1	B	149	GLU	12.2
1	A	192	ILE	12.2
1	B	204	THR	12.2
1	A	374	LEU	12.2
1	B	562	HIS	12.1
1	B	305	THR	12.1
1	B	32	ILE	12.1
1	A	146	ILE	12.0
1	B	431	ASP	12.0
1	A	399	SER	12.0
1	A	306	SER	12.0
1	B	281	PRO	11.9
1	B	108	PHE	11.9
1	B	90	SER	11.9
1	A	298	LEU	11.9
1	B	249	SER	11.9
1	B	261	LEU	11.8
1	A	228	LYS	11.8
1	B	33	ALA	11.8
1	A	368	GLN	11.8
1	B	223	GLN	11.7
1	A	42	THR	11.7
1	A	144	VAL	11.7
1	A	185	VAL	11.7

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Mol	Chain	Res	Type	RSRZ
1	B	128	ILE	11.6
1	B	186	SER	11.6
1	B	436	ASN	11.6
1	B	420	ALA	11.6
1	B	310	ARG	11.6
1	A	92	VAL	11.6
1	B	185	VAL	11.5
1	B	234	SER	11.5
1	A	183	SER	11.5
1	A	94	GLY	11.5
1	A	295	MET	11.4
1	A	467	PRO	11.4
1	B	106	ASN	11.4
1	B	329	ASP	11.4
1	A	548	ILE	11.4
1	A	118	GLN	11.3
1	B	182	ILE	11.3
1	A	365	SER	11.2
1	A	226	GLU	11.2
1	B	398	GLY	11.1
1	A	378	SER	11.0
1	A	325	GLU	11.0
1	B	547	GLU	11.0
1	B	581	GLY	11.0
1	B	480	SER	10.9
1	A	447	ARG	10.9
1	A	323	ASP	10.9
1	A	242	MET	10.9
1	A	251	ALA	10.9
1	B	296	ARG	10.9
1	A	240	GLN	10.9
1	A	369	GLY	10.9
1	A	53	ASP	10.9
1	A	452	GLN	10.8
1	B	222	GLY	10.8
1	B	141	ARG	10.8
1	A	336	GLU	10.8
1	A	482	SER	10.8
1	B	514	GLU	10.8
1	A	28	VAL	10.8
1	A	288	PHE	10.8
1	A	503	ILE	10.7

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Mol	Chain	Res	Type	RSRZ
1	B	150	GLY	10.7
1	A	57	GLY	10.7
1	A	492	ALA	10.7
1	B	336	GLU	10.7
1	A	457	ALA	10.6
1	B	326	THR	10.6
1	A	65	ARG	10.6
1	A	297	PRO	10.6
1	B	208	GLU	10.6
1	B	408	ARG	10.6
1	B	145	SER	10.6
1	B	40	ALA	10.6
1	B	510	ALA	10.5
1	A	466	MET	10.5
1	A	247	ALA	10.5
1	A	333	TYR	10.5
1	B	80	LEU	10.5
1	A	510	ALA	10.4
1	A	404	GLY	10.4
1	B	338	VAL	10.4
1	B	94	GLY	10.3
1	B	550	VAL	10.3
1	A	20	ILE	10.3
1	A	218	LEU	10.3
1	B	301	LEU	10.3
1	B	214	HIS	10.3
1	B	43	TYR	10.3
1	B	509	SER	10.2
1	B	135	VAL	10.2
1	B	215	LYS	10.2
1	B	309	GLN	10.2
1	B	543	GLU	10.2
1	B	236	SER	10.2
1	A	115	PHE	10.1
1	A	397	SER	10.1
1	A	179	ALA	10.1
1	B	132	SER	10.1
1	B	526	LEU	10.1
1	B	571	ALA	10.0
1	A	262	ALA	10.0
1	A	372	VAL	10.0
1	A	33	ALA	10.0

