



wwPDB NMR Structure Validation Summary Report ⓘ

Nov 23, 2019 – 03:55 PM EST

PDB ID : 6CLZ
Title : MT1-MMP HPX domain with Blade 4 Loop Bound to Nanodiscs
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Deposited on : 2018-03-02

This is a wwPDB NMR Structure Validation Summary 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/NMRValidationReportHelp>

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:

Cyrange	:	FAILED
NmrClust	:	FAILED
MolProbity	:	FAILED
Percentile statistics	:	20171227.v01 (using entries in the PDB archive December 27th 2017)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.4
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.4

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 3%.

There are no overall percentile quality scores available for this entry.

The sequence quality summary graphics cannot be shown.

2 Ensemble composition and analysis ⓘ

This entry contains 15 models. The atoms present in the NMR models are not consistent. Some calculations may have failed as a result. All residues are included in the validation scores.

Cyrange was unable to find well-defined residues.

Error message: Cyrange did not run

NmrClust was unable to cluster the ensemble.

Error message: NmrClust did not run

3 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 35924 atoms, of which 20751 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Matrix metalloproteinase-14.

Mol	Chain	Residues	Atoms						Trace
1	A	196	Total	C	H	N	O	S	0
			3202	1067	1565	277	284	9	

- Molecule 2 is a protein called Apolipoprotein A-I.

Mol	Chain	Residues	Atoms						Trace
2	B	211	Total	C	H	N	O	S	0
			3498	1101	1745	308	340	4	
2	C	211	Total	C	H	N	O	S	0
			3498	1101	1745	308	340	4	

There are 44 discrepancies between the modelled and reference sequences:

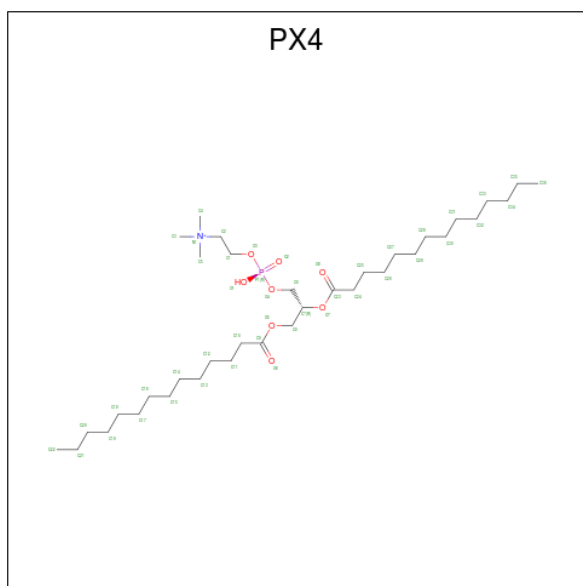
Chain	Residue	Modelled	Actual	Comment	Reference
B	99	PRO	-	insertion	UNP P02647
B	100	TYR	-	insertion	UNP P02647
B	101	LEU	-	insertion	UNP P02647
B	102	ASP	-	insertion	UNP P02647
B	103	ASP	-	insertion	UNP P02647
B	104	PHE	-	insertion	UNP P02647
B	105	GLN	-	insertion	UNP P02647
B	106	LYS	-	insertion	UNP P02647
B	107	LYS	-	insertion	UNP P02647
B	108	TRP	-	insertion	UNP P02647
B	109	GLN	-	insertion	UNP P02647
B	110	GLU	-	insertion	UNP P02647
B	111	GLU	-	insertion	UNP P02647
B	112	MET	-	insertion	UNP P02647
B	113	GLU	-	insertion	UNP P02647
B	114	LEU	-	insertion	UNP P02647
B	115	TYR	-	insertion	UNP P02647
B	116	ARG	-	insertion	UNP P02647
B	117	GLN	-	insertion	UNP P02647
B	118	LYS	-	insertion	UNP P02647
B	119	VAL	-	insertion	UNP P02647
B	120	GLU	-	insertion	UNP P02647
C	99	PRO	-	insertion	UNP P02647

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Chain	Residue	Modelled	Actual	Comment	Reference
C	100	TYR	-	insertion	UNP P02647
C	101	LEU	-	insertion	UNP P02647
C	102	ASP	-	insertion	UNP P02647
C	103	ASP	-	insertion	UNP P02647
C	104	PHE	-	insertion	UNP P02647
C	105	GLN	-	insertion	UNP P02647
C	106	LYS	-	insertion	UNP P02647
C	107	LYS	-	insertion	UNP P02647
C	108	TRP	-	insertion	UNP P02647
C	109	GLN	-	insertion	UNP P02647
C	110	GLU	-	insertion	UNP P02647
C	111	GLU	-	insertion	UNP P02647
C	112	MET	-	insertion	UNP P02647
C	113	GLU	-	insertion	UNP P02647
C	114	LEU	-	insertion	UNP P02647
C	115	TYR	-	insertion	UNP P02647
C	116	ARG	-	insertion	UNP P02647
C	117	GLN	-	insertion	UNP P02647
C	118	LYS	-	insertion	UNP P02647
C	119	VAL	-	insertion	UNP P02647
C	120	GLU	-	insertion	UNP P02647

- Molecule 3 is 1,2-DIMYRISTOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PX4) (formula: C₃₆H₇₃NO₈P).



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Mol	Chain	Residues	Atoms					
3	C	1	Total	C	H	N	O	P
			118	36	72	1	8	1
3	C	1	Total	C	H	N	O	P
			118	36	72	1	8	1
3	C	1	Total	C	H	N	O	P
			118	36	72	1	8	1
3	C	1	Total	C	H	N	O	P
			118	36	72	1	8	1
3	C	1	Total	C	H	N	O	P
			118	36	72	1	8	1
3	C	1	Total	C	H	N	O	P
			118	36	72	1	8	1

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	
4	A	1	Total	Na
			1	1

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

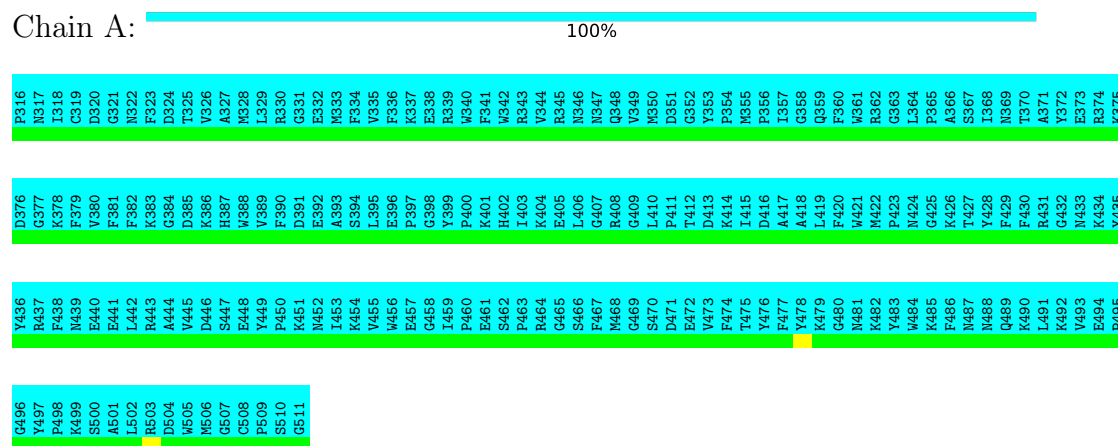
Mol	Chain	Residues	Atoms	
5	A	1	Total	Cl
			1	1

4 Residue-property plots

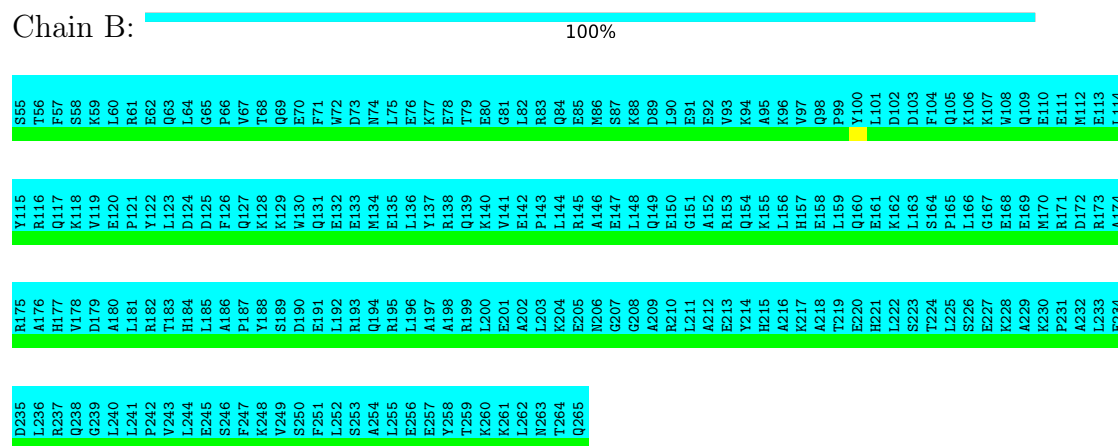
4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA and DNA chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-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. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

- Molecule 1: Matrix metalloproteinase-14



- Molecule 2: Apolipoprotein A-I



- Molecule 2: Apolipoprotein A-I



S55	Y115	R175	D235
T56	R116	A176	L236
F57	Q117	H177	R237
S58	K118	V178	Q238
K59	V119	D179	G239
L60	E120	A180	L240
R61	P121	L181	L241
S62	Y122	R182	P242
Q63	L123	T183	V243
L64	D124	H184	L244
G65	D125	L185	E245
P66	F126	A186	S246
V67	Q127	P187	F247
T68	K128	Y188	K248
Q69	K129	S189	V249
E70	W130	D190	S250
F71	Q131	E191	F251
W72	E132	L192	L252
D73	E133	R193	S253
N74	M134	Q194	A254
L75	E135	R195	L255
E76	L136	L196	E256
K77	Y137	A197	E257
T78	R138	A198	Y258
T79	Q139	R199	T259
S80	K140	L200	K260
G81	V141	E201	K261
L82	E142	A202	L262
R83	P143	L203	N263
Q84	L144	K204	T264
R85	R145	E205	Q265
H86	A146	N206	
S87	E147	G207	
K88	L148	G208	
D89	Q149	A209	
L90	E150	R210	
F91	G151	L211	
E92	A152	A212	
Y93	R153	E213	
K94	Q154	Y214	
A95	K155	H215	
K96	L156	A216	
V97	H157	K217	
Q98	E158	A218	
P99	L159	T219	
Y100	Q160	E220	
L101	E161	H221	
D102	K162	L222	
D103	L163	S223	
F104	S164	T224	
Q105	P165	L225	
K106	L166	S226	
K107	G167	E227	
W108	E168	K228	
Q109	E169	A229	
E110	M170	K230	
E111	R171	P231	
M112	D172	A232	
E113	R173	L233	
L114	A174	E234	

4.2 Residue scores for the representative (author defined) model from the NMR ensemble

The representative model is number 1. Colouring as in section 4.1 above.

- Molecule 1: Matrix metalloproteinase-14

Chain A:

100%

P316	G377	Y436	G496
N317	K378	R437	Y497
L318	F379	P438	P498
C319	V380	N439	K499
D320	F381	E440	S500
G321	F382	E441	A501
N322	K383	L442	L502
F323	D384	R443	R503
D324	D385	A444	D504
T325	D386	V445	W505
V326	V387	D446	M506
A327	H388	S447	G507
M328	V389	E448	C508
L329	F390	Y449	P509
R330	D391	P450	S510
G331	E392	K451	G511
E332	A393	N452	
M333	S394	I453	
F334	L395	K454	
V335	E396	V455	
F336	P397	W456	
K337	G398	E457	
E338	Y399	G458	
R339	P400	I459	
W340	K401	P460	
F341	H402	E461	
W342	I403	S462	
R343	K404	P463	
V344	E405	G464	
R345	L406	G465	
N346	G407	S466	
K347	R408	P467	
Q348	G409	M468	
V349	L410	G469	
M350	P411	S470	
D351	T412	D471	
G352	D413	E472	
Y353	K414	W473	
P354	I415	F474	
M355	D416	T475	
P356	A417	Y476	
I357	A418	F477	
G358	L419	Y478	
Q359	F420	K479	
F360	W421	G480	
W361	N422	N481	
R362	P423	K482	
G363	N424	Y483	
L364	G425	W484	
P365	K426	K485	
A366	T427	F486	
S367	Y428	M487	
I368	F429	N488	
N369	K490	Q489	
T370	F430	K491	
R431	A431	L491	
A371	G432	K492	
Y372	N433	V493	
E373	K434	E494	
R374	Y435	P495	
K375			

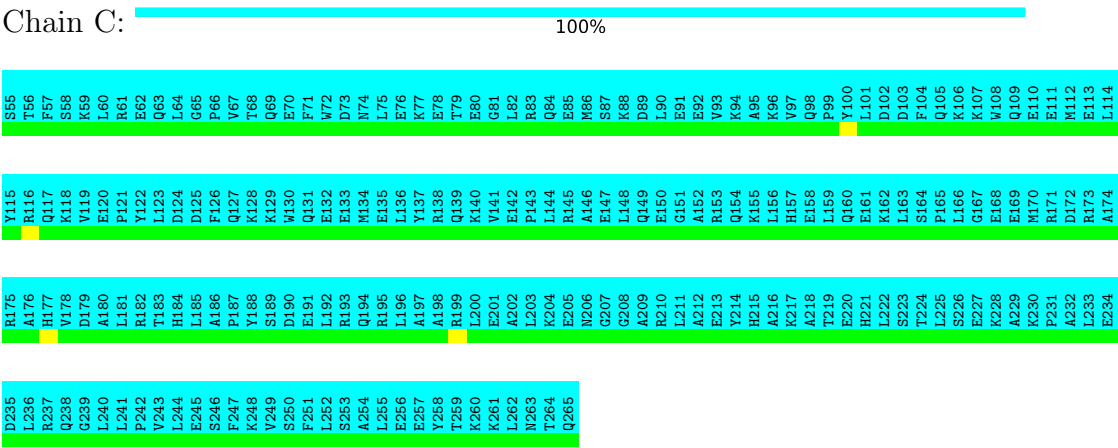
- Molecule 2: Apolipoprotein A-I

Chain B:

100%

S55	Y115	R175	D235
T56	R116	A176	L236
F57	Q117	H177	R237
S58	K118	V178	Q238
K59	V119	D179	G239
L60	E120	A180	L240
R61	P121	L181	L241
S62	Y122	R182	P242
Q63	L123	T183	V243
L64	D124	H184	L244
G65	D125	L185	E245
P66	F126	A186	S246
V67	Q127	P187	F247
T68	K128	Y188	K248
Q69	K129	S189	V249
E70	W130	D190	S250
F71	Q131	E191	F251
W72	E132	L192	L252
D73	E133	R193	S253
N74	M134	Q194	A254
L75	E135	R195	L255
E76	L136	L196	E256
K77	Y137	A197	E257
T78	R138	A198	Y258
T79	Q139	R199	T259
S80	K140	L200	K260
G81	V141	E201	K261
L82	E142	A202	L262
R83	P143	L203	N263
Q84	L144	K204	T264
R85	R145	E205	Q265
H86	A146	N206	
S87	E147	G207	
K88	L148	G208	
D89	Q149	A209	
L90	E150	R210	
F91	G151	L211	
E92	A152	A212	
Y93	R153	E213	
K94	Q154	Y214	
A95	K155	H215	
K96	L156	A216	
V97	H157	K217	
Q98	E158	A218	
P99	L159	T219	
Y100	Q160	E220	
L101	E161	H221	
D102	K162	L222	
D103	L163	S223	
F104	S164	T224	
Q105	P165	L225	
K106	L166	S226	
K107	G167	E227	
W108	E168	K228	
Q109	E169	A229	
E110	M170	K230	
E111	R171	P231	
M112	D172	A232	
E113	R173	L233	
L114	A174	E234	

- Molecule 2: Apolipoprotein A-I



5 Refinement protocol and experimental data overview

The models were refined using the following method: *molecular dynamics*.

Of the 500 calculated structures, 15 were deposited, based on the following criterion: *structures with the lowest energy*.

The following table shows the software used for structure solution, optimisation and refinement.

Software name	Classification	Version
HADDOCK	structure calculation	HADDOCK2.1
NAMD	structure calculation	NAMD2.1 with CUDA GPU processing
NAMD	refinement	NAMD2.1 with CUDA GPU processing

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	6clz_cs.cif
Number of chemical shift lists	1
Total number of shifts	324
Number of shifts mapped to atoms	324
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	3%

No validations of the models with respect to experimental NMR restraints is performed at this time.

6 Model quality [i](#)

6.1 Standard geometry [i](#)

MolProbity failed to run properly - this section will have to be empty.

6.2 Too-close contacts [i](#)

MolProbity failed to run properly - this section will have to be empty.

6.3 Torsion angles [i](#)

6.3.1 Protein backbone [i](#)

MolProbity failed to run properly - this section will have to be empty.

6.3.2 Protein sidechains [i](#)

MolProbity failed to run properly - this section will have to be empty.

6.3.3 RNA [i](#)

MolProbity failed to run properly - this section will have to be empty.

6.4 Non-standard residues in protein, DNA, RNA chains [i](#)

MolProbity failed to run properly - this section will have to be empty.

6.5 Carbohydrates [i](#)

MolProbity failed to run properly - this section will have to be empty.

6.6 Ligand geometry [i](#)

MolProbity failed to run properly - this section will have to be empty.

6.7 Other polymers [i](#)

MolProbity failed to run properly - this section will have to be empty.

6.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

7 Chemical shift validation [i](#)

The completeness of assignment taking into account all chemical shift lists is 3% for the well-defined parts and 3% for the entire structure.

7.1 Chemical shift list 1

File name: 6clz_cs.cif

Chemical shift list name: *showstar5.txt*

7.1.1 Bookkeeping [i](#)

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	324
Number of shifts mapped to atoms	324
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.1.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	0	—	None (insufficient data)
$^{13}\text{C}_\beta$	0	—	None (insufficient data)
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	92	1.11 ± 0.58	None needed (imprecise)

7.1.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 3%, i.e. 262 atoms were assigned a chemical shift out of a possible 8156. 0 out of 99 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	184/3030 (6%)	92/1206 (8%)	0/1236 (0%)	92/588 (16%)
Sidechain	78/4413 (2%)	35/2615 (1%)	43/1561 (3%)	0/237 (0%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	0/713 (0%)	0/377 (0%)	0/310 (0%)	0/26 (0%)
Overall	262/8156 (3%)	127/4198 (3%)	43/3107 (1%)	92/851 (11%)

7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

7.1.5 Random Coil Index (RCI) plots [i](#)

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition.

Random coil index (RCI) for chain A:

