



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 27, 2021 – 10:10 AM JST

PDB ID : 7DW2
Title : Crystal structure of a glutathione S-transferase SbGSTU6 from *Salix babingtonica*
Authors : Zhuge, X.L.; Yang, H.L.
Deposited on : 2021-01-15
Resolution : 1.74 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.22
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.22

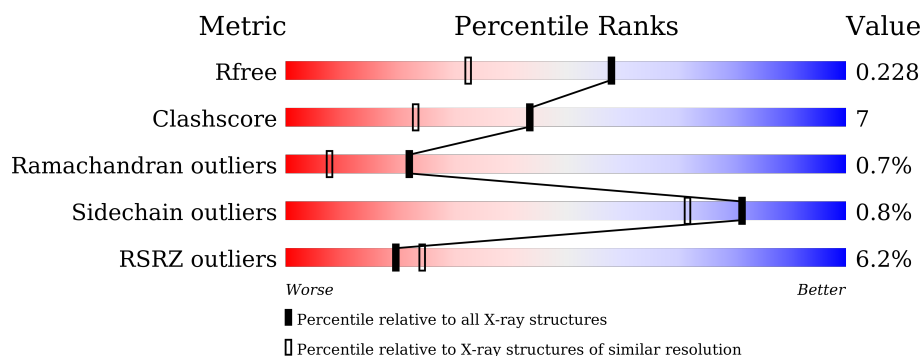
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.74 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}	130704	3764 (1.76-1.72)
Clashscore	141614	3923 (1.76-1.72)
Ramachandran outliers	138981	3878 (1.76-1.72)
Sidechain outliers	138945	3878 (1.76-1.72)
RSRZ outliers	127900	3705 (1.76-1.72)

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	235	<div> <div>5%</div> <div> <div></div> <div>82%</div> <div>10%</div> <div>• 6%</div> </div> </div>
1	B	235	<div> <div>6%</div> <div> <div></div> <div>80%</div> <div>14%</div> <div>6%</div> </div> </div>
1	C	235	<div> <div>7%</div> <div> <div></div> <div>83%</div> <div>11%</div> <div>6%</div> </div> </div>
1	D	235	<div> <div>6%</div> <div> <div></div> <div>82%</div> <div>11%</div> <div>• 6%</div> </div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7631 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 Glutathione S-transferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	220	Total	C	N	O	S	0	0	0
			1734	1131	284	313	6			
1	B	220	Total	C	N	O	S	0	0	0
			1734	1131	284	313	6			
1	C	220	Total	C	N	O	S	0	0	0
			1734	1131	284	313	6			
1	D	220	Total	C	N	O	S	0	0	0
			1734	1131	284	313	6			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	HIS	-	expression tag	UNP A0A4Y5R032
A	-4	HIS	-	expression tag	UNP A0A4Y5R032
A	-3	HIS	-	expression tag	UNP A0A4Y5R032
A	-2	HIS	-	expression tag	UNP A0A4Y5R032
A	-1	HIS	-	expression tag	UNP A0A4Y5R032
A	0	HIS	-	expression tag	UNP A0A4Y5R032
B	-5	HIS	-	expression tag	UNP A0A4Y5R032
B	-4	HIS	-	expression tag	UNP A0A4Y5R032
B	-3	HIS	-	expression tag	UNP A0A4Y5R032
B	-2	HIS	-	expression tag	UNP A0A4Y5R032
B	-1	HIS	-	expression tag	UNP A0A4Y5R032
B	0	HIS	-	expression tag	UNP A0A4Y5R032
C	-5	HIS	-	expression tag	UNP A0A4Y5R032
C	-4	HIS	-	expression tag	UNP A0A4Y5R032
C	-3	HIS	-	expression tag	UNP A0A4Y5R032
C	-2	HIS	-	expression tag	UNP A0A4Y5R032
C	-1	HIS	-	expression tag	UNP A0A4Y5R032
C	0	HIS	-	expression tag	UNP A0A4Y5R032
D	-5	HIS	-	expression tag	UNP A0A4Y5R032
D	-4	HIS	-	expression tag	UNP A0A4Y5R032
D	-3	HIS	-	expression tag	UNP A0A4Y5R032

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-2	HIS	-	expression tag	UNP A0A4Y5R032
D	-1	HIS	-	expression tag	UNP A0A4Y5R032
D	0	HIS	-	expression tag	UNP A0A4Y5R032