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Mol	Chain	Res	Type	RSRZ
1	A	496	LEU	10.0
1	B	17	TRP	9.9
1	A	23	TYR	9.9
1	B	97	VAL	9.9
1	A	154	ILE	9.9
1	B	552	ASP	9.8
1	A	172	ILE	9.8
1	A	366	ILE	9.8
1	B	56	PHE	9.8
1	B	71	ILE	9.8
1	A	149	GLU	9.8
1	B	144	VAL	9.8
1	B	534	VAL	9.8
1	B	34	LEU	9.8
1	A	127	ARG	9.8
1	B	129	THR	9.8
1	A	571	ALA	9.8
1	A	237	MET	9.8
1	B	549	LEU	9.7
1	B	300	ALA	9.7
1	B	167	LEU	9.7
1	B	387	ASN	9.7
1	A	234	SER	9.7
1	B	205	SER	9.7
1	A	291	MET	9.7
1	B	173	VAL	9.6
1	B	76	PHE	9.6
1	B	513	THR	9.6
1	B	193	SER	9.6
1	B	117	ASP	9.6
1	A	401	CYS	9.5
1	B	319	PHE	9.5
1	B	199	ALA	9.5
1	A	76	PHE	9.5
1	A	105	PHE	9.5
1	A	113	VAL	9.5
1	B	42	THR	9.5
1	B	467	PRO	9.5
1	A	517	ARG	9.4
1	A	551	VAL	9.4
1	A	100	MET	9.4
1	A	327	GLU	9.4

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Mol	Chain	Res	Type	RSRZ
1	B	501	VAL	9.4
1	B	328	ARG	9.3
1	B	356	LYS	9.3
1	B	219	SER	9.3
1	A	79	GLY	9.3
1	A	93	SER	9.3
1	B	375	VAL	9.3
1	A	335	ALA	9.3
1	A	377	ARG	9.3
1	B	330	ASN	9.2
1	A	187	LYS	9.2
1	B	548	ILE	9.2
1	B	529	ASN	9.2
1	A	282	GLY	9.2
1	B	390	THR	9.2
1	A	41	ASP	9.2
1	B	203	VAL	9.2
1	A	465	ASN	9.2
1	A	80	LEU	9.2
1	B	380	SER	9.2
1	B	241	THR	9.2
1	B	471	ASP	9.1
1	B	362	VAL	9.1
1	B	19	TYR	9.1
1	A	518	ALA	9.1
1	A	208	GLU	9.1
1	B	507	ALA	9.1
1	A	205	SER	9.0
1	A	497	ARG	9.0
1	A	83	PHE	9.0
1	B	554	GLY	8.9
1	B	576	HIS	8.9
1	A	388	LEU	8.9
1	B	36	ILE	8.9
1	B	154	ILE	8.9
1	B	318	LEU	8.9
1	A	143	LEU	8.8
1	A	140	SER	8.8
1	A	50	PRO	8.8
1	A	480	SER	8.7
1	B	409	ASP	8.7
1	B	335	ALA	8.7

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Mol	Chain	Res	Type	RSRZ
1	B	397	SER	8.7
1	A	464	GLU	8.7
1	A	199	ALA	8.7
1	B	86	SER	8.7
1	B	264	PHE	8.7
1	A	501	VAL	8.7
1	A	126	SER	8.7
1	B	171	LEU	8.6
1	A	252	ASP	8.6
1	B	252	ASP	8.6
1	B	377	ARG	8.6
1	A	244	LEU	8.6
1	A	576	HIS	8.5
1	A	194	ARG	8.5
1	A	526	LEU	8.5
1	B	175	ALA	8.5
1	A	459	ALA	8.5
1	B	27	LEU	8.5
1	B	82	GLY	8.5
1	A	273	ASP	8.5
1	A	509	SER	8.5
1	B	207	ALA	8.5
1	A	521	ALA	8.5
1	B	116	PHE	8.5
1	A	413	THR	8.5
1	B	143	LEU	8.4
1	B	455	ARG	8.4
1	B	443	GLY	8.4
1	B	104	LEU	8.4
1	A	420	ALA	8.3
1	A	578	ILE	8.3
1	A	99	GLN	8.3
1	A	367	PRO	8.3
1	B	266	VAL	8.3
1	B	403	ASP	8.3
1	B	323	ASP	8.2
1	B	20	ILE	8.2
1	A	533	LEU	8.2
1	A	528	LYS	8.2
1	A	531	THR	8.2
1	A	24	LYS	8.2
1	A	529	ASN	8.2

