



Full wwPDB NMR Structure Validation Report ⓘ

Apr 26, 2016 – 11:34 PM BST

PDB ID : 2KRJ
Title : High-Resolution Solid-State NMR Structure of a 17.6 kDa Protein
Authors : Bertini, I.; Bhaumik, A.; De Pa pe, G.; Griffin, R.G.; Lelli, M.; Lewandowski, J.R.; Luchinat, C.
Deposited on : 2009-12-18

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

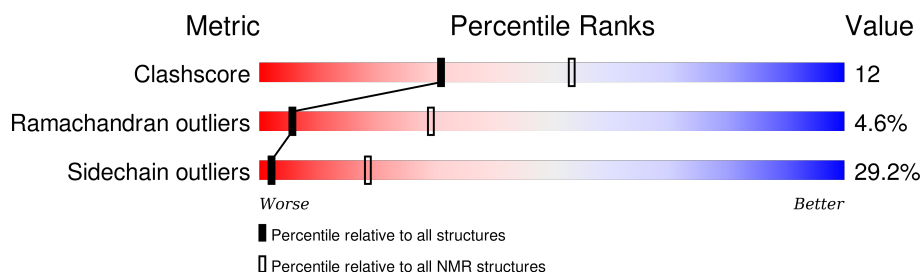
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLID-STATE 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	152	<div> <div>58%</div> <div>38%</div> <div>.</div> </div>

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:115-A:260 (146)	0.71	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 3 clusters and 1 single-model cluster was found.

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

3 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 2299 atoms, of which 1113 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Macrophage metalloelastase.

Mol	Chain	Residues	Atoms						Trace
1	A	152	Total	C	H	N	O	S	0
			2298	754	1113	205	223	3	

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	171	ASP	PHE	CONFLICT	UNP P39900

- Molecule 2 is COBALT (II) ION (three-letter code: CO) (formula: Co).

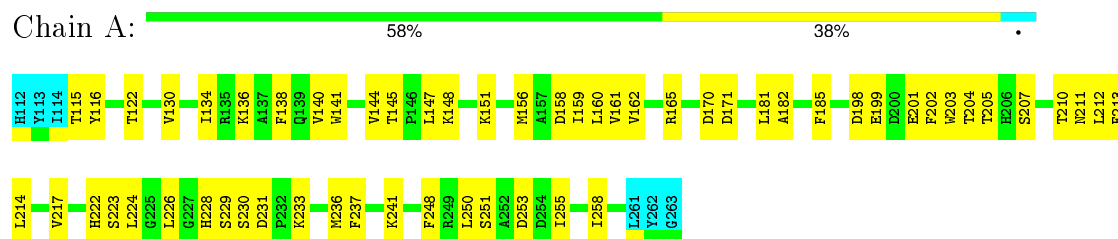
Mol	Chain	Residues	Atoms	
2	A	1	Total	Co
			1	1

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: Macrophage metalloelastase

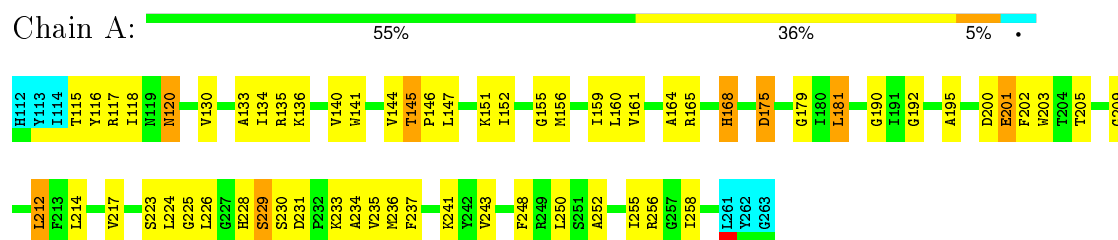


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

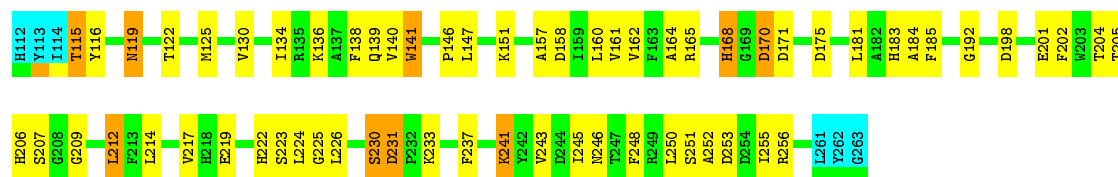
- Molecule 1: Macrophage metalloelastase



4.2.2 Score per residue for model 2

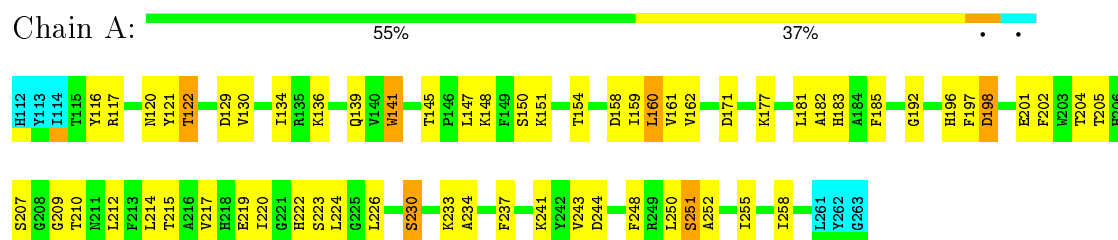
- Molecule 1: Macrophage metalloelastase





