



Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 01:28 pm BST

PDB ID : 5YSK
Title : SdeA mART-C domain EE/AA apo
Authors : Kim, L.; Kwon, D.H.; Song, H.K.
Deposited on : 2017-11-14
Resolution : 2.40 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
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
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) : 2.11

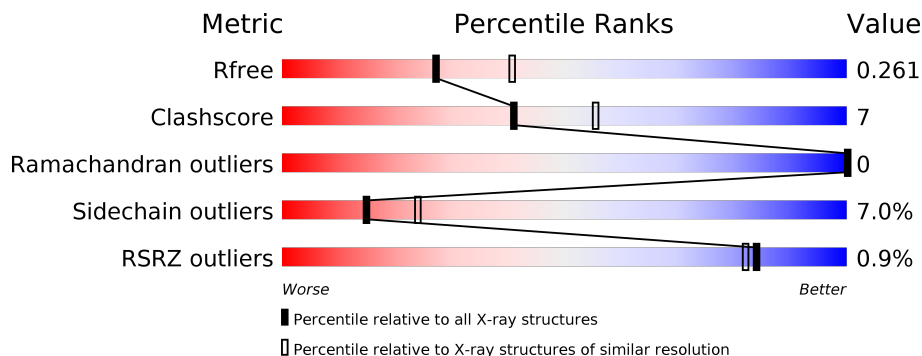
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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 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	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 75%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 12%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 10%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 11%; height: 10px; background-color: grey;"></div> </div> <p style="font-size: small; margin-top: 5px;">2% 75% 12% • 10%</p>
1	B	152	<div style="display: flex; align-items: center;"> <div style="width: 0%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 77%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 11%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 11%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 11%; height: 10px; background-color: grey;"></div> </div> <p style="font-size: small; margin-top: 5px;">% 77% 11% • 11%</p>
1	C	152	<div style="display: flex; align-items: center;"> <div style="width: 0%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 67%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 20%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 11%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 11%; height: 10px; background-color: grey;"></div> </div> <p style="font-size: small; margin-top: 5px;">% 67% 20% • 11%</p>
1	D	152	<div style="display: flex; align-items: center;"> <div style="width: 76%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 15%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 6%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 3%; height: 10px; background-color: grey;"></div> </div> <p style="font-size: small; margin-top: 5px;">76% 15% • 6%</p>

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 8570 atoms, of which 4143 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 Ubiquitinating/deubiquitinating enzyme SdeA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	Se			
1	A	137	2103	680	1033	179	208	3	0	0	0
1	B	135	2089	674	1030	177	205	3	0	0	0
1	C	135	2106	677	1043	178	205	3	0	0	0
1	D	143	2153	705	1037	190	218	3	0	0	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	754	GLY	-	expression tag	UNP Q5ZTK4
A	755	SER	-	expression tag	UNP Q5ZTK4
A	860	ALA	GLU	engineered mutation	UNP Q5ZTK4
A	862	ALA	GLU	engineered mutation	UNP Q5ZTK4
B	754	GLY	-	expression tag	UNP Q5ZTK4
B	755	SER	-	expression tag	UNP Q5ZTK4
B	860	ALA	GLU	engineered mutation	UNP Q5ZTK4
B	862	ALA	GLU	engineered mutation	UNP Q5ZTK4
C	754	GLY	-	expression tag	UNP Q5ZTK4
C	755	SER	-	expression tag	UNP Q5ZTK4
C	860	ALA	GLU	engineered mutation	UNP Q5ZTK4
C	862	ALA	GLU	engineered mutation	UNP Q5ZTK4
D	754	GLY	-	expression tag	UNP Q5ZTK4
D	755	SER	-	expression tag	UNP Q5ZTK4
D	860	ALA	GLU	engineered mutation	UNP Q5ZTK4
D	862	ALA	GLU	engineered mutation	UNP Q5ZTK4

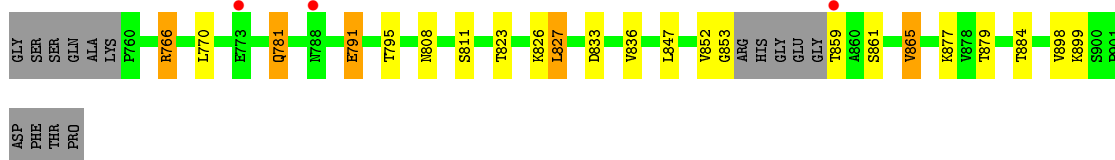
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	28	Total 28	O 28	0	0
2	B	27	Total 27	O 27	0	0
2	C	28	Total 28	O 28	0	0
2	D	36	Total 36	O 36	0	0

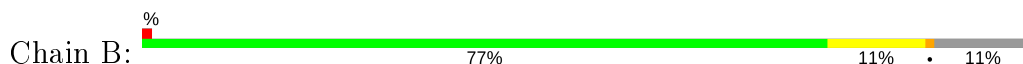
3 Residue-property plots [i](#)

