



Full wwPDB NMR Structure Validation Report ⓘ

Apr 27, 2016 – 04:37 AM BST

PDB ID : 2POJ
Title : NMR Solution Structure of the Inhibitor-Free State of Macrophage Metalloelastase (MMP-12)
Authors : Bhaskaran, R.; Van Doren, S.R.
Deposited on : 2007-04-26

This is a Full wwPDB NMR 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/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 : Kirchner and Güntert (2011)
NmrClust : Kelley et al. (1996)
MolProbity : 4.02b-467
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : rb-20027457
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027457

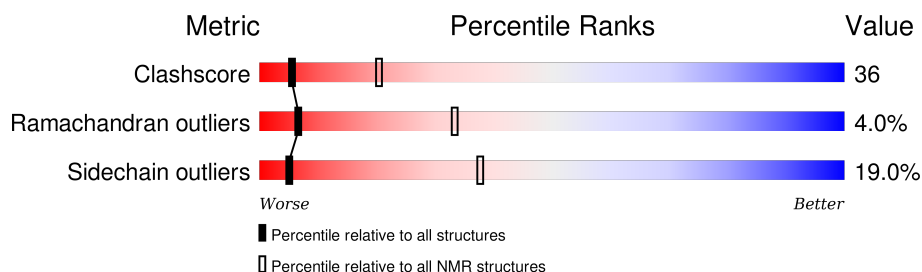
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment was not calculated.

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)	NMR archive (#Entries)
Clashscore	114402	11133
Ramachandran outliers	111179	9975
Sidechain outliers	111093	9958

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and 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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	164	

2 Ensemble composition and analysis

This entry contains 20 models. Model 5 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:112-A:153, A:157-A:263 (149)	0.15	5

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 4 clusters and 4 single-model clusters were found.

Cluster number	Models
1	3, 4, 5, 6, 9, 11, 14, 15
2	8, 10, 16
3	12, 13, 18
4	1, 2
Single-model clusters	7; 17; 19; 20

3 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2510 atoms, of which 1219 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Macrophage metalloelastase.

Mol	Chain	Residues	Atoms						Trace
1	A	164	Total	C	H	N	O	S	0
			2505	824	1219	225	233	4	

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	219	ALA	GLU	ENGINEERED	UNP P39900

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	
2	A	2	Total	Zn
			2	2

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

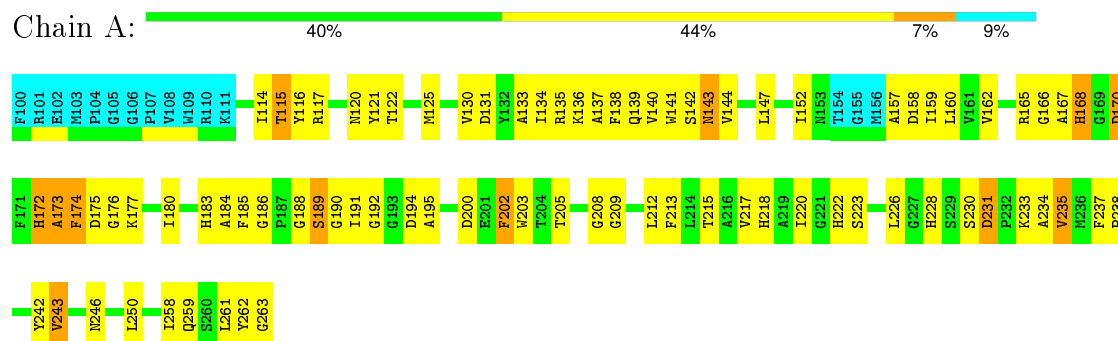
Mol	Chain	Residues	Atoms	
3	A	3	Total	Ca
			3	3

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: Macrophage metalloelastase

