Full wwPDB X-ray Structure Validation Report

Oct 6, 2016 – 03:20 PM EDT

PDB ID	:	5FIG
Title	:	APO-CSP3 (COPPER STORAGE PROTEIN 3) FROM BACILLUS SUBTILIS
Authors	:	Vita, N.; Landolfi, G.; Basle, A.; Platsaki, S.; Waldron, K.; Dennison, C.
Deposited on	:	2015-09-25
Resolution	:	1.70 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

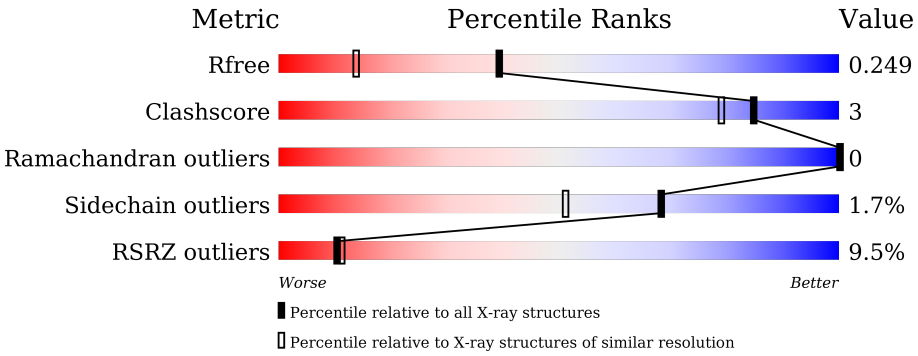
MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027939
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027939

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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}	91344	3190 (1.70-1.70)
Clashscore	102246	3585 (1.70-1.70)
Ramachandran outliers	100387	3527 (1.70-1.70)
Sidechain outliers	100360	3527 (1.70-1.70)
RSRZ outliers	91569	3200 (1.70-1.70)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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 <=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	108	8% 84% 8% 7%
1	B	108	6% 88% 6% • 6%
1	C	108	14% 79% 7% 14%
1	D	108	13% 74% 9% 17%
1	E	108	3% 84% 8% 7%
1	F	108	8% 85% 10% 5%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 4541 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 CSP3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	100	Total	C	N	O	S	0	4	0
			754	454	130	145	25			
1	B	102	Total	C	N	O	S	0	3	0
			770	462	132	151	25			
1	C	93	Total	C	N	O	S	0	3	0
			684	412	115	131	26			
1	D	90	Total	C	N	O	S	0	2	0
			657	397	109	128	23			
1	E	100	Total	C	N	O	S	0	4	0
			761	457	132	149	23			
1	F	103	Total	C	N	O	S	0	3	0
			778	469	135	149	25			

- Molecule 2 is water.

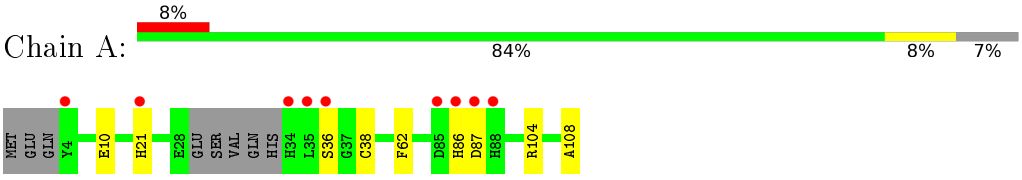
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	28	Total	O	0	0
			28	28		
2	B	25	Total	O	0	0
			25	25		
2	C	17	Total	O	0	0
			17	17		
2	D	23	Total	O	0	0
			23	23		
2	E	27	Total	O	0	0
			27	27		
2	F	17	Total	O	0	0
			17	17		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

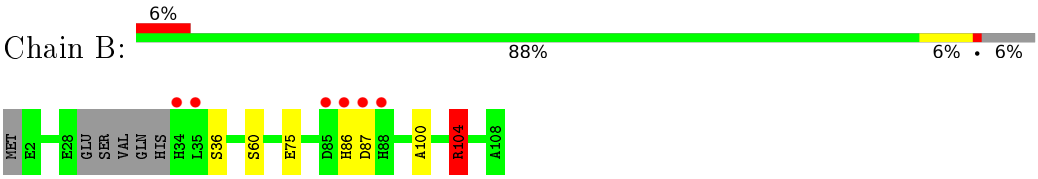
- Molecule 1: CSP3

Chain A:



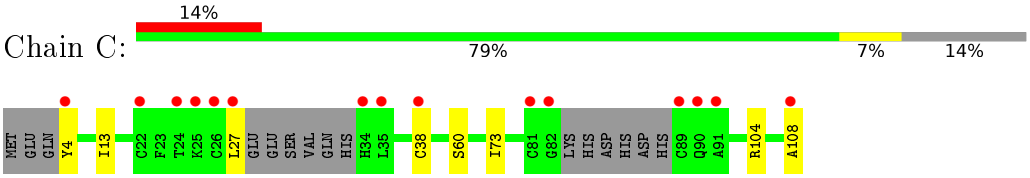
- Molecule 1: CSP3

Chain B:



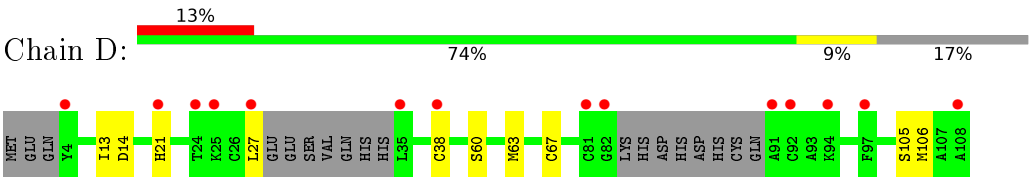
- Molecule 1: CSP3

Chain C:



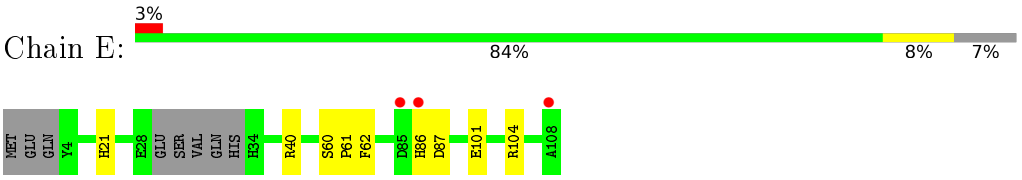
- Molecule 1: CSP3

Chain D:



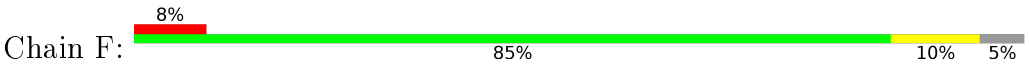
- Molecule 1: CSP3

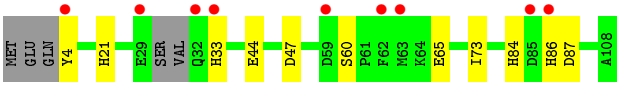
Chain E:



- Molecule 1: CSP3

Chain F:




MET
GLU
GLN
Y4
H21
E29
SER
VAL
Q32
H33
E44
D47
D59
S60
P61
F62
M63
K64
E65
I73
H84
D85
H86
D87
A108

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	107.09Å 126.51Å 85.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	81.74 – 1.70 45.41 – 1.70	Depositor EDS
% Data completeness (in resolution range)	99.7 (81.74-1.70) 99.7 (45.41-1.70)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.80 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.8.0124	Depositor
R, R_{free}	0.220 , 0.243 0.226 , 0.249	Depositor DCC
R_{free} test set	3180 reflections (5.23%)	DCC
Wilson B-factor (Å^2)	16.3	Xtriage
Anisotropy	0.528	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 40.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	4541	wwPDB-VP
Average B, all atoms (Å^2)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 55.86 % of the origin peak, indicating pseudo translational symmetry.The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 2.9776e-05.The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.79	0/775	0.88	2/1034 (0.2%)
1	B	0.86	1/787 (0.1%)	1.03	5/1051 (0.5%)
1	C	0.78	1/698 (0.1%)	0.92	4/930 (0.4%)
1	D	0.83	1/666 (0.2%)	0.91	1/887 (0.1%)
1	E	0.79	0/781	0.84	0/1044
1	F	0.82	1/796 (0.1%)	0.89	4/1065 (0.4%)
All	All	0.81	4/4503 (0.1%)	0.91	16/6011 (0.3%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	60	SER	CB-OG	-5.65	1.34	1.42
1	D	105	SER	CB-OG	-5.42	1.35	1.42
1	F	4	TYR	CG-CD1	5.16	1.45	1.39
1	C	4	TYR	CD2-CE2	-5.00	1.31	1.39

