



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 06:06 PM EDT

PDB ID : 4C0H / pdb_00004c0h
Title : Extended interface between Pcf11p and Clp1p and structural basis for ATP loss in Gly135Arg point mutant
Authors : Dupin, A.F.; Fribourg, S.
Deposited on : 2013-08-02
Resolution : 2.70 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

<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

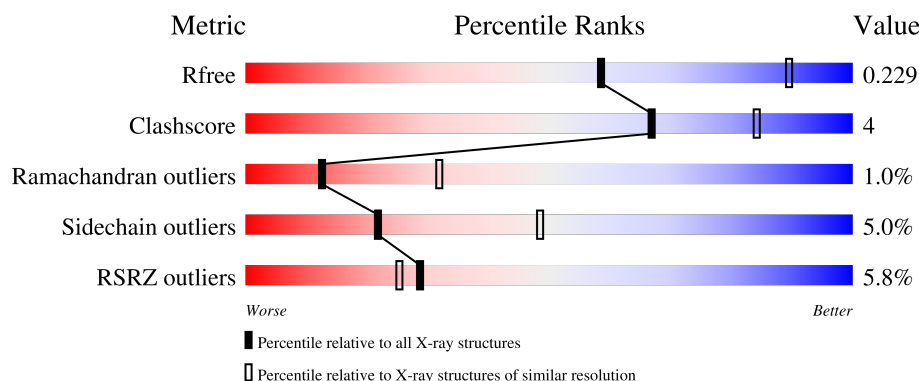
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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 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	445	5% 82% 11% • 5%
1	B	445	3% 82% 12% • • •
2	C	110	5% 20% • • 75%
2	D	110	7% 23% 6% • 70%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7336 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 MRNA CLEAVAGE AND POLYADENYLATION FACTOR CLP1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	422	Total	C	N	O	S	0	1	0
			3391	2180	569	630	12			
1	B	427	Total	C	N	O	S	0	1	0
			3421	2198	574	637	12			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	135	ARG	GLY	engineered mutation	UNP Q08685
B	135	ARG	GLY	engineered mutation	UNP Q08685

- Molecule 2 is a protein called PCF11P.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	28	Total	C	N	O	0	0	0
			231	141	40	50			
2	D	33	Total	C	N	O	0	0	0
			268	165	47	56			

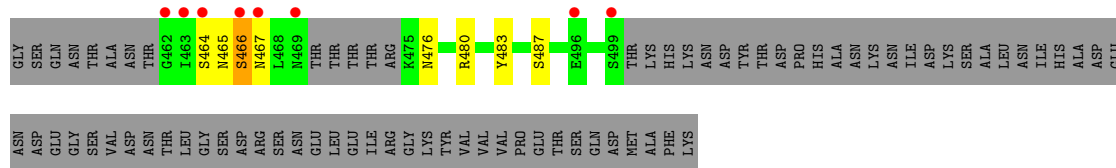
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	8	Total	O	0	0
			8	8		
3	B	14	Total	O	0	0
			14	14		
3	C	1	Total	O	0	0
			1	1		
3	D	2	Total	O	0	0
			2	2		

- Molecule 1: MRNA CLEAVAGE AND POLYADENYLATION FACTOR CLP1



- Molecule 2: PCF11P



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	89.39Å 95.61Å 182.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.80 – 2.70 47.80 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.7 (47.80-2.70) 99.6 (47.80-2.70)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.191 , 0.223 0.201 , 0.229	Depositor DCC
R_{free} test set	2188 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	55.4	Xtriage
Anisotropy	0.048	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 59.5	EDS
L-test for twinning ¹	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.37$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7336	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.41% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Theoretical 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

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	0.83	0/3467	1.30	15/4713 (0.3%)
1	B	0.86	0/3498	1.37	25/4758 (0.5%)
2	C	0.79	0/235	1.25	0/317
2	D	0.98	0/272	1.35	0/366
All	All	0.85	0/7472	1.34	40/10154 (0.4%)

There are no bond length outliers.

