



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:31 AM 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
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : trunk26865

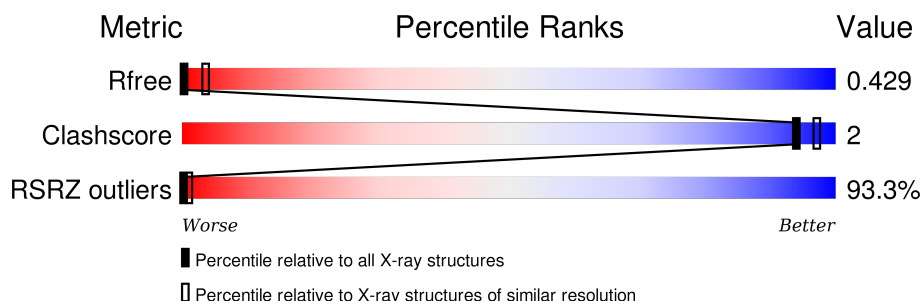
1 Overall quality at a glance

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}	91344	1015 (7.38-3.62)
Clashscore	102246	1020 (7.10-3.70)
RSRZ outliers	91569	1014 (7.38-3.62)

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.

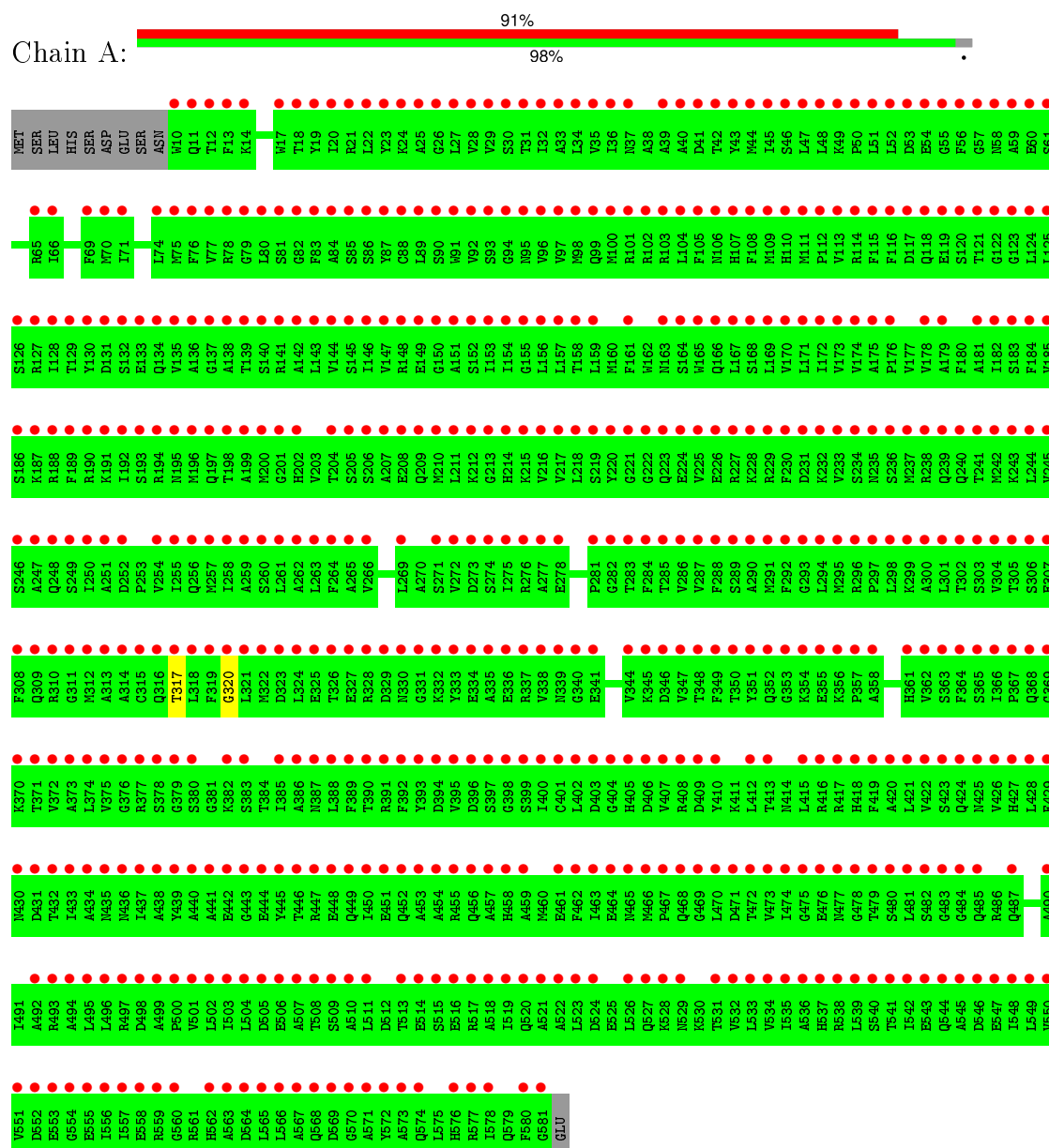
- Molecule 1 is a protein called Lipid A export ATP-binding/permease protein msbA.

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 errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

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



Category	Percentage
Red Bar	92%
Green Bar	98%



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 0.420 , 0.429	Depositor DCC
R_{free} test set	553 reflections (7.31%)	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 , 82.4	EDS
Estimated twinning fraction	0.030 for -h,l,k	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	1 of 7570 reflections (0.013%)	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, 0.375 respectively for untwinned datasets, and 0.333, 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).

