



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:18 PM UTC

PDB ID : 6O30 / pdb_00006o30
Title : Lipid A transporter MsbA from Salmonella typhimurium
Authors : Padayatti, P.S.; Zhang, Q.; Wilson, I.A.; Lee, S.C.; Stanfield, R.L.
Deposited on : 2019-02-25
Resolution : 4.47 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

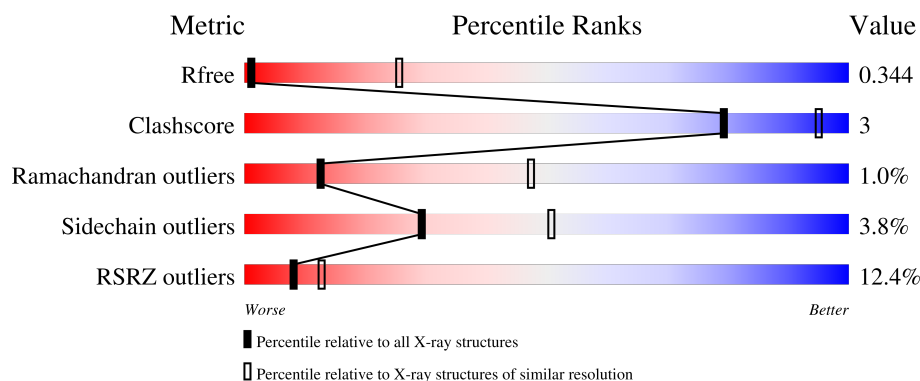
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.47 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	1124 (5.06-3.90)
Clashscore	190562	1028 (5.04-3.92)
Ramachandran outliers	187476	1058 (5.06-3.90)
Sidechain outliers	187428	1041 (5.06-3.90)
RSRZ outliers	180081	1119 (5.06-3.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	576	10% 90% 10%
1	B	576	14% 88% 12%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 8894 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.

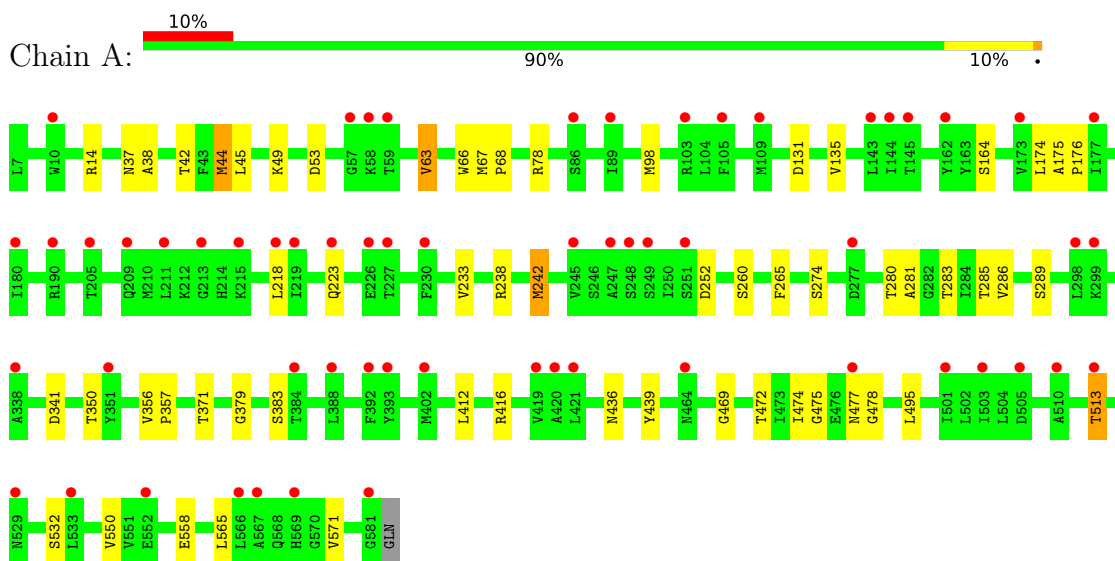
- Molecule 1 is a protein called Lipid A export ATP-binding/permease protein MsbA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	575	Total	C	N	O	S	0	0	0
			4447	2823	770	827	27			
1	B	575	Total	C	N	O	S	0	0	0
			4447	2823	770	827	27			