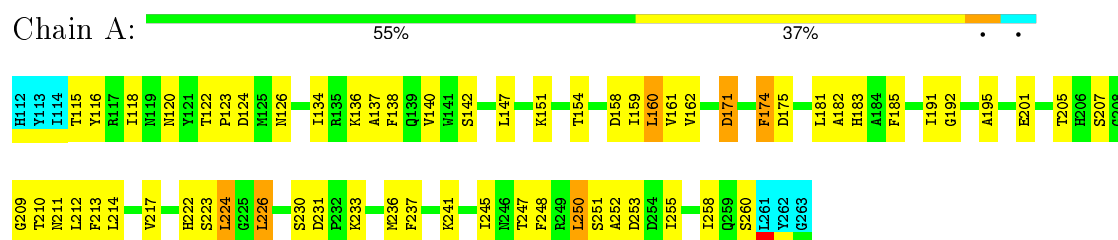
4.2.3 Score per residue for model 3

- Molecule 1: Macrophage metalloelastase



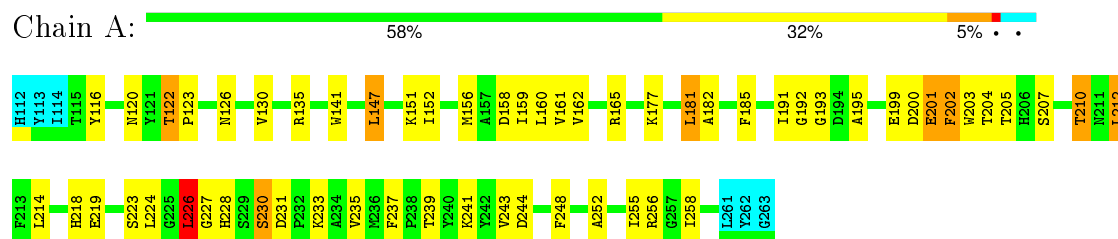
4.2.4 Score per residue for model 4

- Molecule 1: Macrophage metalloelastase



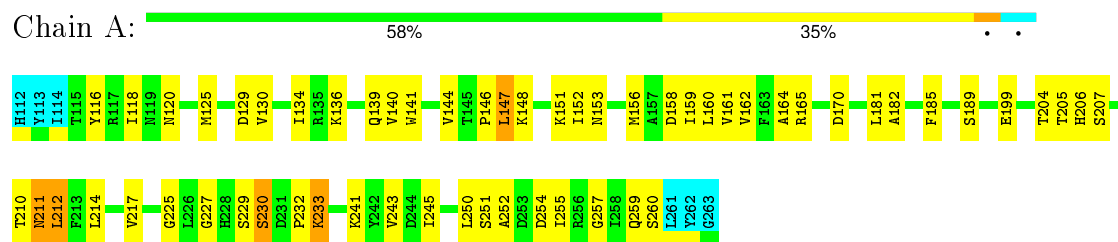
4.2.5 Score per residue for model 5 (medoid)