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 ⓘ

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%)	9.30	532 (93%) 0 1	309, 309, 309, 309	0
1	B	572/582 (98%)	8.58	535 (93%) 0 1	309, 309, 309, 309	0
All	All	1144/1164 (98%)	8.94	1067 (93%) 0 1	309, 309, 309, 309	0

All (1067) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	246	SER	36.3
1	A	31	THR	36.2
1	A	117	ASP	34.8
1	A	147	VAL	34.4
1	A	296	ARG	34.0
1	A	198	THR	33.1
1	A	230	PHE	32.5
1	B	92	VAL	30.1
1	A	231	ASP	29.1
1	B	243	LYS	29.1
1	A	235	ASN	29.1
1	B	198	THR	28.6
1	A	227	ARG	28.5
1	A	299	LYS	27.9
1	B	242	MET	27.5
1	B	505	ASP	26.9
1	A	21	ARG	26.9
1	A	204	THR	26.9
1	A	289	SER	26.2
1	A	137	GLY	26.2
1	B	93	SER	26.1
1	A	236	SER	25.9
1	A	568	GLN	25.7
1	B	235	ASN	25.6

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Mol	Chain	Res	Type	RSRZ
1	A	32	ILE	25.4
1	A	145	SER	25.3
1	A	34	LEU	24.9
1	B	25	ALA	24.6
1	B	133	GLU	24.4
1	B	134	GLN	23.9
1	A	75	MET	23.5
1	A	133	GLU	23.3
1	A	224	GLU	23.3
1	A	78	ARG	23.2
1	B	245	VAL	23.1
1	A	577	ARG	22.8
1	B	183	SER	22.8
1	B	75	MET	22.8
1	A	431	ASP	22.7
1	A	150	GLY	22.6
1	B	152	SER	22.5
1	A	132	SER	22.3
1	B	456	GLN	22.2
1	B	137	GLY	22.0
1	B	112	PRO	21.9
1	B	265	ALA	21.7
1	A	300	ALA	21.7
1	B	157	LEU	21.7
1	A	421	LEU	21.6
1	A	259	ALA	21.6
1	B	262	ALA	21.4
1	A	477	ASN	21.4
1	A	363	SER	21.3
1	B	363	SER	21.2
1	B	248	GLN	21.1
1	B	355	GLU	21.0
1	A	245	VAL	20.9
1	B	422	VAL	20.9
1	A	265	ALA	20.9
1	A	258	ILE	20.9
1	B	227	ARG	20.7
1	A	116	PHE	20.4
1	A	423	SER	20.4
1	A	250	ILE	20.2
1	A	222	GLY	20.1
1	B	542	ILE	20.1

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Mol	Chain	Res	Type	RSRZ
1	B	53	ASP	20.0
1	A	243	LYS	19.9
1	A	425	ASN	19.9
1	A	422	VAL	19.9
1	A	547	GLU	19.9
1	A	470	LEU	19.8
1	A	438	ALA	19.7
1	B	258	ILE	19.7
1	A	527	GLN	19.6
1	B	423	SER	19.6
1	A	18	THR	19.5
1	B	158	THR	19.4
1	A	557	ILE	19.3
1	B	122	GLY	19.3
1	B	473	VAL	19.2
1	B	577	ARG	19.0
1	B	231	ASP	19.0
1	B	425	ASN	19.0
1	A	549	LEU	18.9
1	A	106	ASN	18.9
1	A	284	PHE	18.7
1	A	221	GLY	18.7
1	B	457	ALA	18.6
1	B	21	ARG	18.6
1	A	134	GLN	18.5
1	B	251	ALA	18.4
1	B	454	ALA	18.4
1	A	25	ALA	18.3
1	A	424	GLN	18.3
1	B	140	SER	18.2
1	A	408	ARG	18.1
1	A	202	HIS	18.1
1	B	18	THR	18.0
1	B	26	GLY	18.0
1	B	195	ASN	18.0
1	A	112	PRO	17.9
1	B	276	ARG	17.9
1	B	91	TRP	17.9
1	A	239	GLN	17.8
1	A	514	GLU	17.8
1	B	502	LEU	17.8
1	B	228	LYS	17.7

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Mol	Chain	Res	Type	RSRZ
1	A	505	ASP	17.7
1	B	418	HIS	17.7
1	B	307	GLU	17.7
1	B	354	LYS	17.6
1	A	504	LEU	17.6
1	A	129	THR	17.6
1	A	159	LEU	17.5
1	A	448	GLU	17.5
1	A	37	ASN	17.4
1	A	418	HIS	17.2
1	A	223	GLN	17.2
1	A	215	LYS	17.0
1	A	330	ASN	17.0
1	B	578	ILE	17.0
1	A	22	LEU	16.7
1	A	550	VAL	16.7
1	A	307	GLU	16.6
1	B	11	GLN	16.6
1	B	244	LEU	16.5
1	B	31	THR	16.5
1	B	22	LEU	16.4
1	B	506	GLU	16.3
1	A	329	ASP	16.1
1	B	558	GLU	16.1
1	A	283	THR	16.1
1	A	182	ILE	16.0
1	A	435	ASN	15.9
1	A	285	THR	15.9
1	A	301	LEU	15.8
1	A	483	GLY	15.8
1	A	409	ASP	15.8
1	A	556	ILE	15.7
1	A	506	GLU	15.7
1	A	403	ASP	15.7
1	B	239	GLN	15.7
1	B	30	SER	15.6
1	B	461	GLU	15.6
1	A	238	ARG	15.6
1	A	131	ASP	15.5
1	A	546	ASP	15.5
1	A	96	VAL	15.4
1	A	454	ALA	15.4

