



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 1WP1 / pdb_00001wp1
Title : Crystal structure of the drug-discharge outer membrane protein, OprM
Authors : Akama, H.; Kanemaki, M.; Yoshimura, M.; Tsukihara, T.; Kashiwagi, T.;
Narita, S.; Nakagawa, A.; Nakae, T.
Deposited on : 2004-08-28
Resolution : 2.56 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

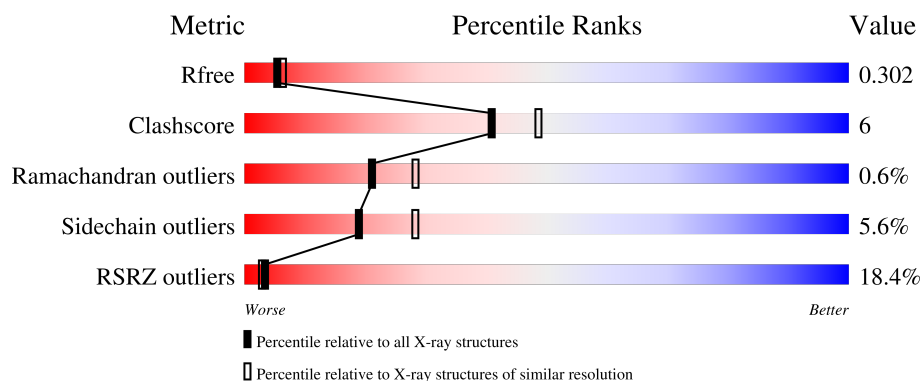
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.56 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	1853 (2.58-2.54)
Clashscore	190562	1897 (2.58-2.54)
Ramachandran outliers	187476	1875 (2.58-2.54)
Sidechain outliers	187428	1875 (2.58-2.54)
RSRZ outliers	180081	1853 (2.58-2.54)

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	474	
1	B	474	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6671 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 Outer membrane protein oprM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	456	Total	C	N	O	S	0	0	0
			3494	2186	622	683	3			
1	B	405	Total	C	N	O	S	0	0	0
			3153	1983	559	609	2			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	469	HIS	-	expression tag	UNP Q51487
A	470	HIS	-	expression tag	UNP Q51487
A	471	HIS	-	expression tag	UNP Q51487
A	472	HIS	-	expression tag	UNP Q51487
A	473	HIS	-	expression tag	UNP Q51487
A	474	HIS	-	expression tag	UNP Q51487
B	469	HIS	-	expression tag	UNP Q51487
B	470	HIS	-	expression tag	UNP Q51487
B	471	HIS	-	expression tag	UNP Q51487
B	472	HIS	-	expression tag	UNP Q51487
B	473	HIS	-	expression tag	UNP Q51487
B	474	HIS	-	expression tag	UNP Q51487

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	17	Total	O	0	0
			17	17		
2	B	7	Total	O	0	0
			7	7		

T454	
T455	
T456	
Q457	
GLN	GLN
THR	THR
ALA	ALA
LYS	LYS
GLU	GLU
ASP	ASP
PRO	PRO
GLN	GLN
ALA	ALA
HIS	HIS
HIS	HIS
HIS	HIS
HIS	HIS
HIS	HIS

4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	85.43Å 85.43Å 1044.30Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	38.63 – 2.56 38.63 – 2.56	Depositor EDS
% Data completeness (in resolution range)	99.2 (38.63-2.56) 99.1 (38.63-2.56)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.82 (at 2.58Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.252 , 0.308 0.249 , 0.302	Depositor DCC
R_{free} test set	2438 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	77.7	Xtriage
Anisotropy	0.023	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 58.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	6671	wwPDB-VP
Average B, all atoms (Å ²)	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.86% 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	A	0.77	0/3550	1.00	4/4829 (0.1%)
1	B	0.95	9/3202 (0.3%)	1.04	10/4353 (0.2%)
All	All	0.86	9/6752 (0.1%)	1.02	14/9182 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	78	ARG	CZ-NH1	27.58	1.71	1.32
1	B	78	ARG	NE-CZ	12.21	1.46	1.33
1	B	81	ARG	CZ-NH1	11.99	1.49	1.32
1	B	81	ARG	NE-CZ	5.84	1.39	1.33
1	B	78	ARG	CD-NE	5.65	1.54	1.46
1	B	78	ARG	CZ-NH2	5.48	1.40	1.33
1	B	136	ARG	CZ-NH1	5.25	1.40	1.32
1	B	141	GLU	CD-OE2	5.24	1.35	1.25
1	B	81	ARG	CZ-NH2	5.00	1.40	1.33

