



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:54 AM UTC

PDB ID : 7KP4 / pdb_00007kp4
Title : Crystal structure of human claudin-4 in complex with Clostridium perfringens enterotoxin C-terminal domain
Authors : Vecchio, A.J.; Stroud, R.M.
Deposited on : 2020-11-10
Resolution : 3.37 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

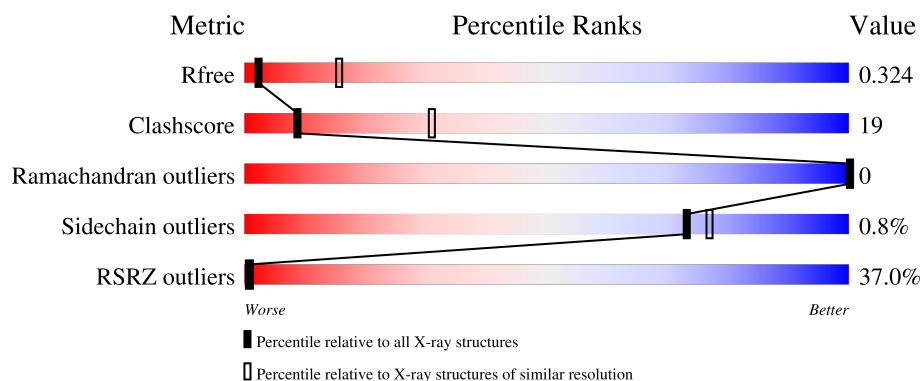
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.37 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	1047 (3.42-3.34)
Clashscore	190562	1067 (3.42-3.34)
Ramachandran outliers	187476	1056 (3.42-3.34)
Sidechain outliers	187428	1056 (3.42-3.34)
RSRZ outliers	180081	1047 (3.42-3.34)

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	214	27% 54% 30% 15%
2	B	134	45% 79% 21%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2375 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 Claudin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	182	Total	C	N	O	S	0	0	0
			1318	854	216	231	17			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	210	GLY	-	expression tag	UNP O14493
A	211	LEU	-	expression tag	UNP O14493
A	212	VAL	-	expression tag	UNP O14493
A	213	PRO	-	expression tag	UNP O14493
A	214	ARG	-	expression tag	UNP O14493

- Molecule 2 is a protein called Heat-labile enterotoxin B chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	134	Total	C	N	O	S	0	0	0
			1057	673	174	208	2			

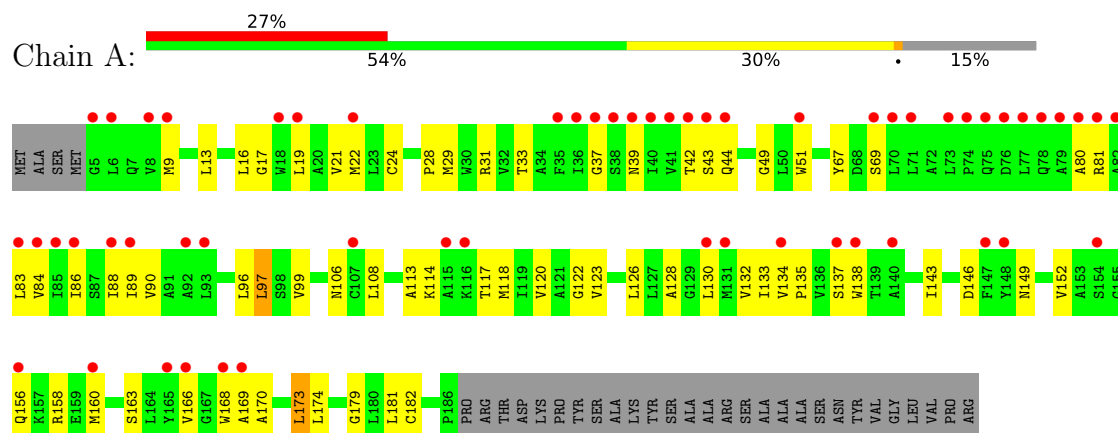
There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	191	MET	-	initiating methionine	UNP P01558
B	320	GLY	-	expression tag	UNP P01558
B	321	LEU	-	expression tag	UNP P01558
B	322	VAL	-	expression tag	UNP P01558
B	323	PRO	-	expression tag	UNP P01558
B	324	ARG	-	expression tag	UNP P01558