- Molecule 1: Macrophage metalloelastase



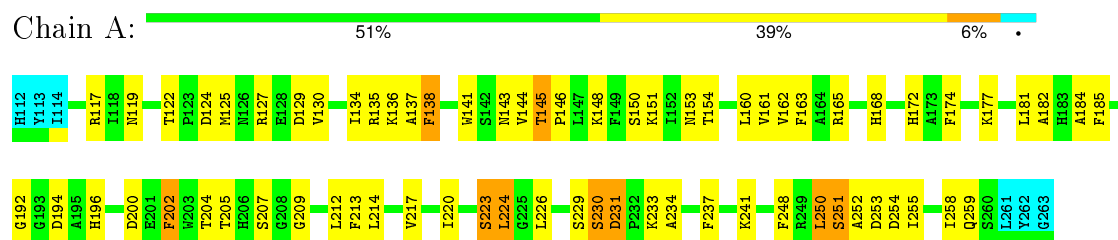
4.2.6 Score per residue for model 6

- Molecule 1: Macrophage metalloelastase



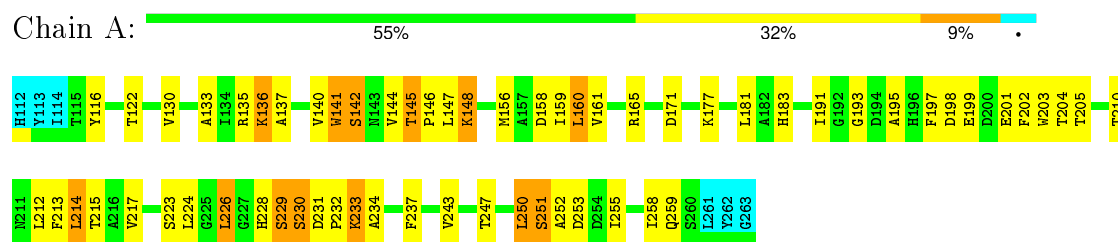
4.2.7 Score per residue for model 7

- Molecule 1: Macrophage metalloelastase



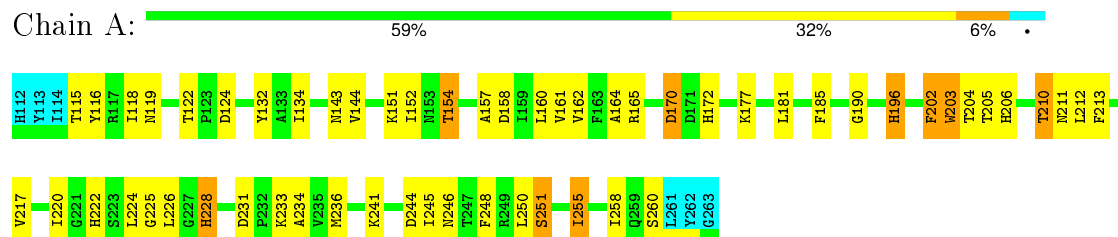
4.2.8 Score per residue for model 8

- Molecule 1: Macrophage metalloelastase



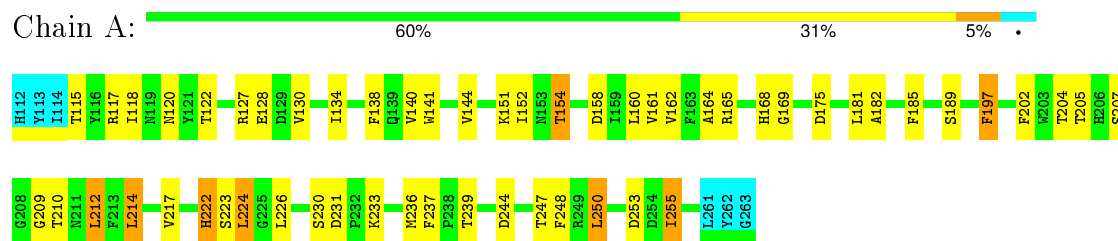
4.2.9 Score per residue for model 9

- Molecule 1: Macrophage metalloelastase



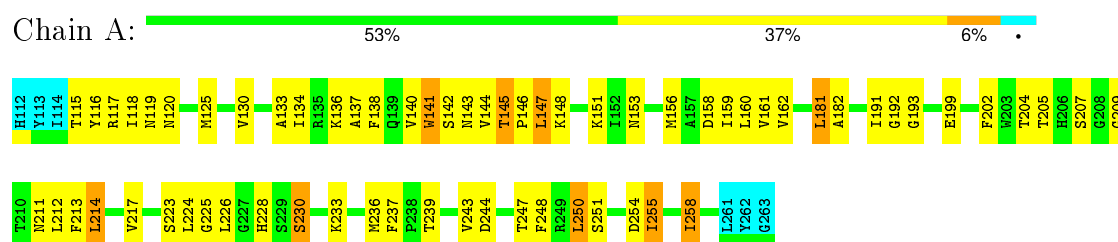
4.2.10 Score per residue for model 10

- Molecule 1: Macrophage metalloelastase



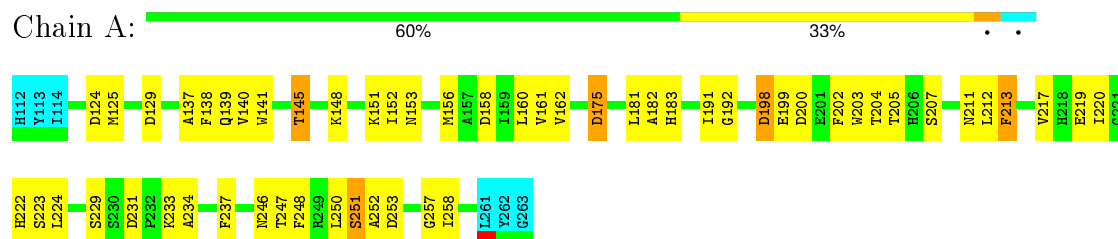
4.2.11 Score per residue for model 11

- Molecule 1: Macrophage metalloelastase



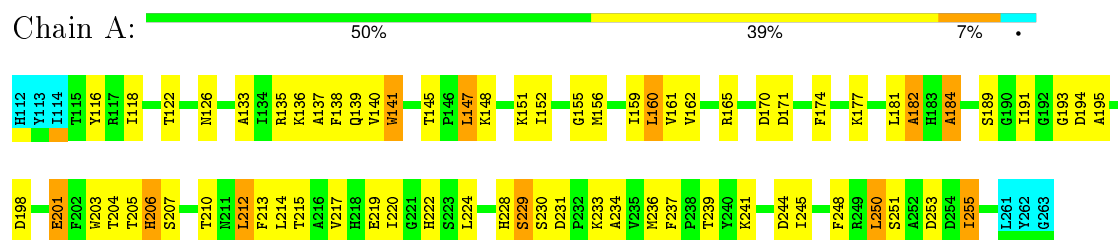
4.2.12 Score per residue for model 12

- Molecule 1: Macrophage metalloelastase



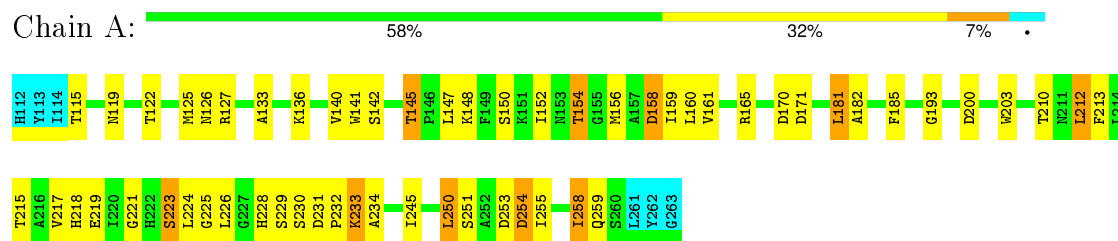
4.2.13 Score per residue for model 13

- Molecule 1: Macrophage metalloelastase



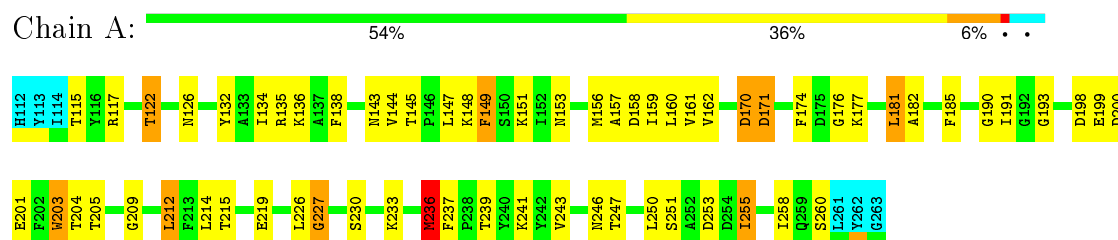
4.2.14 Score per residue for model 14

- Molecule 1: Macrophage metalloelastase



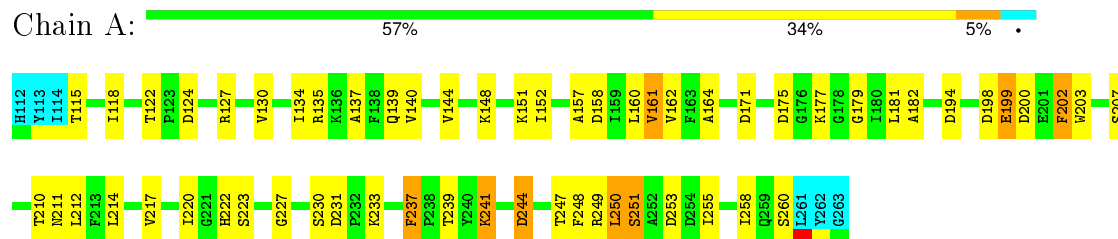
4.2.15 Score per residue for model 15

- Molecule 1: Macrophage metalloelastase



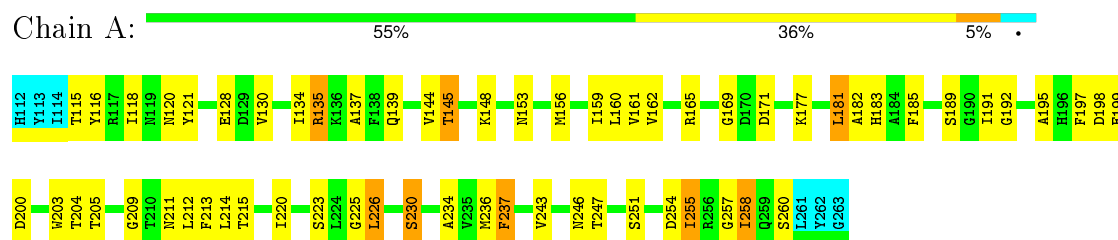
4.2.16 Score per residue for model 16

- Molecule 1: Macrophage metalloelastase



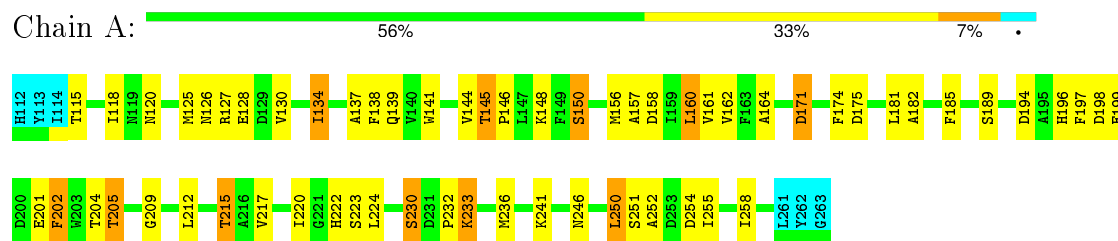
4.2.17 Score per residue for model 17

- Molecule 1: Macrophage metalloelastase



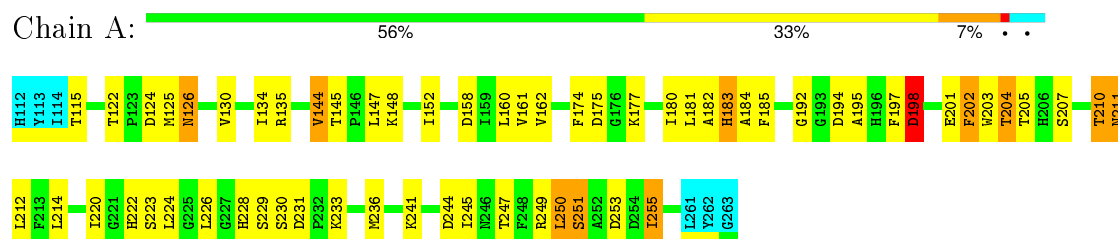
4.2.18 Score per residue for model 18

- Molecule 1: Macrophage metalloelastase



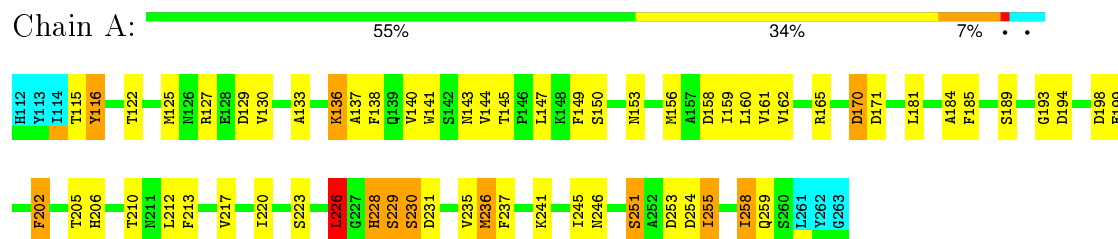
4.2.19 Score per residue for model 19

- 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*.

Of the 2000 calculated structures, 20 were deposited, based on the following criterion: *target function*.

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

Software name	Classification	Version
CYANA	refinement	

No chemical shift data was provided. Note: This is a solid-state NMR structure, where hydrogen atoms are typically not assigned a chemical shift value, which may lead to lower completeness of assignment measure.

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:
CO

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	1131	1063	1063	26±4
2	A	1	0	0	0±0
All	All	22640	21260	21260	510