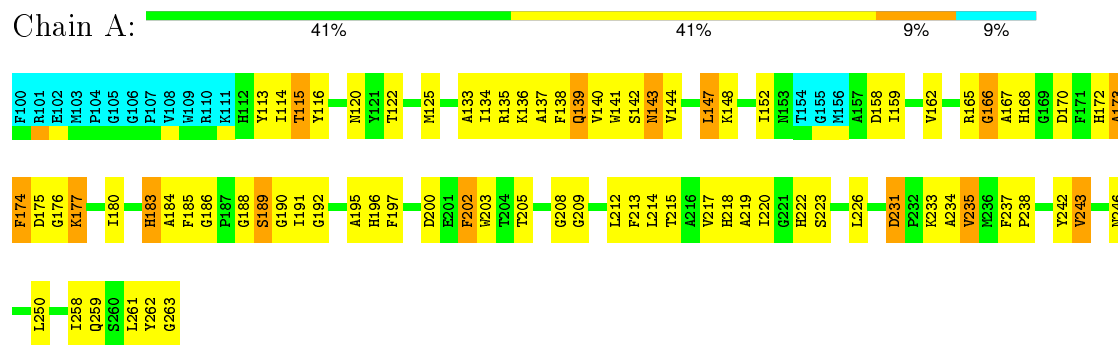


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

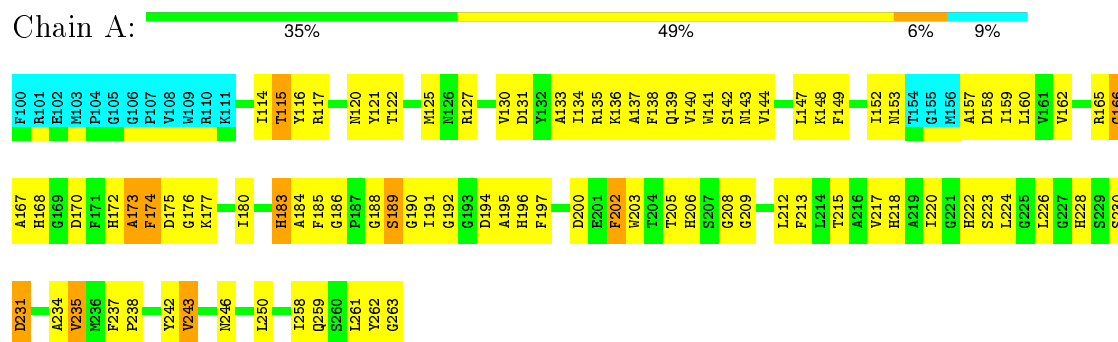
4.2.1 Score per residue for model 1

- Molecule 1: Macrophage metalloelastase



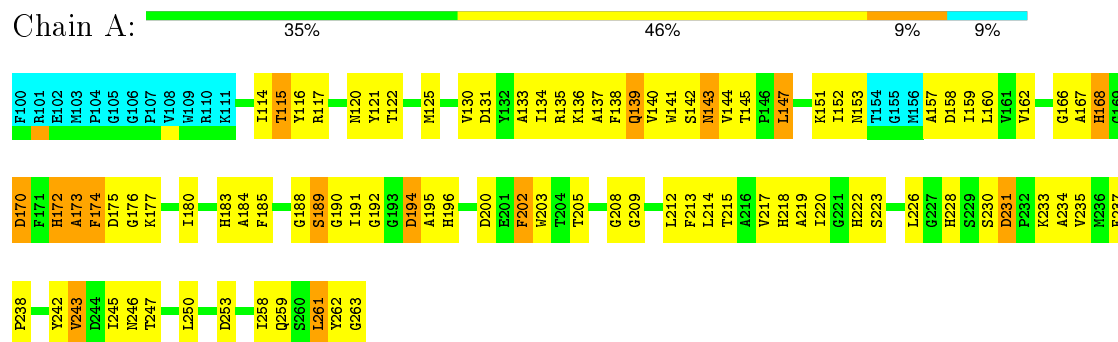
4.2.2 Score per residue for model 2

- Molecule 1: Macrophage metalloelastase



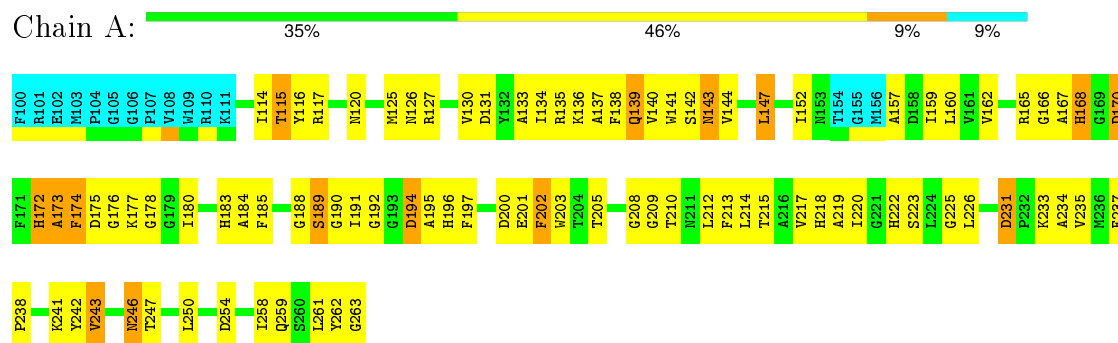
4.2.3 Score per residue for model 3

- Molecule 1: Macrophage metalloelastase



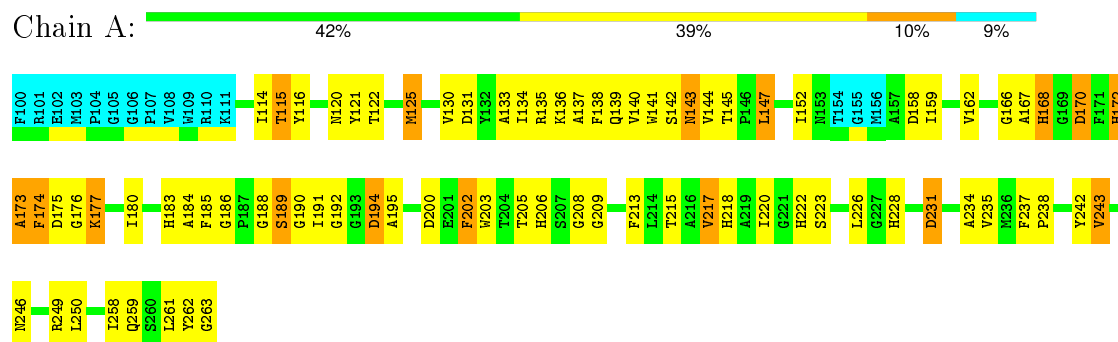
4.2.4 Score per residue for model 4

- Molecule 1: Macrophage metalloelastase



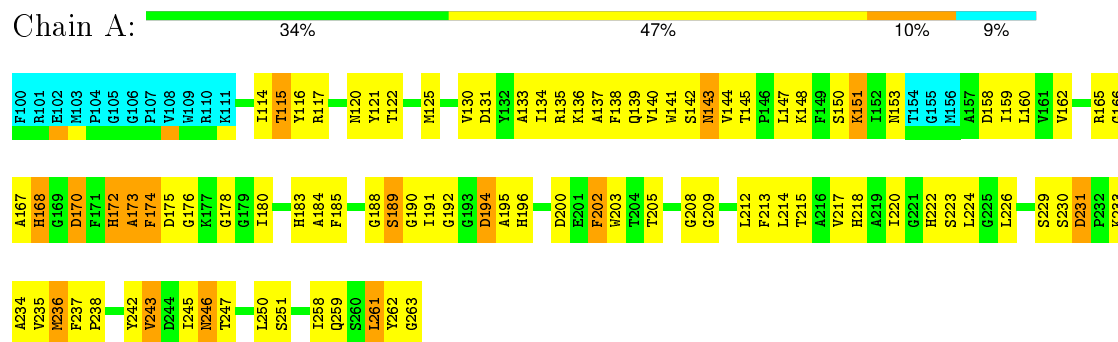
4.2.5 Score per residue for model 5 (medoid)