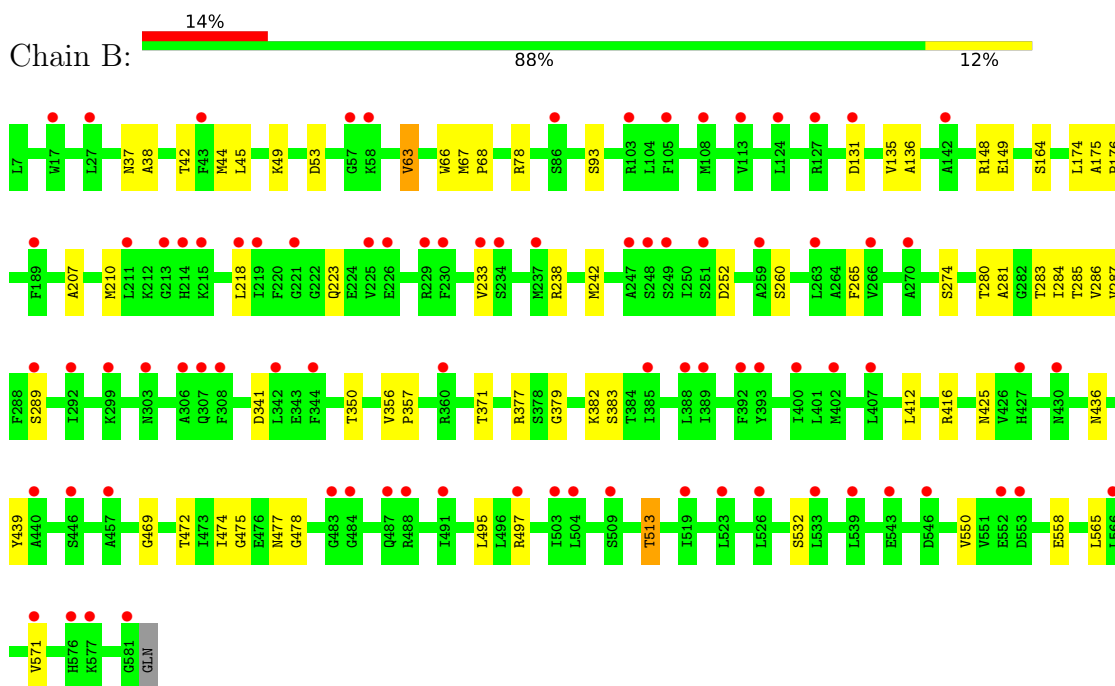
3 Residue-property plots [i](#)

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

- Molecule 1: 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 2	Depositor
Cell constants a, b, c, α , β , γ	82.26Å 153.20Å 232.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.75 – 4.47 46.75 – 4.47	Depositor EDS
% Data completeness (in resolution range)	80.7 (46.75-4.47) 83.2 (46.75-4.47)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.88 (at 4.45Å)	Xtriage
Refinement program	PHENIX (1.12_2829: ???)	Depositor
R, R_{free}	0.307 , 0.340 0.320 , 0.344	Depositor DCC
R_{free} test set	745 reflections (3.50%)	wwPDB-VP
Wilson B-factor (Å ²)	184.6	Xtriage
Anisotropy	0.730	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 222.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	8894	wwPDB-VP
Average B, all atoms (Å ²)	271.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.95% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.20	0/4514	0.53	0/6101
1	B	0.20	0/4514	0.53	0/6101
All	All	0.20	0/9028	0.53	0/12202

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	4447	0	4568	24	0
1	B	4447	0	4568	24	0
All	All	8894	0	9136	48	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 3.

