



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 19, 2016 – 07:49 PM EST

PDB ID : 5M9E
Title : Interactions between the Mal3 EB1-like domain and Dis1
Authors : Zakian, S.; Singleton, M.R.
Deposited on : 2016-11-01
Resolution : 2.83 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028442
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-20028442

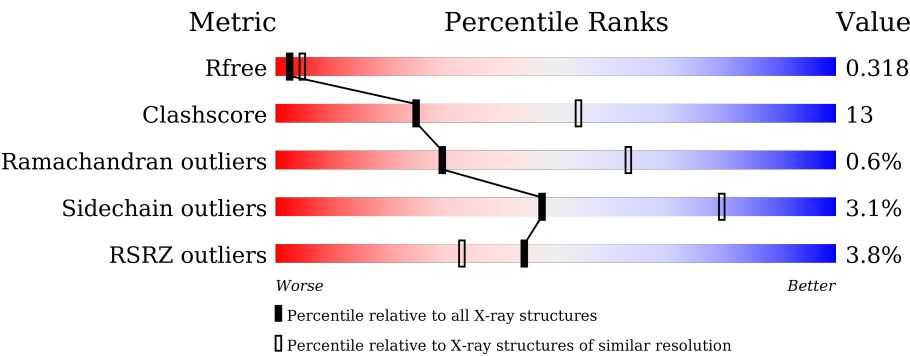
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.83 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	3170 (2.88-2.80)
Clashscore	102246	3658 (2.88-2.80)
Ramachandran outliers	100387	3591 (2.88-2.80)
Sidechain outliers	100360	3594 (2.88-2.80)
RSRZ outliers	91569	3184 (2.88-2.80)

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 $\leq 5\%$. 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	77	<div><div>3%</div><div><div></div><div></div><div></div><div></div></div><div>58%29%•10%</div></div>
1	B	77	<div><div>4%</div><div><div></div><div></div><div></div><div></div></div><div>62%27%•8%</div></div>
1	C	77	<div><div>5%</div><div><div></div><div></div><div></div><div></div></div><div>64%23%•12%</div></div>
1	D	77	<div><div>%</div><div><div></div><div></div><div></div><div></div></div><div>60%31%9%</div></div>
2	E	20	<div><div></div><div><div></div><div></div><div></div><div></div></div><div>85%10%5%</div></div>
2	F	20	<div><div></div><div><div></div><div></div><div></div><div></div></div><div>75%25%</div></div>

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Mol	Chain	Length	Quality of chain
2	G	20	
2	H	20	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2805 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 Microtubule integrity protein mal3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	69	Total	C	N	O	S	0	0	0
			572	359	95	114	4			
1	B	71	Total	C	N	O	S	0	0	0
			585	366	97	118	4			
1	C	68	Total	C	N	O	S	0	0	0
			566	356	94	112	4			
1	D	70	Total	C	N	O	S	0	0	0
			581	364	96	117	4			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	171	SER	-	expression tag	UNP Q10113
A	172	GLY	-	expression tag	UNP Q10113
A	173	SER	-	expression tag	UNP Q10113
B	171	SER	-	expression tag	UNP Q10113
B	172	GLY	-	expression tag	UNP Q10113
B	173	SER	-	expression tag	UNP Q10113
C	171	SER	-	expression tag	UNP Q10113
C	172	GLY	-	expression tag	UNP Q10113
C	173	SER	-	expression tag	UNP Q10113
D	171	SER	-	expression tag	UNP Q10113
D	172	GLY	-	expression tag	UNP Q10113
D	173	SER	-	expression tag	UNP Q10113

- Molecule 2 is a protein called Phosphoprotein p93.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	19	Total	C	N	O	S	0	0	0
			149	91	31	26	1			
2	F	20	Total	C	N	O	S	0	0	0
			160	100	32	27	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	13	Total	C	N	O	S	0	0	0
			97	59	19	18	1			
2	H	12	Total	C	N	O	S	0	0	0
			95	59	18	17	1			

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: Microtubule integrity protein mal3



- Molecule 1: Microtubule integrity protein mal3



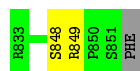
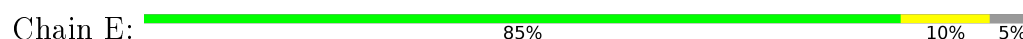
- Molecule 1: Microtubule integrity protein mal3