- Molecule 1: Macrophage metalloelastase



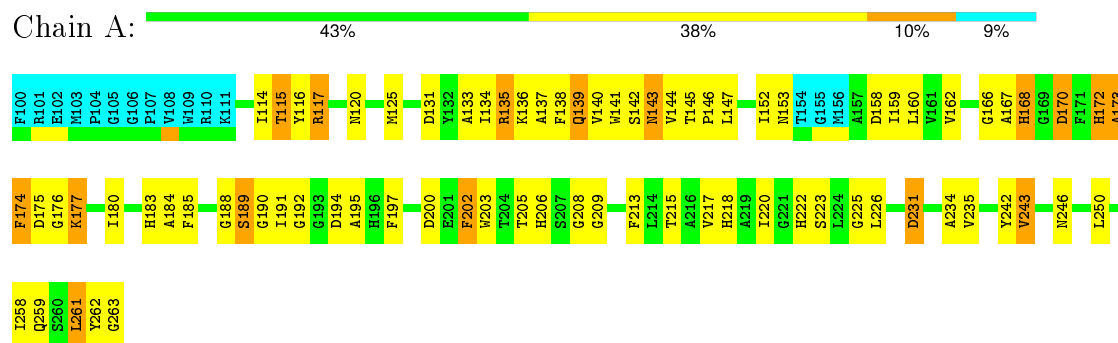
4.2.6 Score per residue for model 6

- Molecule 1: Macrophage metalloelastase



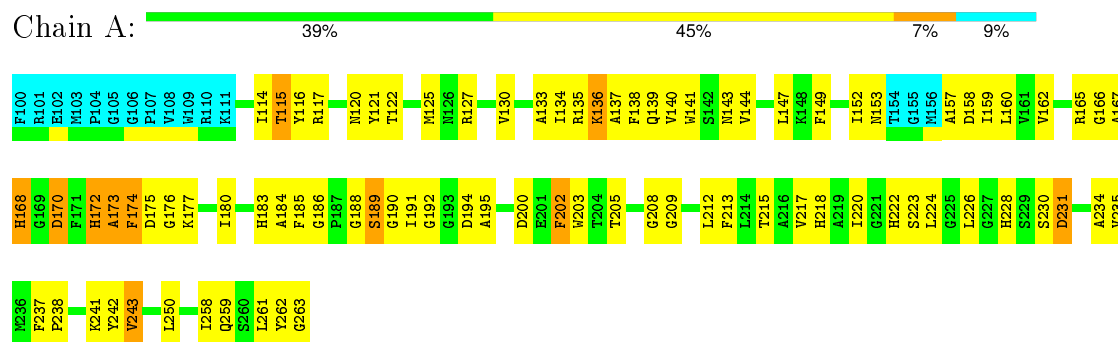
4.2.7 Score per residue for model 7

- Molecule 1: Macrophage metalloelastase



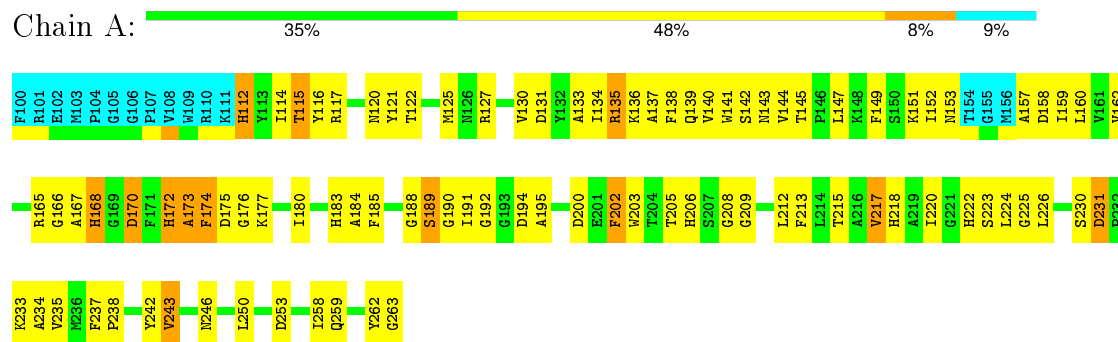
4.2.8 Score per residue for model 8

- Molecule 1: Macrophage metalloelastase



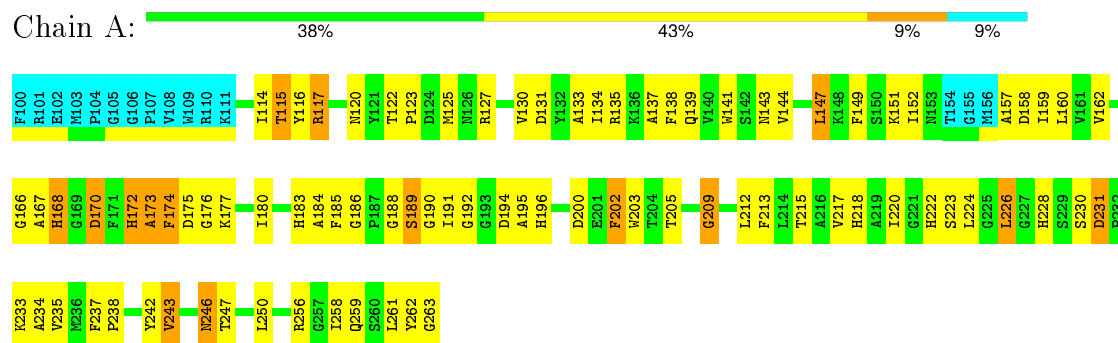
4.2.9 Score per residue for model 9

- Molecule 1: Macrophage metalloelastase



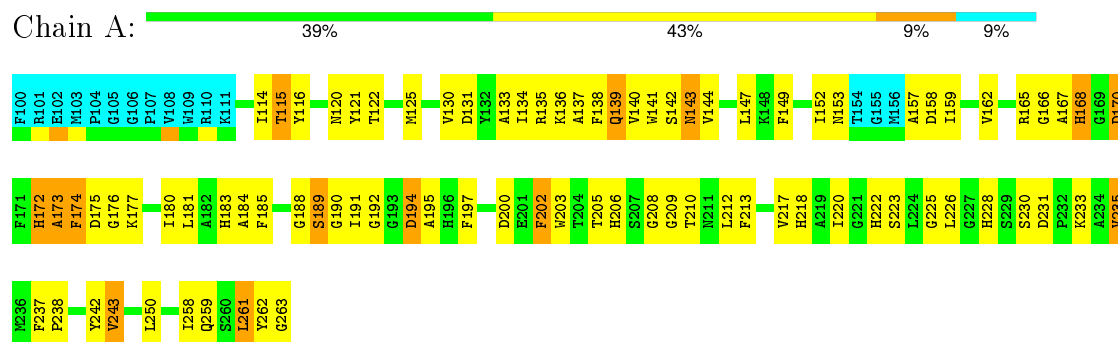
4.2.10 Score per residue for model 10

- Molecule 1: Macrophage metalloelastase



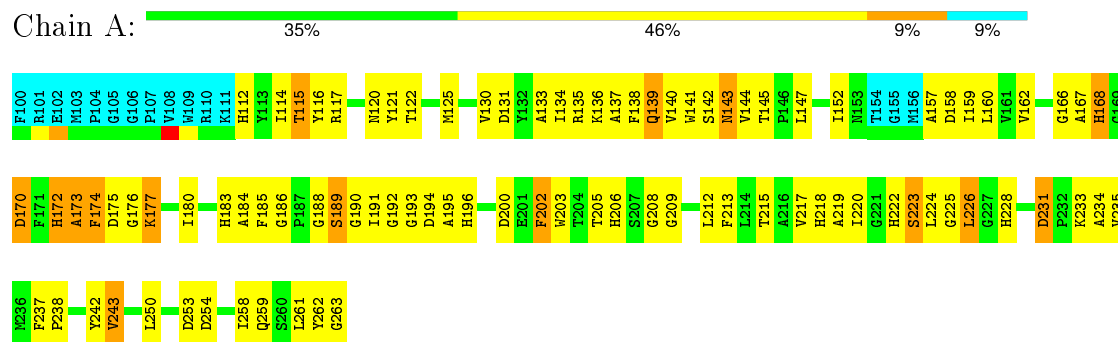
4.2.11 Score per residue for model 11

- Molecule 1: Macrophage metalloelastase



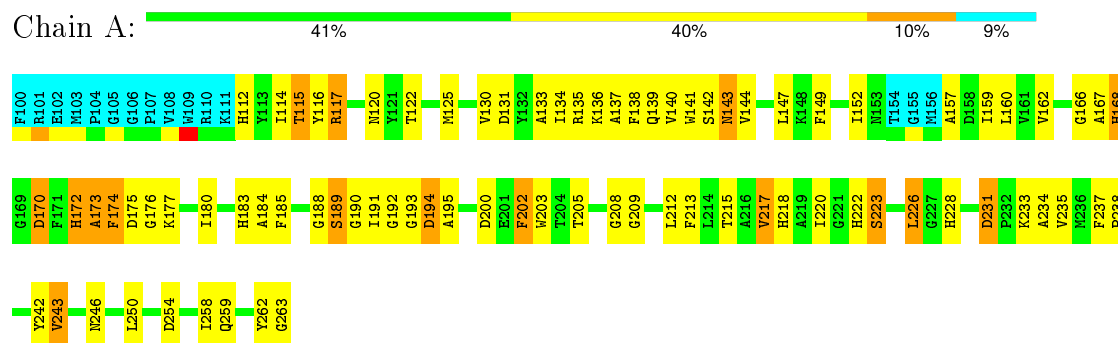
4.2.12 Score per residue for model 12

- Molecule 1: Macrophage metalloelastase



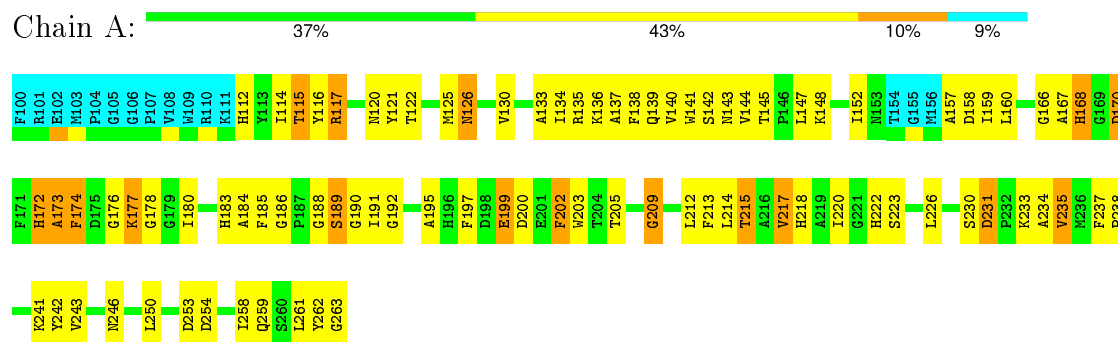
4.2.13 Score per residue for model 13

- Molecule 1: Macrophage metalloelastase



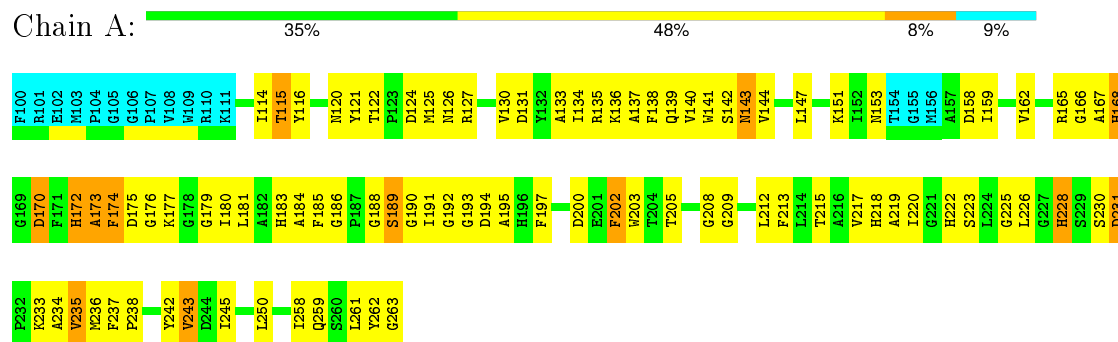
4.2.14 Score per residue for model 14