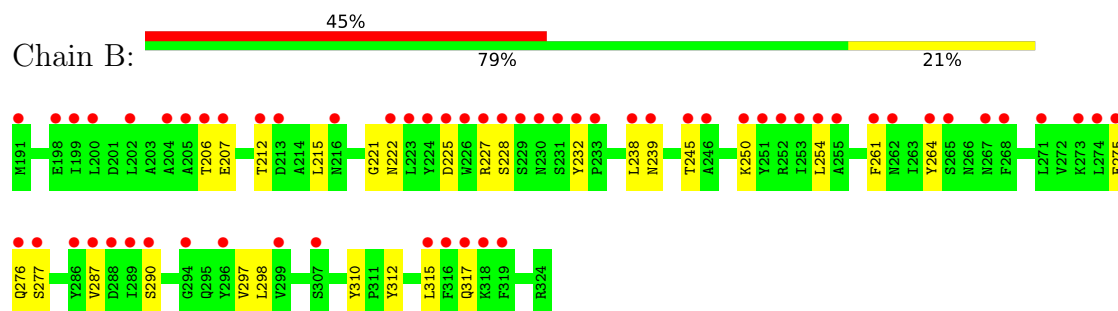
3 Residue-property plots [i](#)

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: Claudin-4



• Molecule 2: Heat-labile enterotoxin B chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	70.36Å 116.23Å 118.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.81 – 3.37 44.81 – 3.37	Depositor EDS
% Data completeness (in resolution range)	91.8 (44.81-3.37) 78.6 (44.81-3.37)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.11 (at 3.26Å)	Xtriage
Refinement program	PHENIX (1.14_3260: ???)	Depositor
R, R_{free}	0.294 , 0.296 0.311 , 0.324	Depositor DCC
R_{free} test set	1433 reflections (9.38%)	wwPDB-VP
Wilson B-factor (Å ²)	111.1	Xtriage
Anisotropy	0.345	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 66.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.054 for -h,l,k	Xtriage
F_o, F_c correlation	0.81	EDS
Total number of atoms	2375	wwPDB-VP
Average B, all atoms (Å ²)	170.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.96% 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	0.30	0/1341	0.55	0/1832
2	B	0.30	0/1079	0.52	0/1467
All	All	0.30	0/2420	0.54	0/3299

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	1318	0	1357	75	0
2	B	1057	0	1026	18	0
All	All	2375	0	2383	89	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 19.