- Molecule 1: Microtubule integrity protein mal3

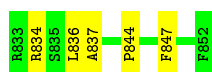


- Molecule 2: Phosphoprotein p93

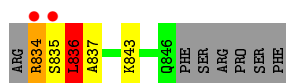


- Molecule 2: Phosphoprotein p93

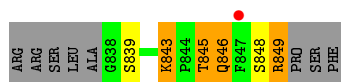




- Molecule 2: Phosphoprotein p93



- Molecule 2: Phosphoprotein p93



4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	93.31Å 93.31Å 196.54Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	80.80 – 2.83 80.80 – 2.83	Depositor EDS
% Data completeness (in resolution range)	97.1 (80.80-2.83) 98.3 (80.80-2.83)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.93 (at 2.82Å)	Xtriage
Refinement program	PHENIX (1.11.1 _2575: ???)	Depositor
R, R_{free}	0.266 , 0.325 0.264 , 0.318	Depositor DCC
R_{free} test set	606 reflections (4.84%)	DCC
Wilson B-factor (Å ²)	79.4	Xtriage
Anisotropy	0.033	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 58.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	2805	wwPDB-VP
Average B, all atoms (Å ²)	92.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.02% 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	0.56	2/579 (0.3%)	0.74	1/779 (0.1%)
1	B	0.73	2/592 (0.3%)	1.22	5/796 (0.6%)
1	C	0.49	0/573	0.76	0/771
1	D	0.53	0/588	0.85	3/791 (0.4%)
2	E	0.40	0/151	0.54	0/200
2	F	0.42	0/163	0.58	0/216
2	G	0.37	0/97	1.05	1/128 (0.8%)
2	H	0.35	0/96	0.64	0/126
All	All	0.56	4/2839 (0.1%)	0.88	10/3807 (0.3%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	233	ARG	CB-CG	8.08	1.74	1.52
1	B	233	ARG	CG-CD	7.12	1.69	1.51
1	A	228	GLU	CG-CD	6.15	1.61	1.51
1	A	232	GLU	CG-CD	-5.28	1.44	1.51

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	233	ARG	NE-CZ-NH2	20.33	130.46	120.30
1	B	233	ARG	NE-CZ-NH1	-13.58	113.51	120.30
1	B	233	ARG	CG-CD-NE	-8.62	93.71	111.80
1	D	176	GLN	CA-CB-CG	8.25	131.54	113.40
2	G	836	LEU	CA-CB-CG	8.09	133.91	115.30
1	B	233	ARG	CD-NE-CZ	7.05	133.47	123.60
1	B	228	GLU	N-CA-CB	-5.93	99.92	110.60
1	D	195	MET	CB-CG-SD	-5.75	95.15	112.40
1	A	238	LEU	CA-CB-CG	5.67	128.34	115.30
1	D	195	MET	CA-CB-CG	5.23	122.18	113.30

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	572	0	566	20	0
1	B	585	0	575	18	0
1	C	566	0	561	15	0
1	D	581	0	572	18	0
2	E	149	0	156	2	0
2	F	160	0	165	9	0
2	G	97	0	104	4	0
2	H	95	0	97	5	0
All	All	2805	0	2796	71	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 13.