- Molecule 1: Macrophage metalloelastase



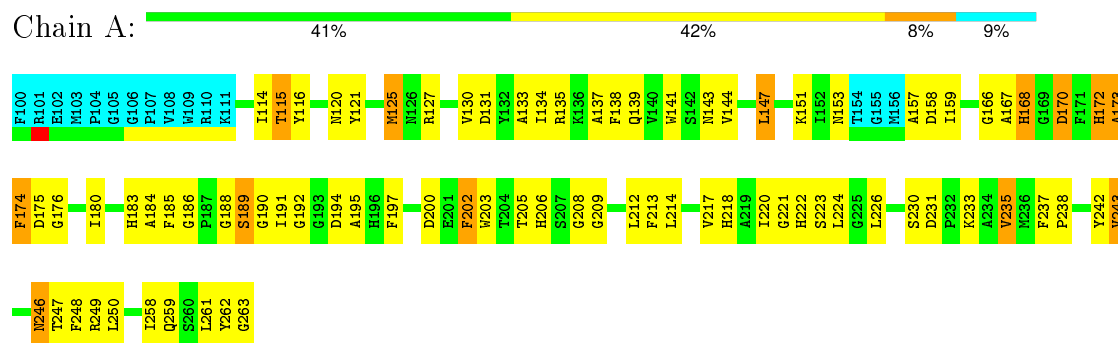
4.2.15 Score per residue for model 15

- Molecule 1: Macrophage metalloelastase



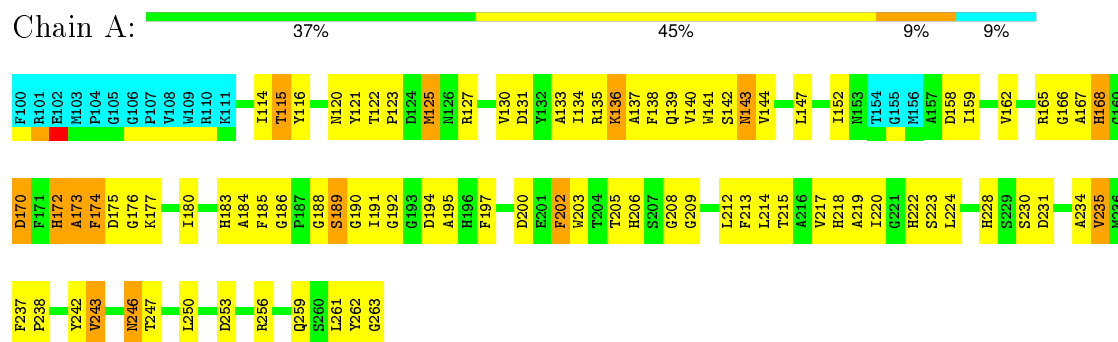
4.2.16 Score per residue for model 16

- Molecule 1: Macrophage metalloelastase



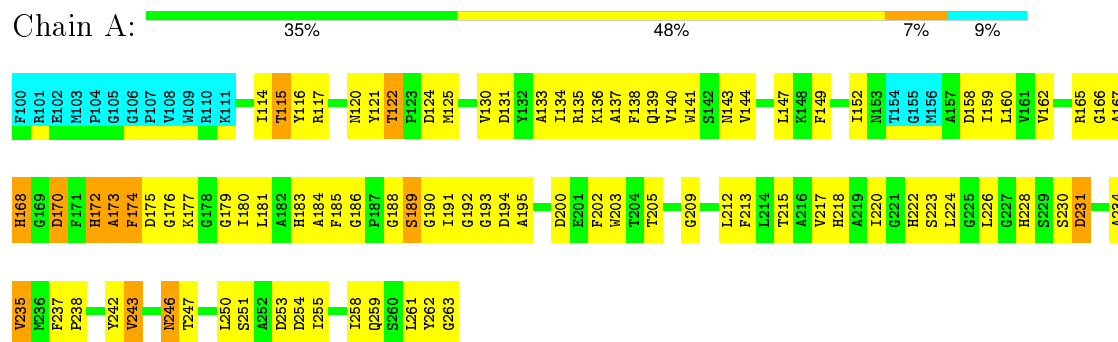
4.2.17 Score per residue for model 17

- Molecule 1: Macrophage metalloelastase



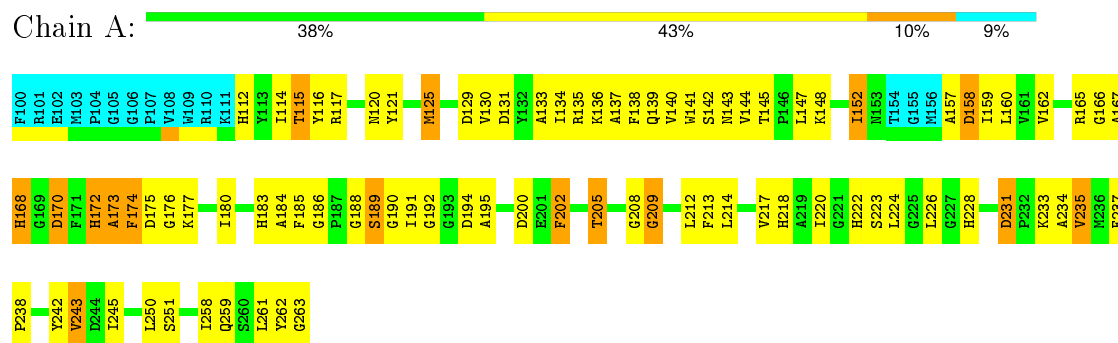
4.2.18 Score per residue for model 18

- Molecule 1: Macrophage metalloelastase



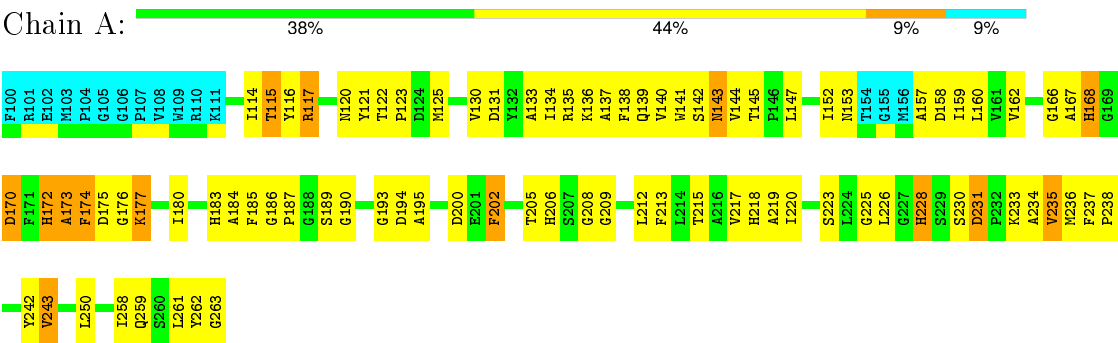
4.2.19 Score per residue for model 19

- Molecule 1: Macrophage metalloelastase



4.2.20 Score per residue for model 20

● Molecule 1: Macrophage metalloelastase



5 Refinement protocol and experimental data overview

The models were refined using the following method: *SIMULATED ANNEALING, TORSION ANGLE DYNAMICS, AUTOMATED ANALYSIS OF NOESY DATA AND 3D STRUCTURES.*

Of the 100 calculated structures, 20 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
CYANA	refinement	2.1

No chemical shift data was provided. No validations of the models with respect to experimental NMR restraints is performed at this time.