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	186	Total 186	O 186	0	0
2	B	181	Total 181	O 181	0	0
2	C	177	Total 177	O 177	0	0
2	D	151	Total 151	O 151	0	0

- Molecule 1: Glutathione S-transferase



K218	K219	L220	A221	K222	LEU	LYS	ALA	THR	PRO	PRO	LYS
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4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	53.15Å 103.15Å 186.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	31.03 – 1.74 42.42 – 1.74	Depositor EDS
% Data completeness (in resolution range)	95.8 (31.03-1.74) 95.2 (42.42-1.74)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.65 (at 1.74Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.193 , 0.227 0.193 , 0.228	Depositor DCC
R_{free} test set	2000 reflections (1.91%)	wwPDB-VP
Wilson B-factor (Å ²)	26.1	Xtriage
Anisotropy	0.289	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 44.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7631	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.42% 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	0.65	0/1779	0.62	0/2408
1	B	0.44	0/1779	0.59	0/2408
1	C	0.43	0/1779	0.60	0/2408
1	D	0.43	0/1779	0.57	0/2408
All	All	0.50	0/7116	0.60	0/9632

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	A	1734	0	1757	26	0
1	B	1734	0	1757	27	0
1	C	1734	0	1757	20	0
1	D	1734	0	1757	23	0
2	A	186	0	0	2	0
2	B	181	0	0	4	0
2	C	177	0	0	2	0
2	D	151	0	0	1	0
All	All	7631	0	7028	94	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 7.