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	104	ARG	CG-CD-NE	-9.60	91.64	111.80
1	B	104	ARG	NE-CZ-NH2	-9.36	115.62	120.30
1	B	104	ARG	NE-CZ-NH1	8.13	124.37	120.30
1	B	104	ARG	CB-CG-CD	7.03	129.88	111.60
1	F	4	TYR	CB-CG-CD1	6.65	124.99	121.00
1	C	104	ARG	NE-CZ-NH1	6.00	123.30	120.30
1	B	104	ARG	CD-NE-CZ	5.77	131.68	123.60
1	F	47	ASP	CB-CG-OD1	5.73	123.46	118.30
1	C	104	ARG	NE-CZ-NH2	-5.44	117.58	120.30
1	D	38	CYS	CA-CB-SG	5.31	123.56	114.00
1	F	4	TYR	CB-CA-C	5.29	120.99	110.40
1	A	38[A]	CYS	CB-CA-C	-5.15	100.10	110.40
1	A	38[B]	CYS	CB-CA-C	-5.15	100.10	110.40
1	F	4	TYR	CB-CG-CD2	-5.02	117.99	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	38	CYS	CA-CB-SG	5.02	123.03	114.00
1	C	108	ALA	CA-C-O	-5.00	109.59	120.10

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	754	0	723	5	1
1	B	770	0	729	4	0
1	C	684	0	661	3	0
1	D	657	0	640	8	1
1	E	761	0	727	8	1
1	F	778	0	741	8	0
2	A	28	0	0	0	0
2	B	25	0	0	0	0
2	C	17	0	0	0	0
2	D	23	0	0	0	1
2	E	27	0	0	1	1
2	F	17	0	0	0	0
All	All	4541	0	4221	25	3

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 (25) 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:C:13:ILE:HD13	1:D:13:ILE:HD13	1.52	0.92
1:D:63[B]:MET:CE	1:D:67:CYS:SG	2.75	0.74
1:D:63[B]:MET:HE3	1:D:67:CYS:SG	2.29	0.72
1:A:108:ALA:O	1:E:40:ARG:HD3	1.94	0.66
1:E:62:PHE:CG	1:F:73[A]:ILE:CD1	2.80	0.64
1:D:63[B]:MET:HE2	1:D:67:CYS:SG	2.37	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:104[B]:ARG:NH1	2:E:2020:HOH:O	2.35	0.57
1:B:36:SER:HB2	1:C:27:LEU:HB3	1.86	0.56
1:A:36:SER:HB2	1:D:27:LEU:HB3	1.90	0.53
1:E:60[B]:SER:HB2	1:F:44:GLU:OE2	2.09	0.52
1:A:62:PHE:CG	1:C:73:ILE:HG12	2.44	0.52
1:E:62:PHE:CD1	1:F:73[A]:ILE:HD13	2.44	0.52
1:D:63[B]:MET:HE3	1:D:106:MET:HB3	1.95	0.48
1:A:104:ARG:NH1	1:F:65:GLU:OE2	2.47	0.48
1:B:75[B]:GLU:HG2	1:B:100:ALA:CB	2.46	0.46
1:E:62:PHE:CG	1:F:73[A]:ILE:HD13	2.52	0.45
1:F:86:HIS:CG	1:F:87:ASP:H	2.35	0.44
1:B:86:HIS:CG	1:B:87:ASP:H	2.36	0.43
1:A:86:HIS:CG	1:A:87:ASP:H	2.36	0.42
1:E:61:PRO:HD2	1:F:44:GLU:OE2	2.20	0.42
1:D:63[B]:MET:CE	1:D:106:MET:HB3	2.49	0.41
1:E:86:HIS:CG	1:E:87:ASP:H	2.39	0.40
1:B:75[A]:GLU:CD	1:B:104:ARG:HH11	2.24	0.40
1:F:33:HIS:CD2	1:F:84:HIS:HD2	2.40	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:2014:HOH:O	2:E:2014:HOH:O[4_556]	1.09	1.11
1:A:10:GLU:OE2	1:D:14:ASP:OD2[6_554]	2.12	0.08
1:E:101:GLU:OE1	2:D:2023:HOH:O[6_554]	2.14	0.06