6 Model quality ⓘ

6.1 Standard geometry ⓘ

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

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 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 each 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 averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	1165	1098	1098	81±8
All	All	23400	21960	21960	1611

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 36.

All unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:152:ILE:HD11	1:A:157:ALA:HB2	1.06	1.15	19	8
1:A:133:ALA:HB3	1:A:212:LEU:HD23	0.80	1.54	4	11
1:A:226:LEU:HD11	1:A:258:ILE:HD13	0.80	1.52	7	12
1:A:137:ALA:HA	1:A:217:VAL:HG22	0.78	1.55	19	20
1:A:141:TRP:NE1	1:A:217:VAL:HG12	0.77	1.95	13	20
1:A:168:HIS:CE1	1:A:172:HIS:CE1	0.77	2.72	1	20
1:A:147:LEU:HD21	1:A:262:TYR:HB3	0.75	1.58	9	4
1:A:152:ILE:CD1	1:A:157:ALA:HB2	0.75	2.05	19	6
1:A:186:GLY:N	1:A:187:PRO:CD	0.74	2.50	20	1
1:A:147:LEU:HD21	1:A:262:TYR:CG	0.73	2.18	1	11
1:A:144:VAL:HG11	1:A:250:LEU:HD12	0.73	1.61	4	18
1:A:226:LEU:HD11	1:A:258:ILE:CD1	0.72	2.14	14	16