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 12.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:222:HIS:CE1	2:A:264:CO:CO	0.90	1.55	10	1
1:A:222:HIS:HE1	2:A:264:CO:CO	0.88	0.74	10	1
1:A:118:ILE:HG22	1:A:161:VAL:HG21	0.88	1.46	4	2
1:A:250:LEU:HD12	1:A:255:ILE:HD12	0.76	1.55	9	2
1:A:234:ALA:HB2	1:A:252:ALA:HB2	0.74	1.60	12	3
1:A:122:THR:HG21	1:A:212:LEU:HD11	0.73	1.59	2	1
1:A:130:VAL:HG23	1:A:212:LEU:HD21	0.71	1.62	10	5
1:A:130:VAL:HG23	1:A:212:LEU:HD22	0.70	1.64	20	1
1:A:195:ALA:HB1	1:A:197:PHE:CE2	0.70	2.21	17	2
1:A:214:LEU:HD22	1:A:243:VAL:HG12	0.68	1.64	6	2
1:A:159:ILE:HG22	1:A:193:GLY:HA3	0.68	1.65	8	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:250:LEU:HD13	1:A:251:SER:N	0.68	2.03	9	2
1:A:160:LEU:HD22	1:A:160:LEU:C	0.67	2.10	8	2
1:A:147:LEU:HD13	1:A:224:LEU:HD23	0.67	1.66	13	2
1:A:144:VAL:HG11	1:A:255:ILE:HG12	0.66	1.67	16	1
1:A:140:VAL:HG11	1:A:217:VAL:HG22	0.66	1.67	2	1
1:A:181:LEU:HD12	1:A:182:ALA:N	0.66	2.06	6	12
1:A:136:LYS:O	1:A:140:VAL:HG23	0.66	1.91	20	5
1:A:116:TYR:CD2	1:A:159:ILE:HG21	0.65	2.27	1	1
1:A:159:ILE:HG22	1:A:193:GLY:CA	0.64	2.22	14	3
1:A:118:ILE:HG23	1:A:161:VAL:HG23	0.64	1.68	11	2
1:A:130:VAL:O	1:A:134:ILE:HD12	0.64	1.92	3	5
1:A:214:LEU:HD12	1:A:248:PHE:CE1	0.64	2.28	4	3
1:A:141:TRP:O	1:A:145:THR:HG22	0.64	1.91	3	2
1:A:140:VAL:HG11	1:A:217:VAL:HG11	0.64	1.67	6	5
1:A:130:VAL:HG23	1:A:212:LEU:CD2	0.64	2.22	16	3
1:A:138:PHE:CZ	1:A:224:LEU:HD11	0.64	2.27	11	1
1:A:231:ASP:HB3	1:A:234:ALA:HB3	0.64	1.70	7	1
1:A:144:VAL:HG11	1:A:255:ILE:HD11	0.63	1.70	6	3
1:A:144:VAL:HG11	1:A:255:ILE:CG1	0.63	2.23	17	6
1:A:250:LEU:HD12	1:A:255:ILE:CD1	0.63	2.23	9	1
1:A:140:VAL:HG11	1:A:217:VAL:CG2	0.63	2.23	2	2
1:A:140:VAL:O	1:A:250:LEU:HD12	0.63	1.94	16	2
1:A:213:PHE:O	1:A:217:VAL:HG23	0.63	1.94	4	9
1:A:203:TRP:CZ3	1:A:210:THR:HG21	0.62	2.30	9	1
1:A:217:VAL:HG21	1:A:248:PHE:CE2	0.62	2.29	13	4
1:A:181:LEU:HD13	1:A:181:LEU:N	0.62	2.10	11	1
1:A:115:THR:O	1:A:157:ALA:HB1	0.61	1.96	18	3
1:A:244:ASP:HB3	1:A:247:THR:HG22	0.61	1.72	16	1
1:A:231:ASP:CG	1:A:252:ALA:HB1	0.61	2.16	12	1
1:A:160:LEU:HD23	1:A:161:VAL:N	0.61	2.11	12	1
1:A:159:ILE:HG23	1:A:193:GLY:O	0.61	1.95	15	2
1:A:144:VAL:HG23	1:A:258:ILE:CG2	0.61	2.26	11	1
1:A:144:VAL:HG21	1:A:255:ILE:HG13	0.60	1.73	6	5
1:A:221:GLY:O	1:A:226:LEU:HD23	0.60	1.96	14	1
1:A:140:VAL:HG21	1:A:217:VAL:CG2	0.60	2.26	10	2
1:A:252:ALA:HB3	1:A:254:ASP:OD2	0.60	1.96	6	2
1:A:250:LEU:HD11	1:A:255:ILE:HD12	0.60	1.71	10	1
1:A:161:VAL:HA	1:A:195:ALA:HB3	0.60	1.73	19	6
1:A:180:ILE:HG21	1:A:183:HIS:CD2	0.60	2.32	19	1
1:A:231:ASP:OD2	1:A:252:ALA:HB1	0.59	1.97	2	1
1:A:145:THR:HG23	1:A:258:ILE:HG13	0.59	1.74	8	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:250:LEU:CD2	1:A:255:ILE:HD12	0.59	2.27	13	1
1:A:116:TYR:HB2	1:A:159:ILE:HD11	0.59	1.72	3	2
1:A:137:ALA:HA	1:A:217:VAL:HG22	0.59	1.72	12	7
1:A:141:TRP:CE2	1:A:224:LEU:HD13	0.59	2.33	12	2
1:A:226:LEU:HD11	1:A:236:MET:HA	0.59	1.74	15	1
1:A:223:SER:O	1:A:224:LEU:HD12	0.59	1.97	14	3
1:A:118:ILE:HG23	1:A:161:VAL:CG2	0.59	2.27	11	2
1:A:160:LEU:HD23	1:A:162:VAL:HG23	0.59	1.71	4	1
1:A:122:THR:HG23	1:A:203:TRP:HB2	0.58	1.75	19	1
1:A:116:TYR:CE2	1:A:159:ILE:HG21	0.58	2.33	6	1
1:A:133:ALA:HB1	1:A:213:PHE:N	0.58	2.13	14	3
1:A:213:PHE:CZ	1:A:214:LEU:HD23	0.58	2.33	11	1
1:A:214:LEU:HD22	1:A:241:LYS:O	0.58	1.99	5	2
1:A:191:ILE:HG23	1:A:194:ASP:CG	0.58	2.19	13	1
1:A:116:TYR:HA	1:A:157:ALA:HB1	0.58	1.73	9	2
1:A:164:ALA:HB3	1:A:199:GLU:OE2	0.58	1.98	6	2
1:A:133:ALA:HB1	1:A:213:PHE:CA	0.58	2.29	20	3
1:A:211:ASN:ND2	1:A:214:LEU:HD23	0.57	2.14	6	1
1:A:152:ILE:HG22	1:A:154:THR:H	0.57	1.60	14	1
1:A:250:LEU:HD23	1:A:255:ILE:CD1	0.57	2.30	15	1
1:A:160:LEU:HD21	1:A:162:VAL:HG23	0.57	1.77	18	4
1:A:160:LEU:HD22	1:A:161:VAL:N	0.57	2.15	18	15
1:A:206:HIS:CB	1:A:245:ILE:HG23	0.56	2.29	9	1
1:A:214:LEU:HD22	1:A:243:VAL:CG1	0.56	2.29	6	2
1:A:160:LEU:HD11	1:A:162:VAL:HG23	0.56	1.77	9	5
1:A:140:VAL:HG21	1:A:217:VAL:HG22	0.56	1.77	10	1
1:A:252:ALA:O	1:A:255:ILE:HG22	0.56	1.99	2	2
1:A:164:ALA:HB1	1:A:168:HIS:NE2	0.56	2.15	2	1
1:A:226:LEU:HD23	1:A:258:ILE:CD1	0.56	2.30	5	1
1:A:205:THR:OG1	1:A:245:ILE:HD12	0.56	2.00	20	1
1:A:117:ARG:CZ	1:A:160:LEU:HD23	0.56	2.30	15	1
1:A:203:TRP:CH2	1:A:215:THR:HG21	0.56	2.35	8	2
1:A:125:MET:HG2	1:A:205:THR:HG23	0.56	1.76	18	1
1:A:118:ILE:HG21	1:A:134:ILE:HG13	0.56	1.78	18	1
1:A:146:PRO:O	1:A:147:LEU:HD22	0.56	2.00	6	1
1:A:220:ILE:O	1:A:224:LEU:HD13	0.56	2.01	3	2
1:A:141:TRP:CZ3	1:A:250:LEU:HD23	0.56	2.36	3	1
1:A:129:ASP:OD2	1:A:212:LEU:HD12	0.56	2.00	20	1
1:A:160:LEU:HD11	1:A:162:VAL:CG2	0.55	2.32	20	9
1:A:121:TYR:HB2	1:A:130:VAL:HG11	0.55	1.78	17	2
1:A:198:ASP:OD1	1:A:210:THR:HG21	0.55	2.02	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:234:ALA:HB2	1:A:252:ALA:CB	0.55	2.31	7	2
1:A:152:ILE:HD12	1:A:154:THR:O	0.55	2.01	10	2
1:A:134:ILE:HD12	1:A:135:ARG:N	0.55	2.17	15	2
1:A:250:LEU:HD11	1:A:255:ILE:CD1	0.55	2.31	10	1
1:A:145:THR:HG21	1:A:258:ILE:HD11	0.55	1.78	14	2
1:A:122:THR:HG21	1:A:203:TRP:CD1	0.54	2.37	15	1
1:A:144:VAL:HG11	1:A:255:ILE:HG13	0.54	1.78	15	4
1:A:226:LEU:HD22	1:A:236:MET:CE	0.54	2.32	11	1
1:A:125:MET:HE3	1:A:204:THR:HG22	0.54	1.79	19	1
1:A:250:LEU:HD21	1:A:254:ASP:OD2	0.54	2.03	11	2
1:A:145:THR:HG22	1:A:146:PRO:HD2	0.53	1.80	8	5
1:A:250:LEU:HD11	1:A:255:ILE:HG13	0.53	1.79	14	1
1:A:147:LEU:HD13	1:A:224:LEU:CD2	0.53	2.33	13	1
1:A:119:ASN:CB	1:A:162:VAL:HG22	0.53	2.33	11	3
1:A:217:VAL:HG21	1:A:248:PHE:CE1	0.53	2.38	1	1
1:A:211:ASN:ND2	1:A:214:LEU:HD22	0.53	2.18	19	1
1:A:152:ILE:HD13	1:A:155:GLY:O	0.53	2.04	1	1
1:A:211:ASN:HD21	1:A:214:LEU:HD22	0.53	1.64	19	1
1:A:160:LEU:HD23	1:A:160:LEU:O	0.53	2.04	13	1
1:A:214:LEU:HD13	1:A:243:VAL:HG21	0.53	1.80	5	1
1:A:226:LEU:HD21	1:A:257:GLY:O	0.52	2.04	17	1
1:A:217:VAL:HG21	1:A:248:PHE:CZ	0.52	2.40	13	6
1:A:226:LEU:HD12	1:A:258:ILE:HB	0.52	1.80	3	1
1:A:140:VAL:HG21	1:A:217:VAL:HG21	0.52	1.80	6	1
1:A:130:VAL:HG22	1:A:134:ILE:HG12	0.52	1.82	10	1
1:A:250:LEU:HD23	1:A:255:ILE:HD12	0.52	1.80	13	2
1:A:160:LEU:HD13	1:A:160:LEU:O	0.52	2.05	3	2
1:A:214:LEU:HD22	1:A:241:LYS:CB	0.52	2.35	16	1
1:A:234:ALA:HB1	1:A:254:ASP:CG	0.52	2.24	14	1
1:A:203:TRP:CZ3	1:A:215:THR:HG21	0.52	2.40	17	3
1:A:140:VAL:HG12	1:A:250:LEU:HD12	0.52	1.82	12	2
1:A:206:HIS:CG	1:A:245:ILE:HG23	0.52	2.39	9	1
1:A:120:ASN:OD1	1:A:161:VAL:HG12	0.52	2.04	1	2
1:A:116:TYR:HB3	1:A:159:ILE:HD11	0.52	1.81	4	2
1:A:250:LEU:HD23	1:A:251:SER:N	0.52	2.20	2	4
1:A:119:ASN:HB2	1:A:162:VAL:HG22	0.51	1.81	11	1
1:A:213:PHE:CZ	1:A:245:ILE:HG22	0.51	2.40	14	1
1:A:225:GLY:O	1:A:226:LEU:HD22	0.51	2.04	9	3
1:A:244:ASP:CB	1:A:247:THR:HG22	0.51	2.35	16	1
1:A:206:HIS:HD1	1:A:245:ILE:HG22	0.51	1.65	13	1
1:A:122:THR:CG2	1:A:212:LEU:HD11	0.51	2.35	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:235:VAL:HG13	1:A:241:LYS:HE2	0.51	1.83	1	1
1:A:181:LEU:HD13	1:A:215:THR:CG2	0.51	2.35	15	1
1:A:160:LEU:O	1:A:160:LEU:HD13	0.51	2.06	18	9
1:A:212:LEU:O	1:A:212:LEU:HD13	0.50	2.06	14	2
1:A:116:TYR:CD2	1:A:159:ILE:HD11	0.50	2.41	17	1
1:A:175:ASP:OD2	1:A:180:ILE:HD12	0.50	2.06	19	1
1:A:137:ALA:HB1	1:A:220:ILE:HD12	0.50	1.84	17	2
1:A:160:LEU:HD21	1:A:162:VAL:CG2	0.50	2.37	13	3
1:A:160:LEU:CD2	1:A:162:VAL:HG23	0.50	2.36	12	3
1:A:118:ILE:HG21	1:A:134:ILE:HG21	0.50	1.83	16	2
1:A:134:ILE:HD12	1:A:197:PHE:CZ	0.49	2.41	19	1
1:A:226:LEU:HD23	1:A:258:ILE:HD13	0.49	1.83	5	1
1:A:214:LEU:HD13	1:A:243:VAL:CG2	0.49	2.36	5	1
1:A:241:LYS:O	1:A:243:VAL:HG23	0.49	2.07	5	3
1:A:115:THR:C	1:A:157:ALA:HB1	0.49	2.28	16	2
1:A:134:ILE:O	1:A:137:ALA:HB3	0.49	2.07	7	1
1:A:118:ILE:HD13	1:A:134:ILE:HB	0.49	1.84	10	1
1:A:220:ILE:O	1:A:224:LEU:HD12	0.48	2.09	12	4
1:A:144:VAL:HG11	1:A:250:LEU:HD13	0.48	1.84	18	1
1:A:201:GLU:OE2	1:A:210:THR:HG21	0.48	2.09	5	1
1:A:203:TRP:CG	1:A:212:LEU:HD23	0.48	2.43	8	1
1:A:115:THR:HG22	1:A:150:SER:HB3	0.48	1.84	18	1
1:A:234:ALA:HB1	1:A:254:ASP:OD1	0.48	2.09	14	1
1:A:126:ASN:O	1:A:130:VAL:HG12	0.47	2.09	19	1
1:A:133:ALA:HB3	1:A:212:LEU:HD12	0.47	1.85	8	1
1:A:250:LEU:HD22	1:A:255:ILE:HG13	0.47	1.85	18	1
1:A:118:ILE:CG2	1:A:134:ILE:HG21	0.47	2.39	1	1
1:A:212:LEU:O	1:A:212:LEU:HD12	0.47	2.08	15	1
1:A:184:ALA:HB2	1:A:219:GLU:OE2	0.47	2.09	2	1
1:A:237:PHE:HB3	1:A:239:THR:HG22	0.47	1.87	16	1
1:A:141:TRP:HE1	1:A:258:ILE:HD11	0.47	1.70	18	1
1:A:133:ALA:CB	1:A:212:LEU:HD22	0.47	2.39	1	2
1:A:160:LEU:C	1:A:160:LEU:HD13	0.47	2.30	18	7
1:A:140:VAL:HG11	1:A:217:VAL:CG1	0.47	2.39	14	1
1:A:218:HIS:HA	1:A:235:VAL:HG12	0.47	1.84	5	1
1:A:214:LEU:O	1:A:214:LEU:HD12	0.47	2.10	6	1
1:A:250:LEU:HD23	1:A:251:SER:H	0.47	1.70	19	4
1:A:122:THR:HG23	1:A:130:VAL:HG21	0.47	1.87	8	1
1:A:130:VAL:HA	1:A:212:LEU:HD13	0.47	1.87	6	1
1:A:118:ILE:HG22	1:A:161:VAL:CG2	0.47	2.31	4	1
1:A:181:LEU:HD22	1:A:215:THR:HG23	0.47	1.86	18	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:118:ILE:HD13	1:A:134:ILE:HG13	0.47	1.85	18	1
1:A:212:LEU:HD23	1:A:212:LEU:O	0.46	2.09	9	1
1:A:122:THR:OG1	1:A:212:LEU:HD11	0.46	2.10	3	1
1:A:145:THR:HG21	1:A:258:ILE:HG13	0.46	1.87	12	1
1:A:203:TRP:CG	1:A:212:LEU:HD13	0.46	2.45	17	1
1:A:119:ASN:CG	1:A:162:VAL:HG22	0.46	2.30	11	1
1:A:145:THR:OG1	1:A:147:LEU:HD12	0.46	2.11	13	1
1:A:141:TRP:HE1	1:A:226:LEU:HD12	0.46	1.69	11	1
1:A:141:TRP:CZ2	1:A:226:LEU:HD12	0.46	2.46	2	1
1:A:203:TRP:CZ2	1:A:215:THR:HG21	0.46	2.45	15	1
1:A:164:ALA:HB1	1:A:168:HIS:CD2	0.46	2.45	10	2
1:A:250:LEU:HD22	1:A:255:ILE:CA	0.46	2.41	7	1
1:A:191:ILE:O	1:A:191:ILE:HG22	0.46	2.10	17	2
1:A:251:SER:O	1:A:255:ILE:HD12	0.46	2.11	14	1
1:A:144:VAL:CG1	1:A:250:LEU:HD13	0.46	2.41	18	1
1:A:147:LEU:HD12	1:A:147:LEU:O	0.46	2.11	11	1
1:A:191:ILE:HG22	1:A:191:ILE:O	0.46	2.11	11	2
1:A:115:THR:HG23	1:A:149:PHE:HB3	0.46	1.87	15	1
1:A:250:LEU:HB3	1:A:255:ILE:HD12	0.46	1.88	19	1
1:A:250:LEU:HD23	1:A:251:SER:O	0.45	2.10	13	1
1:A:184:ALA:HB1	1:A:194:ASP:O	0.45	2.11	19	3
1:A:160:LEU:HD13	1:A:160:LEU:C	0.45	2.32	7	4
1:A:206:HIS:HB3	1:A:245:ILE:HD13	0.45	1.88	2	1
1:A:118:ILE:HD13	1:A:134:ILE:CG1	0.45	2.42	18	1
1:A:226:LEU:HD22	1:A:236:MET:SD	0.45	2.52	20	2
1:A:206:HIS:CG	1:A:245:ILE:HG22	0.45	2.47	6	1
1:A:214:LEU:CD2	1:A:243:VAL:HG22	0.45	2.42	8	1
1:A:145:THR:HG21	1:A:258:ILE:CG1	0.45	2.42	12	1
1:A:160:LEU:C	1:A:160:LEU:CD2	0.45	2.82	8	1
1:A:237:PHE:O	1:A:237:PHE:CG	0.45	2.69	13	1
1:A:182:ALA:HB3	1:A:196:HIS:O	0.45	2.12	7	1
1:A:203:TRP:HB3	1:A:212:LEU:HD23	0.45	1.89	14	1
1:A:152:ILE:O	1:A:152:ILE:HD12	0.45	2.12	6	2
1:A:144:VAL:HG23	1:A:258:ILE:HG22	0.45	1.89	11	1
1:A:181:LEU:HD12	1:A:182:ALA:H	0.45	1.72	17	1
1:A:214:LEU:HD21	1:A:248:PHE:CE1	0.44	2.46	10	1
1:A:133:ALA:HB3	1:A:212:LEU:HD22	0.44	1.89	11	3
1:A:144:VAL:HG23	1:A:258:ILE:HG21	0.44	1.89	11	1
1:A:130:VAL:CG2	1:A:212:LEU:HD22	0.44	2.41	20	1
1:A:137:ALA:CB	1:A:220:ILE:HD12	0.44	2.42	17	1
1:A:234:ALA:HB1	1:A:254:ASP:OD2	0.44	2.11	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:160:LEU:CD1	1:A:162:VAL:HG23	0.44	2.41	9	1
1:A:116:TYR:OH	1:A:118:ILE:HD11	0.44	2.11	13	1
1:A:214:LEU:HD13	1:A:243:VAL:CG1	0.44	2.43	1	1
1:A:142:SER:HB2	1:A:147:LEU:HD11	0.44	1.89	8	1
1:A:213:PHE:CE1	1:A:245:ILE:HG22	0.44	2.47	14	1
1:A:144:VAL:HG11	1:A:255:ILE:CD1	0.44	2.40	6	1
1:A:181:LEU:HD13	1:A:215:THR:HG23	0.44	1.88	15	1
1:A:119:ASN:ND2	1:A:160:LEU:HD21	0.44	2.28	14	1
1:A:214:LEU:HD23	1:A:248:PHE:CD1	0.44	2.48	16	1
1:A:191:ILE:HG23	1:A:194:ASP:CB	0.43	2.44	13	1
1:A:203:TRP:HB3	1:A:212:LEU:HD13	0.43	1.90	17	1
1:A:234:ALA:CB	1:A:252:ALA:HB2	0.43	2.39	12	1
1:A:251:SER:O	1:A:252:ALA:HB2	0.43	2.13	12	1
1:A:181:LEU:HD22	1:A:182:ALA:N	0.43	2.29	11	1
1:A:141:TRP:CE3	1:A:250:LEU:HD11	0.43	2.48	8	1
1:A:164:ALA:HB3	1:A:196:HIS:CD2	0.43	2.48	18	1
1:A:184:ALA:HB2	1:A:219:GLU:CD	0.43	2.33	13	1
1:A:141:TRP:CZ2	1:A:258:ILE:HD13	0.43	2.48	20	1
1:A:144:VAL:HG21	1:A:255:ILE:CG1	0.43	2.41	6	1
1:A:252:ALA:HA	1:A:255:ILE:HD12	0.43	1.91	4	2
1:A:147:LEU:HD12	1:A:148:LYS:N	0.43	2.28	8	1
1:A:130:VAL:HG23	1:A:212:LEU:HD23	0.43	1.88	16	1
1:A:164:ALA:HB1	1:A:168:HIS:ND1	0.43	2.28	1	1
1:A:250:LEU:CD1	1:A:255:ILE:HD12	0.43	2.42	10	1
1:A:181:LEU:HD22	1:A:215:THR:CG2	0.43	2.44	3	1
1:A:118:ILE:HD11	1:A:134:ILE:HG21	0.43	1.90	6	2
1:A:197:PHE:CE2	1:A:212:LEU:HD23	0.43	2.48	10	1
1:A:250:LEU:HD22	1:A:255:ILE:HA	0.43	1.90	7	1
1:A:136:LYS:O	1:A:140:VAL:HG12	0.43	2.14	2	1
1:A:133:ALA:HB1	1:A:213:PHE:HA	0.43	1.90	11	2
1:A:137:ALA:HB1	1:A:220:ILE:HG13	0.43	1.91	16	1
1:A:127:ARG:HA	1:A:130:VAL:HG12	0.42	1.90	10	1
1:A:115:THR:HG23	1:A:158:ASP:H	0.42	1.73	14	1
1:A:144:VAL:O	1:A:144:VAL:HG22	0.42	2.14	20	1
1:A:120:ASN:CG	1:A:161:VAL:HG12	0.42	2.35	10	1
1:A:251:SER:O	1:A:252:ALA:HB3	0.42	2.14	3	1
1:A:161:VAL:HG13	1:A:195:ALA:CB	0.42	2.45	13	1
1:A:191:ILE:HG23	1:A:194:ASP:HB2	0.42	1.91	13	1
1:A:250:LEU:HD11	1:A:255:ILE:CG1	0.42	2.44	10	1
1:A:160:LEU:CD2	1:A:160:LEU:C	0.42	2.83	4	1
1:A:130:VAL:O	1:A:134:ILE:HD13	0.42	2.14	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:116:TYR:CE1	1:A:159:ILE:HD13	0.42	2.50	20	1
1:A:224:LEU:O	1:A:226:LEU:HD12	0.42	2.14	4	1
1:A:161:VAL:HG13	1:A:195:ALA:HB3	0.42	1.91	13	1
1:A:120:ASN:ND2	1:A:161:VAL:HG12	0.42	2.29	10	1
1:A:212:LEU:HD13	1:A:212:LEU:C	0.42	2.35	19	1
1:A:226:LEU:HD13	1:A:236:MET:SD	0.42	2.55	20	1
1:A:203:TRP:CZ3	1:A:212:LEU:HD21	0.42	2.50	1	1
1:A:141:TRP:CH2	1:A:250:LEU:HD23	0.42	2.49	3	1
1:A:203:TRP:CD1	1:A:212:LEU:HD23	0.41	2.50	8	1
1:A:232:PRO:O	1:A:233:LYS:C	0.41	2.59	6	4
1:A:214:LEU:HD13	1:A:243:VAL:HG12	0.41	1.91	1	1
1:A:226:LEU:HD13	1:A:227:GLY:N	0.41	2.30	15	1
1:A:147:LEU:HD22	1:A:224:LEU:HD21	0.41	1.91	4	1
1:A:122:THR:OG1	1:A:212:LEU:HD21	0.41	2.16	20	1
1:A:181:LEU:N	1:A:181:LEU:CD1	0.41	2.81	11	1
1:A:181:LEU:N	1:A:181:LEU:HD13	0.41	2.31	1	1
1:A:214:LEU:HD22	1:A:241:LYS:HB3	0.41	1.91	16	1
1:A:234:ALA:HB2	1:A:251:SER:HB3	0.41	1.92	14	1
1:A:122:THR:HG23	1:A:203:TRP:CB	0.41	2.46	19	1
1:A:122:THR:HG22	1:A:123:PRO:HD2	0.41	1.93	5	1
1:A:214:LEU:HD21	1:A:243:VAL:HG22	0.41	1.92	8	1
1:A:141:TRP:CZ3	1:A:250:LEU:HD12	0.41	2.51	13	1
1:A:118:ILE:HG21	1:A:134:ILE:CG1	0.41	2.45	18	1
1:A:141:TRP:O	1:A:144:VAL:HG12	0.41	2.15	18	1
1:A:206:HIS:ND1	1:A:245:ILE:HG22	0.41	2.30	13	1
1:A:211:ASN:ND2	1:A:243:VAL:H	0.41	2.14	17	1
1:A:181:LEU:O	1:A:182:ALA:HB2	0.40	2.16	13	1
1:A:130:VAL:CA	1:A:212:LEU:HD13	0.40	2.45	6	1
1:A:235:VAL:HG22	1:A:251:SER:OG	0.40	2.15	20	1
1:A:231:ASP:CB	1:A:234:ALA:HB3	0.40	2.43	7	1
1:A:138:PHE:CE1	1:A:220:ILE:HD11	0.40	2.50	7	1
1:A:138:PHE:CD1	1:A:220:ILE:HD12	0.40	2.51	12	1
1:A:134:ILE:HG21	1:A:161:VAL:HG21	0.40	1.93	4	1
1:A:116:TYR:CZ	1:A:159:ILE:HG21	0.40	2.51	20	1
1:A:250:LEU:HD11	1:A:255:ILE:HG12	0.40	1.92	4	1
1:A:164:ALA:HB3	1:A:196:HIS:NE2	0.40	2.31	9	1
1:A:214:LEU:HD13	1:A:243:VAL:HG11	0.40	1.92	15	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	146/152 (96%)	115±4 (79±3%)	25±3 (17±2%)	7±2 (5±1%)	5	29
All	All	2920/3040 (96%)	2294 (79%)	491 (17%)	135 (5%)	5	29

All 35 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	230	SER	17
1	A	202	PHE	10
1	A	192	GLY	10
1	A	209	GLY	10
1	A	198	ASP	7
1	A	229	SER	7
1	A	170	ASP	6
1	A	171	ASP	5
1	A	228	HIS	5
1	A	226	LEU	4
1	A	258	ILE	4
1	A	199	GLU	4
1	A	227	GLY	4
1	A	201	GLU	4
1	A	225	GLY	4
1	A	175	ASP	3
1	A	147	LEU	3
1	A	210	THR	3
1	A	190	GLY	3
1	A	234	ALA	2
1	A	179	GLY	2
1	A	236	MET	2
1	A	174	PHE	2
1	A	169	GLY	2
1	A	191	ILE	2
1	A	176	GLY	1
1	A	224	LEU	1

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Mol	Chain	Res	Type	Models (Total)
1	A	155	GLY	1
1	A	200	ASP	1
1	A	211	ASN	1
1	A	184	ALA	1
1	A	237	PHE	1
1	A	123	PRO	1
1	A	182	ALA	1
1	A	146	PRO	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	117/122 (96%)	83±3 (71±3%)	34±3 (29±3%)	2	18
All	All	2340/2440 (96%)	1656 (71%)	684 (29%)	2	18

All 100 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	233	LYS	18
1	A	205	THR	17
1	A	158	ASP	16
1	A	223	SER	15
1	A	204	THR	15
1	A	251	SER	14
1	A	151	LYS	14
1	A	237	PHE	14
1	A	185	PHE	14
1	A	148	LYS	13
1	A	231	ASP	13
1	A	253	ASP	12
1	A	156	MET	12
1	A	165	ARG	12
1	A	250	LEU	12
1	A	207	SER	12
1	A	202	PHE	11

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Mol	Chain	Res	Type	Models (Total)
1	A	230	SER	11
1	A	212	LEU	11
1	A	181	LEU	11
1	A	145	THR	11
1	A	141	TRP	11
1	A	241	LYS	10
1	A	122	THR	10
1	A	222	HIS	10
1	A	177	LYS	10
1	A	210	THR	9
1	A	171	ASP	9
1	A	115	THR	9
1	A	135	ARG	8
1	A	255	ILE	8
1	A	201	GLU	8
1	A	226	LEU	8
1	A	136	LYS	8
1	A	139	GLN	8
1	A	236	MET	8
1	A	138	PHE	8
1	A	247	THR	8
1	A	244	ASP	8
1	A	160	LEU	8
1	A	120	ASN	7
1	A	246	ASN	7
1	A	200	ASP	7
1	A	126	ASN	7
1	A	125	MET	7
1	A	198	ASP	7
1	A	153	ASN	7
1	A	183	HIS	7
1	A	147	LEU	7
1	A	214	LEU	7
1	A	224	LEU	6
1	A	189	SER	6
1	A	175	ASP	6
1	A	260	SER	6
1	A	124	ASP	6
1	A	211	ASN	6
1	A	229	SER	6
1	A	154	THR	6
1	A	228	HIS	6

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Mol	Chain	Res	Type	Models (Total)
1	A	150	SER	5
1	A	117	ARG	5
1	A	174	PHE	5
1	A	219	GLU	5
1	A	203	TRP	5
1	A	199	GLU	5
1	A	170	ASP	5
1	A	143	ASN	5
1	A	259	GLN	5
1	A	127	ARG	5
1	A	239	THR	5
1	A	129	ASP	4
1	A	152	ILE	4
1	A	142	SER	3
1	A	248	PHE	3
1	A	256	ARG	3
1	A	197	PHE	3
1	A	168	HIS	3
1	A	128	GLU	3
1	A	258	ILE	2
1	A	119	ASN	2
1	A	249	ARG	2
1	A	206	HIS	2
1	A	116	TYR	2
1	A	172	HIS	2
1	A	245	ILE	2
1	A	213	PHE	2
1	A	196	HIS	2
1	A	215	THR	2
1	A	132	TYR	2
1	A	254	ASP	2
1	A	194	ASP	2
1	A	218	HIS	1
1	A	134	ILE	1
1	A	149	PHE	1
1	A	243	VAL	1
1	A	161	VAL	1
1	A	163	PHE	1
1	A	191	ILE	1
1	A	144	VAL	1
1	A	162	VAL	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 1 ligands modelled in this entry, 1 is 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