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	297	PHE	CA-C-N	11.16	133.79	119.84
1	B	297	PHE	C-N-CA	11.16	133.79	119.84
1	B	78	ARG	NE-CZ-NH2	-10.64	109.62	119.20
1	B	78	ARG	CD-NE-CZ	-8.25	112.86	124.40
1	B	81	ARG	NE-CZ-NH2	-7.79	112.19	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	410	ASN	N-CA-C	7.54	120.25	110.53
1	B	332	LEU	CA-C-N	6.97	126.89	119.85
1	B	332	LEU	C-N-CA	6.97	126.89	119.85
1	B	275	ILE	N-CA-C	-5.85	104.62	111.00
1	A	305	ASN	N-CA-C	5.81	117.80	109.14
1	B	297	PHE	N-CA-C	5.42	116.50	109.72
1	A	336	THR	N-CA-C	-5.36	102.11	110.42
1	B	331	ASN	N-CA-C	5.29	116.82	107.61
1	A	302	LEU	N-CA-C	5.24	117.14	108.13

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	447	GLY	Peptide

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	3494	0	3473	44	0
1	B	3153	0	3138	42	0
2	A	17	0	0	2	0
2	B	7	0	0	0	0
All	All	6671	0	6611	86	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 6.

All (86) 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:B:78:ARG:NH1	1:B:78:ARG:CZ	1.71	1.54
1:A:336:THR:HG21	1:A:339:SER:HB3	1.26	1.08
1:A:336:THR:CG2	1:A:339:SER:HB3	1.89	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:87:ARG:HB2	1:B:124:TRP:HB2	1.59	0.84
1:A:336:THR:HG21	1:A:339:SER:CB	2.11	0.79
1:A:336:THR:CG2	1:A:339:SER:CB	2.64	0.76
1:B:435:GLN:HG3	1:B:436:LEU:N	2.00	0.76
1:B:433:LEU:O	1:B:437:THR:HG23	1.86	0.75
1:A:403:ARG:NH1	1:A:409:ASP:OD2	2.21	0.73
1:B:39:GLY:HA2	1:B:451:ASN:O	1.90	0.71
1:A:272:ARG:HD3	1:A:274:ASP:OD1	1.91	0.71
1:A:251:GLY:H	1:A:254:GLN:HE21	1.38	0.70
1:B:289:ILE:HD11	1:B:351:LYS:HD2	1.72	0.70
1:B:67:ALA:HA	1:B:150:GLN:HE21	1.57	0.69
1:A:305:ASN:HB2	1:A:325:LEU:HB3	1.73	0.69
1:A:12:ALA:HB2	1:A:269:LEU:HD11	1.75	0.69
1:A:38:ILE:HD12	1:A:260:VAL:HG22	1.75	0.69
1:B:9:ARG:CD	1:B:279:GLU:OE2	2.42	0.68
1:B:345:ASP:O	1:B:349:ILE:HG12	1.94	0.68
1:B:365:ALA:O	1:B:369:VAL:HG23	1.93	0.68
1:B:9:ARG:HD2	1:B:279:GLU:OE2	1.95	0.67
1:B:282:LEU:HD11	1:B:355:VAL:HG23	1.75	0.67
1:A:121:THR:HG21	1:A:124:TRP:HB2	1.80	0.62
1:A:331:ASN:C	1:A:331:ASN:OD1	2.43	0.62
1:A:336:THR:HG22	1:A:339:SER:H	1.66	0.59
1:B:77:TYR:HA	1:B:139:ALA:HB1	1.85	0.59
1:B:7:TYR:OH	1:B:279:GLU:HG2	2.03	0.57
1:B:272:ARG:NH1	1:B:274:ASP:OD2	2.38	0.57
1:B:9:ARG:HD3	1:B:279:GLU:OE2	2.06	0.55
1:B:70:VAL:HG21	1:B:150:GLN:NE2	2.21	0.55
1:B:41:ARG:HG3	1:B:452:GLN:HG3	1.89	0.55
1:B:397:TYR:HA	1:B:417:ALA:HB1	1.89	0.54
1:A:35:ALA:HB2	1:A:260:VAL:HG13	1.90	0.54