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Mol	Chain	Res	Type	RSRZ
1	B	230	PHE	15.4
1	A	479	THR	15.4
1	B	29	VAL	15.4
1	A	19	TYR	15.3
1	A	386	ALA	15.3
1	B	462	PHE	15.3
1	B	14	LYS	15.3
1	B	23	TYR	15.3
1	A	511	LEU	15.3
1	A	30	SER	15.2
1	A	27	LEU	15.2
1	A	58	ASN	15.2
1	A	456	GLN	15.2
1	A	558	GLU	15.2
1	B	146	ILE	15.2
1	B	466	MET	15.1
1	B	413	THR	15.1
1	B	191	LYS	15.1
1	B	325	GLU	15.0
1	A	232	LYS	15.0
1	A	48	LEU	15.0
1	A	128	ILE	15.0
1	B	232	LYS	14.9
1	A	156	LEU	14.9
1	A	398	GLY	14.8
1	B	188	ARG	14.8
1	B	96	VAL	14.8
1	A	436	ASN	14.7
1	A	515	SER	14.7
1	A	71	ILE	14.7
1	B	446	THR	14.7
1	B	527	GLN	14.7
1	A	387	ASN	14.7
1	A	439	TYR	14.7
1	A	463	ILE	14.6
1	B	131	ASP	14.6
1	A	559	ARG	14.6
1	B	426	VAL	14.6
1	B	404	GLY	14.6
1	A	264	PHE	14.5
1	A	70	MET	14.5
1	B	482	SER	14.5

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Mol	Chain	Res	Type	RSRZ
1	B	202	HIS	14.4
1	A	473	VAL	14.4
1	B	421	LEU	14.4
1	B	371	THR	14.4
1	A	502	LEU	14.3
1	A	407	VAL	14.3
1	B	468	GLN	14.3
1	B	41	ASP	14.2
1	B	174	VAL	14.2
1	B	483	GLY	14.2
1	A	40	ALA	14.2
1	B	447	ARG	14.1
1	A	354	LYS	14.1
1	B	339	ASN	14.1
1	A	148	ARG	14.0
1	B	432	THR	14.0
1	A	97	VAL	13.9
1	A	293	GLY	13.9
1	B	435	ASN	13.8
1	B	224	GLU	13.8
1	B	127	ARG	13.8
1	A	542	ILE	13.8
1	B	424	GLN	13.7
1	B	138	ALA	13.7
1	B	159	LEU	13.7
1	B	557	ILE	13.6
1	B	229	ARG	13.6
1	A	214	HIS	13.5
1	A	29	VAL	13.5
1	B	153	ILE	13.5
1	B	327	GLU	13.4
1	A	122	GLY	13.4
1	B	369	GLY	13.4
1	B	118	GLN	13.4
1	B	218	LEU	13.3
1	A	432	THR	13.3
1	B	113	VAL	13.3
1	A	364	PHE	13.2
1	B	293	GLY	13.2
1	A	406	ASP	13.2
1	B	246	SER	13.2
1	A	35	VAL	13.2

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Mol	Chain	Res	Type	RSRZ
1	A	462	PHE	13.2
1	A	201	GLY	13.1
1	A	337	ARG	13.1
1	A	309	GLN	13.1
1	B	221	GLY	13.1
1	A	334	GLU	13.1
1	B	298	LEU	13.1
1	A	192	ILE	13.1
1	A	157	LEU	13.1
1	A	374	LEU	13.1
1	B	305	THR	13.0
1	B	136	ALA	13.0
1	B	391	ARG	13.0
1	A	304	VAL	13.0
1	A	146	ILE	13.0
1	B	204	THR	13.0
1	B	32	ILE	12.8
1	B	33	ALA	12.8
1	B	401	CYS	12.7
1	B	149	GLU	12.7
1	A	102	ARG	12.7
1	A	298	LEU	12.7
1	B	206	SER	12.7
1	A	339	ASN	12.7
1	B	562	HIS	12.7
1	A	103	ARG	12.6
1	B	128	ILE	12.6
1	B	194	ARG	12.5
1	B	431	ASP	12.5
1	B	37	ASN	12.5
1	A	399	SER	12.5
1	A	42	THR	12.5
1	A	306	SER	12.5
1	B	108	PHE	12.4
1	A	185	VAL	12.4
1	B	185	VAL	12.4
1	A	548	ILE	12.3
1	B	261	LEU	12.3
1	A	144	VAL	12.3
1	A	368	GLN	12.3
1	B	420	ALA	12.3
1	B	281	PRO	12.3