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:121:TYR:CE2	1:A:130:VAL:HG11	0.72	2.19	19	15
1:A:226:LEU:HD11	1:A:258:ILE:HA	0.71	1.62	13	3
1:A:213:PHE:O	1:A:217:VAL:HG23	0.71	1.86	12	20
1:A:147:LEU:HD11	1:A:262:TYR:CD2	0.69	2.22	6	7
1:A:147:LEU:HD11	1:A:262:TYR:CG	0.69	2.21	13	7
1:A:145:THR:CB	1:A:147:LEU:HD23	0.69	2.18	19	4
1:A:140:VAL:O	1:A:250:LEU:HD11	0.68	1.88	7	5
1:A:167:ALA:CA	1:A:173:ALA:HA	0.68	2.18	7	20
1:A:226:LEU:HD21	1:A:258:ILE:HA	0.68	1.65	6	12
1:A:147:LEU:HD21	1:A:262:TYR:CD1	0.68	2.24	10	16
1:A:184:ALA:HB2	1:A:195:ALA:HA	0.67	1.67	2	20
1:A:129:ASP:OD1	1:A:205:THR:HG23	0.67	1.89	19	1
1:A:167:ALA:HB2	1:A:173:ALA:CB	0.67	2.19	14	18
1:A:147:LEU:HD21	1:A:262:TYR:CE1	0.67	2.23	7	3
1:A:167:ALA:HA	1:A:173:ALA:HA	0.67	1.66	7	20
1:A:170:ASP:O	1:A:170:ASP:OD1	0.65	2.14	6	7
1:A:170:ASP:OD1	1:A:170:ASP:O	0.65	2.15	12	11
1:A:116:TYR:CG	1:A:138:PHE:CZ	0.65	2.85	4	20
1:A:112:HIS:HA	1:A:147:LEU:HD12	0.65	1.69	19	3
1:A:122:THR:HG22	1:A:125:MET:HE1	0.64	1.67	2	3
1:A:122:THR:HG22	1:A:125:MET:CE	0.64	2.22	1	9
1:A:120:ASN:OD1	1:A:162:VAL:HG23	0.64	1.93	6	18
1:A:122:THR:HG22	1:A:125:MET:HE2	0.64	1.69	1	7
1:A:126:ASN:O	1:A:130:VAL:HG23	0.64	1.92	4	3
1:A:136:LYS:O	1:A:140:VAL:HG23	0.63	1.92	3	18
1:A:145:THR:OG1	1:A:147:LEU:HD23	0.63	1.94	9	4
1:A:133:ALA:HB1	1:A:213:PHE:CA	0.62	2.24	6	20
1:A:133:ALA:HB1	1:A:213:PHE:N	0.62	2.10	4	16
1:A:117:ARG:NE	1:A:160:LEU:HD11	0.62	2.09	18	2
1:A:141:TRP:CZ3	1:A:258:ILE:HD13	0.62	2.29	10	2
1:A:168:HIS:CE1	1:A:172:HIS:HE1	0.62	2.09	1	20
1:A:159:ILE:HG12	1:A:220:ILE:HG23	0.61	1.72	12	20
1:A:166:GLY:CA	1:A:174:PHE:HB2	0.61	2.26	14	20
1:A:145:THR:HB	1:A:147:LEU:HD23	0.61	1.71	19	4
1:A:226:LEU:HD21	1:A:258:ILE:HD12	0.60	1.72	16	1
1:A:226:LEU:HD11	1:A:258:ILE:CA	0.60	2.26	13	1
1:A:189:SER:O	1:A:191:ILE:N	0.60	2.35	4	19
1:A:125:MET:CE	1:A:130:VAL:HG22	0.60	2.27	14	10
1:A:144:VAL:HG21	1:A:250:LEU:CD1	0.59	2.27	12	8
1:A:139:GLN:O	1:A:143:ASN:ND2	0.59	2.35	10	19
1:A:147:LEU:HD21	1:A:262:TYR:CB	0.59	2.28	19	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:147:LEU:HD11	1:A:262:TYR:CD1	0.59	2.33	19	4
1:A:172:HIS:ND1	1:A:173:ALA:N	0.59	2.51	14	20
1:A:134:ILE:HD13	1:A:212:LEU:HD21	0.58	1.75	13	12
1:A:226:LEU:HD11	1:A:258:ILE:HD12	0.58	1.74	15	4
1:A:234:ALA:HB1	1:A:254:ASP:OD1	0.58	1.98	13	4
1:A:141:TRP:CE3	1:A:258:ILE:HD13	0.58	2.33	16	5
1:A:167:ALA:HB2	1:A:173:ALA:HB2	0.58	1.75	9	18
1:A:218:HIS:HB2	1:A:235:VAL:HG13	0.58	1.75	19	18
1:A:218:HIS:HB2	1:A:235:VAL:HG22	0.58	1.73	12	1
1:A:137:ALA:O	1:A:217:VAL:HG13	0.57	2.00	13	20
1:A:237:PHE:CG	1:A:238:PRO:HD2	0.57	2.34	13	19
1:A:215:THR:O	1:A:219:ALA:HB2	0.56	2.00	12	7
1:A:145:THR:HG23	1:A:146:PRO:HD2	0.56	1.77	7	1
1:A:125:MET:SD	1:A:212:LEU:HD22	0.56	2.40	20	17
1:A:115:THR:OG1	1:A:152:ILE:HD12	0.56	2.00	19	1
1:A:231:ASP:CB	1:A:234:ALA:HB2	0.56	2.31	12	16
1:A:246:ASN:ND2	1:A:247:THR:HG23	0.56	2.16	10	6
1:A:159:ILE:HG23	1:A:223:SER:OG	0.55	2.02	1	13
1:A:114:ILE:HG22	1:A:115:THR:N	0.55	2.16	13	20
1:A:134:ILE:CD1	1:A:212:LEU:HD21	0.55	2.32	8	9
1:A:185:PHE:O	1:A:222:HIS:O	0.54	2.25	15	19
1:A:152:ILE:HD11	1:A:157:ALA:N	0.54	2.17	3	9
1:A:144:VAL:HG23	1:A:145:THR:HG23	0.54	1.77	14	4
1:A:145:THR:HG21	1:A:258:ILE:CG1	0.54	2.32	19	3
1:A:141:TRP:CD1	1:A:217:VAL:HG12	0.54	2.38	9	5
1:A:147:LEU:HD21	1:A:262:TYR:CD2	0.54	2.38	1	4
1:A:202:PHE:O	1:A:209:GLY:HA3	0.53	2.03	2	19
1:A:125:MET:HE2	1:A:212:LEU:HD22	0.53	1.79	19	1
1:A:117:ARG:HD2	1:A:160:LEU:HD11	0.53	1.80	13	11
1:A:185:PHE:O	1:A:223:SER:HA	0.53	2.03	20	13
1:A:125:MET:HE3	1:A:130:VAL:HG22	0.53	1.80	15	6
1:A:138:PHE:CZ	1:A:220:ILE:HG12	0.53	2.39	18	20
1:A:130:VAL:O	1:A:134:ILE:HD13	0.53	2.04	8	5
1:A:144:VAL:HG21	1:A:250:LEU:HD13	0.53	1.80	7	1
1:A:138:PHE:CE2	1:A:220:ILE:HG21	0.53	2.39	12	10
1:A:184:ALA:HB1	1:A:223:SER:HB2	0.53	1.81	12	1
1:A:203:TRP:CZ3	1:A:215:THR:HG21	0.52	2.39	13	12
1:A:145:THR:HB	1:A:147:LEU:CD2	0.52	2.34	19	3
1:A:141:TRP:CH2	1:A:250:LEU:HD22	0.52	2.39	9	14
1:A:145:THR:HG21	1:A:258:ILE:HG13	0.52	1.80	3	7
1:A:143:ASN:HD22	1:A:143:ASN:N	0.52	2.02	3	8