1:A:16:ALA:O	1:A:265:PRO:HG2	2.09	0.52
1:B:67:ALA:HA	1:B:150:GLN:NE2	2.24	0.52
1:B:67:ALA:O	1:B:70:VAL:HB	2.11	0.51
1:B:399:LEU:O	1:B:403:ARG:HG3	2.11	0.50
1:A:41:ARG:HD2	1:A:50:GLN:OE1	2.11	0.50
1:B:403:ARG:NH1	1:B:409:ASP:OD2	2.45	0.50
1:A:174:GLN:HE22	1:A:426:GLN:HA	1.76	0.50
1:A:46:ASP:OD1	1:A:46:ASP:C	2.54	0.49
1:A:3:LEU:O	1:A:293:ARG:NH1	2.36	0.49
1:B:60:ASN:ND2	1:B:157:LEU:HD11	2.28	0.48
1:A:171:ASP:OD2	1:A:230:ASP:OD2	2.31	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:140:LEU:O	1:B:143:TYR:HB3	2.15	0.47
1:A:41:ARG:CD	1:A:50:GLN:OE1	2.64	0.46
1:B:298:PRO:HB3	1:B:331:ASN:H	1.79	0.46
1:B:349:ILE:HA	1:B:352:ASP:HB2	1.98	0.46
1:A:174:GLN:HE22	1:A:426:GLN:HG2	1.81	0.46
1:A:435:GLN:HG3	1:A:436:LEU:N	2.30	0.46
1:A:46:ASP:OD1	1:A:48:GLN:N	2.46	0.46
1:A:391:LYS:O	1:A:395:GLU:HG2	2.17	0.45
1:A:120:GLY:HA3	1:A:304:ALA:O	2.17	0.45
1:A:71:GLU:OE1	1:A:74:ARG:NH1	2.44	0.44
1:B:83:ASP:C	1:B:132:LEU:HD11	2.42	0.44
1:B:84:LEU:O	1:B:124:TRP:HZ2	2.01	0.44
1:A:10:PRO:HD2	1:A:358:TYR:CE2	2.53	0.43
1:B:7:TYR:OH	1:B:279:GLU:CG	2.65	0.43
1:A:35:ALA:CB	1:A:260:VAL:HG13	2.48	0.43
1:A:245:ASN:HB3	2:A:477:HOH:O	2.17	0.43
1:A:300:ILE:H	1:A:300:ILE:HG13	1.59	0.43
1:A:13:PRO:HG3	1:A:359:GLU:HG2	2.00	0.43
1:A:336:THR:HG22	1:A:337:ALA:N	2.34	0.43
1:A:58:GLU:O	1:A:64:ARG:NH2	2.52	0.42
1:B:238:LEU:C	1:B:240:SER:H	2.26	0.42
1:A:189:PHE:CD2	1:A:189:PHE:C	2.97	0.42
1:A:272:ARG:HB3	1:A:275:ILE:HD12	2.00	0.42
1:B:8:GLN:H	1:B:8:GLN:HG3	1.65	0.42
1:B:242:ILE:HA	1:B:243:PRO:HD3	1.88	0.42
1:A:155:THR:HG22	1:A:449:GLY:H	1.85	0.42
1:B:64:ARG:O	1:B:68:LEU:HG	2.20	0.42
1:A:46:ASP:HA	1:A:47:PRO:HD3	1.95	0.42
1:B:13:PRO:HB2	1:B:363:GLN:HE21	1.84	0.42
1:B:452:GLN:HG2	1:B:453:GLN:HG2	2.01	0.41
1:B:9:ARG:HA	1:B:10:PRO:HD3	1.93	0.41
1:A:19:PRO:HB2	1:A:24:TYR:CZ	2.55	0.41
1:B:271:ARG:O	1:B:273:PRO:HD3	2.20	0.41
1:B:383:LEU:CD1	1:B:435:GLN:HE21	2.33	0.41
1:A:121:THR:HG22	1:A:122:THR:N	2.35	0.41
1:B:148:GLN:NE2	1:B:273:PRO:HA	2.36	0.41
1:A:87:ARG:O	1:A:121:THR:HG23	2.19	0.41
1:A:174:GLN:HE21	1:A:174:GLN:HA	1.86	0.40
1:A:272:ARG:HA	1:A:273:PRO:HD3	1.87	0.40
1:B:48:GLN:HE21	1:B:165:TYR:HE1	1.69	0.40
1:A:331:ASN:HB2	2:A:479:HOH:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:18:TYR:CZ	1:B:369:VAL:HG11	2.57	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	454/474 (96%)	432 (95%)	20 (4%)	2 (0%)	30	39
1	B	397/474 (84%)	368 (93%)	26 (6%)	3 (1%)	16	22
All	All	851/948 (90%)	800 (94%)	46 (5%)	5 (1%)	21	28