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Mol	Chain	Res	Type	RSRZ
1	B	249	SER	12.2
1	B	223	GLN	12.2
1	A	92	VAL	12.1
1	A	228	LYS	12.0
1	B	90	SER	12.0
1	B	182	ILE	12.0
1	A	94	GLY	12.0
1	A	183	SER	12.0
1	B	186	SER	12.0
1	B	234	SER	12.0
1	A	295	MET	12.0
1	A	251	ALA	11.9
1	B	436	ASN	11.9
1	B	310	ARG	11.9
1	B	329	ASP	11.8
1	A	118	GLN	11.7
1	B	398	GLY	11.7
1	A	365	SER	11.7
1	B	106	ASN	11.7
1	A	467	PRO	11.7
1	A	457	ALA	11.6
1	A	226	GLU	11.6
1	B	510	ALA	11.5
1	A	325	GLU	11.5
1	A	242	MET	11.5
1	B	581	GLY	11.5
1	B	326	THR	11.5
1	A	369	GLY	11.5
1	B	547	GLU	11.5
1	A	323	ASP	11.5
1	A	503	ILE	11.5
1	B	480	SER	11.5
1	A	378	SER	11.4
1	A	247	ALA	11.4
1	A	28	VAL	11.4
1	B	222	GLY	11.4
1	A	57	GLY	11.4
1	A	333	TYR	11.4
1	A	240	GLN	11.3
1	A	510	ALA	11.3
1	A	452	GLN	11.3
1	B	40	ALA	11.3

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Mol	Chain	Res	Type	RSRZ
1	A	53	ASP	11.3
1	A	492	ALA	11.3
1	A	288	PHE	11.3
1	A	336	GLU	11.3
1	B	150	GLY	11.3
1	A	447	ARG	11.3
1	A	482	SER	11.2
1	B	141	ARG	11.2
1	B	80	LEU	11.2
1	B	514	GLU	11.2
1	B	336	GLU	11.1
1	B	296	ARG	11.1
1	B	208	GLU	11.1
1	B	43	TYR	11.1
1	B	145	SER	11.1
1	B	338	VAL	11.0
1	A	218	LEU	11.0
1	A	466	MET	11.0
1	A	179	ALA	11.0
1	B	571	ALA	11.0
1	B	301	LEU	11.0
1	A	20	ILE	11.0
1	A	65	ARG	10.9
1	B	550	VAL	10.9
1	A	404	GLY	10.9
1	A	297	PRO	10.9
1	B	135	VAL	10.9
1	B	408	ARG	10.9
1	B	214	HIS	10.8
1	B	94	GLY	10.8
1	A	33	ALA	10.8
1	B	526	LEU	10.8
1	A	262	ALA	10.8
1	A	372	VAL	10.7
1	A	571	ALA	10.7
1	A	23	TYR	10.7
1	A	496	LEU	10.7
1	A	115	PHE	10.6
1	B	309	GLN	10.6
1	B	132	SER	10.6
1	B	300	ALA	10.6
1	B	509	SER	10.6

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Mol	Chain	Res	Type	RSRZ
1	A	172	ILE	10.6
1	A	397	SER	10.6
1	A	366	ILE	10.6
1	A	154	ILE	10.5
1	B	17	TRP	10.5
1	B	543	GLU	10.5
1	B	236	SER	10.5
1	B	71	ILE	10.5
1	B	129	THR	10.5
1	B	167	LEU	10.5
1	B	34	LEU	10.4
1	B	97	VAL	10.4
1	B	534	VAL	10.4
1	B	215	LYS	10.4
1	B	56	PHE	10.4
1	B	549	LEU	10.4
1	B	144	VAL	10.3
1	B	199	ALA	10.3
1	B	173	VAL	10.3
1	A	237	MET	10.2
1	B	552	ASP	10.2
1	A	149	GLU	10.2
1	B	76	PHE	10.2
1	A	291	MET	10.2
1	A	234	SER	10.1
1	A	335	ALA	10.1
1	B	42	THR	10.1
1	A	127	ARG	10.1
1	B	117	ASP	10.1
1	B	205	SER	10.1
1	B	319	PHE	10.1
1	B	19	TYR	10.0
1	B	513	THR	10.0
1	B	507	ALA	10.0
1	A	76	PHE	10.0
1	A	113	VAL	9.9
1	A	551	VAL	9.9
1	A	105	PHE	9.9
1	B	548	ILE	9.9
1	B	387	ASN	9.9
1	A	327	GLU	9.9
1	A	518	ALA	9.9

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Mol	Chain	Res	Type	RSRZ
1	B	193	SER	9.9
1	B	501	VAL	9.9
1	A	100	MET	9.9
1	B	375	VAL	9.9
1	B	390	THR	9.8
1	A	80	LEU	9.8
1	B	241	THR	9.8
1	A	79	GLY	9.8
1	A	517	ARG	9.8
1	B	219	SER	9.7
1	B	203	VAL	9.7
1	A	282	GLY	9.7
1	A	41	ASP	9.7
1	B	467	PRO	9.6
1	A	93	SER	9.6
1	A	199	ALA	9.6
1	B	328	ARG	9.6
1	A	388	LEU	9.5
1	A	401	CYS	9.5
1	B	380	SER	9.5
1	B	335	ALA	9.5
1	B	471	ASP	9.5
1	B	356	LYS	9.5
1	B	318	LEU	9.5
1	B	330	ASN	9.5
1	B	362	VAL	9.5
1	B	154	ILE	9.5
1	B	576	HIS	9.4
1	B	36	ILE	9.4
1	A	187	LYS	9.4
1	A	377	ARG	9.4
1	A	208	GLU	9.4
1	A	83	PHE	9.4
1	A	465	ASN	9.4
1	B	529	ASN	9.4
1	A	459	ALA	9.3
1	A	497	ARG	9.3
1	A	143	LEU	9.3
1	B	207	ALA	9.3
1	A	521	ALA	9.3
1	B	171	LEU	9.3
1	A	205	SER	9.3