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Mol	Chain	Res	Type	RSRZ
1	B	160	MET	8.1
1	A	46	SER	8.1
1	A	520	GLN	8.1
1	A	554	GLY	8.1
1	B	419	PHE	8.1
1	B	439	TYR	8.1
1	B	541	THR	8.1
1	B	556	ILE	8.1
1	A	119	GLU	8.1
1	A	77	VAL	8.0
1	B	334	GLU	8.0
1	B	210	MET	8.0
1	A	308	PHE	8.0
1	A	158	THR	8.0
1	A	61	SER	8.0
1	A	233	VAL	8.0
1	B	324	LEU	7.9
1	B	337	ARG	7.9
1	B	83	PHE	7.9
1	A	534	VAL	7.9
1	B	452	GLN	7.9
1	B	494	ALA	7.9
1	B	372	VAL	7.9
1	A	206	SER	7.9
1	A	469	GLY	7.9
1	B	57	GLY	7.8
1	B	350	THR	7.8
1	A	81	SER	7.8
1	A	305	THR	7.8
1	A	442	GLU	7.8
1	B	156	LEU	7.8
1	B	24	LYS	7.8
1	B	275	ILE	7.8
1	A	45	ILE	7.7
1	B	538	ARG	7.7
1	B	192	ILE	7.7
1	B	28	VAL	7.7
1	B	373	ALA	7.7
1	B	518	ALA	7.7
1	A	155	GLY	7.7
1	A	560	GLY	7.7
1	B	250	ILE	7.7

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Mol	Chain	Res	Type	RSRZ
1	A	311	GLY	7.7
1	B	444	GLU	7.7
1	A	89	LEU	7.7
1	A	419	PHE	7.7
1	B	370	LYS	7.7
1	A	426	VAL	7.6
1	B	289	SER	7.6
1	A	74	LEU	7.6
1	A	136	ALA	7.6
1	A	564	ASP	7.5
1	B	123	GLY	7.5
1	A	135	VAL	7.5
1	B	566	LEU	7.5
1	A	391	ARG	7.5
1	B	511	LEU	7.5
1	B	304	VAL	7.5
1	B	184	PHE	7.5
1	A	532	VAL	7.5
1	B	434	ALA	7.5
1	B	259	ALA	7.5
1	B	559	ARG	7.5
1	B	396	ASP	7.4
1	B	74	LEU	7.4
1	B	109	MET	7.4
1	B	332	LYS	7.4
1	B	477	ASN	7.4
1	A	402	LEU	7.4
1	A	104	LEU	7.4
1	B	437	ILE	7.4
1	B	361	HIS	7.4
1	A	322	MET	7.4
1	A	248	GLN	7.4
1	A	212	LYS	7.3
1	B	212	LYS	7.3
1	B	322	MET	7.3
1	B	393	TYR	7.3
1	B	209	GLN	7.3
1	B	286	VAL	7.3
1	A	338	VAL	7.3
1	B	283	THR	7.3
1	B	357	PRO	7.3
1	A	412	LEU	7.3

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Mol	Chain	Res	Type	RSRZ
1	A	539	LEU	7.2
1	A	351	TYR	7.2
1	B	48	LEU	7.2
1	A	565	LEU	7.2
1	B	163	ASN	7.2
1	B	374	LEU	7.2
1	B	35	VAL	7.2
1	A	193	SER	7.2
1	B	564	ASP	7.2
1	B	292	PHE	7.2
1	A	114	ARG	7.2
1	A	373	ALA	7.2
1	A	276	ARG	7.2
1	B	238	ARG	7.2
1	A	481	LEU	7.2
1	A	383	SER	7.2
1	A	313	ALA	7.1
1	A	56	PHE	7.1
1	A	455	ARG	7.1
1	A	290	ALA	7.1
1	B	463	ILE	7.1
1	B	124	LEU	7.1
1	B	313	ALA	7.1
1	B	102	ARG	7.1
1	A	395	VAL	7.1
1	A	171	LEU	7.1
1	A	111	MET	7.1
1	A	310	ARG	7.0
1	A	484	GLY	7.0
1	B	100	MET	7.0
1	A	43	TYR	7.0
1	A	396	ASP	7.0
1	B	45	ILE	7.0
1	A	95	ASN	7.0
1	B	492	ALA	7.0
1	A	275	ILE	7.0
1	B	288	PHE	7.0
1	A	196	MET	6.9
1	B	516	GLU	6.9
1	A	538	ARG	6.9
1	B	365	SER	6.9
1	A	493	ARG	6.9