All (48) 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:474:ILE:HG22	1:A:478:GLY:HA2	1.82	0.60
1:B:49:LYS:NZ	1:B:53:ASP:OD2	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:474:ILE:HG22	1:B:478:GLY:HA2	1.87	0.57
1:A:550:VAL:HG11	1:A:571:VAL:HG23	1.87	0.56
1:B:37:ASN:OD1	1:B:78:ARG:HG2	2.07	0.54
1:B:175:ALA:HB3	1:B:176:PRO:HD3	1.90	0.54
1:B:350:THR:HG22	1:B:357:PRO:HA	1.91	0.53
1:B:550:VAL:HG11	1:B:571:VAL:HG23	1.91	0.53
1:A:412:LEU:HD22	1:A:416:ARG:CZ	2.40	0.52
1:B:281:ALA:O	1:B:285:THR:HG23	2.10	0.51
1:B:412:LEU:HD22	1:B:416:ARG:CZ	2.39	0.51
1:A:350:THR:HG22	1:A:357:PRO:HA	1.93	0.51
1:A:281:ALA:O	1:A:285:THR:HG23	2.11	0.50
1:B:67:MET:HB3	1:B:68:PRO:HD3	1.93	0.50
1:A:67:MET:HB3	1:A:68:PRO:HD3	1.95	0.49
1:A:218:LEU:HD23	1:A:223:GLN:HE21	1.77	0.49
1:B:63:VAL:HA	1:B:66:TRP:NE1	2.28	0.49
1:A:175:ALA:HB3	1:A:176:PRO:HD3	1.95	0.48
1:A:558:GLU:HB3	1:A:565:LEU:HD22	1.96	0.48
1:A:38:ALA:O	1:A:42:THR:HG23	2.14	0.48
1:A:37:ASN:OD1	1:A:78:ARG:HG2	2.14	0.48
1:A:45:LEU:HD11	1:A:289:SER:HB3	1.95	0.48
1:A:238:ARG:O	1:A:242:MET:HG2	2.14	0.48
1:B:38:ALA:O	1:B:42:THR:HG23	2.14	0.48
1:B:218:LEU:HD23	1:B:223:GLN:HE21	1.80	0.47
1:A:131:ASP:O	1:A:135:VAL:HG23	2.15	0.47
1:B:238:ARG:O	1:B:242:MET:HG2	2.15	0.46
1:A:49:LYS:NZ	1:A:53:ASP:OD2	2.45	0.46
1:B:280:THR:OG1	1:B:283:THR:HG23	2.15	0.46
1:B:207:ALA:HA	1:B:210:MET:HE3	1.97	0.45
1:A:63:VAL:HA	1:A:66:TRP:NE1	2.33	0.44
1:A:280:THR:OG1	1:A:283:THR:HG23	2.17	0.44
1:B:174:LEU:HD11	1:B:265:PHE:CD2	2.53	0.44
1:B:174:LEU:HD11	1:B:265:PHE:HD2	1.81	0.44
1:B:37:ASN:HD22	1:B:148:ARG:HE	1.65	0.44
1:B:558:GLU:HB3	1:B:565:LEU:HD22	1.99	0.44
1:B:469:GLY:O	1:B:472:THR:OG1	2.36	0.43
1:B:131:ASP:O	1:B:135:VAL:HG23	2.17	0.43
1:A:44:MET:HE3	1:A:44:MET:HB2	1.87	0.43
1:B:45:LEU:HD11	1:B:289:SER:HB3	2.00	0.43
1:A:14:ARG:HA	1:A:14:ARG:HD2	1.79	0.42
1:A:174:LEU:HD11	1:A:265:PHE:HD2	1.83	0.42
1:A:174:LEU:HD11	1:A:265:PHE:CD2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:283:THR:O	1:B:287:VAL:HG23	2.21	0.41
1:B:93:SER:HB2	1:B:136:ALA:HB1	2.02	0.41
1:A:98:MET:HE2	1:A:98:MET:HB3	1.90	0.41
1:A:469:GLY:O	1:A:472:THR:OG1	2.38	0.41
1:A:242:MET:HE2	1:A:242:MET:HA	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	573/576 (100%)	537 (94%)	30 (5%)	6 (1%)	12	47
1	B	573/576 (100%)	535 (93%)	32 (6%)	6 (1%)	12	47
All	All	1146/1152 (100%)	1072 (94%)	62 (5%)	12 (1%)	12	47

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	513	THR
1	B	513	THR
1	A	356	VAL
1	B	356	VAL
1	A	164	SER
1	B	164	SER
1	B	379	GLY
1	B	439	TYR
1	A	379	GLY
1	A	439	TYR
1	A	475	GLY
1	B	475	GLY

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	485/487 (100%)	469 (97%)	16 (3%)	33	55
1	B	485/487 (100%)	464 (96%)	21 (4%)	26	48
All	All	970/974 (100%)	933 (96%)	37 (4%)	29	51

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	MET
1	A	63	VAL
1	A	233	VAL
1	A	242	MET
1	A	252	ASP
1	A	260	SER
1	A	274	SER
1	A	286	VAL
1	A	341	ASP
1	A	371	THR
1	A	383	SER
1	A	436	ASN
1	A	477	ASN
1	A	495	LEU
1	A	513	THR
1	A	532	SER
1	B	44	MET
1	B	63	VAL
1	B	149	GLU
1	B	233	VAL
1	B	252	ASP
1	B	260	SER
1	B	274	SER
1	B	284	ILE
1	B	286	VAL
1	B	341	ASP
1	B	371	THR

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Mol	Chain	Res	Type
1	B	377	ARG
1	B	382	LYS
1	B	383	SER
1	B	425	ASN
1	B	436	ASN
1	B	477	ASN
1	B	495	LEU
1	B	497	ARG
1	B	513	THR
1	B	532	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	307	GLN
1	A	405	HIS
1	A	418	GLN
1	A	424	GLN
1	B	11	GLN
1	B	405	HIS
1	B	424	GLN
1	B	427	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	575/576 (99%)	0.54	60 (10%)	11 16	168, 258, 319, 375	0
1	B	575/576 (99%)	0.72	83 (14%)	6 11	206, 280, 327, 365	0
All	All	1150/1152 (99%)	0.63	143 (12%)	8 13	168, 269, 324, 375	0

All (143) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	569	HIS	9.9
1	A	59	THR	8.6
1	A	57	GLY	8.2
1	B	57	GLY	6.5
1	A	86	SER	6.2
1	B	233	VAL	6.2
1	B	215	LYS	6.0
1	A	567	ALA	6.0
1	B	251	SER	5.8
1	B	108	MET	5.8
1	A	248	SER	5.8
1	B	392	PHE	5.8
1	A	421	LEU	5.4
1	A	177	ILE	5.4
1	A	226	GLU	5.3
1	A	477	ASN	5.0
1	A	105	PHE	5.0
1	A	219	ILE	4.9
1	B	237	MET	4.9
1	A	505	ASP	4.9
1	B	533	LEU	4.9
1	A	384	THR	4.8
1	A	298	LEU	4.8
1	B	113	VAL	4.8

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Mol	Chain	Res	Type	RSRZ
1	A	503	ILE	4.7
1	A	58	LYS	4.7
1	A	566	LEU	4.7
1	A	513	THR	4.7
1	B	292	ILE	4.6
1	B	400	ILE	4.5
1	B	576	HIS	4.4
1	A	419	VAL	4.3
1	A	144	ILE	4.2
1	B	344	PHE	4.2
1	B	189	PHE	4.2
1	B	483	GLY	4.2
1	A	277	ASP	4.2
1	B	389	ILE	4.2
1	B	263	LEU	4.2
1	B	289	SER	4.1
1	B	484	GLY	4.1
1	B	218	LEU	4.1
1	A	180	ILE	4.0
1	B	234	SER	4.0
1	A	247	ALA	4.0
1	A	245	VAL	4.0
1	A	89	ILE	3.9
1	B	388	LEU	3.9
1	A	402	MET	3.9
1	B	230	PHE	3.9
1	A	213	GLY	3.9
1	B	487	GLN	3.8
1	B	393	TYR	3.8
1	B	248	SER	3.8
1	A	393	TYR	3.8
1	A	215	LYS	3.7
1	A	392	PHE	3.6
1	B	566	LEU	3.6
1	B	86	SER	3.5
1	A	388	LEU	3.5
1	B	266	VAL	3.5
1	A	162	TYR	3.4
1	B	247	ALA	3.3
1	A	109	MET	3.3
1	B	219	ILE	3.3
1	B	457	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	307	GLN	3.3
1	B	503	ILE	3.3
1	A	230	PHE	3.3
1	A	223	GLN	3.3
1	B	226	GLU	3.2
1	B	577	LYS	3.2
1	A	249	SER	3.2
1	B	427	HIS	3.2
1	B	103	ARG	3.2
1	A	227	THR	3.1
1	B	213	GLY	3.1
1	B	491	ILE	3.1
1	B	221	GLY	3.0
1	B	342	LEU	3.0
1	B	306	ALA	3.0
1	A	211	LEU	2.9
1	B	519	ILE	2.9
1	A	209	GLN	2.9
1	B	58	LYS	2.9
1	A	351	TYR	2.9
1	B	504	LEU	2.8
1	B	303	ASN	2.8
1	B	407	LEU	2.8
1	A	299	LYS	2.8
1	B	17	TRP	2.7
1	B	526	LEU	2.7
1	A	581	GLY	2.7
1	A	464	ASN	2.7
1	B	440	ALA	2.7
1	A	190	ARG	2.7
1	B	229	ARG	2.7
1	B	225	VAL	2.6
1	A	251	SER	2.6
1	B	124	LEU	2.5
1	B	127	ARG	2.5
1	A	529	ASN	2.5
1	A	338	ALA	2.5
1	B	523	LEU	2.5
1	B	249	SER	2.5
1	A	143	LEU	2.5
1	B	308	PHE	2.5
1	A	420	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	270	ALA	2.4
1	A	510	ALA	2.4
1	A	501	ILE	2.4
1	B	259	ALA	2.4
1	B	105	PHE	2.3
1	B	546	ASP	2.3
1	B	571	VAL	2.3
1	B	27	LEU	2.3
1	B	488	ARG	2.3
1	B	509	SER	2.3
1	B	552	GLU	2.2
1	B	497	ARG	2.2
1	B	581	GLY	2.2
1	B	43	PHE	2.2
1	B	553	ASP	2.2
1	A	173	VAL	2.2
1	B	543	GLU	2.2
1	B	211	LEU	2.2
1	B	142	ALA	2.1
1	B	539	LEU	2.1
1	A	205	THR	2.1
1	B	446	SER	2.1
1	B	385	ILE	2.1
1	A	103	ARG	2.1
1	A	533	LEU	2.1
1	B	360	ARG	2.1
1	B	131	ASP	2.1
1	B	214	HIS	2.1
1	A	552	GLU	2.1
1	A	145	THR	2.0
1	B	402	MET	2.0
1	A	218	LEU	2.0
1	B	299	LYS	2.0
1	A	10	TRP	2.0
1	B	430	ASN	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.