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Mol	Chain	Res	Type	RSRZ
1	B	554	GLY	9.3
1	B	175	ALA	9.2
1	B	264	PHE	9.2
1	A	140	SER	9.2
1	A	50	PRO	9.1
1	B	409	ASP	9.1
1	B	397	SER	9.1
1	A	244	LEU	9.1
1	A	480	SER	9.1
1	B	27	LEU	9.1
1	A	501	VAL	9.1
1	A	576	HIS	9.1
1	B	82	GLY	9.0
1	A	526	LEU	9.0
1	A	464	GLU	9.0
1	A	252	ASP	9.0
1	A	420	ALA	9.0
1	B	143	LEU	9.0
1	B	86	SER	9.0
1	A	126	SER	9.0
1	A	413	THR	8.9
1	A	578	ILE	8.9
1	B	116	PHE	8.9
1	B	104	LEU	8.9
1	B	252	ASP	8.9
1	A	273	ASP	8.9
1	A	533	LEU	8.9
1	B	439	TYR	8.9
1	B	443	GLY	8.8
1	B	377	ARG	8.8
1	A	194	ARG	8.8
1	B	20	ILE	8.8
1	B	266	VAL	8.8
1	A	509	SER	8.8
1	B	323	ASP	8.7
1	A	99	GLN	8.7
1	B	494	ALA	8.7
1	B	403	ASP	8.7
1	B	541	THR	8.6
1	A	367	PRO	8.6
1	B	455	ARG	8.6
1	B	556	ILE	8.6

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Mol	Chain	Res	Type	RSRZ
1	A	531	THR	8.6
1	B	419	PHE	8.6
1	B	160	MET	8.5
1	B	373	ALA	8.5
1	A	158	THR	8.5
1	A	46	SER	8.5
1	A	554	GLY	8.5
1	B	324	LEU	8.5
1	A	308	PHE	8.5
1	A	520	GLN	8.4
1	B	210	MET	8.4
1	A	119	GLU	8.4
1	B	518	ALA	8.4
1	A	77	VAL	8.4
1	B	83	PHE	8.4
1	A	233	VAL	8.4
1	A	534	VAL	8.4
1	B	350	THR	8.4
1	A	529	ASN	8.3
1	A	61	SER	8.3
1	A	469	GLY	8.3
1	B	275	ILE	8.3
1	B	57	GLY	8.3
1	A	305	THR	8.3
1	B	372	VAL	8.3
1	A	528	LYS	8.3
1	A	24	LYS	8.3
1	A	45	ILE	8.3
1	A	89	LEU	8.3
1	B	250	ILE	8.3
1	B	192	ILE	8.3
1	B	156	LEU	8.3
1	B	334	GLU	8.3
1	B	452	GLN	8.2
1	B	566	LEU	8.2
1	A	155	GLY	8.2
1	A	206	SER	8.2
1	B	337	ARG	8.2
1	B	434	ALA	8.2
1	A	136	ALA	8.2
1	A	442	GLU	8.1
1	A	74	LEU	8.1

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Mol	Chain	Res	Type	RSRZ
1	A	419	PHE	8.1
1	B	259	ALA	8.1
1	A	311	GLY	8.1
1	A	560	GLY	8.1
1	B	28	VAL	8.0
1	A	81	SER	8.0
1	A	426	VAL	8.0
1	B	444	GLU	8.0
1	A	135	VAL	8.0
1	B	393	TYR	8.0
1	B	511	LEU	8.0
1	B	304	VAL	8.0
1	B	74	LEU	8.0
1	B	538	ARG	8.0
1	B	24	LYS	8.0
1	A	104	LEU	8.0
1	A	351	TYR	7.9
1	B	184	PHE	7.9
1	B	437	ILE	7.9
1	B	123	GLY	7.9
1	A	373	ALA	7.9
1	B	283	THR	7.9
1	A	564	ASP	7.9
1	A	532	VAL	7.9
1	B	289	SER	7.9
1	B	396	ASP	7.8
1	A	391	ARG	7.8
1	B	109	MET	7.8
1	B	374	LEU	7.8
1	B	559	ARG	7.8
1	B	48	LEU	7.8
1	A	565	LEU	7.8
1	B	361	HIS	7.8
1	A	412	LEU	7.8
1	A	402	LEU	7.8
1	B	286	VAL	7.8
1	A	322	MET	7.8
1	A	539	LEU	7.7
1	B	313	ALA	7.7
1	A	481	LEU	7.7
1	A	338	VAL	7.7
1	B	370	LYS	7.7

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Mol	Chain	Res	Type	RSRZ
1	A	290	ALA	7.7
1	B	35	VAL	7.7
1	B	322	MET	7.7
1	A	313	ALA	7.7
1	A	43	TYR	7.6
1	A	248	GLN	7.6
1	B	463	ILE	7.6
1	B	492	ALA	7.6
1	B	209	GLN	7.6
1	B	292	PHE	7.6
1	B	477	ASN	7.6
1	B	124	LEU	7.5
1	A	171	LEU	7.5
1	A	276	ARG	7.5
1	B	332	LYS	7.5
1	B	564	ASP	7.5
1	B	45	ILE	7.5
1	B	357	PRO	7.5
1	A	193	SER	7.5
1	A	395	VAL	7.5
1	A	114	ARG	7.5
1	B	212	LYS	7.5
1	A	212	LYS	7.4
1	A	56	PHE	7.4
1	B	238	ARG	7.4
1	A	455	ARG	7.4
1	A	275	ILE	7.4
1	B	89	LEU	7.4
1	A	383	SER	7.4
1	A	211	LEU	7.4
1	A	484	GLY	7.4
1	A	111	MET	7.4
1	B	163	ASN	7.4
1	A	91	TRP	7.3
1	A	396	ASP	7.3
1	B	288	PHE	7.3
1	B	247	ALA	7.3
1	B	100	MET	7.3
1	B	412	LEU	7.3
1	B	438	ALA	7.3
1	A	572	TYR	7.3
1	B	102	ARG	7.3