All (89) 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:17:GLY:N	1:A:173:LEU:HD11	1.44	1.32
1:A:17:GLY:HA2	1:A:173:LEU:HD21	1.20	1.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:LEU:C	1:A:173:LEU:HD11	1.86	1.00
1:A:17:GLY:N	1:A:173:LEU:CD1	2.24	0.99
1:A:17:GLY:HA2	1:A:173:LEU:CD2	1.98	0.93
1:A:170:ALA:HA	1:A:173:LEU:CD2	2.00	0.91
1:A:17:GLY:CA	1:A:173:LEU:HD11	2.06	0.85
1:A:9:MET:HE3	1:A:13:LEU:HD13	1.71	0.72
1:A:17:GLY:CA	1:A:173:LEU:HD21	2.11	0.71
1:A:17:GLY:CA	1:A:173:LEU:CG	2.69	0.71
1:A:170:ALA:O	1:A:173:LEU:HD23	1.91	0.71
1:A:170:ALA:HA	1:A:173:LEU:HD21	1.77	0.67
1:A:122:GLY:HA3	1:A:182:CYS:HB2	1.78	0.65
1:A:17:GLY:HA3	1:A:173:LEU:HG	1.80	0.64
1:A:17:GLY:CA	1:A:173:LEU:CD1	2.72	0.62
1:A:17:GLY:CA	1:A:173:LEU:CD2	2.76	0.62
1:A:170:ALA:HA	1:A:173:LEU:HD23	1.82	0.61
1:A:146:ASP:OD1	2:B:227:ARG:NH1	2.31	0.61
1:A:130:LEU:HA	1:A:133:ILE:HG22	1.83	0.60
1:A:21:VAL:HG22	1:A:132:VAL:HG11	1.84	0.60
2:B:264:TYR:HB2	2:B:297:VAL:HG12	1.84	0.59
1:A:24:CYS:SG	1:A:163:SER:O	2.56	0.58
1:A:17:GLY:HA2	1:A:173:LEU:CG	2.34	0.57
1:A:170:ALA:C	1:A:173:LEU:HD23	2.29	0.57
1:A:17:GLY:CA	1:A:173:LEU:HG	2.34	0.56
1:A:170:ALA:CA	1:A:173:LEU:HD23	2.36	0.56
1:A:120:VAL:HA	1:A:123:VAL:HG12	1.87	0.56
1:A:128:ALA:O	1:A:132:VAL:HG23	2.06	0.55
2:B:261:PHE:CE1	2:B:277:SER:HB3	2.41	0.55
2:B:275:GLU:HG2	2:B:287:VAL:HG21	1.88	0.55
1:A:123:VAL:HA	1:A:126:LEU:HD12	1.90	0.54
1:A:83:LEU:HD23	1:A:135:PRO:HB3	1.90	0.54
1:A:22:MET:HG2	1:A:88:ILE:HD12	1.90	0.53
1:A:86:ILE:HD13	1:A:89:ILE:HD11	1.91	0.53
1:A:132:VAL:O	1:A:135:PRO:HD2	2.10	0.52
1:A:42:THR:HG21	2:B:222:ASN:ND2	2.25	0.51
1:A:90:VAL:HG12	1:A:128:ALA:HB2	1.91	0.51
1:A:39:ASN:OD1	2:B:317:GLN:NE2	2.36	0.51
1:A:84:VAL:O	1:A:88:ILE:HG12	2.10	0.51
1:A:113:ALA:O	1:A:117:THR:HG23	2.11	0.50
1:A:21:VAL:HG21	1:A:132:VAL:HG21	1.94	0.49
1:A:17:GLY:O	1:A:21:VAL:HG23	2.13	0.49
1:A:134:VAL:O	1:A:138:TRP:HB2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:THR:OG1	1:A:44:GLN:NE2	2.47	0.48
1:A:28:PRO:HA	1:A:49:GLY:HA3	1.96	0.48
