



Full wwPDB NMR Structure Validation Report ⓘ

Mar 7, 2026 – 12:46 AM UTC

PDB ID : 2K9C / pdb_00002k9c
Title : Paramagnetic shifts in solid-state NMR of Proteins to elicit structural information
Authors : Balayssac, S.; Bertini, I.; Bhaumik, A.; Lelli, M.; Luchinat, C.
Deposited on : 2008-10-08

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

<https://www.wwpdb.org/validation/2017/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

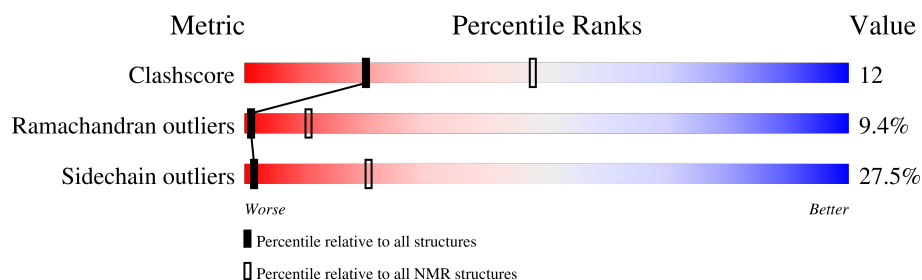
1 Overall quality at a glance

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	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

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	37% 43% . 18%

2 Ensemble composition and analysis

This entry contains 20 models. Model 6 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative.

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:114-A:152, A:157-A:174, A:181-A:187, A:195-A:228, A:233-A:258 (124)	2.99	6

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 7 single-model clusters were found.

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

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	engineered mutation	UNP P39900

- Molecule 2 is COBALT (II) ION (CCD ID: CO) (formula: Co).

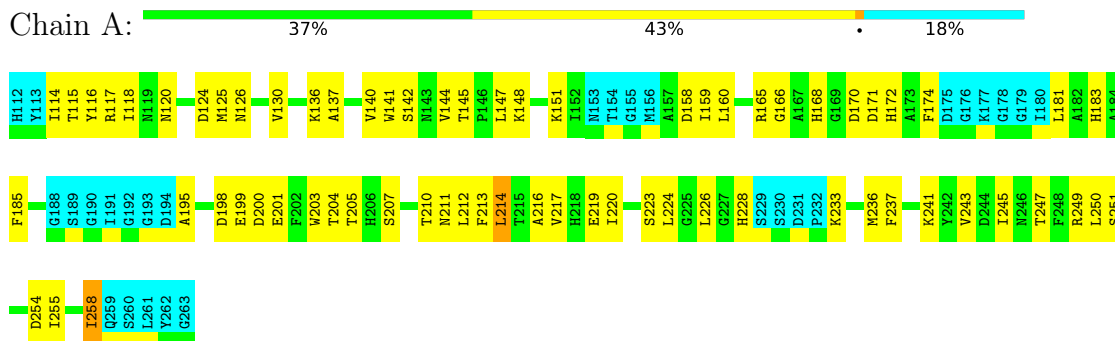
Mol	Chain	Residues	Atoms	
2	A	1	Total	Co
			1	1

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide 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