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Mol	Chain	Res	Type	RSRZ
1	B	105	PHE	6.9
1	A	91	TRP	6.9
1	A	188	ARG	6.9
1	A	211	LEU	6.9
1	B	89	LEU	6.9
1	B	299	LYS	6.9
1	B	465	ASN	6.9
1	B	464	GLU	6.9
1	B	412	LEU	6.8
1	B	247	ALA	6.8
1	A	90	SER	6.8
1	B	273	ASP	6.8
1	A	451	GLU	6.8
1	A	286	VAL	6.7
1	B	546	ASP	6.7
1	B	475	GLY	6.7
1	A	152	SER	6.7
1	B	303	SER	6.7
1	B	438	ALA	6.7
1	B	448	GLU	6.7
1	B	470	LEU	6.7
1	B	139	THR	6.7
1	B	415	LEU	6.7
1	A	572	TYR	6.7
1	A	348	THR	6.6
1	A	508	THR	6.6
1	A	434	ALA	6.6
1	B	442	GLU	6.6
1	A	153	ILE	6.6
1	A	324	LEU	6.6
1	B	197	GLN	6.6
1	B	580	PHE	6.5
1	B	553	GLU	6.5
1	A	229	ARG	6.5
1	A	207	ALA	6.5
1	B	358	ALA	6.5
1	A	197	GLN	6.5
1	B	121	THR	6.5
1	A	393	TYR	6.5
1	A	292	PHE	6.4
1	B	469	GLY	6.4
1	A	458	HIS	6.4

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Mol	Chain	Res	Type	RSRZ
1	A	494	ALA	6.4
1	A	318	LEU	6.4
1	A	87	TYR	6.4
1	A	98	MET	6.4
1	A	219	SER	6.4
1	B	274	SER	6.4
1	B	148	ARG	6.4
1	B	525	GLU	6.3
1	B	472	THR	6.3
1	B	103	ARG	6.3
1	A	476	GLU	6.3
1	A	121	THR	6.3
1	B	168	SER	6.3
1	B	255	ILE	6.3
1	A	82	GLY	6.2
1	A	567	ALA	6.2
1	B	81	SER	6.2
1	B	416	ARG	6.2
1	B	333	TYR	6.1
1	A	263	LEU	6.1
1	B	176	PRO	6.1
1	B	481	LEU	6.1
1	B	569	ASP	6.1
1	A	319	PHE	6.1
1	B	493	ARG	6.1
1	B	282	GLY	6.1
1	B	386	ALA	6.1
1	B	445	TYR	6.1
1	A	269	LEU	6.1
1	B	10	TRP	6.0
1	B	237	MET	6.0
1	A	332	LYS	6.0
1	B	285	THR	6.0
1	B	306	SER	6.0
1	B	98	MET	5.9
1	B	407	VAL	5.9
1	A	59	ALA	5.9
1	A	186	SER	5.9
1	B	351	TYR	5.9
1	A	141	ARG	5.9
1	B	78	ARG	5.9
1	A	375	VAL	5.9

