



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 27, 2025 – 04:08 pm BST

PDB ID : 9F8F / pdb_00009f8f
Title : SLPL/SLPH (H/L) complex C. difficile Opt2472 strain (SLCT2)
Authors : Barwinska-Sendra, A.; Salgado, P.S.
Deposited on : 2024-05-06
Resolution : 3.07 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 Phenix2.0rc1
Xtriage (Phenix) : 2.0rc1
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.006 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.45.1

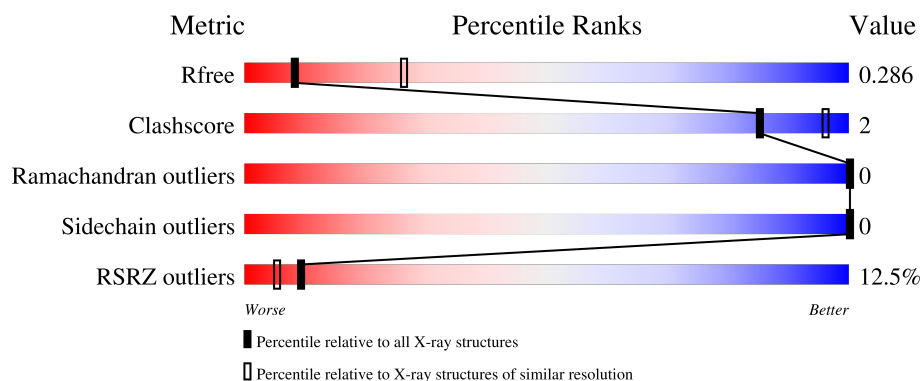
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.07 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}	164625	1842 (3.10-3.06)
Clashscore	180529	1965 (3.10-3.06)
Ramachandran outliers	177936	1859 (3.10-3.06)
Sidechain outliers	177891	1858 (3.10-3.06)
RSRZ outliers	164620	1842 (3.10-3.06)

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	B	394	<div> <div>11%</div> <div> <div></div> <div>95%</div> <div>5%</div> </div> </div>
1	D	394	<div> <div>13%</div> <div> <div></div> <div>94%</div> <div>6%</div> </div> </div>
2	A	324	<div> <div>11%</div> <div> <div></div> <div>93%</div> <div>• •</div> </div> </div>
2	C	324	<div> <div>14%</div> <div> <div></div> <div>89%</div> <div>7% 5%</div> </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10638 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 SLPH - S-layer protein HMW.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	394	Total	C	N	O	S	0	0	0
			2921	1795	483	635	8			
1	D	394	Total	C	N	O	S	0	0	0
			2921	1795	483	635	8			

- Molecule 2 is a protein called S-layer protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	309	Total	C	N	O	S	0	0	0
			2373	1489	383	499	2			
2	A	310	Total	C	N	O	S	0	0	0
			2370	1485	381	502	2			

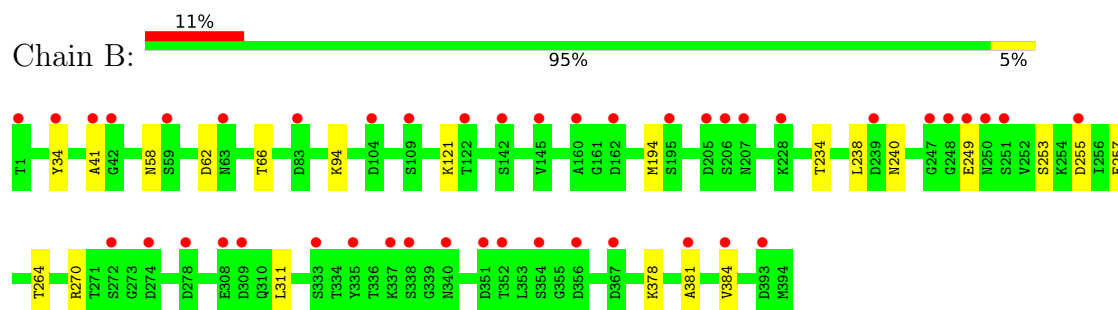
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	17	Total	O	0	0
			17	17		
3	D	13	Total	O	0	0
			13	13		
3	C	12	Total	O	0	0
			12	12		
3	A	11	Total	O	0	0
			11	11		

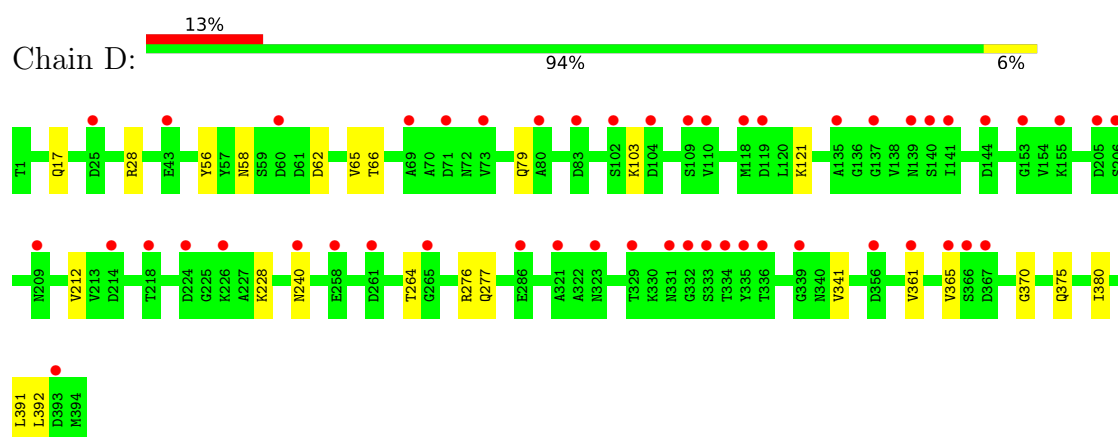
3 Residue-property plots [i](#)

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.

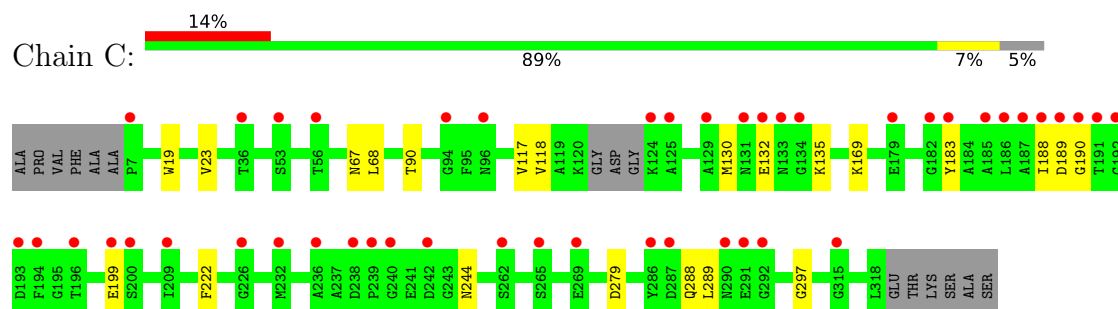
- Molecule 1: SLPH - S-layer protein HMW



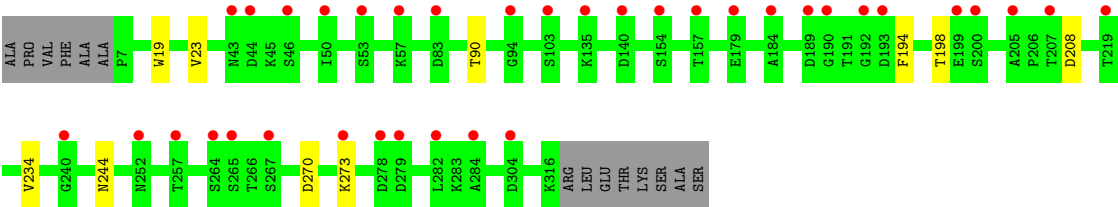
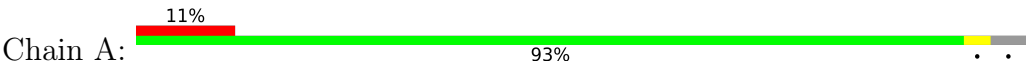
- Molecule 1: SLPH - S-layer protein HMW



- Molecule 2: S-layer protein



- Molecule 2: S-layer protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	75.32Å 76.48Å 78.23Å 81.80° 78.86° 66.78°	Depositor
Resolution (Å)	35.78 – 3.07 35.78 – 3.07	Depositor EDS
% Data completeness (in resolution range)	99.0 (35.78-3.07) 99.3 (35.78-3.07)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.32 (at 3.06Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.231 , 0.283 0.232 , 0.286	Depositor DCC
R_{free} test set	1489 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å ²)	14.2	Xtriage
Anisotropy	1.008	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 54.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.024 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.79	EDS
Total number of atoms	10638	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.46% 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	B	0.13	0/2947	0.29	0/3991
1	D	0.12	0/2947	0.28	0/3991
2	A	0.13	0/2399	0.31	0/3239
2	C	0.13	0/2401	0.33	0/3240
All	All	0.13	0/10694	0.30	0/14461

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	B	2921	0	2883	15	0
1	D	2921	0	2883	15	0
2	A	2370	0	2358	6	0
2	C	2373	0	2371	14	0
3	A	11	0	0	0	0
3	B	17	0	0	1	0
3	C	12	0	0	1	0
3	D	13	0	0	0	0
All	All	10638	0	10495	45	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 (45) 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:94:LYS:NZ	3:B:401:HOH:O	2.19	0.75
1:B:253:SER:OG	1:B:255:ASP:OD1	2.06	0.71
1:B:34:TYR:HE2	2:A:273:LYS:HG2	1.56	0.70
1:D:58:ASN:H	1:D:66:THR:HG23	1.62	0.63
2:A:194:PHE:O	2:A:198:THR:OG1	2.18	0.59
2:C:288:GLN:NE2	2:C:297:GLY:HA3	2.19	0.57
2:C:183:TYR:N	2:C:199:GLU:O	2.26	0.57
1:B:58:ASN:H	1:B:66:THR:HG23	1.70	0.56
1:D:370:GLY:HA3	1:D:392:LEU:HD12	1.87	0.56
2:C:132:GLU:O	2:C:132:GLU:HG3	2.06	0.56
1:D:17:GLN:HG3	2:C:289:LEU:HD12	1.88	0.54
1:B:41:ALA:HB1	1:B:378:LYS:HG3	1.89	0.53
1:B:194:MET:HG3	1:B:311:LEU:HD12	1.90	0.53
1:B:240:ASN:HA	1:B:264:THR:HG23	1.91	0.52
1:D:361:VAL:HG21	1:D:391:LEU:HD13	1.92	0.52
1:B:121:LYS:NZ	1:D:62:ASP:OD1	2.30	0.51
1:B:257:GLU:OE1	1:B:270:ARG:NH2	2.46	0.48
1:D:361:VAL:O	1:D:365:VAL:HG13	2.14	0.48
1:B:194:MET:HE3	1:B:194:MET:HA	1.94	0.48
2:C:67:ASN:OD1	2:C:68:LEU:N	2.46	0.47
2:C:135:LYS:HG2	2:C:190:GLY:O	2.13	0.47
2:A:270:ASP:HA	2:A:273:LYS:HG3	1.96	0.47
2:C:117:VAL:HG23	2:C:118:VAL:HG22	1.97	0.47
1:D:228:LYS:HE3	1:D:228:LYS:HB2	1.82	0.46
1:D:212:VAL:HG23	1:D:341:VAL:HG21	1.97	0.46
1:B:381:ALA:O	1:B:384:VAL:HG22	2.17	0.44
1:D:240:ASN:HA	1:D:264:THR:HG23	1.99	0.44
1:B:62:ASP:H	1:D:121:LYS:HE3	1.83	0.43
1:D:28:ARG:NH2	2:C:279:ASP:OD1	2.51	0.43
2:C:130:MET:HE2	2:C:130:MET:HB3	1.88	0.43
1:B:234:THR:O	1:B:238:LEU:HD12	2.17	0.43
2:A:208:ASP:HB3	2:A:234:VAL:HG22	2.01	0.43
2:C:90:THR:HA	2:C:244:ASN:O	2.18	0.43
2:C:169:LYS:HE2	3:C:403:HOH:O	2.18	0.43
2:C:19:TRP:O	2:C:23:VAL:HG23	2.20	0.42
1:B:249:GLU:HG2	1:B:270:ARG:NH1	2.34	0.42
1:B:249:GLU:HG2	1:B:270:ARG:HH12	1.84	0.41
2:C:117:VAL:HG12	2:C:222:PHE:HB3	2.03	0.41
2:A:19:TRP:O	2:A:23:VAL:HG23	2.21	0.41
1:D:79:GLN:HE22	1:D:103:LYS:HB3	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:188:ILE:HG13	2:C:189:ASP:OD1	2.20	0.41
1:D:276:ARG:HG3	1:D:277:GLN:N	2.36	0.40
2:A:90:THR:HA	2:A:244:ASN:O	2.22	0.40
1:D:56:TYR:HB3	1:D:65:VAL:HG23	2.02	0.40
1:D:375:GLN:HE21	1:D:380:ILE:HB	1.87	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	B	392/394 (100%)	384 (98%)	8 (2%)	0	100	100
1	D	392/394 (100%)	384 (98%)	8 (2%)	0	100	100
2	A	308/324 (95%)	300 (97%)	8 (3%)	0	100	100
2	C	305/324 (94%)	294 (96%)	11 (4%)	0	100	100
All	All	1397/1436 (97%)	1362 (98%)	35 (2%)	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	B	325/325 (100%)	325 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	325/325 (100%)	325 (100%)	0	100	100
2	A	261/271 (96%)	261 (100%)	0	100	100
2	C	262/271 (97%)	262 (100%)	0	100	100
All	All	1173/1192 (98%)	1173 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	375	GLN
1	D	323	ASN
1	D	375	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	B	394/394 (100%)	0.93	44 (11%) 11 7	9, 19, 38, 51	0
1	D	394/394 (100%)	1.05	50 (12%) 9 5	12, 21, 41, 58	0
2	A	310/324 (95%)	0.96	36 (11%) 11 6	6, 18, 35, 54	0
2	C	309/324 (95%)	1.01	46 (14%) 7 3	8, 20, 43, 68	0
All	All	1407/1436 (97%)	0.99	176 (12%) 9 5	6, 19, 40, 68	0