All (71) 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:A:212:ILE:HG13	1:A:237:ILE:HD11	1.57	0.86
1:A:173:SER:HA	1:B:174:ALA:HB2	1.62	0.82
1:A:225:MET:HB3	1:A:229:ASN:HD22	1.51	0.75
1:B:215:LEU:HD11	1:B:233:ARG:HD2	1.71	0.72
2:G:835:SER:H	2:G:836:LEU:HD13	1.57	0.69
2:H:843:LYS:H	2:H:843:LYS:HD2	1.60	0.67
1:B:210:ARG:HH21	2:H:839:SER:HB2	1.60	0.66
1:A:175:LYS:HA	1:A:178:GLN:OE1	1.97	0.64
1:C:188:LEU:HD11	1:D:187:GLN:HG2	1.80	0.64
1:B:215:LEU:CD1	1:B:233:ARG:HD2	2.28	0.64
1:A:226:SER:O	1:A:229:ASN:HB2	1.97	0.64
1:C:188:LEU:HD12	1:D:188:LEU:HG	1.80	0.62
1:A:235:GLN:HA	1:A:238:LEU:HD13	1.81	0.62
1:D:228:GLU:N	1:D:228:GLU:OE1	2.28	0.61
1:A:188:LEU:HD12	1:B:188:LEU:HG	1.84	0.60
1:C:240:SER:O	1:C:241:THR:OG1	2.19	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:190:GLU:HB2	2:F:837:ALA:HB3	1.87	0.57
1:A:215:LEU:HD11	1:A:233:ARG:HD3	1.86	0.56
1:A:222:THR:HG22	1:A:223:SER:HB3	1.87	0.55
1:B:219:HIS:HD2	1:B:225:MET:H	1.55	0.55
2:E:848:SER:HB2	2:F:834:ARG:HB3	1.90	0.54
1:C:212:ILE:HG13	1:C:237:ILE:HG21	1.90	0.54
1:D:178:GLN:O	1:D:181:ILE:HG13	2.07	0.54
1:C:219:HIS:CD2	1:C:225:MET:H	2.27	0.52
1:B:219:HIS:CD2	1:B:225:MET:H	2.27	0.52
1:C:180:GLN:HA	1:C:183:SER:HB3	1.91	0.52
1:D:234:ILE:O	1:D:238:LEU:HG	2.10	0.52
1:A:212:ILE:CG1	1:A:237:ILE:HD11	2.36	0.52
1:B:234:ILE:O	1:B:238:LEU:HG	2.10	0.52
1:C:187:GLN:HA	1:C:190:GLU:OE1	2.09	0.52
1:C:231:LEU:O	1:C:235:GLN:HG3	2.10	0.51
1:D:182:THR:O	1:D:186:THR:HG23	2.11	0.51
1:A:228:GLU:O	1:A:228:GLU:OE1	2.28	0.51
1:A:179:GLN:HA	1:A:182:THR:HG22	1.92	0.51
1:A:234:ILE:O	1:A:238:LEU:HD12	2.10	0.51
1:B:194:THR:OG1	2:F:837:ALA:HB2	2.11	0.50
1:C:181:ILE:O	1:C:185:GLU:HG3	2.12	0.50
1:A:188:LEU:HA	1:A:191:VAL:HG22	1.95	0.48
1:B:203:ASP:O	1:B:207:ASN:ND2	2.45	0.48
1:D:240:SER:O	1:D:241:THR:HB	2.13	0.48
1:A:187:GLN:O	1:A:191:VAL:HG13	2.14	0.48
1:D:241:THR:O	1:D:241:THR:HG22	2.14	0.47
1:B:210:ARG:NH2	2:H:839:SER:HB2	2.27	0.47
1:A:188:LEU:HD11	1:B:187:GLN:HG2	1.96	0.47
1:B:216:VAL:O	1:B:220:LEU:HB2	2.14	0.47
1:A:241:THR:O	1:A:241:THR:HG23	2.14	0.47
1:D:219:HIS:HD2	1:D:220:LEU:HD23	1.80	0.46
2:G:843:LYS:HD2	2:G:843:LYS:N	2.31	0.45
1:C:185:GLU:HG2	1:D:184:LEU:HD11	1.98	0.45
1:D:180:GLN:O	1:D:184:LEU:HD23	2.16	0.45
1:D:188:LEU:HD23	1:D:188:LEU:HA	1.73	0.45
1:A:234:ILE:O	1:A:237:ILE:HG12	2.17	0.45
1:D:228:GLU:O	1:D:232:GLU:HG3	2.16	0.45
1:C:210:ARG:HH21	2:F:836:LEU:HA	1.81	0.45
1:D:207:ASN:HB3	2:G:834:ARG:NH1	2.33	0.44
1:A:212:ILE:HG13	1:A:237:ILE:CD1	2.40	0.44
1:B:190:GLU:HB2	2:F:837:ALA:CB	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:843:LYS:HD2	2:G:843:LYS:H	1.83	0.43
1:D:194:THR:HG23	2:F:847:PHE:HB3	2.00	0.43
2:E:849:ARG:HG3	2:F:836:LEU:HD21	2.00	0.43
1:B:221:THR:OG1	1:B:222:THR:N	2.52	0.43
1:C:206:PHE:CE1	2:F:844:PRO:HD3	2.53	0.42
1:D:231:LEU:O	1:D:235:GLN:HG3	2.19	0.42
2:H:845:THR:HG22	2:H:846:GLN:H	1.84	0.42
1:C:177:ALA:HB1	1:D:177:ALA:HB1	2.01	0.42
1:A:185:GLU:HG3	1:B:184:LEU:HD11	2.02	0.41
2:H:848:SER:O	2:H:849:ARG:HG3	2.21	0.41
1:B:227:MET:HG2	1:B:227:MET:O	2.18	0.41
1:C:210:ARG:O	1:C:214:ILE:HG22	2.21	0.40
1:D:219:HIS:CD2	1:D:220:LEU:HD23	2.55	0.40
1:C:210:ARG:HE	2:F:836:LEU:HD23	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	67/77 (87%)	65 (97%)	2 (3%)	0	100	100
1	B	69/77 (90%)	66 (96%)	3 (4%)	0	100	100
1	C	66/77 (86%)	62 (94%)	4 (6%)	0	100	100
1	D	68/77 (88%)	64 (94%)	4 (6%)	0	100	100
2	E	17/20 (85%)	17 (100%)	0	0	100	100
2	F	18/20 (90%)	18 (100%)	0	0	100	100
2	G	11/20 (55%)	8 (73%)	2 (18%)	1 (9%)	1	1
2	H	10/20 (50%)	7 (70%)	2 (20%)	1 (10%)	1	1
All	All	326/388 (84%)	307 (94%)	17 (5%)	2 (1%)	30	63

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	845	THR
2	G	837	ALA

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	65/71 (92%)	65 (100%)	0	100	100
1	B	66/71 (93%)	63 (96%)	3 (4%)	34	67
1	C	64/71 (90%)	63 (98%)	1 (2%)	70	91
1	D	66/71 (93%)	65 (98%)	1 (2%)	72	92
2	E	17/18 (94%)	17 (100%)	0	100	100
2	F	18/18 (100%)	18 (100%)	0	100	100
2	G	11/18 (61%)	9 (82%)	2 (18%)	2	5
2	H	11/18 (61%)	8 (73%)	3 (27%)	0	1
All	All	318/356 (89%)	308 (97%)	10 (3%)	47	79

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	175	LYS
1	B	192	ASN
1	B	210	ARG
1	C	210	ARG
1	D	210	ARG
2	G	834	ARG
2	G	836	LEU
2	H	843	LYS
2	H	846	GLN
2	H	849	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	229	ASN
1	B	219	HIS
1	C	219	HIS
2	E	846	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 ⓘ

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	69/77 (89%)	0.34	2 (2%) 55 45	51, 78, 121, 130	0
1	B	71/77 (92%)	0.45	3 (4%) 40 29	57, 90, 145, 174	0
1	C	68/77 (88%)	0.48	4 (5%) 26 17	51, 103, 152, 166	0
1	D	70/77 (90%)	0.35	1 (1%) 78 71	54, 80, 141, 147	0
2	E	19/20 (95%)	0.05	0 100 100	53, 65, 102, 105	0
2	F	20/20 (100%)	-0.06	0 100 100	58, 75, 115, 121	0
2	G	13/20 (65%)	0.39	2 (15%) 3 2	90, 108, 143, 143	0
2	H	12/20 (60%)	0.73	1 (8%) 14 7	105, 131, 177, 188	0
All	All	342/388 (88%)	0.37	13 (3%) 44 33	51, 89, 145, 188	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	192	ASN	4.0
2	H	847	PHE	3.4
2	G	835	SER	2.7
1	B	222	THR	2.7
1	B	223	SER	2.6
1	C	222	THR	2.3
1	C	174	ALA	2.3
2	G	834	ARG	2.2
1	D	229	ASN	2.2
1	A	235	GLN	2.2
1	C	193	GLU	2.1
1	A	179	GLN	2.1
1	C	189	TYR	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 [i](#)

There are no such residues in this entry.