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	152	ALA	N-CA-C	8.30	120.62	110.91
1	B	135	ARG	N-CA-C	-7.08	103.62	112.90
1	B	411	ILE	CA-C-N	6.79	129.93	120.29
1	B	411	ILE	C-N-CA	6.79	129.93	120.29
1	B	137	THR	CB-CA-C	6.70	123.76	110.42
1	B	133	GLN	CA-C-N	6.40	133.12	121.41
1	B	133	GLN	C-N-CA	6.40	133.12	121.41
1	B	136	LYS	N-CA-C	-6.22	102.16	110.55
1	B	259	ASP	CA-CB-CG	6.22	118.82	112.60
1	A	350	TYR	CA-C-N	6.12	129.09	120.28
1	A	350	TYR	C-N-CA	6.12	129.09	120.28
1	B	350	TYR	CA-C-N	6.04	128.98	120.28
1	B	350	TYR	C-N-CA	6.04	128.98	120.28
1	B	134	THR	N-CA-C	-5.99	105.53	114.64
1	B	149	LYS	N-CA-C	5.98	117.80	111.28
1	A	259	ASP	CA-CB-CG	5.96	118.56	112.60
1	A	186	LEU	N-CA-C	5.93	118.89	109.64
1	A	216	ASN	CA-CB-CG	5.83	118.43	112.60
1	A	310	LEU	N-CA-CB	5.83	120.41	110.50
1	B	338	ASP	CA-CB-CG	5.77	118.37	112.60
1	B	186	LEU	N-CA-C	5.74	118.60	109.64
1	B	240	ASP	CA-CB-CG	5.74	118.34	112.60
1	B	216	ASN	CA-CB-CG	5.69	118.29	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	338	ASP	CA-CB-CG	5.59	118.19	112.60
1	A	240	ASP	CA-CB-CG	5.56	118.16	112.60
1	A	381	LEU	N-CA-C	5.52	121.03	113.97
1	B	444	LEU	CA-C-N	5.49	131.58	121.70
1	B	444	LEU	C-N-CA	5.49	131.58	121.70
1	B	381	LEU	N-CA-C	5.47	120.97	113.97
1	A	309	LYS	N-CA-C	5.45	122.41	110.80
1	B	173	ILE	N-CA-C	-5.36	100.75	108.53
1	B	246	SER	N-CA-C	-5.25	101.98	110.32
1	B	121	PHE	CA-CB-CG	5.20	119.00	113.80
1	A	121	PHE	CA-CB-CG	5.20	119.00	113.80
1	A	173	ILE	N-CA-C	-5.17	101.03	108.53
1	B	210	PHE	N-CA-C	-5.13	104.65	112.04
1	A	127	VAL	N-CA-CB	5.10	120.65	111.21
1	B	140	SER	CA-C-N	5.07	127.07	120.28
1	B	140	SER	C-N-CA	5.07	127.07	120.28
1	A	196	GLY	N-CA-C	5.05	118.22	111.20

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	3391	0	3430	21	0
1	B	3421	0	3459	25	0
2	C	231	0	200	10	0
2	D	268	0	244	4	0
3	A	8	0	0	0	0
3	B	14	0	0	0	0
3	C	1	0	0	0	0
3	D	2	0	0	0	0
All	All	7336	0	7333	54	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 4.

All (54) 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:343:PRO:O	2:C:467:ASN:HA	1.70	0.91
1:B:168:THR:HG23	2:D:483:TYR:OH	1.75	0.85
1:A:345:ALA:HB3	2:C:466:SER:HA	1.62	0.80
1:A:127:VAL:HG22	1:A:274:VAL:HG11	1.66	0.78
2:C:467:ASN:ND2	2:C:467:ASN:H	1.87	0.72
1:B:348:VAL:HG11	1:B:431:LEU:HD22	1.70	0.72
2:D:466:SER:OG	2:D:467:ASN:N	2.22	0.71
1:B:412:THR:HG21	1:B:422:ARG:HE	1.56	0.70
1:B:135:ARG:HH22	1:B:253:PRO:C	1.99	0.69
1:A:53:VAL:HG13	1:A:75:ILE:HG23	1.82	0.62
2:C:467:ASN:H	2:C:467:ASN:HD22	1.47	0.62
1:B:124:PRO:O	1:B:247:GLY:HA3	2.00	0.60
1:A:348:VAL:HG11	1:A:431:LEU:HD22	1.84	0.59
1:B:137:THR:HG23	1:B:138:SER:H	1.70	0.57
2:C:465:ASN:ND2	2:C:466:SER:OG	2.37	0.56
1:B:137:THR:O	1:B:138:SER:C	2.50	0.54
1:B:148:LEU:HD21	1:B:180:ASP:C	2.33	0.53
1:A:371:LEU:HG	1:A:401:ILE:HD12	1.91	0.53
1:B:412:THR:HG21	1:B:422:ARG:NE	2.22	0.53
1:B:134:THR:O	1:B:138:SER:HB3	2.09	0.53
1:B:243:VAL:O	1:B:246:SER:O	2.27	0.52
1:A:357:LYS:HB2	1:A:374:VAL:HG22	1.92	0.52
1:A:55:ILE:HD12	1:A:60:LEU:HD21	1.92	0.51
1:B:55:ILE:HD12	1:B:60:LEU:HD21	1.91	0.51
1:B:128:ILE:CG2	1:B:135:ARG:HB2	2.40	0.51
1:B:371:LEU:HG	1:B:401:ILE:HD12	1.92	0.50
1:A:135:ARG:HB3	1:A:280:LEU:HD22	1.94	0.50
1:B:109:LEU:HD21	1:B:278:LEU:HD21	1.95	0.49
1:A:53:VAL:CG1	1:A:75:ILE:HG23	2.42	0.49
1:B:168:THR:HG22	1:B:169:VAL:H	1.78	0.48
2:D:465:ASN:O	2:D:466:SER:HB3	2.12	0.48
1:B:357:LYS:HB2	1:B:374:VAL:HG22	1.95	0.48
2:C:467:ASN:ND2	2:C:467:ASN:N	2.60	0.48
1:A:426:PRO:HB2	2:C:480:ARG:HB3	1.96	0.47
1:B:253:PRO:HG2	1:B:258:LEU:HD21	1.95	0.47
1:B:139:LEU:HD22	1:B:280:LEU:HD11	1.98	0.45
1:A:418:ARG:O	1:A:420:LYS:N	2.50	0.45
1:B:137:THR:CG2	1:B:138:SER:H	2.29	0.45
2:C:467:ASN:HD22	2:C:467:ASN:N	2.15	0.45
1:B:40:ALA:HB3	1:B:41:GLU:OE1	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:465:ASN:HA	2:C:466:SER:HA	1.73	0.43
1:B:418:ARG:O	1:B:420:LYS:N	2.50	0.43
1:A:135:ARG:HH21	1:A:254:SER:HA	1.83	0.43
1:B:136:LYS:HD3	1:B:164:GLN:HG2	2.00	0.43
1:A:377:THR:HG22	1:A:379:SER:H	1.83	0.42
1:A:135:ARG:HG3	1:A:136:LYS:N	2.35	0.41
1:B:427:VAL:HG22	2:D:480:ARG:O	2.20	0.41
1:A:102:THR:OG1	1:A:310:LEU:HB3	2.20	0.41
1:B:377:THR:HG22	1:B:379:SER:H	1.83	0.41
1:A:107:TYR:N	1:A:107:TYR:CD1	2.88	0.41
1:A:102:THR:HG21	1:A:310:LEU:HA	2.03	0.41
1:A:215:ILE:HG22	1:A:219:LYS:HD3	2.03	0.41
1:A:278:LEU:HB3	1:A:307:ILE:CD1	2.51	0.41
1:A:345:ALA:H	2:C:466:SER:HB3	1.86	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	419/445 (94%)	395 (94%)	21 (5%)	3 (1%)	18	41
1	B	426/445 (96%)	408 (96%)	15 (4%)	3 (1%)	18	41
2	C	24/110 (22%)	20 (83%)	3 (12%)	1 (4%)	2	4
2	D	29/110 (26%)	25 (86%)	2 (7%)	2 (7%)	1	1
All	All	898/1110 (81%)	848 (94%)	41 (5%)	9 (1%)	12	32

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	309	LYS

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Mol	Chain	Res	Type
1	A	419	ARG
1	B	138	SER
1	B	419	ARG
2	D	464	SER
2	C	465	ASN
2	D	466	SER
1	B	40	ALA
1	A	138	SER

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	383/401 (96%)	365 (95%)	18 (5%)	23	51
1	B	386/401 (96%)	369 (96%)	17 (4%)	25	53
2	C	26/98 (26%)	22 (85%)	4 (15%)	2	7
2	D	30/98 (31%)	28 (93%)	2 (7%)	15	36
All	All	825/998 (83%)	784 (95%)	41 (5%)	22	48

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	LYS
1	A	53	VAL
1	A	95	ILE
1	A	107	TYR
1	A	109	LEU
1	A	112	MET
1	A	118	MET
1	A	127	VAL
1	A	214	ARG
1	A	224	GLU
1	A	260	GLU
1	A	283	GLU
1	A	310	LEU

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Mol	Chain	Res	Type
1	A	323	SER
1	A	380	ASN
1	A	394	ARG
1	A	418	ARG
1	A	422	ARG
1	B	41	GLU
1	B	53	VAL
1	B	95	ILE
1	B	109	LEU
1	B	118	MET
1	B	136	LYS
1	B	137	THR
1	B	168	THR
1	B	219	LYS
1	B	224	GLU
1	B	232	VAL
1	B	245	ARG
1	B	246	SER
1	B	323	SER
1	B	364	ASN
1	B	380	ASN
1	B	418	ARG
2	C	464	SER
2	C	465	ASN
2	C	467	ASN
2	C	487	SER
2	D	476	ASN
2	D	487	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	101	HIS
1	A	209	ASN
1	A	238	HIS
1	A	301	ASN
1	B	101	HIS
1	B	151	ASN
1	B	209	ASN
2	C	465	ASN
2	C	467	ASN
2	D	465	ASN

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Mol	Chain	Res	Type
2	D	481	ASN
2	D	488	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 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 [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	422/445 (94%)	0.28	24 (5%)	29 26	32, 62, 102, 122	1 (0%)
1	B	427/445 (95%)	0.03	15 (3%)	47 43	19, 49, 90, 113	1 (0%)
2	C	28/110 (25%)	0.84	6 (21%)	2 2	32, 49, 102, 111	0
2	D	33/110 (30%)	0.63	8 (24%)	2 1	27, 40, 99, 105	0
All	All	910/1110 (81%)	0.19	53 (5%)	29 25	19, 55, 98, 122	2 (0%)

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	466	SER	7.0
1	B	137	THR	6.3
2	C	467	ASN	5.1
2	C	499	SER	4.8
2	D	463	ILE	4.8
1	B	136	LYS	4.7
1	A	136	LYS	4.5
1	A	137	THR	4.3
1	B	135	ARG	3.7
2	D	469	ASN	3.7
1	B	19	GLY	3.6
2	C	465	ASN	3.4
1	B	134	THR	3.3
1	A	134	THR	3.3
1	A	39	LYS	3.3
1	A	316	VAL	3.3
2	C	464	SER	3.2
2	D	462	GLY	3.2
1	A	133	GLN	3.2
2	C	477	ILE	3.2
1	B	257	GLN	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	257	GLN	3.1
1	A	19	GLY	3.0
1	B	418	ARG	3.0
1	A	366	VAL	2.9
2	D	467	ASN	2.9
1	B	39	LYS	2.9
1	A	310	LEU	2.9
1	B	42	GLY	2.8
2	D	466	SER	2.8
1	B	445	GLU	2.8
1	B	133	GLN	2.7
1	A	21	ASN	2.6
1	B	41	GLU	2.5
1	A	43	LYS	2.5
2	D	499	SER	2.5
1	A	130	GLY	2.5
1	B	284	THR	2.3
2	D	464	SER	2.3
1	A	417	LYS	2.3
1	B	313	VAL	2.3
2	D	496	GLU	2.2
1	A	72	LYS	2.2
1	A	118	MET	2.2
1	A	79	GLU	2.2
1	A	394	ARG	2.2
1	A	107	TYR	2.2
1	A	131	GLY	2.2
1	A	309	LYS	2.1
1	A	41	GLU	2.1
1	B	315	ALA	2.1
1	A	63[A]	ASP	2.0
1	A	445	GLU	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.