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	298	PRO
1	B	296	PHE
1	B	82	ALA
1	A	94	GLY
1	A	116	GLY

5.3.2 Protein sidechains [i](#)

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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	359/375 (96%)	344 (96%)	15 (4%)	26	38
1	B	324/375 (86%)	301 (93%)	23 (7%)	13	19
All	All	683/750 (91%)	645 (94%)	38 (6%)	19	28

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	84	LEU
1	A	95	THR
1	A	126	LEU
1	A	198	VAL
1	A	204	LEU
1	A	211	THR
1	A	240	SER
1	A	260	VAL
1	A	272	ARG
1	A	334	ILE
1	A	406	THR
1	A	408	VAL
1	A	435	GLN
1	A	444	LYS
1	A	452	GLN
1	B	3	LEU
1	B	4	ILE
1	B	8	GLN
1	B	33	VAL
1	B	61	ARG
1	B	74	ARG
1	B	125	GLU
1	B	134	SER
1	B	136	ARG
1	B	146	THR
1	B	152	SER
1	B	169	LYS
1	B	174	GLN
1	B	211	THR
1	B	260	VAL
1	B	270	GLN
1	B	272	ARG

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Mol	Chain	Res	Type
1	B	293	ARG
1	B	355	VAL
1	B	409	ASP
1	B	435	GLN
1	B	456	THR
1	B	457	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	GLN
1	A	26	GLN
1	A	48	GLN
1	A	51	GLN
1	A	150	GLN
1	A	174	GLN
1	A	186	GLN
1	A	193	GLN
1	A	254	GLN
1	A	281	GLN
1	A	427	GLN
1	A	441	ASN
1	A	453	GLN
1	B	8	GLN
1	B	48	GLN
1	B	150	GLN
1	B	154	GLN
1	B	174	GLN
1	B	229	GLN
1	B	286	ASN
1	B	350	GLN
1	B	354	ASN
1	B	363	GLN
1	B	435	GLN

5.3.3 RNA ⓘ

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	A	456/474 (96%)	0.85	39 (8%) 16 16	54, 70, 95, 99	0
1	B	405/474 (85%)	1.64	119 (29%) 1 1	66, 88, 133, 167	0
All	All	861/948 (90%)	1.22	158 (18%) 3 3	54, 78, 116, 167	0