All (94) 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:55:ILE:H	1:C:55:ILE:HD13	1.25	0.99
1:A:55:ILE:HD13	1:A:55:ILE:H	1.25	0.98
1:D:55:ILE:H	1:D:55:ILE:HD13	1.30	0.96
1:A:11:ALA:H	1:A:55:ILE:HG13	1.31	0.94
1:D:105:GLU:HG3	1:D:106:LYS:HG2	1.48	0.93
1:B:93:ARG:HD3	2:B:414:HOH:O	1.68	0.92
1:B:55:ILE:H	1:B:55:ILE:HD13	1.35	0.92
1:C:11:ALA:H	1:C:55:ILE:HG13	1.36	0.91
1:D:11:ALA:H	1:D:55:ILE:HG13	1.38	0.88
1:A:221:ALA:O	1:A:222:LYS:NZ	2.07	0.87
1:A:93:ARG:HD3	2:A:413:HOH:O	1.82	0.77
1:B:11:ALA:H	1:B:55:ILE:HG13	1.53	0.73
1:A:183:ASP:OD1	1:A:184:GLU:N	2.24	0.70
1:B:55:ILE:HB	1:B:56:PRO:HA	1.71	0.70
1:C:55:ILE:HD13	1:C:55:ILE:N	2.05	0.70
1:A:91:TYR:CZ	1:B:63:LYS:HG2	2.29	0.68
1:D:55:ILE:H	1:D:55:ILE:CD1	2.06	0.68
1:A:55:ILE:HD13	1:A:55:ILE:N	2.05	0.65
1:A:183:ASP:O	1:A:191:LEU:HD11	1.97	0.64
1:A:172:ALA:O	1:A:176:MET:HG3	1.98	0.63
1:B:119:ASP:HB2	1:B:122:ALA:H	1.65	0.62
1:C:55:ILE:H	1:C:55:ILE:CD1	2.05	0.62
1:D:220:LEU:O	1:D:222:LYS:N	2.31	0.62
1:A:91:TYR:CE1	1:B:63:LYS:HG2	2.36	0.61
1:A:55:ILE:H	1:A:55:ILE:CD1	2.06	0.61
1:C:117:ALA:HB3	1:C:123:ARG:HG3	1.82	0.60
1:D:111:MET:HG2	1:D:173:ILE:HD13	1.83	0.60
1:A:183:ASP:OD1	1:A:185:THR:N	2.35	0.59
1:B:111:MET:HG2	1:B:173:ILE:HD13	1.86	0.57
1:B:55:ILE:HD13	1:B:55:ILE:N	2.14	0.56
1:D:101:ALA:O	1:D:105:GLU:HG2	2.07	0.55
1:B:209:GLU:HG3	2:B:311:HOH:O	2.07	0.55
1:C:103:LEU:HD21	1:C:137:LEU:HD11	1.88	0.55
1:A:220:LEU:O	1:A:222:LYS:N	2.40	0.55
1:B:55:ILE:H	1:B:55:ILE:CD1	2.14	0.54
1:D:55:ILE:HB	1:D:56:PRO:HA	1.90	0.54
1:C:63:LYS:HE3	2:C:331:HOH:O	2.08	0.54
1:C:3:LYS:HE2	1:C:30:GLU:OE2	2.09	0.53
1:D:55:ILE:HD13	1:D:55:ILE:N	2.10	0.53
1:A:3:LYS:N	2:A:310:HOH:O	2.41	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:128:ASP:O	1:B:132:GLU:HG3	2.09	0.52
1:A:43:GLN:HE21	1:A:47:GLU:HG3	1.75	0.52
1:A:148:LYS:HD3	1:A:154:ASP:CG	2.30	0.52
1:A:66:CYS:O	1:A:67:GLU:HB2	2.09	0.51
1:D:209:GLU:O	1:D:212:LYS:HB3	2.10	0.51
1:D:105:GLU:CG	1:D:106:LYS:HG2	2.33	0.50
1:A:183:ASP:O	1:A:184:GLU:HB2	2.12	0.50
1:D:80:SER:N	1:D:81:PRO:HD2	2.27	0.50
1:D:123:ARG:HH21	1:D:123:ARG:HG3	1.77	0.50
1:B:35:GLU:HG2	1:B:37:THR:HG23	1.93	0.49
1:B:139:ASP:O	1:B:143:LYS:HG2	2.11	0.49
1:B:218:LYS:NZ	2:B:302:HOH:O	2.22	0.49
1:D:95:LEU:HD21	1:D:143:LYS:HD3	1.95	0.48
1:D:179:VAL:O	1:D:180:LYS:HE2	2.12	0.48
1:D:3:LYS:HA	1:D:30:GLU:HG2	1.95	0.48
1:B:36:GLU:O	2:B:301:HOH:O	2.20	0.48
1:C:175:LYS:NZ	1:C:211:GLU:OE1	2.47	0.47
1:A:201:PRO:HA	1:A:204:LYS:HE2	1.96	0.47
1:A:11:ALA:N	1:A:55:ILE:HG13	2.13	0.47
1:D:55:ILE:CD1	1:D:55:ILE:N	2.72	0.46
1:C:9:LEU:HD23	1:C:34:LEU:HD12	1.98	0.46
1:B:182:MET:HE2	1:B:191:LEU:HD23	1.98	0.46
1:D:211:GLU:H	1:D:211:GLU:CD	2.19	0.46
1:C:54:LYS:NZ	2:D:301:HOH:O	2.40	0.46
1:C:55:ILE:N	1:C:55:ILE:CD1	2.72	0.45
1:B:220:LEU:O	1:B:222:LYS:N	2.50	0.45
1:A:55:ILE:N	1:A:55:ILE:CD1	2.73	0.45
1:A:221:ALA:O	1:A:222:LYS:HD3	2.17	0.45
1:B:48:SER:HB3	1:B:57:VAL:HG11	1.99	0.44
1:C:111:MET:HG2	1:C:173:ILE:HD13	1.99	0.44
1:B:11:ALA:N	1:B:55:ILE:HG13	2.28	0.43
1:C:36:GLU:OE2	1:C:42:SER:OG	2.33	0.43
1:A:87:PRO:O	1:A:93:ARG:HG3	2.17	0.43
1:B:10:GLY:HA2	1:B:55:ILE:HG13	2.00	0.43
1:B:55:ILE:N	1:B:55:ILE:CD1	2.79	0.43
1:C:9:LEU:HD12	1:C:57:VAL:HB	2.01	0.43
1:C:55:ILE:HB	1:C:56:PRO:HA	2.01	0.42
1:D:111:MET:CG	1:D:173:ILE:HD13	2.47	0.42
1:B:112:ARG:HH11	1:B:112:ARG:HG3	1.84	0.42
1:D:9:LEU:HD11	1:D:44:LEU:HG	2.01	0.42
1:B:66:CYS:O	1:B:67:GLU:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:73:GLU:OE1	1:C:86:LEU:HD11	2.19	0.41
1:A:10:GLY:HA2	1:A:55:ILE:HB	2.02	0.41
1:C:111:MET:HG2	1:C:173:ILE:CD1	2.49	0.41
1:A:55:ILE:HB	1:A:56:PRO:HA	2.02	0.41
1:C:221:ALA:O	1:C:222:LYS:HB2	2.21	0.41
1:B:148:LYS:HD3	1:B:154:ASP:OD1	2.20	0.41
1:D:221:ALA:O	1:D:222:LYS:NZ	2.44	0.41
1:A:222:LYS:HD3	1:A:222:LYS:HA	1.91	0.41
1:B:111:MET:CG	1:B:173:ILE:HD13	2.49	0.41
1:B:103:LEU:HD21	1:B:137:LEU:HD11	2.03	0.40
1:D:214:VAL:HG12	1:D:218:LYS:HE2	2.03	0.40
1:C:63:LYS:NZ	2:C:310:HOH:O	2.54	0.40
1:D:11:ALA:N	1:D:55:ILE:HG13	2.20	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	218/235 (93%)	212 (97%)	4 (2%)	2 (1%)	17	5
1	B	218/235 (93%)	215 (99%)	2 (1%)	1 (0%)	29	12
1	C	218/235 (93%)	214 (98%)	2 (1%)	2 (1%)	17	5
1	D	218/235 (93%)	213 (98%)	4 (2%)	1 (0%)	29	12
All	All	872/940 (93%)	854 (98%)	12 (1%)	6 (1%)	22	8