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Mol	Chain	Res	Type	RSRZ
1	B	515	SER	5.9
1	B	427	HIS	5.8
1	B	196	MET	5.8
1	B	402	LEU	5.8
1	A	101	ARG	5.8
1	A	12	THR	5.8
1	A	281	PRO	5.8
1	A	394	ASP	5.8
1	B	226	GLU	5.8
1	B	256	GLN	5.8
1	A	108	PHE	5.8
1	B	392	PHE	5.8
1	B	500	PRO	5.8
1	B	539	LEU	5.8
1	A	385	ILE	5.8
1	A	417	ARG	5.7
1	B	490	ALA	5.7
1	B	54	GLU	5.6
1	A	210	MET	5.6
1	A	390	THR	5.6
1	B	161	PHE	5.6
1	A	416	ARG	5.6
1	B	302	THR	5.6
1	A	356	LYS	5.6
1	B	317	THR	5.6
1	B	364	PHE	5.6
1	B	451	GLU	5.6
1	A	516	GLU	5.6
1	A	328	ARG	5.5
1	A	184	PHE	5.5
1	B	125	LEU	5.5
1	B	381	GLY	5.5
1	B	563	ALA	5.5
1	B	574	GLN	5.5
1	A	109	MET	5.5
1	A	400	ILE	5.5
1	A	44	MET	5.4
1	A	195	ASN	5.4
1	A	553	GLU	5.4
1	B	58	ASN	5.4
1	B	269	LEU	5.4
1	A	125	LEU	5.4

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Mol	Chain	Res	Type	RSRZ
1	A	445	TYR	5.4
1	B	459	ALA	5.4
1	A	255	ILE	5.4
1	A	430	ASN	5.4
1	A	468	GLN	5.4
1	A	443	GLY	5.3
1	B	47	LEU	5.3
1	A	39	ALA	5.3
1	B	484	GLY	5.3
1	B	366	ILE	5.3
1	A	176	PRO	5.3
1	B	107	HIS	5.3
1	A	543	GLU	5.3
1	B	240	GLN	5.2
1	A	490	ALA	5.2
1	B	530	LYS	5.2
1	B	378	SER	5.2
1	A	107	HIS	5.2
1	A	541	THR	5.2
1	A	326	THR	5.2
1	B	272	VAL	5.2
1	A	47	LEU	5.1
1	B	536	ALA	5.1
1	B	70	MET	5.1
1	B	39	ALA	5.1
1	A	427	HIS	5.1
1	B	44	MET	5.1
1	B	521	ALA	5.1
1	A	10	TRP	5.1
1	B	50	PRO	5.1
1	B	414	ASN	5.1
1	A	69	PHE	5.1
1	B	388	LEU	5.1
1	A	315	CYS	5.1
1	A	277	ALA	5.1
1	A	581	GLY	5.0
1	B	533	LEU	5.0
1	B	49	LYS	5.0
1	B	115	PHE	5.0
1	B	260	SER	5.0
1	B	61	SER	5.0
1	A	54	GLU	5.0

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Mol	Chain	Res	Type	RSRZ
1	A	340	GLY	5.0
1	B	353	GLY	5.0
1	B	560	GLY	4.9
1	A	209	GLN	4.9
1	A	415	LEU	4.9
1	A	441	ALA	4.9
1	A	200	MET	4.9
1	A	478	GLY	4.9
1	A	124	LEU	4.9
1	B	189	PHE	4.9
1	B	225	VAL	4.9
1	B	496	LEU	4.9
1	B	545	ALA	4.9
1	A	317	THR	4.8
1	A	26	GLY	4.8
1	B	537	HIS	4.8
1	B	85	SER	4.8
1	A	321	LEU	4.8
1	A	170	VAL	4.8
1	B	101	ARG	4.8
1	B	572	TYR	4.8
1	A	540	SER	4.8
1	A	49	LYS	4.8
1	A	55	GLY	4.8
1	B	114	ARG	4.8
1	B	295	MET	4.7
1	B	119	GLU	4.7
1	A	138	ALA	4.7
1	B	405	HIS	4.7
1	B	60	GLU	4.7
1	B	499	ALA	4.7
1	A	537	HIS	4.7
1	A	294	LEU	4.7
1	B	211	LEU	4.7
1	A	241	THR	4.7
1	A	178	VAL	4.7
1	B	46	SER	4.7
1	A	405	HIS	4.7
1	B	453	ALA	4.7
1	A	303	SER	4.6
1	A	256	GLN	4.6
1	B	395	VAL	4.6