All (158) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	335	PHE	7.9
1	B	90	VAL	6.8
1	B	339	SER	6.4
1	B	325	LEU	6.3
1	B	140	LEU	6.3
1	B	344	LEU	6.2
1	A	241	GLY	6.0
1	B	349	ILE	5.5
1	B	353	ILE	5.2
1	B	449	GLY	4.9
1	B	334	ILE	4.8
1	B	68	LEU	4.8
1	B	84	LEU	4.7
1	B	287	ALA	4.7
1	B	18	TYR	4.6
1	B	23	ALA	4.5
1	B	296	PHE	4.5
1	B	19	PRO	4.5
1	B	79	ILE	4.4
1	B	291	ALA	4.4
1	B	300	ILE	4.4
1	B	332	LEU	4.3
1	B	132	LEU	4.3
1	B	126	LEU	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	366	PHE	4.1
1	B	139	ALA	4.0
1	B	340	LEU	4.0
1	B	323	SER	3.9
1	B	326	PHE	3.9
1	B	82	ALA	3.8
1	B	404	TYR	3.8
1	B	292	ALA	3.8
1	B	295	ALA	3.8
1	B	455	VAL	3.7
1	B	290	GLY	3.7
1	A	268	LEU	3.7
1	B	362	ILE	3.7
1	A	240	SER	3.6
1	B	75	ALA	3.6
1	B	127	ASP	3.6
1	A	210	GLN	3.5
1	B	333	PRO	3.5
1	B	4	ILE	3.5
1	B	274	ASP	3.4
1	B	302	LEU	3.4
1	A	57	LEU	3.3
1	B	412	LEU	3.3
1	B	192	THR	3.3
1	B	361	ALA	3.3
1	B	128	LEU	3.3
1	B	328	PRO	3.3
1	B	355	VAL	3.3
1	B	324	TRP	3.3
1	B	343	SER	3.3
1	B	15	ALA	3.2
1	B	213	VAL	3.2
1	B	294	ALA	3.2
1	B	85	PHE	3.1
1	B	348	LYS	3.1
1	B	77	TYR	3.1
1	A	242	ILE	3.1
1	A	325	LEU	3.1
1	B	341	ARG	3.1
1	A	379	PHE	3.0
1	B	351	LYS	3.0
1	B	22	GLN	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	283	MET	2.9
1	B	16	ALA	2.9
1	B	216	ALA	2.9
1	A	86	PRO	2.9
1	B	5	PRO	2.9
1	B	450	TRP	2.9
1	A	382	GLN	2.9
1	B	446	LEU	2.9
1	B	411	TYR	2.9
1	B	24	TYR	2.8
1	B	86	PRO	2.8
1	B	269	LEU	2.8
1	B	414	LEU	2.8
1	B	40	TRP	2.8
1	A	247	PRO	2.8
1	B	284	ALA	2.8
1	B	13	PRO	2.7
1	B	14	VAL	2.7
1	B	200	VAL	2.7
1	B	330	ILE	2.7
1	A	203	ALA	2.7
1	B	215	GLY	2.6
1	B	206	LEU	2.6
1	A	246	LEU	2.6
1	A	40	TRP	2.6
1	B	130	GLY	2.6
1	A	275	ILE	2.6
1	A	362	ILE	2.6
1	A	60	ASN	2.6
1	B	285	ALA	2.6
1	B	342	ALA	2.6
1	B	10	PRO	2.6
1	B	331	ASN	2.6
1	A	83	ASP	2.5
1	B	354	ASN	2.5
1	B	392	ALA	2.5
1	A	55	VAL	2.5
1	B	456	THR	2.5
1	A	121	THR	2.5
1	B	289	ILE	2.4
1	B	396	TYR	2.4
1	A	213	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	239	GLY	2.4
1	B	209	ALA	2.4
1	B	211	THR	2.4
1	A	117	VAL	2.4
1	B	21	GLY	2.4
1	A	196	TYR	2.4
1	B	397	TYR	2.4
1	B	329	SER	2.3
1	B	88	ILE	2.3
1	B	327	GLN	2.3
1	A	24	TYR	2.3
1	A	118	THR	2.3
1	B	303	THR	2.3
1	B	65	VAL	2.3
1	B	70	VAL	2.3
1	B	185	TYR	2.3
1	B	408	VAL	2.3
1	B	405	ARG	2.3
1	B	122	THR	2.2
1	B	273	PRO	2.2
1	A	212	ALA	2.2
1	B	134	SER	2.1
1	B	188	SER	2.1
1	B	217	ARG	2.1
1	A	231	GLN	2.1
1	B	347	ALA	2.1
1	A	269	LEU	2.1
1	B	63	LEU	2.1
1	B	276	LEU	2.1
1	B	447	GLY	2.1
1	A	214	GLU	2.1
1	B	357	GLN	2.1
1	A	219	THR	2.1
1	B	129	PHE	2.1
1	A	209	ALA	2.1
1	B	135	LEU	2.1
1	B	293	ARG	2.1
1	A	211	THR	2.1
1	B	137	ASP	2.1
1	B	20	GLN	2.0
1	A	217	ARG	2.0
1	A	311	ARG	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	67	ALA	2.0
1	B	250	LEU	2.0
1	A	330	ILE	2.0
1	A	369	VAL	2.0
1	A	455	VAL	2.0
1	B	73	PHE	2.0
1	B	198	VAL	2.0
1	B	262	ALA	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 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.