2:B:250:LYS:HA	2:B:290:SER:HA	1.96	0.47
2:B:212:THR:HG21	2:B:245:THR:HB	1.96	0.47
2:B:207:GLU:HG3	2:B:238:LEU:HD11	1.95	0.47
1:A:114:LYS:O	1:A:118:MET:HG2	2.14	0.47
1:A:19:LEU:HA	1:A:22:MET:HE3	1.96	0.46
1:A:29:MET:HB2	1:A:163:SER:H	1.80	0.46
2:B:232:TYR:N	2:B:310:TYR:O	2.43	0.46
1:A:96:LEU:O	1:A:99:VAL:HG12	2.15	0.46
1:A:179:GLY:C	1:A:181:LEU:H	2.24	0.46
1:A:31:ARG:HD3	1:A:158:ARG:NE	2.32	0.45
1:A:37:GLY:C	1:A:39:ASN:H	2.24	0.45
1:A:13:LEU:O	1:A:173:LEU:HD12	2.17	0.45
1:A:108:LEU:HD21	1:A:113:ALA:HB3	1.99	0.45
2:B:254:LEU:HB3	2:B:315:LEU:HB3	1.98	0.45
1:A:24:CYS:HB2	1:A:166:VAL:HG12	1.98	0.45
1:A:169:ALA:O	1:A:173:LEU:HD23	2.17	0.45
1:A:80:ALA:O	1:A:84:VAL:HG12	2.18	0.44
2:B:275:GLU:HG3	2:B:276:GLN:N	2.33	0.44
1:A:170:ALA:O	1:A:173:LEU:CD2	2.65	0.43
1:A:33:THR:HG22	1:A:158:ARG:HG2	2.01	0.43
1:A:21:VAL:HG23	1:A:170:ALA:HB1	2.00	0.43
1:A:67:TYR:O	1:A:69:SER:N	2.52	0.43
1:A:173:LEU:HG	1:A:174:LEU:N	2.32	0.43
2:B:225:ASP:OD2	2:B:227:ARG:NH2	2.51	0.43
1:A:51:TRP:C	1:A:67:TYR:HD1	2.27	0.43
1:A:17:GLY:HA2	1:A:173:LEU:HD11	1.93	0.43
1:A:97:LEU:HD11	1:A:120:VAL:HG13	2.01	0.43
1:A:17:GLY:H	1:A:173:LEU:CD1	2.24	0.42
1:A:149:ASN:O	1:A:152:VAL:HG12	2.19	0.42
1:A:83:LEU:HD12	1:A:83:LEU:HA	1.85	0.42
2:B:215:LEU:O	2:B:221:GLY:HA2	2.20	0.42
1:A:37:GLY:C	1:A:39:ASN:N	2.76	0.41
1:A:117:THR:HA	1:A:120:VAL:HG12	2.03	0.41
1:A:51:TRP:NE1	1:A:81:ARG:HD2	2.36	0.41
2:B:261:PHE:CD2	2:B:298:LEU:HD11	2.56	0.41
1:A:156:GLN:OE1	2:B:225:ASP:HB2	2.21	0.41
1:A:134:VAL:HG13	1:A:135:PRO:HD3	2.02	0.41
2:B:228:SER:OG	2:B:312:TYR:N	2.53	0.41
1:A:42:THR:O	1:A:43:SER:C	2.65	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:VAL:C	1:A:135:PRO:HD2	2.46	0.40
1:A:137:SER:N	1:A:168:TRP:HE1	2.18	0.40
1:A:143:ILE:HD11	1:A:160:MET:HA	2.03	0.40
1:A:106:ASN:OD1	1:A:106:ASN:N	2.55	0.40
2:B:206:THR:HA	2:B:239:ASN:O	2.22	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	180/214 (84%)	168 (93%)	12 (7%)	0	100	100
2	B	132/134 (98%)	131 (99%)	1 (1%)	0	100	100
All	All	312/348 (90%)	299 (96%)	13 (4%)	0	100	100

There are no Ramachandran outliers to report.

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.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	139/168 (83%)	137 (99%)	2 (1%)	59	70
2	B	116/118 (98%)	116 (100%)	0	100	100
All	All	255/286 (89%)	253 (99%)	2 (1%)	73	77

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	97	LEU
1	A	173	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	GLN
1	A	156	GLN
2	B	230	ASN
2	B	249	GLN
2	B	276	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	182/214 (85%)	1.95	57 (31%) ⓘ ⓘ	114, 189, 247, 262	0
2	B	134/134 (100%)	2.50	60 (44%) ⓘ ⓘ	106, 143, 237, 266	0
All	All	316/348 (90%)	2.19	117 (37%) ⓘ ⓘ	106, 166, 242, 266	0

All (117) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	229	SER	20.2
1	A	75	GLN	19.6
1	A	8	VAL	15.2
2	B	275	GLU	14.3
2	B	230	ASN	12.7
1	A	79	ALA	12.4
2	B	317	GLN	12.4
1	A	78	GLN	12.1
1	A	5	GLY	10.7
2	B	254	LEU	10.1
1	A	82	ALA	9.9
1	A	89	ILE	9.6
1	A	36	ILE	9.5
1	A	148	TYR	9.4
2	B	251	TYR	8.8
1	A	22	MET	8.6
2	B	250	LYS	8.5
1	A	85	ILE	8.5
2	B	239	ASN	8.0
1	A	130	LEU	8.0
1	A	37	GLY	7.6
1	A	138	TRP	7.3
1	A	42	THR	7.2
1	A	39	ASN	6.9

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Mol	Chain	Res	Type	RSRZ
1	A	76	ASP	6.6
2	B	315	LEU	6.5
1	A	83	LEU	6.3
2	B	316	PHE	6.3
2	B	207	GLU	6.1
2	B	226	TRP	6.0
1	A	35	PHE	6.0
1	A	86	ILE	5.8
2	B	287	VAL	5.8
1	A	18	TRP	5.7
2	B	224	TYR	5.6
1	A	41	VAL	5.6
1	A	88	ILE	5.5
2	B	252	ARG	5.5
1	A	6	LEU	5.3
2	B	205	ALA	5.3
2	B	276	GLN	5.2
2	B	223	LEU	5.2
2	B	286	TYR	5.1
2	B	288	ASP	5.0
2	B	216	ASN	5.0
1	A	169	ALA	4.9
1	A	40	ILE	4.9
1	A	154	SER	4.8
1	A	168	TRP	4.8
1	A	74	PRO	4.8
2	B	289	ILE	4.7
1	A	131	MET	4.7
2	B	277	SER	4.4
2	B	273	LYS	4.2
1	A	147	PHE	4.2
2	B	199	ILE	4.2
2	B	319	PHE	4.2
2	B	246	ALA	4.1
1	A	134	VAL	4.1
1	A	165	TYR	4.1
1	A	38	SER	4.0
1	A	43	SER	4.0
2	B	245	THR	4.0
2	B	274	LEU	4.0
2	B	268	PHE	3.8
1	A	69	SER	3.7

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Mol	Chain	Res	Type	RSRZ
2	B	267	ASN	3.7
2	B	290	SER	3.7
2	B	204	ALA	3.7
1	A	81	ARG	3.7
2	B	222	ASN	3.7
2	B	200	LEU	3.6
2	B	212	THR	3.6
2	B	225	ASP	3.6
2	B	191	MET	3.4
2	B	206	THR	3.3
2	B	228	SER	3.3
2	B	264	TYR	3.3
2	B	318	LYS	3.1
1	A	70	LEU	3.0
1	A	80	ALA	3.0
1	A	51	TRP	3.0
2	B	238	LEU	3.0
2	B	261	PHE	3.0
2	B	296	TYR	3.0
1	A	9	MET	3.0
1	A	116	LYS	2.9
2	B	198	GLU	2.9
2	B	213	ASP	2.8
1	A	77	LEU	2.8
1	A	115	ALA	2.7
1	A	166	VAL	2.6
2	B	271	LEU	2.6
2	B	255	ALA	2.6
1	A	156	GLN	2.5
2	B	262	ASN	2.5
2	B	299	VAL	2.5
1	A	84	VAL	2.5
1	A	19	LEU	2.5
2	B	231	SER	2.5
1	A	140	ALA	2.4
1	A	137	SER	2.4
1	A	160	MET	2.3
1	A	92	ALA	2.3
1	A	71	LEU	2.3
2	B	253	ILE	2.2
2	B	233	PRO	2.2
2	B	307	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	107	CYS	2.2
1	A	93	LEU	2.2
1	A	73	LEU	2.1
2	B	265	SER	2.1
2	B	294	GLY	2.1
2	B	227	ARG	2.1
2	B	202	LEU	2.0
2	B	232	TYR	2.0
1	A	44	GLN	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.