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Mol	Chain	Res	Type	RSRZ
1	A	437	ILE	4.6
1	A	312	MET	4.6
1	A	471	ASP	4.6
1	B	130	TYR	4.6
1	A	376	GLY	4.6
1	A	513	THR	4.6
1	B	517	ARG	4.6
1	A	123	GLY	4.6
1	A	85	SER	4.6
1	A	544	GLN	4.6
1	A	552	ASP	4.6
1	B	406	ASP	4.6
1	A	474	ILE	4.6
1	B	181	ALA	4.6
1	A	353	GLY	4.5
1	A	566	LEU	4.5
1	B	551	VAL	4.5
1	B	535	ILE	4.5
1	B	110	HIS	4.5
1	A	287	VAL	4.5
1	B	277	ALA	4.5
1	B	95	ASN	4.5
1	B	474	ILE	4.5
1	B	284	PHE	4.4
1	A	345	LYS	4.4
1	A	507	ALA	4.4
1	A	302	THR	4.4
1	B	99	GLN	4.4
1	A	169	LEU	4.4
1	B	179	ALA	4.4
1	B	314	ALA	4.4
1	A	191	LYS	4.4
1	B	504	LEU	4.4
1	A	446	THR	4.4
1	B	458	HIS	4.4
1	A	355	GLU	4.4
1	B	147	VAL	4.4
1	A	257	MET	4.3
1	B	376	GLY	4.3
1	B	531	THR	4.3
1	A	453	ALA	4.3
1	B	383	SER	4.3