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

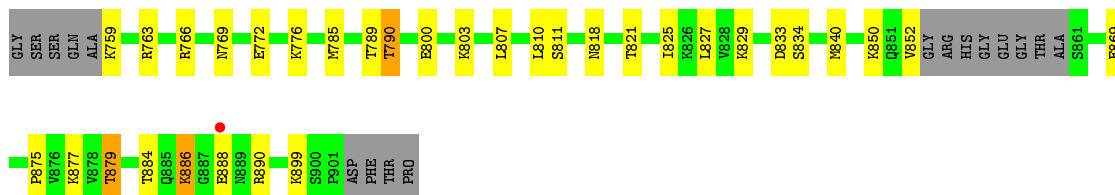
- Molecule 1: Ubiquitinating/deubiquitinating enzyme SdeA



- Molecule 1: Ubiquitinating/deubiquitinating enzyme SdeA



- Molecule 1: Ubiquitinating/deubiquitinating enzyme SdeA



- Molecule 1: Ubiquitinating/deubiquitinating enzyme SdeA



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	43.75Å 85.36Å 70.80Å 90.00° 97.11° 90.00°	Depositor
Resolution (Å)	32.42 – 2.40 39.16 – 2.40	Depositor EDS
% Data completeness (in resolution range)	98.0 (32.42-2.40) 98.0 (39.16-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.59 (at 2.39Å)	Xtrriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.185 , 0.261 0.185 , 0.261	Depositor DCC
R_{free} test set	1980 reflections (10.00%)	wwPDB-VP
Wilson B-factor (Å ²)	23.0	Xtrriage
Anisotropy	0.184	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.44 , 60.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8570	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 65.54 % 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 6.9717e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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	0.59	0/1086	0.74	1/1464 (0.1%)
1	B	0.63	0/1075	0.75	1/1449 (0.1%)
1	C	0.62	0/1079	0.72	0/1454
1	D	0.62	0/1134	0.74	0/1529
All	All	0.62	0/4374	0.74	2/5896 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	827	LEU	CA-CB-CG	5.33	127.55	115.30
1	A	827	LEU	CA-CB-CG	5.01	126.83	115.30