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:125:MET:CE	1:A:212:LEU:HD22	0.52	2.34	19	1
1:A:231:ASP:HB2	1:A:234:ALA:HB2	0.52	1.81	12	8
1:A:188:GLY:C	1:A:192:GLY:HA3	0.51	2.26	9	19
1:A:141:TRP:HE1	1:A:217:VAL:HG12	0.51	1.63	12	17
1:A:143:ASN:N	1:A:143:ASN:HD22	0.51	2.02	1	7
1:A:170:ASP:OD2	1:A:172:HIS:ND1	0.51	2.43	20	18
1:A:184:ALA:HB1	1:A:223:SER:CB	0.51	2.34	12	1
1:A:176:GLY:HA2	1:A:200:ASP:HB2	0.51	1.83	9	20
1:A:186:GLY:N	1:A:187:PRO:HD3	0.51	2.18	20	1
1:A:176:GLY:HA2	1:A:200:ASP:CB	0.51	2.36	4	20
1:A:137:ALA:CA	1:A:217:VAL:HG22	0.51	2.32	19	15
1:A:115:THR:HG23	1:A:157:ALA:HA	0.51	1.83	19	2
1:A:254:ASP:O	1:A:258:ILE:HG22	0.51	2.05	14	1
1:A:138:PHE:CE2	1:A:220:ILE:HG12	0.50	2.41	16	4
1:A:242:TYR:O	1:A:243:VAL:HG13	0.50	2.07	16	20
1:A:145:THR:CG2	1:A:147:LEU:HD13	0.50	2.36	7	1
1:A:166:GLY:N	1:A:174:PHE:HB2	0.50	2.21	1	20
1:A:214:LEU:HD21	1:A:243:VAL:CG2	0.50	2.36	19	5
1:A:246:ASN:HD22	1:A:247:THR:HG23	0.50	1.65	4	3
1:A:166:GLY:HA2	1:A:174:PHE:HB2	0.50	1.84	1	19
1:A:115:THR:OG1	1:A:152:ILE:CD1	0.50	2.59	19	1
1:A:246:ASN:HD21	1:A:247:THR:HG23	0.49	1.66	10	3
1:A:141:TRP:CZ2	1:A:235:VAL:HG11	0.49	2.43	12	1
1:A:184:ALA:CB	1:A:195:ALA:HA	0.49	2.37	6	18
1:A:116:TYR:O	1:A:152:ILE:HD13	0.49	2.07	19	1
1:A:134:ILE:HG22	1:A:135:ARG:N	0.49	2.23	4	20
1:A:184:ALA:HB1	1:A:223:SER:HB3	0.49	1.84	13	1
1:A:138:PHE:CE1	1:A:220:ILE:HG21	0.49	2.43	6	5
1:A:147:LEU:HD22	1:A:147:LEU:N	0.48	2.22	19	2
1:A:112:HIS:HA	1:A:147:LEU:CD1	0.48	2.37	19	4
1:A:170:ASP:OD2	1:A:196:HIS:CE1	0.48	2.67	2	2
1:A:115:THR:O	1:A:159:ILE:HD12	0.48	2.09	5	4
1:A:181:LEU:HD11	1:A:210:THR:HG21	0.47	1.85	11	1
1:A:259:GLN:O	1:A:263:GLY:N	0.47	2.48	17	20
1:A:121:TYR:CD2	1:A:130:VAL:HG11	0.47	2.45	12	3
1:A:136:LYS:HD3	1:A:245:ILE:HD11	0.47	1.86	15	3
1:A:159:ILE:CG1	1:A:220:ILE:HG23	0.47	2.38	12	11
1:A:213:PHE:CD2	1:A:214:LEU:HD23	0.47	2.44	16	3
1:A:185:PHE:O	1:A:193:GLY:HA2	0.47	2.09	20	1
1:A:197:PHE:HB3	1:A:203:TRP:CZ2	0.47	2.45	11	9
1:A:114:ILE:HD12	1:A:114:ILE:N	0.47	2.24	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:170:ASP:OD2	1:A:172:HIS:CG	0.46	2.69	14	18
1:A:158:ASP:O	1:A:192:GLY:O	0.46	2.33	19	1
1:A:116:TYR:N	1:A:116:TYR:CD1	0.46	2.84	16	8
1:A:193:GLY:O	1:A:223:SER:HB3	0.46	2.11	18	2
1:A:202:PHE:O	1:A:210:THR:N	0.46	2.49	11	2
1:A:116:TYR:CD1	1:A:138:PHE:CE1	0.46	3.04	19	3
1:A:251:SER:O	1:A:255:ILE:HD12	0.46	2.11	18	1
1:A:147:LEU:N	1:A:147:LEU:HD22	0.46	2.25	9	1
1:A:193:GLY:O	1:A:223:SER:CB	0.46	2.64	13	4
1:A:142:SER:OG	1:A:149:PHE:CD2	0.46	2.68	2	1
1:A:176:GLY:O	1:A:177:LYS:C	0.45	2.54	15	17
1:A:234:ALA:O	1:A:237:PHE:HB2	0.45	2.11	17	10
1:A:125:MET:SD	1:A:212:LEU:HD13	0.45	2.51	1	12
1:A:159:ILE:HA	1:A:193:GLY:O	0.45	2.12	20	2
1:A:215:THR:O	1:A:219:ALA:CB	0.45	2.64	12	1
1:A:116:TYR:CD1	1:A:138:PHE:CZ	0.45	3.04	19	4
1:A:186:GLY:HA2	1:A:223:SER:O	0.45	2.11	12	1
1:A:172:HIS:CD2	1:A:183:HIS:CE1	0.45	3.05	2	2
1:A:170:ASP:OD1	1:A:170:ASP:C	0.45	2.54	20	10
1:A:114:ILE:CG2	1:A:115:THR:N	0.45	2.80	6	20
1:A:226:LEU:CG	1:A:258:ILE:HD12	0.45	2.41	12	1
1:A:117:ARG:HE	1:A:160:LEU:HD11	0.45	1.72	9	1
1:A:114:ILE:HD13	1:A:149:PHE:HE1	0.45	1.72	2	7
1:A:117:ARG:CZ	1:A:160:LEU:HD11	0.45	2.41	18	1
1:A:220:ILE:HA	1:A:223:SER:OG	0.45	2.12	20	2
1:A:226:LEU:CD2	1:A:258:ILE:HD12	0.45	2.41	16	1
1:A:172:HIS:CG	1:A:183:HIS:CE1	0.45	3.05	15	20
1:A:133:ALA:HB1	1:A:213:PHE:HA	0.45	1.87	19	4
1:A:122:THR:HG22	1:A:124:ASP:H	0.45	1.71	18	1
1:A:192:GLY:O	1:A:194:ASP:N	0.45	2.50	17	15
1:A:218:HIS:HB2	1:A:235:VAL:CG1	0.45	2.43	7	1
1:A:231:ASP:HB3	1:A:234:ALA:HB2	0.44	1.89	5	3
1:A:170:ASP:C	1:A:170:ASP:OD1	0.44	2.55	12	6
1:A:183:HIS:CD2	1:A:196:HIS:HB2	0.44	2.46	3	5
1:A:145:THR:HG21	1:A:147:LEU:HD22	0.44	1.89	7	1
1:A:114:ILE:HD13	1:A:149:PHE:CE1	0.44	2.47	9	2
1:A:185:PHE:O	1:A:193:GLY:CA	0.44	2.66	20	1
1:A:172:HIS:CG	1:A:173:ALA:N	0.44	2.86	17	20
1:A:172:HIS:CD2	1:A:183:HIS:NE2	0.44	2.85	6	18
1:A:122:THR:CG2	1:A:123:PRO:HD2	0.44	2.43	20	3
1:A:116:TYR:CD1	1:A:138:PHE:CE2	0.43	3.06	4	9