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	100/108 (93%)	100 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	101/108 (94%)	101 (100%)	0	0	100	100
1	C	90/108 (83%)	90 (100%)	0	0	100	100
1	D	86/108 (80%)	86 (100%)	0	0	100	100
1	E	100/108 (93%)	100 (100%)	0	0	100	100
1	F	102/108 (94%)	102 (100%)	0	0	100	100
All	All	579/648 (89%)	579 (100%)	0	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	85/89 (96%)	84 (99%)	1 (1%)	78	65
1	B	86/89 (97%)	85 (99%)	1 (1%)	78	65
1	C	77/89 (86%)	76 (99%)	1 (1%)	76	62
1	D	73/89 (82%)	71 (97%)	2 (3%)	52	31
1	E	85/89 (96%)	84 (99%)	1 (1%)	78	65
1	F	87/89 (98%)	85 (98%)	2 (2%)	58	37
All	All	493/534 (92%)	485 (98%)	8 (2%)	68	54

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	HIS
1	B	104	ARG
1	C	60	SER
1	D	21	HIS
1	D	60	SER
1	E	21	HIS
1	F	21	HIS
1	F	60	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	33	HIS
1	F	84	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 carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

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, 95^{th} 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	100/108 (92%)	0.56	9 (9%) 12 13	11, 19, 33, 45	0
1	B	102/108 (94%)	0.61	6 (5%) 26 27	12, 20, 33, 42	0
1	C	93/108 (86%)	0.91	15 (16%) 3 3	13, 23, 39, 52	0
1	D	90/108 (83%)	0.88	14 (15%) 3 3	12, 21, 40, 46	0
1	E	100/108 (92%)	0.47	3 (3%) 54 58	12, 20, 37, 51	0
1	F	103/108 (95%)	0.50	9 (8%) 13 14	11, 18, 39, 55	0
All	All	588/648 (90%)	0.65	56 (9%) 10 11	11, 20, 39, 55	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	4	TYR	7.8
1	C	34	HIS	6.1
1	C	27	LEU	6.1
1	A	34	HIS	5.6
1	D	35	LEU	5.3
1	C	89	CYS	5.3
1	B	35	LEU	5.2
1	A	86	HIS	4.8
1	B	34	HIS	4.7
1	D	38	CYS	4.5
1	F	32	GLN	4.3
1	B	88	HIS	4.3
1	C	81[A]	CYS	4.0
1	F	4	TYR	4.0
1	C	35	LEU	4.0
1	C	90	GLN	3.8
1	E	85	ASP	3.8
1	A	87	ASP	3.8
1	B	86	HIS	3.5

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Mol	Chain	Res	Type	RSRZ
1	D	25	LYS	3.5
1	D	81	CYS	3.5
1	C	4	TYR	3.4
1	D	94	LYS	3.3
1	D	24	THR	3.1
1	D	21	HIS	3.0
1	A	4	TYR	3.0
1	F	86	HIS	2.9
1	F	63	MET	2.9
1	C	22[A]	CYS	2.8
1	C	38	CYS	2.8
1	F	85	ASP	2.8
1	D	27	LEU	2.7
1	A	21	HIS	2.7
1	A	88	HIS	2.7
1	B	87	ASP	2.6
1	C	82	GLY	2.6
1	B	85	ASP	2.6
1	C	26	CYS	2.6
1	F	59	ASP	2.5
1	E	108	ALA	2.5
1	C	24	THR	2.5
1	D	97	PHE	2.5
1	A	36	SER	2.4
1	D	108	ALA	2.4
1	D	91	ALA	2.4
1	C	25	LYS	2.3
1	C	91	ALA	2.3
1	A	85	ASP	2.2
1	A	35	LEU	2.2
1	C	108	ALA	2.2
1	F	33	HIS	2.1
1	E	86	HIS	2.1
1	D	92	CYS	2.1
1	F	62	PHE	2.1
1	F	29	GLU	2.0
1	D	82	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

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.