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	184	GLU
1	A	221	ALA

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Mol	Chain	Res	Type
1	C	118	LYS
1	D	221	ALA
1	B	221	ALA
1	C	67	GLU

5.3.2 Protein sidechains ⓘ

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	185/198 (93%)	182 (98%)	3 (2%)	62	44
1	B	185/198 (93%)	184 (100%)	1 (0%)	88	83
1	C	185/198 (93%)	184 (100%)	1 (0%)	88	83
1	D	185/198 (93%)	184 (100%)	1 (0%)	88	83
All	All	740/792 (93%)	734 (99%)	6 (1%)	81	72

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55	ILE
1	A	118	LYS
1	A	218	LYS
1	B	55	ILE
1	C	55	ILE
1	D	55	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	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 monosaccharides 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	220/235 (93%)	0.36	11 (5%) 28 33	17, 30, 51, 59	0
1	B	220/235 (93%)	0.20	14 (6%) 19 23	17, 28, 46, 61	0
1	C	220/235 (93%)	0.30	16 (7%) 15 19	19, 30, 49, 64	0
1	D	220/235 (93%)	0.29	14 (6%) 19 23	19, 30, 49, 61	0
All	All	880/940 (93%)	0.29	55 (6%) 20 24	17, 30, 49, 64	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	118	LYS	4.9
1	C	117	ALA	4.7
1	B	37	THR	4.6
1	D	219	VAL	4.5
1	A	61	GLY	4.4
1	A	221	ALA	4.4
1	A	118	LYS	4.3
1	C	118	LYS	4.0
1	D	4	SER	4.0
1	B	221	ALA	3.8
1	B	4	SER	3.7
1	C	4	SER	3.6
1	A	121	GLU	3.5
1	B	61	GLY	3.5
1	C	122	ALA	3.4
1	D	122	ALA	3.1
1	C	124	LYS	3.0
1	A	220	LEU	3.0
1	C	116	ALA	3.0
1	D	116	ALA	3.0
1	C	221	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	62	GLY	2.8
1	A	117	ALA	2.8
1	D	117	ALA	2.8
1	C	119	ASP	2.8
1	B	115	ALA	2.8
1	B	118	LYS	2.8
1	D	221	ALA	2.7
1	C	61	GLY	2.6
1	B	122	ALA	2.6
1	B	62	GLY	2.5
1	A	62	GLY	2.5
1	D	30	GLU	2.4
1	A	115	ALA	2.4
1	C	211	GLU	2.4
1	D	121	GLU	2.4
1	D	81	PRO	2.4
1	B	121	GLU	2.4
1	C	121	GLU	2.4
1	C	39	GLY	2.3
1	B	219	VAL	2.3
1	D	119	ASP	2.3
1	D	80	SER	2.3
1	B	116	ALA	2.2
1	A	183	ASP	2.2
1	C	94	ALA	2.2
1	D	185	THR	2.2
1	B	117	ALA	2.2
1	C	9	LEU	2.2
1	A	69	LEU	2.1
1	C	40	SER	2.1
1	A	112	ARG	2.1
1	B	44	LEU	2.1
1	B	5	ASP	2.0
1	D	69	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates [i](#)

There are no monosaccharides 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.