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:116:TYR:CD1	1:A:116:TYR:N	0.43	2.86	10	8
1:A:246:ASN:OD1	1:A:247:THR:HG23	0.43	2.13	3	1
1:A:229:SER:N	1:A:236:MET:HB3	0.43	2.28	6	1
1:A:224:LEU:HD22	1:A:262:TYR:OH	0.43	2.13	9	1
1:A:172:HIS:NE2	1:A:174:PHE:CG	0.43	2.84	12	13
1:A:144:VAL:HG21	1:A:250:LEU:HD12	0.43	1.91	14	1
1:A:220:ILE:HG22	1:A:224:LEU:CD1	0.43	2.43	12	1
1:A:193:GLY:O	1:A:223:SER:HB2	0.43	2.13	12	1
1:A:179:GLY:O	1:A:181:LEU:HD22	0.43	2.13	15	2
1:A:226:LEU:CD1	1:A:258:ILE:HD12	0.42	2.44	12	1
1:A:153:ASN:N	1:A:153:ASN:HD22	0.42	2.12	7	1
1:A:188:GLY:CA	1:A:192:GLY:HA3	0.42	2.44	9	10
1:A:228:HIS:CD2	1:A:236:MET:O	0.42	2.72	15	2
1:A:214:LEU:HD21	1:A:243:VAL:HG23	0.42	1.89	3	2
1:A:159:ILE:HG12	1:A:223:SER:OG	0.42	2.15	15	4
1:A:221:GLY:CA	1:A:226:LEU:HD12	0.42	2.44	16	1
1:A:213:PHE:CE2	1:A:245:ILE:HD12	0.42	2.49	3	1
1:A:122:THR:HG22	1:A:124:ASP:N	0.42	2.30	18	1
1:A:152:ILE:HD11	1:A:157:ALA:CB	0.42	2.45	3	1
1:A:192:GLY:C	1:A:194:ASP:N	0.41	2.73	16	11
1:A:176:GLY:HA2	1:A:200:ASP:CG	0.41	2.36	15	1
1:A:231:ASP:O	1:A:237:PHE:CD1	0.41	2.74	13	1
1:A:199:GLU:CD	1:A:199:GLU:O	0.41	2.59	14	1
1:A:144:VAL:CG1	1:A:250:LEU:HD12	0.41	2.42	4	1
1:A:125:MET:HE1	1:A:130:VAL:HG22	0.41	1.93	13	1
1:A:134:ILE:HG23	1:A:138:PHE:CE1	0.41	2.51	18	1
1:A:214:LEU:HD22	1:A:248:PHE:CD2	0.40	2.51	16	1
1:A:116:TYR:CZ	1:A:151:LYS:HB2	0.40	2.51	6	1
1:A:138:PHE:HE2	1:A:159:ILE:HD13	0.40	1.77	12	1
1:A:149:PHE:N	1:A:149:PHE:CD1	0.40	2.89	2	1
1:A:166:GLY:HA2	1:A:174:PHE:CB	0.40	2.45	5	1
1:A:143:ASN:ND2	1:A:143:ASN:N	0.40	2.70	11	1

6.3 Torsion angles ⓘ

6.3.1 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 PDB entries followed by that with respect to all NMR entries. 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	148/164 (90%)	122±2 (83±1%)	20±2 (13±2%)	6±1 (4±0%)	6	33
All	All	2960/3280 (90%)	2449 (83%)	393 (13%)	118 (4%)	6	33

All 10 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	180	ILE	20
1	A	174	PHE	20
1	A	190	GLY	20
1	A	173	ALA	20
1	A	208	GLY	17
1	A	186	GLY	11
1	A	209	GLY	4
1	A	178	GLY	3
1	A	166	GLY	2
1	A	189	SER	1

6.3.2 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 PDB entries followed by that with respect to all NMR entries. 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	119/131 (91%)	96±2 (81±2%)	23±2 (19±2%)	5	38
All	All	2380/2620 (91%)	1927 (81%)	453 (19%)	5	38

All 55 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	202	PHE	20
1	A	115	THR	20
1	A	231	ASP	20
1	A	205	THR	20
1	A	189	SER	19
1	A	175	ASP	19
1	A	243	VAL	19
1	A	170	ASP	18

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Mol	Chain	Res	Type	Models (Total)
1	A	158	ASP	18
1	A	168	HIS	18
1	A	172	HIS	18
1	A	131	ASP	17
1	A	142	SER	15
1	A	233	LYS	14
1	A	228	HIS	13
1	A	230	SER	13
1	A	143	ASN	13
1	A	246	ASN	13
1	A	165	ARG	11
1	A	235	VAL	10
1	A	206	HIS	9
1	A	153	ASN	9
1	A	127	ARG	8
1	A	194	ASP	8
1	A	139	GLN	7
1	A	177	LYS	7
1	A	147	LEU	6
1	A	151	LYS	6
1	A	253	ASP	6
1	A	148	LYS	5
1	A	117	ARG	5
1	A	125	MET	5
1	A	217	VAL	4
1	A	261	LEU	4
1	A	226	LEU	3
1	A	122	THR	3
1	A	241	LYS	3
1	A	135	ARG	2
1	A	251	SER	2
1	A	256	ARG	2
1	A	120	ASN	2
1	A	183	HIS	2
1	A	112	HIS	2
1	A	223	SER	2
1	A	136	LYS	2
1	A	249	ARG	2
1	A	152	ILE	1
1	A	201	GLU	1
1	A	236	MET	1
1	A	124	ASP	1

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Mol	Chain	Res	Type	Models (Total)
1	A	150	SER	1
1	A	215	THR	1
1	A	126	ASN	1
1	A	113	TYR	1
1	A	199	GLU	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 5 are monoatomic - leaving 0 for Mogul analysis.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided