wwPDB X-ray Structure Validation Summary Report (i)

Oct 23, 2021 – 09:22 AM EDT

PDB ID	:	1UEA
Title	:	MMP-3/TIMP-1 COMPLEX
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Deposited on	:	1997-06-06
Resolution	:	2.80 Å(reported)

This is a wwPDB X-ray 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/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

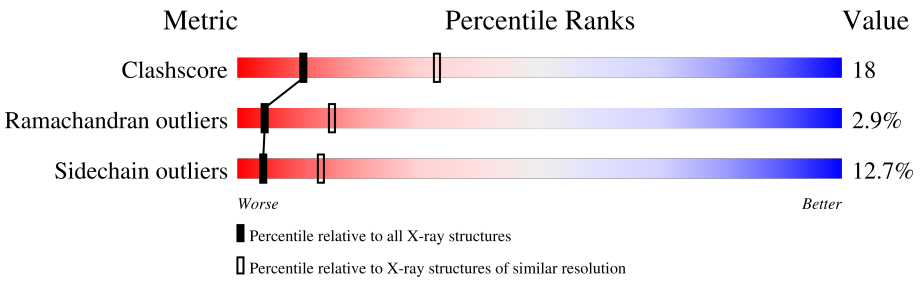
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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 2.80 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))
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)

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 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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	173	68% 28% • •
1	C	173	54% 37% 5% • •
2	B	184	52% 39% 8% •
2	D	184	54% 35% 9% •

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 6039 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 MATRIX METALLOPROTEINASE-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	Se			
1	A	168	1338	861	223	252	2	0	0	0
1	C	168	1338	861	223	252	2	43	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	143	MSE	MET	engineered mutation	UNP P08254
A	219	MSE	MET	engineered mutation	UNP P08254
C	143	MSE	MET	engineered mutation	UNP P08254
C	219	MSE	MET	engineered mutation	UNP P08254

- Molecule 2 is a protein called TISSUE INHIBITOR OF METALLOPROTEINASE-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	181	1421	902	247	257	15	33	0	0
2	D	181	1421	902	247	257	15	30	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	30	ALA	ASN	engineered mutation	UNP P01033
B	78	ALA	ASN	engineered mutation	UNP P01033
D	30	ALA	ASN	engineered mutation	UNP P01033
D	78	ALA	ASN	engineered mutation	UNP P01033

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
3	A	2	2	2	0	0
			Total	Zn		
3	C	2	2	2	0	0

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
4	A	3	3	3	0	0
			Total	Ca		
4	C	3	3	3	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	127	127	127	0	0
			Total	O		
5	B	117	117	117	0	0
			Total	O		
5	C	136	136	136	0	0
			Total	O		
5	D	131	131	131	0	0

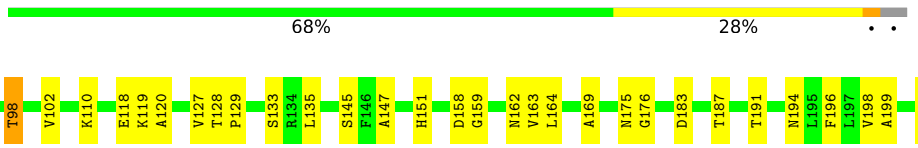
3 Residue-property plots (i)

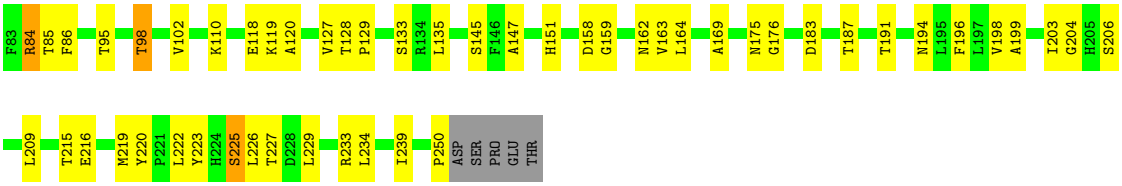
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

Note EDS was not executed.

• Molecule 1: MATRIX METALLOPROTEINASE-3

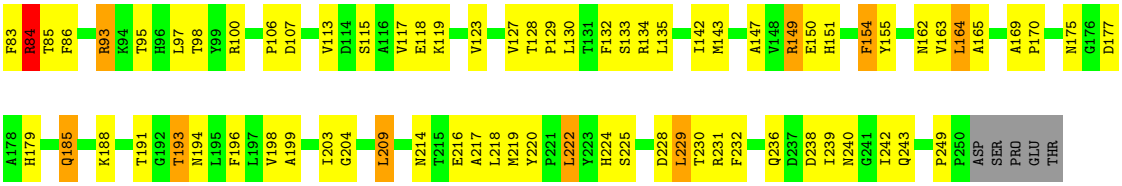
Chain A:





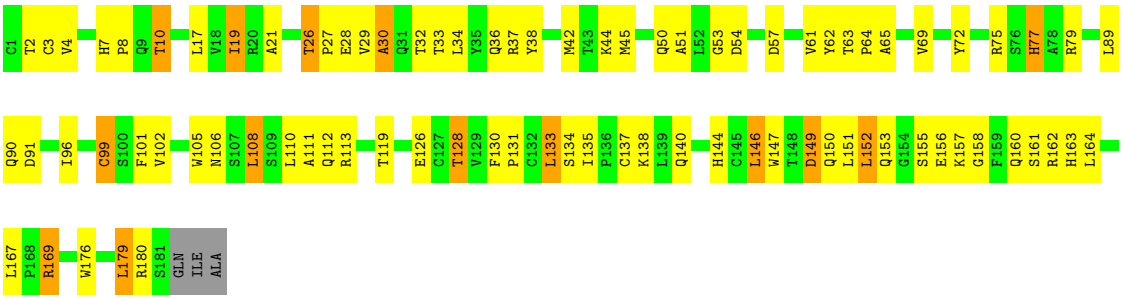
• Molecule 1: MATRIX METALLOPROTEINASE-3

Chain C:



• Molecule 2: TISSUE INHIBITOR OF METALLOPROTEINASE-1

Chain B:



• Molecule 2: TISSUE INHIBITOR OF METALLOPROTEINASE-1

Chain D:

C1
T2
C3
V4
P5
P6
H7
T10
I19
R20
V24
G25
A30
Q31
T32
T33
L34
K41
M42
T43
K44
M45
F49
L52
G53
D54
A55
A56
D57
I58
P64
A65
M66
V69
Y72
F73
H74
H77
A78
R79
L84
I85
Q90
D91
H95
I96
C99
S100
F101
V102
A103
P104
S107
L108
R114
G115
F116
T117
K118
T119
Y120
T121
C127
T128
V129
F130
P131
C132
L133
S134
C137
K138
L139
Q140
S141
C145
L146
W147
T148
L152
Q153
G154
S155
E156
K157
G158
F159
Q160
S161
R162
H163
L164
A165
C166
L167
P168
R169
E170
L173
W176
L179
R180
S181
GLN
ILE
ALA

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α, β, γ	80.62Å 80.62Å 157.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	100.00 – 2.80	Depositor
% Data completeness (in resolution range)	(Not available) (100.00-2.80)	Depositor
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.197 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6039	wwPDB-VP
Average B, all atoms (Å^2)	42.0	wwPDB-VP

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, CA

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	0.41	0/1380	0.64	0/1882
1	C	0.45	0/1380	0.73	1/1882 (0.1%)
2	B	0.46	0/1458	0.79	2/1977 (0.1%)
2	D	0.46	0/1458	0.80	1/1977 (0.1%)
All	All	0.45	0/5676	0.74	4/7718 (0.1%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	84	ARG	NE-CZ-NH2	-6.40	117.10	120.30
2	B	89	LEU	CA-CB-CG	5.42	127.76	115.30
2	B	119	THR	N-CA-C	5.38	125.53	111.00
2	D	57	ASP	N-CA-C	5.37	125.49	111.00

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	1338	0	1266	33	0
1	C	1338	0	1266	54	0
2	B	1421	0	1389	59	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	1421	0	1389	60	0
3	A	2	0	0	0	0
3	C	2	0	0	0	0
4	A	3	0	0	0	0
4	C	3	0	0	0	0
5	A	127	0	0	3	0
5	B	117	0	0	3	0
5	C	136	0	0	0	0
5	D	131	0	0	4	0
All	All	6039	0	5310	189	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 18.

The worst 5 of 189 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)
2:B:53:GLY:HA2	2:B:57:ASP:HB3	1.47	0.96
2:B:96:ILE:HD11	2:B:102:VAL:HG21	1.51	0.92
2:D:115:GLY:HA2	2:D:119:THR:HG23	1.59	0.85
2:D:10:THR:HG21	5:D:1045:HOH:O	1.79	0.83
1:C:84:ARG:HG2	1:C:85:THR:H	1.42	0.83

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	166/173 (96%)	148 (89%)	16 (10%)	2 (1%)	13 39
1	C	166/173 (96%)	142 (86%)	21 (13%)	3 (2%)	8 28

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	B	179/184 (97%)	152 (85%)	22 (12%)	5 (3%)	5 17
2	D	179/184 (97%)	150 (84%)	19 (11%)	10 (6%)	2 5
All	All	690/714 (97%)	592 (86%)	78 (11%)	20 (3%)	4 15

5 of 20 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	225	SER
1	A	227	THR
2	B	54	ASP
2	B	150	GLN
1	C	229	LEU

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	142/145 (98%)	132 (93%)	10 (7%)	15 40
1	C	142/145 (98%)	126 (89%)	16 (11%)	6 18
2	B	157/159 (99%)	131 (83%)	26 (17%)	2 7
2	D	157/159 (99%)	133 (85%)	24 (15%)	2 8
All	All	598/608 (98%)	522 (87%)	76 (13%)	4 14

5 of 76 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	54	ASP
2	D	141	SER
2	D	66	MET
2	D	119	THR
2	D	181	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	162	ASN
1	C	175	ASN
2	D	160	GLN
2	D	77	HIS
2	B	140	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 10 ligands modelled in this entry, 10 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.