



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:43 PM UTC

PDB ID : 8ONB / pdb_00008onb
Title : Structure of the C-terminal beta helix domain of the Bdellovibrio bacteriovorus Bd3182 fibre
Authors : Caulton, S.G.; Lovering, A.L.
Deposited on : 2023-04-01
Resolution : 1.12 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

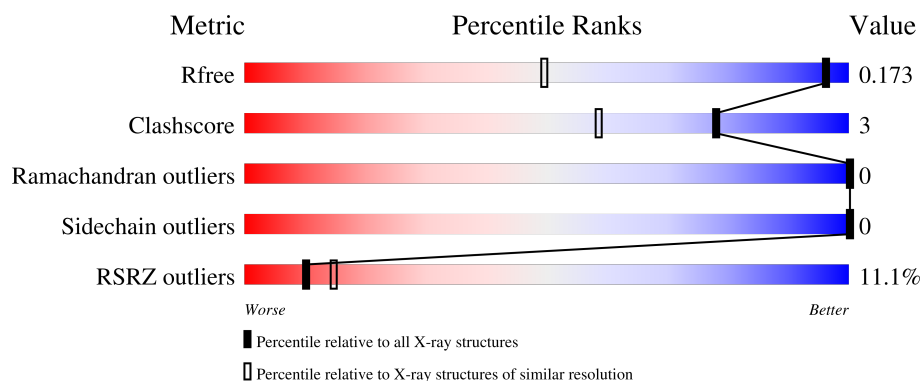
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.12 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	1985 (1.14-1.10)
Clashscore	190562	2021 (1.14-1.10)
Ramachandran outliers	187476	1978 (1.14-1.10)
Sidechain outliers	187428	1974 (1.14-1.10)
RSRZ outliers	180081	1984 (1.14-1.10)

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	152	5% 75% 24%
1	B	152	7% 78% 5% 16%
1	C	152	7% 72% 5% 24%
1	D	152	12% 75% 9% 16%
1	E	152	9% 72% 24%

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Mol	Chain	Length	Quality of chain
1	F	152	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6042 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 Cell wall surface anchor family protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	116	Total	C	N	O	S	0	5	0
			867	537	152	176	2			
1	B	127	Total	C	N	O	S	11	9	0
			969	599	173	194	3			
1	C	116	Total	C	N	O	S	0	4	0
			859	532	151	173	3			
1	D	127	Total	C	N	O	S	0	4	0
			932	578	165	186	3			
1	E	116	Total	C	N	O	S	0	2	0
			847	526	149	169	3			
1	F	126	Total	C	N	O	S	0	6	0
			941	583	166	189	3			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	631	GLY	-	expression tag	UNP Q6MIH5
B	631	GLY	-	expression tag	UNP Q6MIH5
C	631	GLY	-	expression tag	UNP Q6MIH5
D	631	GLY	-	expression tag	UNP Q6MIH5
E	631	GLY	-	expression tag	UNP Q6MIH5
F	631	GLY	-	expression tag	UNP Q6MIH5

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	114	Total	O	0	0
			114	114		
2	B	112	Total	O	0	0
			112	112		
2	C	107	Total	O	0	0
			107	107		

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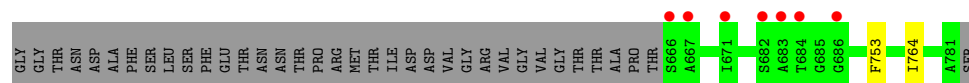
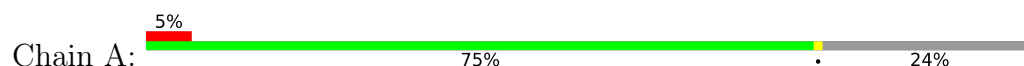
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	100	Total 100	O 100	0	0
2	E	111	Total 111	O 111	0	0
2	F	83	Total 83	O 83	0	0

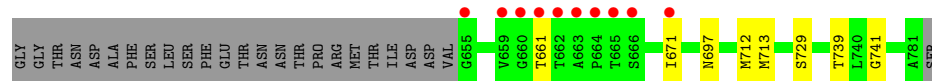
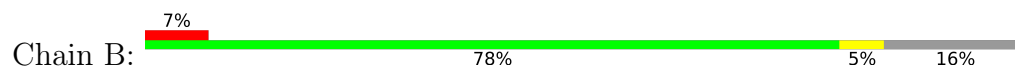
3 Residue-property plots [i](#)

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.

