Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:42 AM GMT

PDB ID	:	2E2D
Title	:	Flexibility and variability of TIMP binding: X-ray structure of the complex between collagenase-3/MMP-13 and TIMP-2
Authors	:	Maskos, K.; Lang, R.; Tschesche, H.; Bode, W.
Deposited on	:	2006-11-11
Resolution	:	2.00 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:

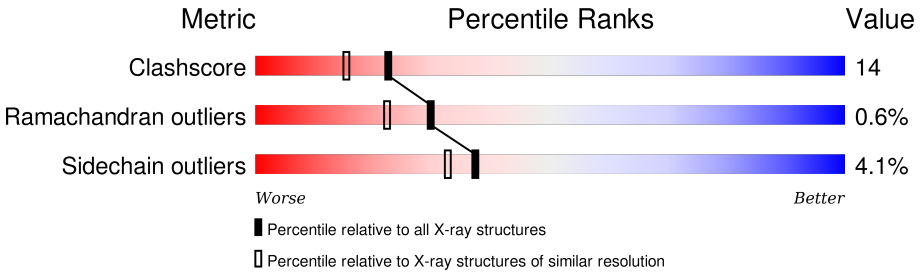
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.00 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	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)

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 <=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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	165	78% 18% .
2	C	180	71% 28% .

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 3052 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 metallopeptidase 13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	165	Total	C	N	O	S	19	0	0
			1317	855	213	244	5			

- Molecule 2 is a protein called Metalloproteinase inhibitor 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	180	Total	C	N	O	S	9	0	0
			1408	889	243	259	17			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	1001	CYS	-	CLONING ARTIFACT	UNP P16368

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

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Ca	0	0
			2	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	149	Total	O	0	0
			149	149		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	174	Total	O	0	0
			174	174		

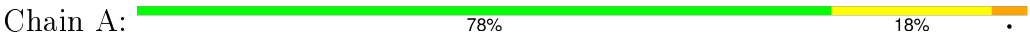
3 Residue-property plots (i)

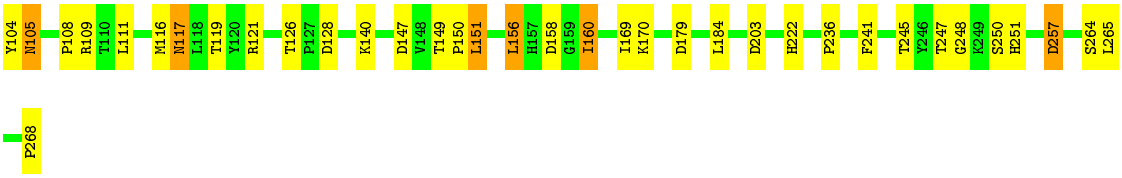
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

Note EDS was not executed.

- Molecule 1: Matrix metallopeptidase 13

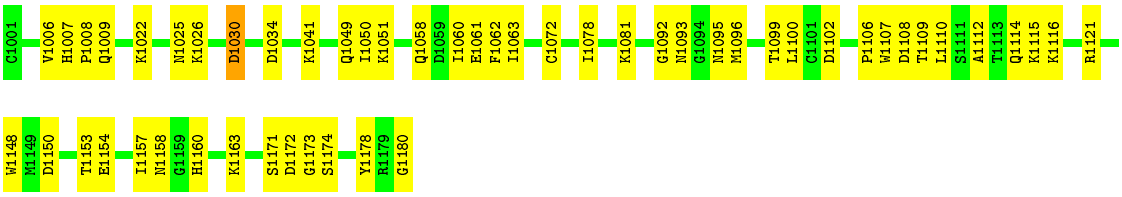
Chain A:





- Molecule 2: Metalloproteinase inhibitor 2

Chain C:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α, β, γ	72.53Å 72.53Å 181.38Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	23.77 – 2.00	Depositor
% Data completeness (in resolution range)	100.0 (23.77-2.00)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
Refinement program	REFMAC 5	Depositor
R, R_{free}	0.200 , 0.231	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3052	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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	0.80	2/1365 (0.1%)	0.92	8/1856 (0.4%)
2	C	0.56	0/1441	0.85	4/1944 (0.2%)
All	All	0.69	2/2806 (0.1%)	0.88	12/3800 (0.3%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	250	SER	C-N	-17.03	0.94	1.34
1	A	247	THR	C-N	6.75	1.45	1.33

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	250	SER	O-C-N	-12.02	103.47	122.70
1	A	250	SER	CA-C-N	8.72	136.38	117.20
2	C	1102	ASP	CB-CG-OD2	6.99	124.59	118.30
1	A	203	ASP	CB-CG-OD2	6.59	124.23	118.30
2	C	1034	ASP	CB-CG-OD2	6.36	124.02	118.30
2	C	1108	ASP	CB-CG-OD2	6.20	123.88	118.30
1	A	257	ASP	CB-CG-OD2	5.55	123.29	118.30
1	A	147	ASP	CB-CG-OD2	5.51	123.26	118.30
2	C	1030	ASP	CB-CG-OD2	5.29	123.06	118.30
1	A	128	ASP	CB-CG-OD2	5.17	122.96	118.30
1	A	121	ARG	NE-CZ-NH2	-5.11	117.74	120.30
1	A	158	ASP	CB-CG-OD2	5.07	122.86	118.30

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	1317	0	1232	22	1
2	C	1408	0	1373	50	1
3	A	2	0	0	0	0
4	A	2	0	0	0	0
5	A	149	0	0	5	0
5	C	174	0	0	14	0
All	All	3052	0	2605	72	1

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 14.

All (72) 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:C:1058:GLN:NE2	2:C:1093:ASN:HB2	1.37	1.36
1:A:117:ASN:OD1	1:A:117:ASN:O	1.64	1.15
2:C:1061:GLU:HG3	5:C:294:HOH:O	1.41	1.15
2:C:1092:GLY:HA3	5:C:153:HOH:O	1.60	1.01
2:C:1058:GLN:NE2	2:C:1093:ASN:CB	2.24	0.99
2:C:1058:GLN:HE22	2:C:1093:ASN:CB	1.77	0.98
2:C:1173:GLY:HA2	5:C:307:HOH:O	1.66	0.95
1:A:117:ASN:C	1:A:117:ASN:OD1	2.04	0.95
2:C:1072:CYS:HB3	2:C:1099:THR:CG2	2.01	0.91
1:A:245:THR:HG21	5:A:629:HOH:O	1.75	0.86
1:A:184:LEU:N	1:A:184:LEU:HD12	1.88	0.85
2:C:1058:GLN:HE22	2:C:1093:ASN:HB2	1.03	0.83
2:C:1092:GLY:CA	5:C:153:HOH:O	2.23	0.83
2:C:1007:HIS:CD2	2:C:1008:PRO:HD2	2.15	0.81
2:C:1072:CYS:CB	2:C:1099:THR:HG23	2.12	0.80
1:A:109:ARG:NH2	1:A:264:SER:OG	2.17	0.76
2:C:1093:ASN:HB3	5:C:130:HOH:O	1.86	0.74
1:A:184:LEU:CD1	1:A:184:LEU:N	2.51	0.74
2:C:1072:CYS:CB	2:C:1099:THR:CG2	2.65	0.73
2:C:1072:CYS:HB3	2:C:1099:THR:HG23	1.68	0.70
2:C:1030:ASP:OD1	2:C:1041:LYS:NZ	2.25	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:184:LEU:H	1:A:184:LEU:CD1	2.04	0.69
1:A:268:PRO:HG2	5:A:642:HOH:O	1.92	0.69
2:C:1058:GLN:CD	2:C:1093:ASN:HB2	2.12	0.69
1:A:179:ASP:OD2	1:A:184:LEU:HD13	1.91	0.69
2:C:1158:ASN:O	2:C:1163:LYS:HE3	1.94	0.67
2:C:1178:TYR:CZ	2:C:1180:GLY:HA2	2.33	0.64
2:C:1072:CYS:HB2	2:C:1099:THR:HG23	1.79	0.63
2:C:1026:LYS:NZ	5:C:248:HOH:O	2.23	0.63
2:C:1121:ARG:CZ	5:C:229:HOH:O	2.47	0.62
1:A:184:LEU:H	1:A:184:LEU:HD12	1.64	0.62
2:C:1072:CYS:HB3	2:C:1099:THR:HG22	1.79	0.61
2:C:1115:LYS:HG3	2:C:1116:LYS:N	2.15	0.59
2:C:1049:GLN:NE2	2:C:1060:ILE:H	2.03	0.55
2:C:1114:GLN:HE22	2:C:1158:ASN:HD21	1.54	0.55
2:C:1007:HIS:HD2	2:C:1009:GLN:H	1.54	0.55
2:C:1007:HIS:CD2	2:C:1008:PRO:CD	2.87	0.54
2:C:1092:GLY:N	5:C:153:HOH:O	2.36	0.54
2:C:1050:ILE:O	2:C:1051:LYS:HD3	2.06	0.54
1:A:251:HIS:CG	1:A:251:HIS:O	2.61	0.53
2:C:1112:ALA:HA	2:C:1115:LYS:HG2	1.93	0.51
2:C:1063:ILE:HA	2:C:1096:MET:O	2.11	0.51
1:A:169:ILE:HG22	1:A:170:LYS:HD2	1.94	0.50
2:C:1062:PHE:HB2	2:C:1095:ASN:HD22	1.78	0.49
2:C:1099:THR:HG22	2:C:1100:LEU:N	2.28	0.48
2:C:1180:GLY:HA3	5:C:150:HOH:O	2.13	0.48
1:A:119:THR:HB	1:A:156:LEU:HD22	1.95	0.48
2:C:1026:LYS:HB2	2:C:1078:ILE:HD13	1.94	0.48
2:C:1050:ILE:HG22	2:C:1051:LYS:HG2	1.94	0.47
1:A:105:ASN:ND2	5:A:628:HOH:O	2.47	0.47
2:C:1148:TRP:HZ2	2:C:1157:ILE:O	1.98	0.47
1:A:109:ARG:HE	1:A:265:LEU:HD23	1.81	0.45
2:C:1171:SER:OG	2:C:1172:ASP:N	2.50	0.45
2:C:1095:ASN:ND2	5:C:169:HOH:O	2.39	0.45
1:A:116:MET:SD	1:A:151:LEU:HD13	2.57	0.45
1:A:104:TYR:N	1:A:257:ASP:OD1	2.50	0.45
2:C:1121:ARG:NH2	5:C:229:HOH:O	2.51	0.44
1:A:140:LYS:NZ	5:A:543:HOH:O	2.51	0.43
1:A:236:PRO:HA	1:A:241:PHE:CG	2.54	0.43
2:C:1148:TRP:CH2	2:C:1157:ILE:HG23	2.54	0.43
2:C:1150:ASP:O	2:C:1154:GLU:O	2.37	0.43
2:C:1115:LYS:HG3	2:C:1116:LYS:H	1.81	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1178:TYR:CE2	2:C:1180:GLY:CA	3.02	0.42
2:C:1107:TRP:HA	2:C:1110:LEU:HD23	2.02	0.42
2:C:1093:ASN:CB	5:C:130:HOH:O	2.57	0.41
1:A:140:LYS:NZ	5:A:650:HOH:O	2.38	0.41
1:A:149:THR:HB	1:A:150:PRO:CD	2.51	0.41
2:C:1180:GLY:C	5:C:150:HOH:O	2.58	0.41
2:C:1007:HIS:CD2	2:C:1009:GLN:H	2.37	0.40
2:C:1106:PRO:HB2	2:C:1109:THR:HG23	2.03	0.40
1:A:222:HIS:C	1:A:222:HIS:CD2	2.95	0.40
2:C:1160:HIS:HE1	5:C:268:HOH:O	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:ILE:CD1	2:C:1153:THR:O[6_654]	2.19	0.01

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	163/165 (99%)	154 (94%)	7 (4%)	2 (1%)	16 8
2	C	178/180 (99%)	167 (94%)	11 (6%)	0	100 100
All	All	341/345 (99%)	321 (94%)	18 (5%)	2 (1%)	30 22

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	248	GLY
1	A	108	PRO

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	141/141 (100%)	134 (95%)	7 (5%)	30 24
2	C	153/153 (100%)	148 (97%)	5 (3%)	45 43
All	All	294/294 (100%)	282 (96%)	12 (4%)	37 32

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	105	ASN
1	A	111	LEU
1	A	117	ASN
1	A	126	THR
1	A	151	LEU
1	A	156	LEU
1	A	160	ILE
2	C	1006	VAL
2	C	1022	LYS
2	C	1025	ASN
2	C	1081	LYS
2	C	1174	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	117	ASN
1	A	260	GLN
2	C	1007	HIS
2	C	1025	ASN
2	C	1049	GLN
2	C	1058	GLN
2	C	1093	ASN
2	C	1095	ASN
2	C	1158	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 4 ligands modelled in this entry, 4 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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.