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	1070	1033	1079	18	0
1	B	1059	1030	1069	9	0
1	C	1063	1043	1076	20	0
1	D	1116	1037	1116	22	0
2	A	28	0	0	2	0
2	B	27	0	0	2	0
2	C	28	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	36	0	0	7	0
All	All	4427	4143	4340	61	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 (61) 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:D:766:ARG:NH2	1:D:811:SER:O	1.87	1.08
1:A:766:ARG:NH2	1:A:811:SER:O	1.91	1.04
1:D:854:ARG:HB2	1:D:857:GLU:HG3	1.50	0.91
1:C:766:ARG:NH2	1:C:811:SER:O	2.04	0.90
1:C:772:GLU:OE1	2:C:1001:HOH:O	1.90	0.89
1:D:854:ARG:HB2	1:D:857:GLU:CG	2.11	0.81
1:A:791:GLU:OE1	1:A:795:THR:OG1	2.01	0.79
1:B:766:ARG:NH2	1:B:811:SER:O	2.18	0.76
1:D:780:ASP:OD1	2:D:1001:HOH:O	2.07	0.72
1:C:869:GLU:OE2	2:C:1002:HOH:O	2.08	0.70
1:C:769:ASN:ND2	2:C:1003:HOH:O	2.22	0.69
1:A:791:GLU:HG2	1:C:763:ARG:HH21	1.68	0.59
1:A:823:THR:OG1	1:A:861:SER:HB2	2.06	0.56
1:D:816:ARG:NH1	2:D:1004:HOH:O	2.27	0.56
1:C:829:LYS:HE3	1:C:890:ARG:CZ	2.38	0.54
1:D:808:ASN:HB2	2:D:1005:HOH:O	2.07	0.53
1:A:781:GLN:OE1	1:A:808:ASN:OD1	2.26	0.53
1:C:825:ILE:HG12	1:C:829:LYS:HD2	1.91	0.53
1:B:877:LYS:HG2	1:D:879:THR:HG21	1.90	0.53
1:A:853:GLY:O	2:A:1002:HOH:O	2.19	0.52
1:A:859:THR:HG22	1:A:859:THR:O	2.09	0.52
1:D:877:LYS:HG3	1:D:879:THR:HG22	1.93	0.51
1:B:845:GLY:O	2:B:1001:HOH:O	2.20	0.50
1:C:886:LYS:HE2	1:C:888:GLU:OE1	2.13	0.49
1:D:790:THR:HG21	1:D:875:PRO:O	2.13	0.49
1:C:852:VAL:HG12	1:C:852:VAL:O	2.14	0.48
1:A:879:THR:HG21	1:C:877:LYS:HG2	1.95	0.48
1:D:760:PRO:N	2:D:1011:HOH:O	2.47	0.48
1:C:785:MSE:SE	1:C:810:LEU:HD11	2.65	0.47
1:D:785:MSE:HE1	2:D:1027:HOH:O	2.14	0.46
1:D:760:PRO:N	2:D:1012:HOH:O	2.47	0.46
1:C:790:THR:HG21	1:C:875:PRO:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:852:VAL:O	1:D:852:VAL:HG13	2.16	0.45
1:B:852:VAL:HG12	1:B:852:VAL:O	2.16	0.45
1:D:806:LYS:NZ	2:D:1002:HOH:O	2.14	0.45
1:A:847:LEU:HB3	1:A:865:VAL:HG22	1.97	0.45
1:A:877:LYS:HG2	1:C:879:THR:HG21	1.98	0.45
1:C:833:ASP:OD2	1:C:884:THR:HB	2.16	0.45
1:D:857:GLU:O	1:D:859:THR:HG23	2.17	0.44
1:B:879:THR:HG21	1:D:877:LYS:HG2	2.00	0.44
1:A:879:THR:HG21	1:C:877:LYS:CG	2.48	0.43
1:D:855:HIS:ND1	1:D:855:HIS:N	2.59	0.43
1:C:821:THR:HG21	1:C:840:MSE:HE1	1.99	0.43
1:B:877:LYS:CG	1:D:879:THR:HG21	2.47	0.43
1:B:873:LEU:O	2:B:1002:HOH:O	2.21	0.42
1:D:765:PHE:CE1	1:D:839:GLU:HG3	2.54	0.42
1:A:879:THR:HG23	2:A:1010:HOH:O	2.17	0.42
1:C:821:THR:CG2	1:C:840:MSE:HE1	2.49	0.42
1:C:818:ASN:CG	1:C:818:ASN:O	2.58	0.42
1:A:833:ASP:OD2	1:A:884:THR:HB	2.19	0.42
1:A:877:LYS:CG	1:C:879:THR:HG21	2.50	0.42
1:A:770:LEU:HD12	1:A:836:VAL:HG21	2.02	0.41
1:A:852:VAL:O	1:A:852:VAL:HG12	2.20	0.41
1:D:821:THR:HG21	1:D:840:MSE:HE1	2.02	0.41
1:A:859:THR:CG2	1:A:859:THR:O	2.68	0.41
1:B:809:ASP:OD2	1:B:812:LYS:HA	2.20	0.41
1:D:853:GLY:HA3	1:D:859:THR:O	2.21	0.41
1:C:800:GLU:HA	1:C:803:LYS:HE2	2.03	0.40
1:A:898:VAL:HG12	1:A:899:LYS:O	2.21	0.40
1:D:781:GLN:NE2	1:D:808:ASN:OD1	2.45	0.40
1:B:848:HIS:HB2	1:B:866:TYR:HB3	2.03	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	133/152 (88%)	127 (96%)	6 (4%)	0	100	100
1	B	131/152 (86%)	123 (94%)	8 (6%)	0	100	100
1	C	131/152 (86%)	127 (97%)	4 (3%)	0	100	100
1	D	141/152 (93%)	137 (97%)	4 (3%)	0	100	100
All	All	536/608 (88%)	514 (96%)	22 (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	121/129 (94%)	115 (95%)	6 (5%)	24	40
1	B	120/129 (93%)	113 (94%)	7 (6%)	20	32
1	C	121/129 (94%)	110 (91%)	11 (9%)	9	14
1	D	125/129 (97%)	115 (92%)	10 (8%)	12	18
All	All	487/516 (94%)	453 (93%)	34 (7%)	15	24

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	766	ARG
1	A	781	GLN
1	A	791	GLU
1	A	826	LYS
1	A	827	LEU
1	A	865	VAL
1	B	776	LYS
1	B	791	GLU
1	B	803	LYS
1	B	827	LEU
1	B	861	SER
1	B	886	LYS
1	B	899	LYS

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Mol	Chain	Res	Type
1	C	759	LYS
1	C	776	LYS
1	C	789	THR
1	C	790	THR
1	C	807	LEU
1	C	827	LEU
1	C	834	SER
1	C	850	LYS
1	C	879	THR
1	C	886	LYS
1	C	899	LYS
1	D	766	ARG
1	D	804	GLN
1	D	807	LEU
1	D	826	LYS
1	D	827	LEU
1	D	852	VAL
1	D	855	HIS
1	D	857	GLU
1	D	879	THR
1	D	888	GLU

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

Mol	Chain	Res	Type
1	A	781	GLN
1	A	797	HIS
1	C	781	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 carbohydrates 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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	134/152 (88%)	-0.10	3 (2%) 62 60	17, 27, 43, 60	0
1	B	132/152 (86%)	-0.18	1 (0%) 86 84	14, 27, 42, 57	0
1	C	132/152 (86%)	-0.16	1 (0%) 86 84	14, 27, 44, 50	0
1	D	140/152 (92%)	-0.19	0 100 100	13, 24, 43, 62	0
All	All	538/608 (88%)	-0.15	5 (0%) 84 82	13, 26, 43, 62	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	859	THR	3.0
1	B	860	ALA	2.8
1	A	788	ASN	2.2
1	C	888	GLU	2.1
1	A	773	GLU	2.1

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 carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.