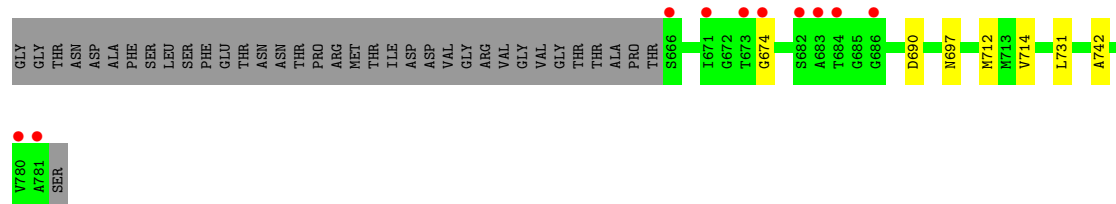
- Molecule 1: Cell wall surface anchor family protein



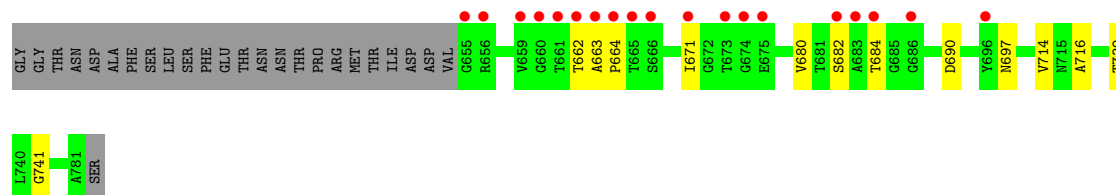
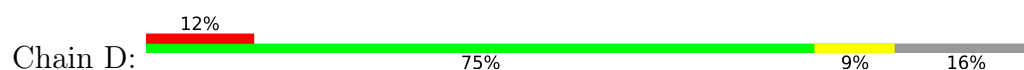
- Molecule 1: Cell wall surface anchor family protein



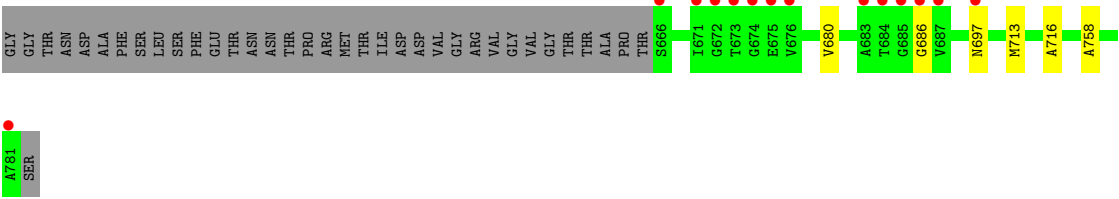
- Molecule 1: Cell wall surface anchor family protein



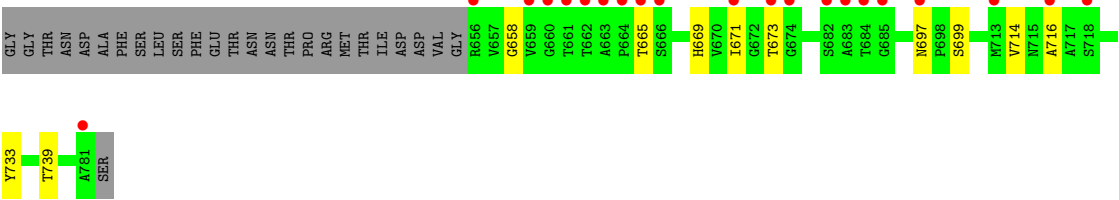
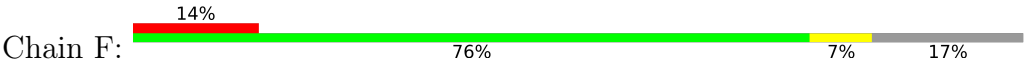
- Molecule 1: Cell wall surface anchor family protein



- Molecule 1: Cell wall surface anchor family protein



● Molecule 1: Cell wall surface anchor family protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	86.56Å 48.40Å 92.96Å 90.00° 102.98° 90.00°	Depositor
Resolution (Å)	84.35 – 1.12 84.35 – 1.12	Depositor EDS
% Data completeness (in resolution range)	61.4 (84.35-1.12) 61.4 (84.35-1.12)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.36 (at 1.12Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.149 , 0.172 0.151 , 0.173	Depositor DCC
R_{free} test set	8754 reflections (3.04%)	wwPDB-VP
Wilson B-factor (Å ²)	14.4	Xtriage
Anisotropy	0.056	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 46.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	6042	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.19% 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	0.52	0/881	0.72	0/1203
1	B	0.58	0/984	0.73	0/1343
1	C	0.64	0/873	0.84	1/1191 (0.1%)
1	D	0.59	2/947 (0.2%)	0.73	3/1294 (0.2%)
1	E	0.57	0/861	0.78	0/1175
1	F	0.49	0/956	0.80	0/1307
All	All	0.57	2/5502 (0.0%)	0.77	4/7513 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	664	PRO	C-O	-7.33	1.15	1.23
1	D	663	ALA	C-O	-5.67	1.17	1.24

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	690	ASP	CA-CB-CG	5.91	118.51	112.60
1	C	690	ASP	CA-CB-CG	5.88	118.48	112.60
1	D	662	THR	CA-C-N	-5.65	116.31	123.15
1	D	662	THR	C-N-CA	-5.65	116.31	123.15

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	867	0	838	1	0
1	B	969	0	949	10	0
1	C	859	0	835	4	0
1	D	932	0	915	7	0
1	E	847	0	826	6	0
1	F	941	0	922	8	0
2	A	114	0	0	0	0
2	B	112	0	0	3	0
2	C	107	0	0	1	0
2	D	100	0	0	0	0
2	E	111	0	0	1	0
2	F	83	0	0	0	0
All	All	6042	0	5285	30	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 (30) 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:671[B]:ILE:HD11	2:B:852:HOH:O	1.83	0.78
1:F:665:THR:HG22	1:F:665:THR:O	2.01	0.59
1:B:671[B]:ILE:CD1	2:B:852:HOH:O	2.43	0.59
1:B:739[B]:THR:HG22	1:B:741:GLY:H	1.68	0.58
1:C:697:ASN:HB3	1:C:714:VAL:O	2.04	0.58
1:D:697:ASN:HD21	1:D:716:ALA:HB2	1.72	0.55
1:C:731:LEU:HD23	1:C:742:ALA:HA	1.90	0.52
1:C:674:GLY:N	2:C:801:HOH:O	2.43	0.51
1:F:733:TYR:CE2	1:F:739[B]:THR:HG22	2.45	0.51
1:F:658:GLY:HA2	1:F:669:HIS:O	2.11	0.50
1:E:686:GLY:HA3	1:F:699:SER:O	2.12	0.49
1:B:697:ASN:ND2	1:B:713[A]:MET:HE1	2.30	0.47
1:D:697:ASN:HB3	1:D:714:VAL:O	2.13	0.47
1:F:697:ASN:OD1	1:F:716:ALA:HB2	2.14	0.47
1:B:661:THR:HB	1:B:671[B]:ILE:HD12	1.96	0.47
1:D:671[A]:ILE:HD12	1:E:680:VAL:O	2.15	0.47
1:D:682:SER:OG	1:F:673[A]:THR:HG22	2.14	0.46
1:E:697:ASN:OD1	1:E:716:ALA:HB2	2.16	0.46
1:F:697:ASN:HB3	1:F:714:VAL:O	2.16	0.46
1:D:680:VAL:HB	1:F:671[B]:ILE:HG12	1.98	0.45
1:E:697:ASN:HB3	1:E:713[B]:MET:CE	2.47	0.45
1:A:753:PHE:O	1:A:764[B]:ILE:HD12	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:684:THR:HG23	1:E:697:ASN:HB2	1.99	0.44
1:B:712:MET:HE1	1:C:712[B]:MET:HE2	2.00	0.44
1:B:739[B]:THR:HG21	2:B:858:HOH:O	2.18	0.44
1:D:739[A]:THR:HG22	1:D:741:GLY:H	1.83	0.43
1:B:661:THR:HB	1:B:671[B]:ILE:CD1	2.49	0.43
1:B:697:ASN:HD22	1:B:713[A]:MET:HE1	1.83	0.43
1:E:758:ALA:O	2:E:801:HOH:O	2.21	0.43
1:B:713[B]:MET:SD	1:B:729[B]:SER:OG	2.77	0.43

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	118/152 (78%)	115 (98%)	3 (2%)	0	100	100
1	B	134/152 (88%)	132 (98%)	2 (2%)	0	100	100
1	C	118/152 (78%)	115 (98%)	3 (2%)	0	100	100
1	D	129/152 (85%)	127 (98%)	2 (2%)	0	100	100
1	E	116/152 (76%)	114 (98%)	2 (2%)	0	100	100
1	F	130/152 (86%)	126 (97%)	4 (3%)	0	100	100
All	All	745/912 (82%)	729 (98%)	16 (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	A	90/114 (79%)	90 (100%)	0	100	100
1	B	101/114 (89%)	101 (100%)	0	100	100
1	C	89/114 (78%)	89 (100%)	0	100	100
1	D	96/114 (84%)	96 (100%)	0	100	100
1	E	87/114 (76%)	87 (100%)	0	100	100
1	F	98/114 (86%)	98 (100%)	0	100	100
All	All	561/684 (82%)	561 (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 (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	697	ASN

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 ⓘ

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	116/152 (76%)	0.26	7 (6%)	27 34	5, 15, 25, 34	5 (4%)
1	B	126/152 (82%)	0.48	10 (7%)	18 25	5, 15, 32, 44	8 (6%)
1	C	116/152 (76%)	0.33	10 (8%)	16 22	5, 15, 26, 46	4 (3%)
1	D	127/152 (83%)	0.80	19 (14%)	5 9	8, 19, 37, 45	4 (3%)
1	E	116/152 (76%)	0.59	14 (12%)	8 12	5, 17, 34, 40	2 (1%)
1	F	126/152 (82%)	1.02	21 (16%)	4 8	8, 20, 38, 46	6 (4%)
All	All	727/912 (79%)	0.59	81 (11%)	10 15	5, 17, 35, 46	29 (3%)

All (81) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	662	THR	10.0
1	F	661	THR	9.5
1	E	686	GLY	7.6
1	F	665	THR	7.6
1	F	663	ALA	7.3
1	E	684	THR	7.1
1	D	662	THR	6.5
1	B	662	THR	6.4
1	F	664	PRO	5.6
1	C	666	SER	5.4
1	A	684	THR	5.3
1	B	660	GLY	5.3
1	B	665	THR	5.2
1	F	684	THR	5.2
1	D	660	GLY	5.1
1	E	685	GLY	5.0
1	C	673	THR	5.0
1	D	671[A]	ILE	4.9
1	D	664	PRO	4.7

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Mol	Chain	Res	Type	RSRZ
1	D	665	THR	4.6
1	B	671[A]	ILE	4.5
1	B	664	PRO	4.5
1	D	661	THR	4.4
1	B	661	THR	4.4
1	E	674	GLY	4.4
1	F	660	GLY	4.4
1	F	671[A]	ILE	4.3
1	E	683	ALA	4.2
1	E	673	THR	4.0
1	B	663	ALA	4.0
1	F	656	ARG	3.9
1	D	655	GLY	3.9
1	B	655	GLY	3.8
1	F	716	ALA	3.8
1	B	659	VAL	3.8
1	D	684	THR	3.7
1	D	663	ALA	3.7
1	A	682	SER	3.6
1	E	781	ALA	3.5
1	D	666	SER	3.5
1	E	666	SER	3.4
1	F	659	VAL	3.3
1	C	674	GLY	3.2
1	A	666[A]	SER	3.1
1	C	684	THR	3.1
1	E	687	VAL	3.1
1	F	682	SER	3.1
1	C	682	SER	3.1
1	F	683	ALA	3.0
1	A	667	ALA	2.9
1	C	683	ALA	2.9
1	E	676	VAL	2.8
1	D	686	GLY	2.8
1	C	781	ALA	2.7
1	D	673	THR	2.7
1	D	656	ARG	2.6
1	F	666	SER	2.5
1	E	697	ASN	2.5
1	D	683	ALA	2.5
1	C	671	ILE	2.4
1	F	713[A]	MET	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	682	SER	2.4
1	F	673[A]	THR	2.4
1	F	674	GLY	2.3
1	E	671	ILE	2.3
1	E	675	GLU	2.3
1	F	781	ALA	2.3
1	D	674	GLY	2.3
1	F	697	ASN	2.2
1	C	686	GLY	2.2
1	D	659	VAL	2.2
1	D	675	GLU	2.2
1	B	666	SER	2.2
1	A	683	ALA	2.2
1	F	718[A]	SER	2.2
1	A	686	GLY	2.1
1	A	671	ILE	2.1
1	C	780	VAL	2.1
1	D	696	TYR	2.1
1	E	672	GLY	2.1
1	F	685	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.