All (176) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	189	ASP	5.7
2	A	284	ALA	5.4
2	C	187	ALA	4.8
2	C	132	GLU	4.6
2	C	240	GLY	4.6
2	C	290	ASN	4.5
2	C	186	LEU	4.4
2	C	265	SER	4.3
2	A	192	GLY	4.3
2	A	190	GLY	4.2
1	D	339	GLY	4.2
1	D	206	SER	4.2
2	C	188	ILE	4.2
1	B	122	THR	4.1
2	A	43	ASN	4.1
1	D	366	SER	4.1
2	A	154	SER	4.1
1	D	139	ASN	3.9
1	D	140	SER	3.8
2	C	189	ASP	3.8
1	D	333	SER	3.8

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Mol	Chain	Res	Type	RSRZ
1	D	261	ASP	3.8
2	A	279	ASP	3.8
1	B	42	GLY	3.8
2	A	205	ALA	3.7
2	C	179	GLU	3.6
2	A	199	GLU	3.6
1	B	63	ASN	3.5
2	C	183	TYR	3.5
2	C	129	ALA	3.4
1	D	334	THR	3.4
1	D	365	VAL	3.4
1	B	247	GLY	3.4
1	B	367	ASP	3.3
2	A	219	THR	3.3
1	B	384	VAL	3.3
2	A	193	ASP	3.3
1	D	367	ASP	3.3
1	B	333	SER	3.3
2	C	131	ASN	3.3
2	C	134	GLY	3.3
1	D	393	ASP	3.2
1	B	352	THR	3.2
1	D	265	GLY	3.1
1	D	356	ASP	3.1
2	C	200	SER	3.1
1	B	251	SER	3.1
1	B	278	ASP	3.0
2	C	291	GLU	3.0
1	D	60	ASP	3.0
1	D	83	ASP	3.0
1	D	144	ASP	3.0
2	A	240	GLY	2.9
1	B	145	VAL	2.9
2	A	83	ASP	2.9
2	C	182	GLY	2.9
1	D	135	ALA	2.9
1	B	104	ASP	2.9
1	D	119	ASP	2.9
1	B	249	GLU	2.8
1	D	137	GLY	2.8
2	C	199	GLU	2.8
1	D	329	THR	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	25	ASP	2.8
2	A	267	SER	2.8
2	A	44	ASP	2.8
1	D	104	ASP	2.8
1	D	224	ASP	2.8
1	D	335	TYR	2.8
2	A	184	ALA	2.8
2	A	265	SER	2.8
2	C	185	ALA	2.7
2	C	125	ALA	2.7
1	B	274	ASP	2.7
1	B	309	ASP	2.7
2	C	7	PRO	2.7
1	B	308	GLU	2.7
2	C	133	ASN	2.7
2	C	53	SER	2.6
2	C	192	GLY	2.6
1	D	73	VAL	2.6
1	B	34	TYR	2.6
2	C	292	GLY	2.6
2	C	96	ASN	2.6
2	A	207	THR	2.6
1	D	214	ASP	2.6
2	C	232	MET	2.6
2	A	179	GLU	2.6
1	D	331	ASN	2.6
2	A	157	THR	2.6
2	A	94	GLY	2.6
1	B	83	ASP	2.6
1	B	255	ASP	2.6
1	B	248	GLY	2.5
2	C	190	GLY	2.5
1	B	340	ASN	2.5
1	B	272	SER	2.5
2	C	196	THR	2.5
2	C	194	PHE	2.5
2	A	264	SER	2.5
2	C	193	ASP	2.5
2	A	278	ASP	2.5
2	C	236	ALA	2.5
1	B	351	ASP	2.5
1	D	209	ASN	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	240	ASN	2.5
2	C	238	ASP	2.5
1	D	110	VAL	2.5
1	D	336	THR	2.4
1	B	142	SER	2.4
2	A	257	THR	2.4
1	B	109	SER	2.4
1	B	228	LYS	2.4
1	D	361	VAL	2.4
1	D	218	THR	2.4
1	B	207	ASN	2.4
1	B	356	ASP	2.4
1	D	332	GLY	2.4
1	D	109	SER	2.3
1	D	69	ALA	2.3
1	D	258	GLU	2.3
1	D	286	GLU	2.3
2	A	273	LYS	2.3
1	D	43	GLU	2.3
1	D	153	GLY	2.3
1	D	141	ILE	2.3
1	B	206	SER	2.3
2	A	252	ASN	2.2
2	A	135	LYS	2.2
2	A	53	SER	2.2
2	A	103	SER	2.2
1	D	71	ASP	2.2
2	C	191	THR	2.2
1	B	41	ALA	2.2
1	D	102	SER	2.2
1	B	162	ASP	2.2
1	B	239	ASP	2.2
2	C	262	SER	2.2
2	C	239	PRO	2.2
1	D	323	ASN	2.2
1	B	1	THR	2.2
2	C	36	THR	2.2
1	B	338	SER	2.2
2	A	46	SER	2.2
1	B	250	ASN	2.2
1	B	393	ASP	2.2
1	D	118	MET	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	160	ALA	2.1
1	B	205	ASP	2.1
2	C	226	GLY	2.1
2	A	304	ASP	2.1
2	A	57	LYS	2.1
1	D	155	LYS	2.1
2	C	286	TYR	2.1
2	C	315	GLY	2.1
2	A	282	LEU	2.1
1	D	80	ALA	2.1
1	D	321	ALA	2.1
1	D	226	LYS	2.1
2	A	50	ILE	2.1
2	C	56	THR	2.1
1	B	195	SER	2.1
2	A	200	SER	2.1
1	D	205	ASP	2.1
2	A	140	ASP	2.1
1	B	381	ALA	2.0
2	C	287	ASP	2.0
1	B	337	LYS	2.0
2	C	124	LYS	2.0
2	C	269	GLU	2.0
1	B	335	TYR	2.0
1	B	59	SER	2.0
1	B	354	SER	2.0
2	C	242	ASP	2.0
2	C	209	ILE	2.0
2	C	94	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 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.