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Mol	Chain	Res	Type	RSRZ
1	B	365	SER	7.3
1	B	105	PHE	7.3
1	A	310	ARG	7.3
1	A	434	ALA	7.2
1	A	196	MET	7.2
1	B	470	LEU	7.2
1	B	516	GLU	7.2
1	B	464	GLU	7.2
1	B	475	GLY	7.2
1	A	95	ASN	7.1
1	B	415	LEU	7.1
1	A	538	ARG	7.1
1	A	207	ALA	7.1
1	B	139	THR	7.1
1	B	273	ASP	7.1
1	A	153	ILE	7.1
1	B	546	ASP	7.1
1	B	358	ALA	7.1
1	B	121	THR	7.0
1	B	465	ASN	7.0
1	A	286	VAL	7.0
1	A	348	THR	7.0
1	A	451	GLU	7.0
1	A	324	LEU	7.0
1	A	393	TYR	7.0
1	A	493	ARG	7.0
1	A	188	ARG	7.0
1	B	448	GLU	7.0
1	B	197	GLN	7.0
1	A	87	TYR	7.0
1	A	494	ALA	7.0
1	A	152	SER	7.0
1	B	303	SER	7.0
1	B	299	LYS	6.9
1	A	90	SER	6.9
1	A	508	THR	6.9
1	B	442	GLU	6.9
1	B	580	PHE	6.9
1	A	318	LEU	6.9
1	A	458	HIS	6.9
1	A	197	GLN	6.9
1	A	292	PHE	6.8

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Mol	Chain	Res	Type	RSRZ
1	B	469	GLY	6.8
1	B	553	GLU	6.8
1	B	472	THR	6.7
1	A	567	ALA	6.7
1	A	121	THR	6.7
1	A	229	ARG	6.7
1	B	255	ILE	6.7
1	B	445	TYR	6.7
1	A	219	SER	6.7
1	B	333	TYR	6.7
1	A	98	MET	6.6
1	B	525	GLU	6.6
1	A	476	GLU	6.6
1	A	82	GLY	6.6
1	B	10	TRP	6.6
1	B	386	ALA	6.6
1	B	274	SER	6.5
1	B	481	LEU	6.5
1	B	168	SER	6.5
1	B	148	ARG	6.5
1	B	103	ARG	6.5
1	B	351	TYR	6.5
1	B	81	SER	6.5
1	A	59	ALA	6.5
1	B	237	MET	6.4
1	A	319	PHE	6.4
1	A	269	LEU	6.4
1	B	416	ARG	6.4
1	A	263	LEU	6.4
1	B	285	THR	6.4
1	B	282	GLY	6.3
1	A	375	VAL	6.3
1	B	569	ASP	6.3
1	B	493	ARG	6.3
1	B	407	VAL	6.3
1	B	490	ALA	6.3
1	B	306	SER	6.2
1	A	12	THR	6.2
1	B	402	LEU	6.2
1	B	98	MET	6.2
1	B	539	LEU	6.2
1	A	332	LYS	6.2

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Mol	Chain	Res	Type	RSRZ
1	A	186	SER	6.2
1	B	427	HIS	6.2
1	A	385	ILE	6.2
1	B	176	PRO	6.2
1	B	392	PHE	6.1
1	B	515	SER	6.1
1	A	108	PHE	6.1
1	B	161	PHE	6.1
1	B	196	MET	6.1
1	A	394	ASP	6.1
1	B	226	GLU	6.0
1	A	141	ARG	6.0
1	B	563	ALA	6.0
1	B	78	ARG	6.0
1	A	101	ARG	6.0
1	B	256	GLN	6.0
1	A	390	THR	6.0
1	A	281	PRO	5.9
1	B	54	GLU	5.9
1	B	125	LEU	5.9
1	B	364	PHE	5.9
1	B	459	ALA	5.9
1	A	210	MET	5.9
1	A	445	TYR	5.9
1	A	417	ARG	5.9
1	B	500	PRO	5.9
1	B	302	THR	5.9
1	B	317	THR	5.9
1	A	184	PHE	5.9
1	A	125	LEU	5.8
1	A	400	ILE	5.8
1	A	516	GLU	5.8
1	B	451	GLU	5.8
1	A	39	ALA	5.8
1	B	381	GLY	5.8
1	A	328	ARG	5.8
1	A	416	ARG	5.8
1	A	255	ILE	5.8
1	B	269	LEU	5.7
1	A	109	MET	5.7
1	B	47	LEU	5.7
1	B	574	GLN	5.7