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Mol	Chain	Res	Type	RSRZ
1	B	394	ASP	4.3
1	B	340	GLY	4.3
1	A	120	SER	4.3
1	A	379	GLY	4.3
1	B	568	GLN	4.2
1	B	316	GLN	4.2
1	B	520	GLN	4.2
1	B	111	MET	4.2
1	B	172	ILE	4.2
1	A	349	PHE	4.1
1	B	294	LEU	4.1
1	A	580	PHE	4.1
1	A	66	ILE	4.1
1	B	441	ALA	4.1
1	B	485	GLN	4.1
1	B	399	SER	4.1
1	B	400	ILE	4.1
1	A	545	ALA	4.1
1	B	352	GLN	4.0
1	A	350	THR	4.0
1	B	478	GLY	4.0
1	A	314	ALA	4.0
1	B	567	ALA	4.0
1	B	321	LEU	4.0
1	A	449	GLN	3.9
1	A	13	PHE	3.9
1	A	555	GLU	3.9
1	B	503	ILE	3.9
1	B	417	ARG	3.9
1	B	349	PHE	3.9
1	B	544	GLN	3.9
1	B	497	ARG	3.9
1	A	382	LYS	3.9
1	B	151	ALA	3.8
1	A	380	SER	3.8
1	A	562	HIS	3.8
1	A	151	ALA	3.8
1	A	36	ILE	3.7
1	B	268	PHE	3.7
1	B	55	GLY	3.7
1	B	155	GLY	3.7
1	A	14	LYS	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	574	GLN	3.7
1	B	79	GLY	3.7
1	A	167	LEU	3.7
1	A	500	PRO	3.7
1	B	190	ARG	3.7
1	B	460	MET	3.7
1	A	139	THR	3.7
1	A	428	LEU	3.6
1	B	315	CYS	3.6
1	B	201	GLY	3.6
1	B	433	ILE	3.6
1	A	217	VAL	3.6
1	B	87	TYR	3.6
1	A	84	ALA	3.6
1	B	267	LEU	3.6
1	A	475	GLY	3.6
1	A	524	ASP	3.6
1	A	110	HIS	3.6
1	A	569	ASP	3.6
1	B	385	ILE	3.5
1	A	523	LEU	3.5
1	B	382	LYS	3.5
1	A	362	VAL	3.5
1	B	347	VAL	3.5
1	A	164	SER	3.5
1	B	540	SER	3.5
1	A	272	VAL	3.5
1	A	142	ALA	3.5
1	A	175	ALA	3.5
1	B	489	VAL	3.5
1	B	67	LEU	3.4
1	B	142	ALA	3.4
1	A	266	VAL	3.4
1	B	200	MET	3.4
1	A	11	GLN	3.4
1	A	261	LEU	3.4
1	A	358	ALA	3.4
1	A	174	VAL	3.4
1	B	523	LEU	3.4
1	B	187	LYS	3.3
1	B	555	GLU	3.3
1	A	536	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	563	ALA	3.3
1	B	120	SER	3.3
1	B	532	VAL	3.2
1	A	535	ILE	3.2
1	A	254	VAL	3.2
1	A	130	TYR	3.2
1	A	60	GLU	3.2
1	A	249	SER	3.2
1	B	254	VAL	3.2
1	B	428	LEU	3.1
1	A	88	CYS	3.1
1	B	476	GLU	3.1
1	B	297	PRO	3.1
1	A	370	LYS	3.1
1	A	168	SER	3.1
1	B	311	GLY	3.1
1	A	433	ILE	3.1
1	A	51	LEU	3.1
1	A	278	GLU	3.1
1	B	570	GLY	3.1
1	A	461	GLU	3.1
1	A	392	PHE	3.1
1	A	52	LEU	3.1
1	A	499	ALA	3.0
1	B	524	ASP	3.0
1	A	189	PHE	3.0
1	B	308	PHE	3.0
1	A	498	ASP	3.0
1	A	357	PRO	3.0
1	B	348	THR	2.9
1	A	347	VAL	2.9
1	B	561	ARG	2.9
1	A	352	GLN	2.9
1	B	220	TYR	2.9
1	B	178	VAL	2.9
1	B	522	ALA	2.9
1	B	389	PHE	2.8
1	B	575	LEU	2.8
1	B	15	ARG	2.8
1	A	166	GLN	2.8
1	A	346	ASP	2.8
1	B	291	MET	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	260	SER	2.8
1	A	570	GLY	2.8
1	A	165	TRP	2.8
1	B	508	THR	2.8
1	A	225	VAL	2.8
1	A	274	SER	2.7
1	A	161	PHE	2.7
1	A	522	ALA	2.7
1	B	16	LEU	2.7
1	A	86	SER	2.7
1	A	163	ASN	2.7
1	A	213	GLY	2.7
1	B	498	ASP	2.6
1	A	371	THR	2.6
1	A	17	TRP	2.6
1	A	429	PHE	2.6
1	A	316	GLN	2.6
1	B	379	GLY	2.6
1	B	12	THR	2.6
1	B	73	GLY	2.5
1	B	368	GLN	2.5
1	A	341	GLU	2.5
1	B	290	ALA	2.5
1	A	344	VAL	2.5
1	B	565	LEU	2.5
1	B	170	VAL	2.5
1	B	180	PHE	2.5
1	B	65	ARG	2.5
1	A	271	SER	2.5
1	B	213	GLY	2.5
1	B	126	SER	2.4
1	A	361	HIS	2.4
1	B	216	VAL	2.4
1	B	280	THR	2.4
1	B	162	TRP	2.4
1	B	217	VAL	2.4
1	A	389	PHE	2.4
1	A	220	TYR	2.4
1	B	491	ILE	2.3
1	B	52	LEU	2.3
1	A	495	LEU	2.3
1	A	190	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	166	GLN	2.3
1	B	440	ALA	2.3
1	B	13	PHE	2.3
1	A	331	GLY	2.3
1	B	278	GLU	2.2
1	B	487	GLN	2.2
1	B	528	LYS	2.2
1	B	62	ASN	2.2
1	A	485	GLN	2.2
1	B	342	VAL	2.2
1	A	444	GLU	2.2
1	B	479	THR	2.2
1	A	440	ALA	2.2
1	A	216	VAL	2.1
1	A	573	ALA	2.1
1	A	519	ILE	2.1
1	B	512	ASP	2.1
1	A	173	VAL	2.1
1	A	181	ALA	2.0
1	A	320	GLY	2.0
1	A	410	TYR	2.0
1	A	450	ILE	2.0
1	B	360	SER	2.0
1	B	287	VAL	2.0
1	B	320	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no carbohydrates 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.