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Mol	Chain	Res	Type	RSRZ
1	A	356	LYS	5.7
1	A	490	ALA	5.7
1	A	44	MET	5.7
1	B	536	ALA	5.7
1	B	366	ILE	5.7
1	A	468	GLN	5.6
1	B	484	GLY	5.6
1	A	443	GLY	5.6
1	B	39	ALA	5.6
1	A	10	TRP	5.6
1	A	553	GLU	5.6
1	B	521	ALA	5.6
1	A	195	ASN	5.6
1	B	107	HIS	5.6
1	A	277	ALA	5.6
1	A	326	THR	5.5
1	B	272	VAL	5.5
1	A	107	HIS	5.5
1	A	430	ASN	5.5
1	B	58	ASN	5.5
1	B	388	LEU	5.5
1	A	47	LEU	5.5
1	A	541	THR	5.5
1	B	44	MET	5.5
1	A	543	GLU	5.5
1	B	378	SER	5.5
1	B	240	GLN	5.4
1	A	427	HIS	5.4
1	B	70	MET	5.4
1	A	69	PHE	5.4
1	A	581	GLY	5.4
1	B	533	LEU	5.4
1	B	545	ALA	5.4
1	A	441	ALA	5.4
1	B	115	PHE	5.4
1	A	176	PRO	5.4
1	B	530	LYS	5.3
1	B	496	LEU	5.3
1	A	415	LEU	5.3
1	B	353	GLY	5.3
1	B	560	GLY	5.2
1	B	260	SER	5.2

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Mol	Chain	Res	Type	RSRZ
1	B	414	ASN	5.2
1	A	124	LEU	5.2
1	A	54	GLU	5.2
1	A	478	GLY	5.2
1	B	572	TYR	5.2
1	B	499	ALA	5.2
1	A	321	LEU	5.2
1	B	50	PRO	5.2
1	B	189	PHE	5.2
1	A	340	GLY	5.2
1	B	61	SER	5.2
1	A	317	THR	5.2
1	A	315	CYS	5.1
1	B	225	VAL	5.1
1	B	49	LYS	5.1
1	A	200	MET	5.1
1	A	138	ALA	5.1
1	A	209	GLN	5.1
1	B	453	ALA	5.1
1	B	537	HIS	5.1
1	A	26	GLY	5.1
1	B	130	TYR	5.1
1	B	181	ALA	5.1
1	A	170	VAL	5.1
1	B	85	SER	5.1
1	A	540	SER	5.0
1	B	211	LEU	5.0
1	A	294	LEU	5.0
1	A	55	GLY	5.0
1	A	241	THR	5.0
1	B	277	ALA	5.0
1	B	114	ARG	5.0
1	A	537	HIS	5.0
1	B	101	ARG	4.9
1	B	119	GLU	4.9
1	B	295	MET	4.9
1	A	566	LEU	4.9
1	A	49	LYS	4.9
1	A	178	VAL	4.9
1	A	376	GLY	4.9
1	A	405	HIS	4.9
1	B	405	HIS	4.9

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Mol	Chain	Res	Type	RSRZ
1	A	474	ILE	4.9
1	B	46	SER	4.9
1	A	507	ALA	4.9
1	A	513	THR	4.9
1	A	353	GLY	4.9
1	A	312	MET	4.9
1	A	437	ILE	4.9
1	B	395	VAL	4.9
1	A	544	GLN	4.9
1	B	60	GLU	4.9
1	B	535	ILE	4.9
1	A	123	GLY	4.8
1	A	85	SER	4.8
1	B	179	ALA	4.8
1	A	471	ASP	4.8
1	B	110	HIS	4.8
1	B	284	PHE	4.8
1	A	256	GLN	4.8
1	A	287	VAL	4.8
1	A	303	SER	4.8
1	A	552	ASP	4.8
1	B	406	ASP	4.8
1	B	551	VAL	4.8
1	A	453	ALA	4.8
1	A	169	LEU	4.8
1	B	314	ALA	4.8
1	B	474	ILE	4.8
1	B	504	LEU	4.8
1	B	517	ARG	4.7
1	A	446	THR	4.7
1	B	458	HIS	4.7
1	A	302	THR	4.7
1	B	95	ASN	4.6
1	B	147	VAL	4.6
1	B	376	GLY	4.6
1	A	355	GLU	4.6
1	B	99	GLN	4.6
1	A	257	MET	4.6
1	B	531	THR	4.6
1	A	379	GLY	4.6
1	A	345	LYS	4.6
1	A	545	ALA	4.5

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Mol	Chain	Res	Type	RSRZ
1	B	340	GLY	4.5
1	A	349	PHE	4.5
1	B	394	ASP	4.5
1	A	120	SER	4.5
1	A	191	LYS	4.5
1	B	172	ILE	4.5
1	B	294	LEU	4.5
1	B	383	SER	4.5
1	B	316	GLN	4.5
1	B	568	GLN	4.4
1	B	111	MET	4.4
1	A	66	ILE	4.4
1	A	580	PHE	4.4
1	B	441	ALA	4.4
1	B	520	GLN	4.4
1	B	400	ILE	4.3
1	B	567	ALA	4.3
1	A	314	ALA	4.3
1	A	350	THR	4.3
1	B	321	LEU	4.3
1	B	352	GLN	4.3
1	B	399	SER	4.3
1	B	485	GLN	4.2
1	B	503	ILE	4.2
1	B	478	GLY	4.2
1	B	151	ALA	4.2
1	B	349	PHE	4.2
1	A	13	PHE	4.1
1	A	151	ALA	4.1
1	A	449	GLN	4.1
1	B	544	GLN	4.1
1	A	555	GLU	4.1
1	B	417	ARG	4.1
1	A	562	HIS	4.0
1	B	87	TYR	4.0
1	B	268	PHE	4.0
1	A	36	ILE	4.0
1	B	497	ARG	4.0
1	A	84	ALA	4.0
1	B	155	GLY	3.9
1	A	167	LEU	3.9
1	A	139	THR	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	79	GLY	3.9
1	B	267	LEU	3.9
1	B	55	GLY	3.9
1	A	380	SER	3.9
1	A	428	LEU	3.9
1	A	382	LYS	3.9
1	B	433	ILE	3.9
1	A	475	GLY	3.9
1	B	460	MET	3.9
1	A	574	GLN	3.8
1	B	385	ILE	3.8
1	A	217	VAL	3.8
1	B	190	ARG	3.8
1	A	523	LEU	3.8
1	B	201	GLY	3.8
1	A	500	PRO	3.8
1	A	14	LYS	3.8
1	A	110	HIS	3.8
1	A	175	ALA	3.8
1	B	142	ALA	3.8
1	A	524	ASP	3.8
1	A	142	ALA	3.7
1	A	569	ASP	3.7
1	A	272	VAL	3.7
1	B	347	VAL	3.7
1	A	362	VAL	3.7
1	A	266	VAL	3.7
1	A	164	SER	3.7
1	B	540	SER	3.7
1	B	67	LEU	3.7
1	B	489	VAL	3.7
1	A	358	ALA	3.7
1	B	315	CYS	3.7
1	A	536	ALA	3.7
1	A	563	ALA	3.7
1	B	200	MET	3.6
1	A	261	LEU	3.6
1	B	523	LEU	3.6
1	A	174	VAL	3.6
1	A	11	GLN	3.6
1	A	130	TYR	3.6
1	B	382	LYS	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	535	ILE	3.5
1	B	532	VAL	3.5
1	B	187	LYS	3.5
1	B	555	GLU	3.4
1	A	254	VAL	3.4
1	B	428	LEU	3.4
1	B	120	SER	3.4
1	A	499	ALA	3.4
1	B	254	VAL	3.4
1	A	433	ILE	3.4
1	A	60	GLU	3.4
1	A	51	LEU	3.3
1	B	476	GLU	3.3
1	A	168	SER	3.3
1	B	570	GLY	3.3
1	A	52	LEU	3.3
1	A	249	SER	3.3
1	A	392	PHE	3.3
1	B	311	GLY	3.3
1	A	278	GLU	3.3
1	B	297	PRO	3.2
1	A	88	CYS	3.2
1	A	461	GLU	3.2
1	B	522	ALA	3.2
1	B	220	TYR	3.2
1	B	308	PHE	3.2
1	B	524	ASP	3.2
1	A	189	PHE	3.2
1	B	348	THR	3.2
1	A	498	ASP	3.1
1	A	370	LYS	3.1
1	A	347	VAL	3.1
1	B	575	LEU	3.1
1	A	352	GLN	3.1
1	B	178	VAL	3.1
1	B	389	PHE	3.1
1	A	357	PRO	3.0
1	A	165	TRP	3.0
1	B	561	ARG	3.0
1	A	570	GLY	3.0
1	A	522	ALA	3.0
1	A	346	ASP	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	15	ARG	3.0
1	A	161	PHE	3.0
1	B	291	MET	3.0
1	B	508	THR	3.0
1	A	260	SER	2.9
1	A	166	GLN	2.9
1	A	225	VAL	2.9
1	A	274	SER	2.9
1	B	16	LEU	2.9
1	A	371	THR	2.9
1	B	498	ASP	2.9
1	A	17	TRP	2.8
1	A	429	PHE	2.8
1	A	86	SER	2.8
1	B	12	THR	2.8
1	A	213	GLY	2.8
1	B	379	GLY	2.8
1	A	163	ASN	2.7
1	A	316	GLN	2.7
1	B	290	ALA	2.7
1	B	73	GLY	2.7
1	B	565	LEU	2.7
1	B	170	VAL	2.7
1	B	368	GLN	2.7
1	B	180	PHE	2.7
1	A	220	TYR	2.7
1	A	344	VAL	2.6
1	B	440	ALA	2.6
1	B	162	TRP	2.6
1	B	213	GLY	2.6
1	A	341	GLU	2.6
1	A	361	HIS	2.6
1	A	271	SER	2.6
1	B	65	ARG	2.6
1	B	280	THR	2.6
1	B	216	VAL	2.6
1	A	389	PHE	2.6
1	B	52	LEU	2.6
1	B	491	ILE	2.5
1	B	217	VAL	2.5
1	B	126	SER	2.5
1	A	495	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	440	ALA	2.5
1	B	13	PHE	2.4
1	A	190	ARG	2.4
1	A	331	GLY	2.4
1	B	342	VAL	2.4
1	B	487	GLN	2.4
1	B	278	GLU	2.4
1	B	166	GLN	2.4
1	B	479	THR	2.4
1	A	573	ALA	2.4
1	A	444	GLU	2.3
1	A	485	GLN	2.3
1	B	62	ASN	2.3
1	B	528	LYS	2.3
1	A	181	ALA	2.3
1	A	216	VAL	2.3
1	A	410	TYR	2.3
1	A	519	ILE	2.3
1	A	173	VAL	2.3
1	B	512	ASP	2.2
1	A	320	GLY	2.2
1	A	450	ILE	2.2
1	B	429	PHE	2.2
1	B	320	GLY	2.2
1	B	287	VAL	2.1
1	B	360	SER	2.1
1	B	519	ILE	2.1
1	B	77	VAL	2.1
1	B	430	ASN	2.1
1	A	472	THR	2.1
1	B	169	LEU	2.1
1	A	487	GLN	2.0
1	B	59	ALA	2.0
1	B	38	ALA	2.0
1	B	367	PRO	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 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.