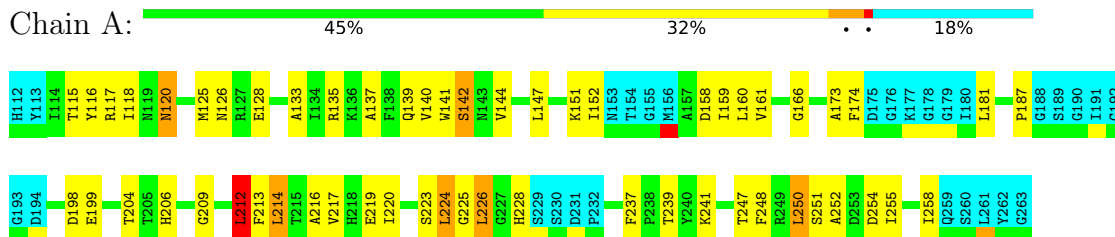


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

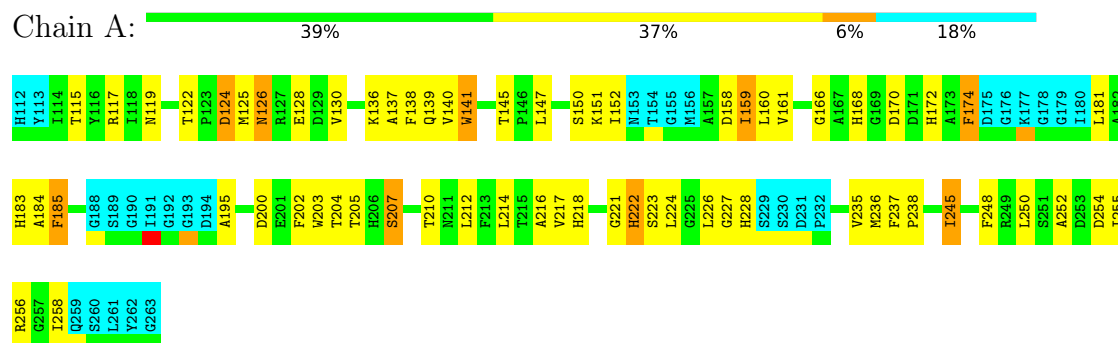
4.2.1 Score per residue for model 1

- Molecule 1: Macrophage metalloelastase



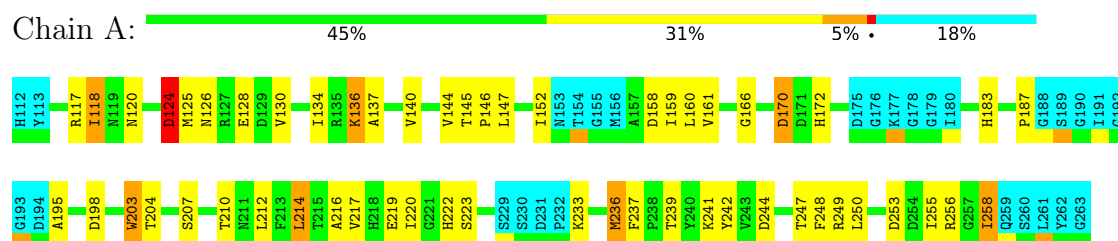
4.2.2 Score per residue for model 2

- Molecule 1: Macrophage metalloelastase



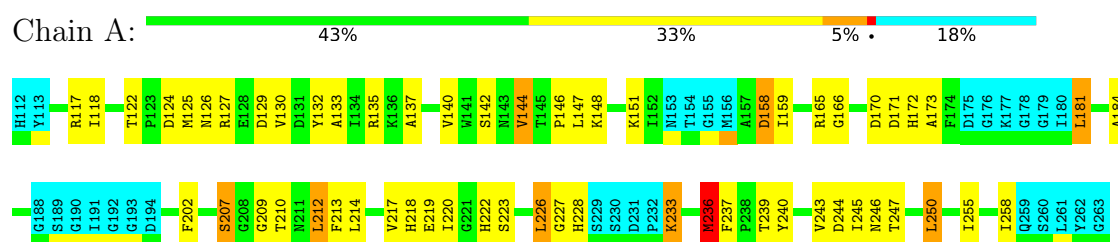
4.2.3 Score per residue for model 3

- Molecule 1: Macrophage metalloelastase



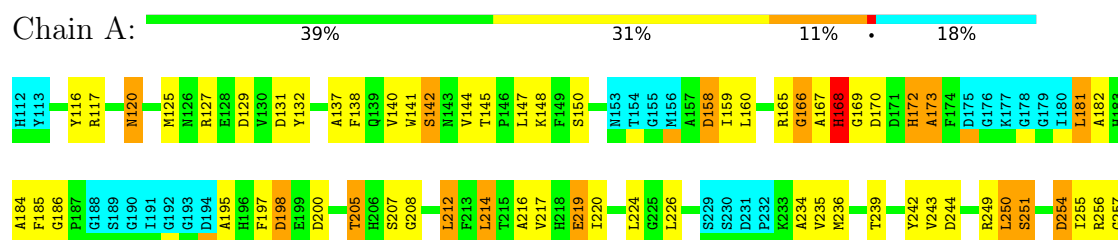
4.2.4 Score per residue for model 4

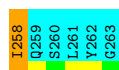
- Molecule 1: Macrophage metalloelastase



4.2.5 Score per residue for model 5

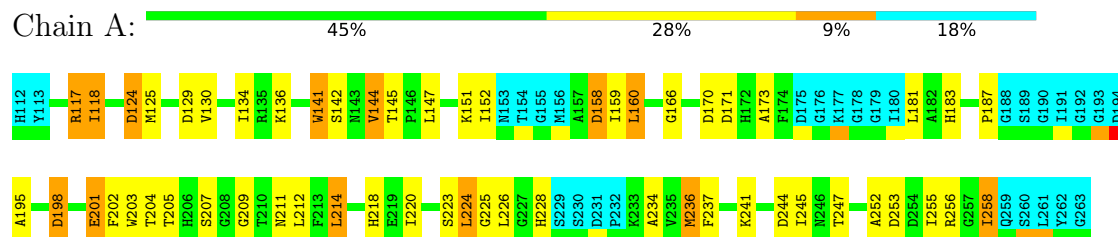
- Molecule 1: Macrophage metalloelastase





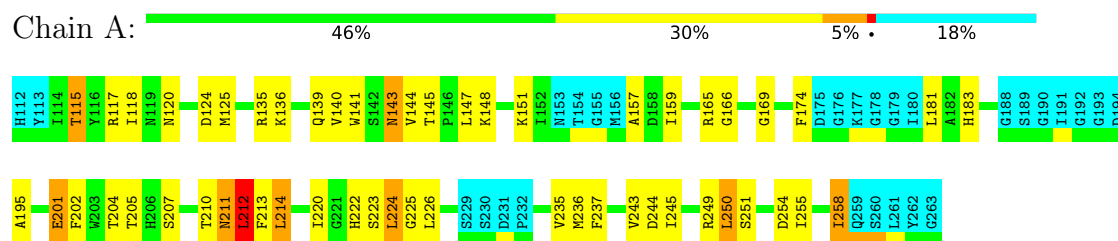
4.2.6 Score per residue for model 6 (medoid)

- Molecule 1: Macrophage metalloelastase



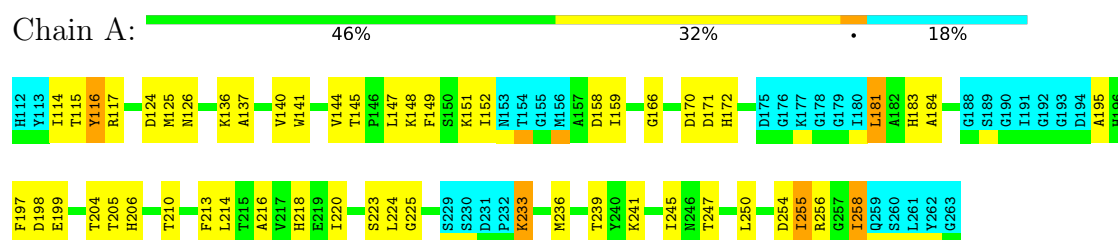
4.2.7 Score per residue for model 7

- Molecule 1: Macrophage metalloelastase



4.2.8 Score per residue for model 8

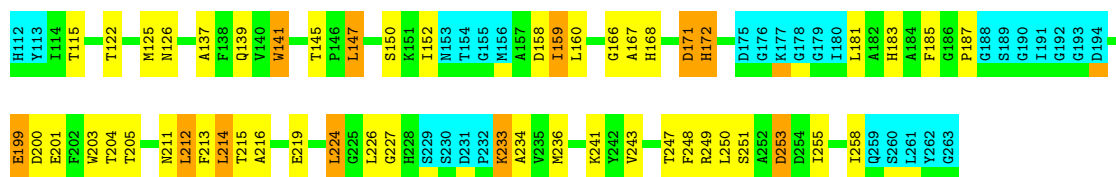
- Molecule 1: Macrophage metalloelastase



4.2.9 Score per residue for model 9

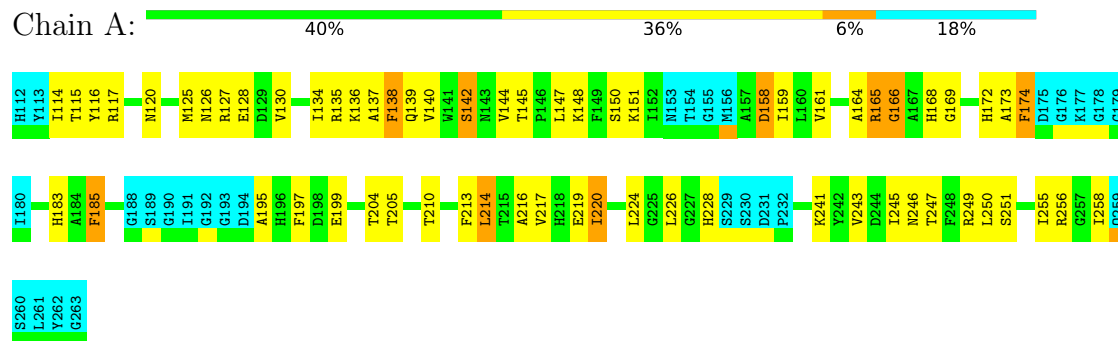
- Molecule 1: Macrophage metalloelastase





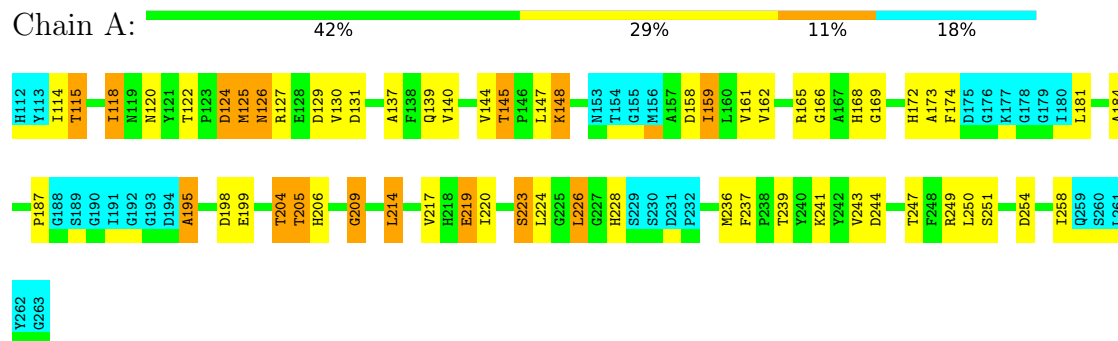
4.2.10 Score per residue for model 10

- Molecule 1: Macrophage metalloelastase



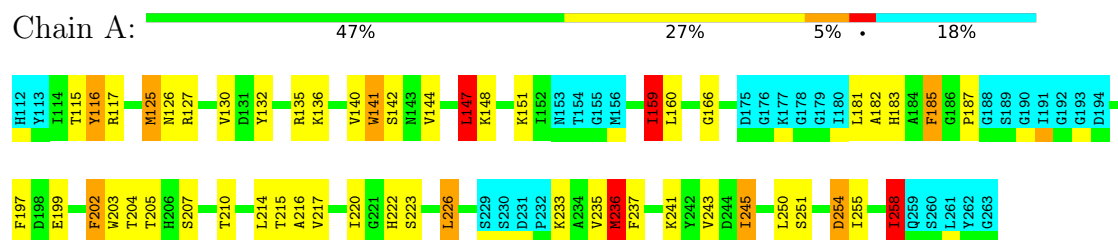
4.2.11 Score per residue for model 11

- Molecule 1: Macrophage metalloelastase



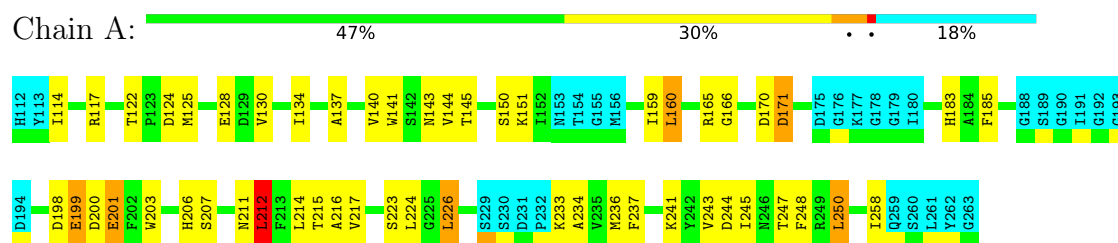
4.2.12 Score per residue for model 12

- Molecule 1: Macrophage metalloelastase



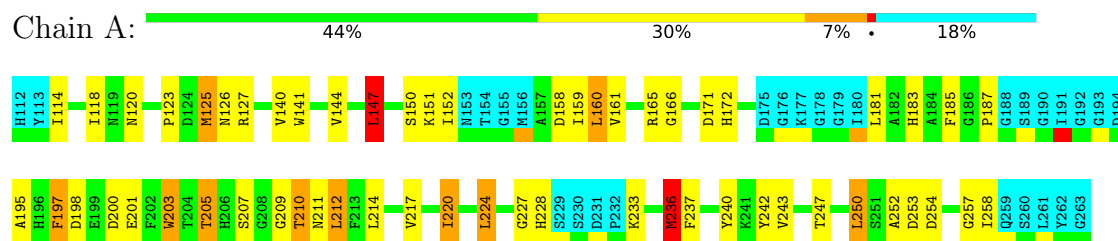
4.2.13 Score per residue for model 13

- Molecule 1: Macrophage metalloelastase



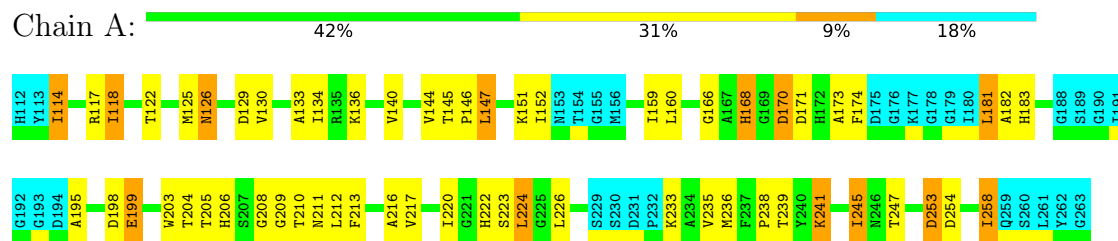
4.2.14 Score per residue for model 14

- Molecule 1: Macrophage metalloelastase



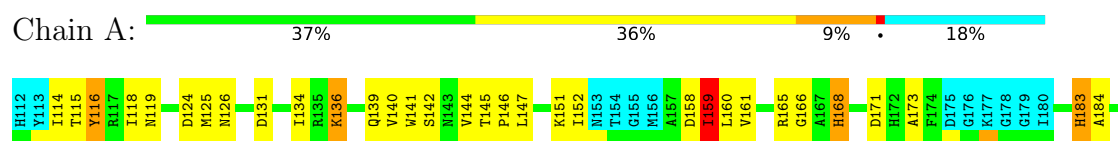
4.2.15 Score per residue for model 15

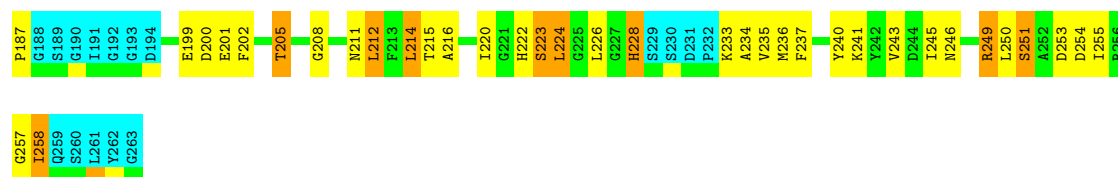
- Molecule 1: Macrophage metalloelastase



4.2.16 Score per residue for model 16

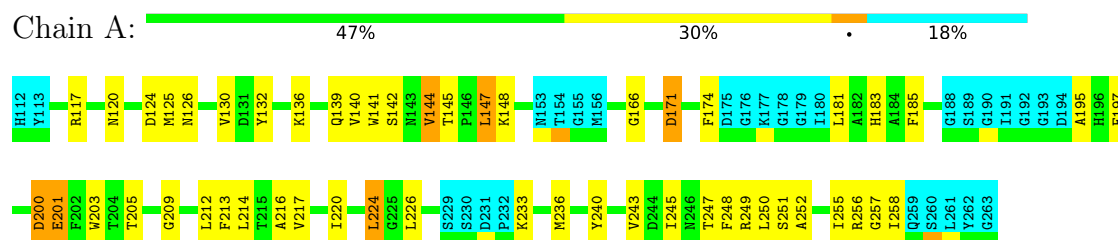
- Molecule 1: Macrophage metalloelastase





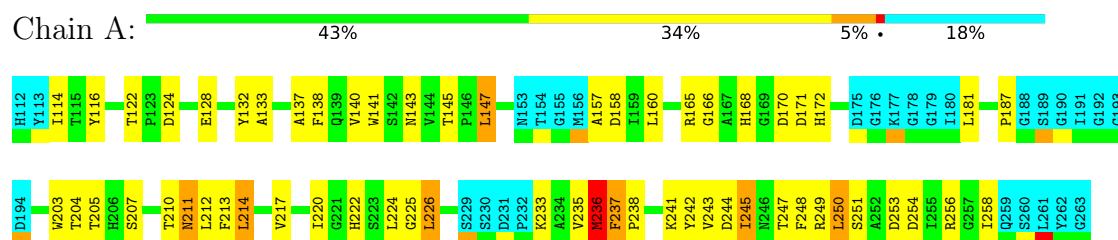
4.2.17 Score per residue for model 17

- Molecule 1: Macrophage metalloelastase



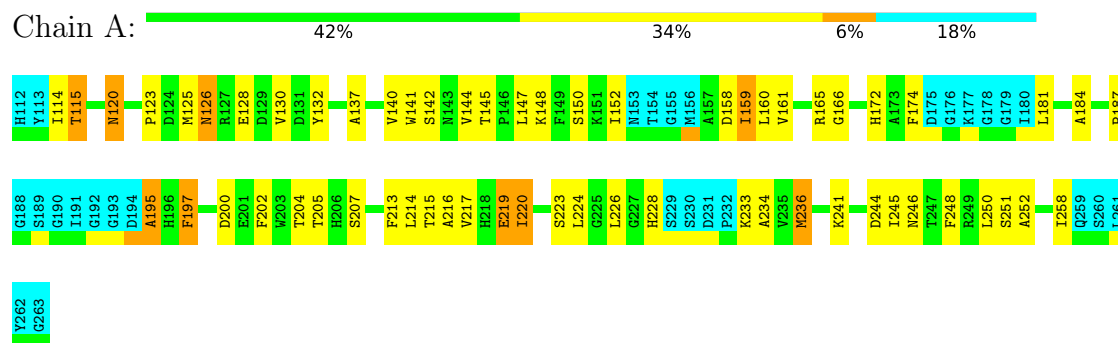
4.2.18 Score per residue for model 18

- Molecule 1: Macrophage metalloelastase



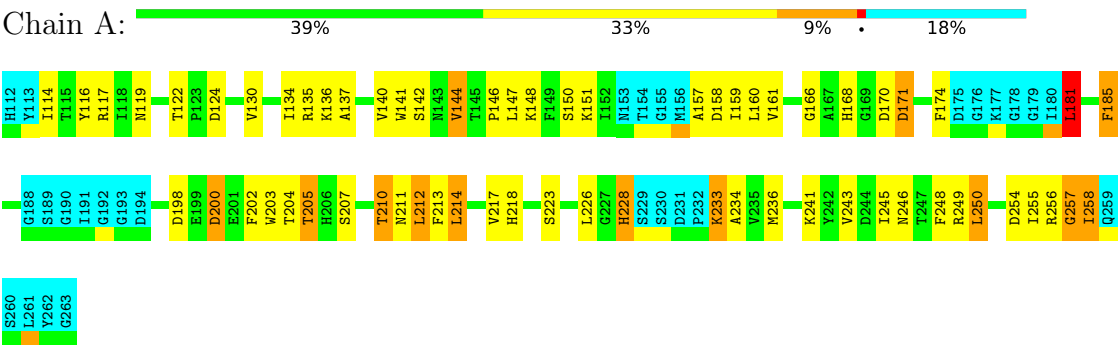
4.2.19 Score per residue for model 19

- 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	structure solution	ParamagneticCyana
CYANA	refinement	ParamagneticCyana

No chemical shift data was provided.

6 Model quality [i](#)

6.1 Standard geometry [i](#)

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 [i](#)

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	995	946	946	24±6
All	All	19920	18920	18920	476

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:214:LEU:HD11	1:A:243:VAL:HG12	0.97	1.35	7	1
1:A:137:ALA:HB2	1:A:216:ALA:HB1	0.93	1.40	3	2
1:A:212:LEU:HD11	1:A:214:LEU:HD12	0.93	1.39	6	1
1:A:144:VAL:HG13	1:A:145:THR:HG23	0.87	1.46	10	1
1:A:144:VAL:HG11	1:A:258:ILE:HG23	0.84	1.47	13	1
1:A:140:VAL:HG11	1:A:217:VAL:HG13	0.80	1.51	14	6
1:A:214:LEU:HD22	1:A:243:VAL:HG22	0.78	1.55	17	1
1:A:250:LEU:HD22	1:A:250:LEU:C	0.75	2.07	20	3
1:A:214:LEU:HD21	1:A:243:VAL:HG22	0.74	1.57	5	2
1:A:144:VAL:HG11	1:A:258:ILE:HG22	0.73	1.60	12	1
1:A:140:VAL:HG13	1:A:250:LEU:HD13	0.72	1.61	12	1
1:A:140:VAL:HG21	1:A:217:VAL:HG13	0.72	1.60	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:118:ILE:HG22	1:A:161:VAL:HG21	0.72	1.59	11	1
1:A:140:VAL:HG13	1:A:250:LEU:HD22	0.70	1.62	16	1
1:A:145:THR:HG22	1:A:147:LEU:HD23	0.70	1.63	15	1
1:A:212:LEU:HD13	1:A:245:ILE:HG22	0.69	1.65	6	1
1:A:140:VAL:HG21	1:A:217:VAL:HG22	0.67	1.65	14	4
1:A:213:PHE:CD1	1:A:245:ILE:HD13	0.67	2.24	19	1
1:A:141:TRP:CZ3	1:A:258:ILE:HD13	0.67	2.24	20	1
1:A:250:LEU:HD13	1:A:255:ILE:HD11	0.67	1.67	7	1
1:A:235:VAL:HG12	1:A:243:VAL:HG12	0.66	1.66	12	1
1:A:140:VAL:HG22	1:A:258:ILE:HG22	0.66	1.65	17	1
1:A:250:LEU:HD13	1:A:250:LEU:N	0.66	2.06	5	1
1:A:235:VAL:HG13	1:A:241:LYS:HB2	0.65	1.68	15	1
1:A:205:THR:HG21	1:A:212:LEU:HD23	0.65	1.68	20	1
1:A:137:ALA:O	1:A:140:VAL:HG12	0.64	1.92	13	7
1:A:130:VAL:HG13	1:A:213:PHE:CE1	0.64	2.28	17	1
1:A:126:ASN:O	1:A:130:VAL:HG23	0.64	1.91	12	7
1:A:164:ALA:HB1	1:A:169:GLY:CA	0.64	2.23	10	1
1:A:114:ILE:HG21	1:A:148:LYS:HE2	0.64	1.68	11	1
1:A:140:VAL:HG23	1:A:255:ILE:HG12	0.64	1.67	7	1
1:A:249:ARG:O	1:A:250:LEU:HD23	0.64	1.93	16	1
1:A:226:LEU:CA	1:A:258:ILE:HD13	0.63	2.24	15	1
1:A:203:TRP:CB	1:A:210:THR:HG22	0.63	2.23	20	1
1:A:217:VAL:HG11	1:A:235:VAL:HG21	0.63	1.71	18	1
1:A:205:THR:HG22	1:A:209:GLY:CA	0.62	2.24	15	1
1:A:224:LEU:HD23	1:A:258:ILE:HD11	0.62	1.72	13	1
1:A:205:THR:O	1:A:212:LEU:HD22	0.62	1.94	16	2
1:A:133:ALA:HB1	1:A:213:PHE:CG	0.62	2.30	4	1
1:A:141:TRP:O	1:A:145:THR:HG23	0.62	1.95	13	3
1:A:197:PHE:CE1	1:A:215:THR:HG21	0.62	2.29	12	1
1:A:225:GLY:HA3	1:A:258:ILE:HG23	0.61	1.71	7	1
1:A:186:GLY:HA2	1:A:224:LEU:HD23	0.61	1.72	5	1
1:A:122:THR:HG21	1:A:203:TRP:NE1	0.61	2.11	18	1
1:A:115:THR:CG2	1:A:152:ILE:HD13	0.61	2.25	1	1
1:A:144:VAL:HG12	1:A:255:ILE:O	0.61	1.96	7	1
1:A:122:THR:HG21	1:A:203:TRP:CE2	0.61	2.30	18	1
1:A:224:LEU:HD22	1:A:258:ILE:CG2	0.60	2.26	5	1
1:A:136:LYS:O	1:A:140:VAL:HG23	0.60	1.96	3	4
1:A:144:VAL:HG22	1:A:255:ILE:O	0.60	1.96	4	2
1:A:181:LEU:HD22	1:A:212:LEU:HD12	0.60	1.72	5	1
1:A:144:VAL:HG23	1:A:145:THR:HG23	0.60	1.73	3	1
1:A:211:ASN:ND2	1:A:215:THR:HG21	0.60	2.11	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:114:ILE:HG21	1:A:148:LYS:CE	0.59	2.26	11	1
1:A:252:ALA:O	1:A:255:ILE:HG22	0.59	1.96	6	1
1:A:164:ALA:HB1	1:A:169:GLY:HA2	0.59	1.71	10	1
1:A:214:LEU:CD2	1:A:243:VAL:HG22	0.59	2.27	17	2
1:A:203:TRP:HB2	1:A:210:THR:HG22	0.59	1.73	20	1
1:A:146:PRO:O	1:A:147:LEU:HD22	0.59	1.97	20	1
1:A:181:LEU:HD21	1:A:240:TYR:CZ	0.59	2.32	17	1
1:A:140:VAL:O	1:A:144:VAL:HG23	0.59	1.96	8	3
1:A:224:LEU:HB3	1:A:258:ILE:HD11	0.59	1.75	11	1
1:A:140:VAL:HG11	1:A:217:VAL:CG1	0.59	2.26	14	2
1:A:195:ALA:HB2	1:A:220:ILE:HA	0.59	1.74	7	1
1:A:144:VAL:HG22	1:A:255:ILE:HA	0.59	1.74	8	1
1:A:114:ILE:HD13	1:A:159:ILE:HD13	0.59	1.74	15	1
1:A:250:LEU:CB	1:A:255:ILE:HD11	0.59	2.28	9	1
1:A:144:VAL:HG21	1:A:258:ILE:HD13	0.58	1.74	14	1
1:A:161:VAL:HG23	1:A:195:ALA:CB	0.58	2.28	14	1
1:A:216:ALA:O	1:A:220:ILE:HG22	0.58	1.98	12	7
1:A:214:LEU:HD22	1:A:242:TYR:HA	0.58	1.74	5	1
1:A:144:VAL:CG1	1:A:258:ILE:HG22	0.58	2.27	12	1
1:A:224:LEU:HB3	1:A:258:ILE:HD12	0.58	1.75	18	1
1:A:116:TYR:HB2	1:A:159:ILE:HG23	0.58	1.74	10	1
1:A:115:THR:HB	1:A:152:ILE:HG21	0.58	1.76	1	1
1:A:214:LEU:HD13	1:A:243:VAL:CG2	0.58	2.28	14	1
1:A:214:LEU:HD22	1:A:243:VAL:HG13	0.58	1.75	14	1
1:A:145:THR:CG2	1:A:147:LEU:HD23	0.58	2.28	15	1
1:A:133:ALA:HB1	1:A:213:PHE:CE1	0.58	2.34	1	1
1:A:165:ARG:O	1:A:166:GLY:C	0.58	2.44	5	2
1:A:137:ALA:O	1:A:140:VAL:HG22	0.58	1.99	10	1
1:A:214:LEU:HB2	1:A:245:ILE:HG22	0.57	1.76	2	1
1:A:144:VAL:HG21	1:A:258:ILE:HG13	0.57	1.74	3	1
1:A:151:LYS:O	1:A:152:ILE:HD13	0.57	1.99	6	3
1:A:197:PHE:CZ	1:A:215:THR:HG21	0.57	2.33	12	2
1:A:130:VAL:O	1:A:134:ILE:HG22	0.57	1.99	13	1
1:A:213:PHE:O	1:A:217:VAL:HG23	0.57	1.99	20	1
1:A:250:LEU:HD13	1:A:258:ILE:HG13	0.57	1.76	2	1
1:A:144:VAL:HG12	1:A:255:ILE:HD13	0.57	1.75	3	1
1:A:116:TYR:CB	1:A:159:ILE:HG23	0.57	2.29	10	1
1:A:140:VAL:HG21	1:A:217:VAL:CG2	0.57	2.28	14	1
1:A:161:VAL:HG23	1:A:195:ALA:HB3	0.57	1.75	14	1
1:A:217:VAL:HG21	1:A:248:PHE:CE1	0.57	2.34	20	1
1:A:217:VAL:HG12	1:A:250:LEU:HD21	0.57	1.75	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:116:TYR:HA	1:A:159:ILE:HD11	0.57	1.76	1	2
1:A:137:ALA:CB	1:A:216:ALA:HB1	0.57	2.28	2	2
1:A:220:ILE:HG12	1:A:224:LEU:HD12	0.57	1.75	7	2
1:A:144:VAL:CG1	1:A:258:ILE:HG23	0.57	2.26	13	1
1:A:159:ILE:HG12	1:A:224:LEU:HD23	0.57	1.76	9	1
1:A:136:LYS:HD2	1:A:245:ILE:HD12	0.57	1.76	10	1
1:A:226:LEU:HD13	1:A:228:HIS:CE1	0.57	2.35	11	1
1:A:214:LEU:HD13	1:A:243:VAL:HG21	0.57	1.77	14	1
1:A:214:LEU:HD22	1:A:240:TYR:CB	0.57	2.30	16	1
1:A:116:TYR:CZ	1:A:157:ALA:HB3	0.57	2.35	20	1
1:A:224:LEU:HD12	1:A:258:ILE:CG2	0.57	2.30	14	3
1:A:140:VAL:HG22	1:A:258:ILE:CG2	0.57	2.29	17	2
1:A:161:VAL:HG23	1:A:195:ALA:HB1	0.56	1.77	19	1
1:A:118:ILE:CG2	1:A:161:VAL:HG21	0.56	2.30	11	1
1:A:223:SER:HB2	1:A:224:LEU:HD22	0.56	1.75	15	1
1:A:115:THR:HG22	1:A:150:SER:HB3	0.56	1.75	2	2
1:A:181:LEU:HD22	1:A:212:LEU:CD1	0.56	2.30	5	1
1:A:116:TYR:CE1	1:A:157:ALA:HB3	0.56	2.34	20	1
1:A:142:SER:HA	1:A:147:LEU:HD11	0.56	1.76	1	1
1:A:120:ASN:O	1:A:161:VAL:HG21	0.56	2.00	3	1
1:A:250:LEU:O	1:A:255:ILE:HD11	0.56	2.01	3	1
1:A:145:THR:HG22	1:A:147:LEU:CD1	0.56	2.30	9	1
1:A:115:THR:O	1:A:152:ILE:HG22	0.56	2.00	19	1
1:A:250:LEU:HD13	1:A:255:ILE:CD1	0.56	2.30	7	1
1:A:217:VAL:CG1	1:A:235:VAL:HG21	0.56	2.31	18	1
1:A:141:TRP:CE3	1:A:258:ILE:HD13	0.56	2.36	8	1
1:A:125:MET:HE2	1:A:129:ASP:OD2	0.55	2.02	4	1
1:A:181:LEU:HD22	1:A:238:PRO:HB2	0.55	1.78	18	1
1:A:212:LEU:HD23	1:A:213:PHE:CE1	0.55	2.36	1	1
1:A:115:THR:CG2	1:A:152:ILE:HG21	0.55	2.31	16	1
1:A:212:LEU:CD1	1:A:245:ILE:HG22	0.55	2.31	6	1
1:A:212:LEU:HD12	1:A:213:PHE:CD2	0.55	2.36	7	1
1:A:137:ALA:HB2	1:A:213:PHE:O	0.55	2.01	10	1
1:A:250:LEU:C	1:A:250:LEU:CD2	0.55	2.80	14	3
1:A:213:PHE:CE1	1:A:245:ILE:HD13	0.55	2.36	19	1
1:A:254:ASP:OD2	1:A:255:ILE:HG23	0.55	2.01	2	1
1:A:124:ASP:OD2	1:A:204:THR:HG23	0.55	2.01	6	1
1:A:213:PHE:HB2	1:A:245:ILE:HG23	0.55	1.77	20	1
1:A:162:VAL:HG13	1:A:172:HIS:CB	0.55	2.32	11	1
1:A:182:ALA:HB1	1:A:222:HIS:CG	0.55	2.37	12	1
1:A:116:TYR:CB	1:A:152:ILE:HD13	0.54	2.32	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:114:ILE:HD13	1:A:159:ILE:CD1	0.54	2.32	15	1
1:A:141:TRP:HB3	1:A:224:LEU:HD13	0.54	1.77	7	2
1:A:141:TRP:CD1	1:A:224:LEU:HD13	0.54	2.38	1	1
1:A:184:ALA:HB3	1:A:223:SER:HA	0.54	1.79	11	2
1:A:211:ASN:O	1:A:212:LEU:HD23	0.54	2.02	7	1
1:A:241:LYS:O	1:A:243:VAL:HG13	0.54	2.03	9	1
1:A:184:ALA:CB	1:A:226:LEU:HD21	0.54	2.32	2	1
1:A:212:LEU:HD21	1:A:240:TYR:CD2	0.53	2.38	4	1
1:A:124:ASP:O	1:A:130:VAL:HG21	0.53	2.04	6	1
1:A:243:VAL:O	1:A:245:ILE:HG23	0.53	2.03	12	2
1:A:205:THR:HG23	1:A:208:GLY:O	0.53	2.04	16	1
1:A:144:VAL:HG22	1:A:257:GLY:C	0.53	2.28	17	1
1:A:182:ALA:HB2	1:A:219:GLU:OE1	0.53	2.04	5	1
1:A:160:LEU:O	1:A:195:ALA:HB2	0.53	2.04	6	1
1:A:141:TRP:CB	1:A:224:LEU:HD13	0.53	2.33	7	1
1:A:136:LYS:CD	1:A:245:ILE:HD12	0.53	2.32	10	1
1:A:234:ALA:HB3	1:A:251:SER:HB2	0.53	1.80	16	1
1:A:140:VAL:HG23	1:A:255:ILE:CG1	0.53	2.34	7	1
1:A:214:LEU:HD11	1:A:242:TYR:CB	0.53	2.33	3	1
1:A:167:ALA:O	1:A:168:HIS:C	0.53	2.51	9	2
1:A:221:GLY:HA3	1:A:235:VAL:HG21	0.53	1.80	2	1
1:A:144:VAL:HG13	1:A:145:THR:CG2	0.53	2.29	10	1
1:A:214:LEU:HD21	1:A:243:VAL:C	0.53	2.29	13	1
1:A:212:LEU:HD23	1:A:213:PHE:CD1	0.53	2.38	1	1
1:A:220:ILE:HG13	1:A:224:LEU:HD12	0.53	1.81	19	1
1:A:140:VAL:CG1	1:A:250:LEU:HD22	0.52	2.34	16	1
1:A:214:LEU:CG	1:A:243:VAL:HG12	0.52	2.34	18	1
1:A:140:VAL:HA	1:A:250:LEU:HD23	0.52	1.80	18	1
1:A:137:ALA:HB1	1:A:220:ILE:HD12	0.52	1.80	4	1
1:A:243:VAL:HG21	1:A:249:ARG:HG3	0.52	1.80	10	1
1:A:133:ALA:HB1	1:A:213:PHE:CD2	0.52	2.39	18	1
1:A:141:TRP:CH2	1:A:258:ILE:HD13	0.52	2.39	20	1
1:A:137:ALA:HB1	1:A:220:ILE:HG13	0.52	1.82	3	1
1:A:195:ALA:HB1	1:A:219:GLU:CG	0.52	2.35	3	1
1:A:114:ILE:HG23	1:A:158:ASP:HB2	0.52	1.82	14	1
1:A:118:ILE:HG21	1:A:134:ILE:CG2	0.52	2.35	15	1
1:A:140:VAL:O	1:A:258:ILE:HG23	0.52	2.05	17	1
1:A:140:VAL:HG22	1:A:250:LEU:HD11	0.52	1.80	11	1
1:A:160:LEU:HD12	1:A:160:LEU:O	0.52	2.05	16	1
1:A:138:PHE:CE1	1:A:184:ALA:HB2	0.52	2.40	5	1
1:A:137:ALA:CB	1:A:216:ALA:HB3	0.52	2.35	10	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:138:PHE:CD1	1:A:220:ILE:HG21	0.52	2.40	5	1
1:A:140:VAL:HG23	1:A:250:LEU:HG	0.52	1.81	5	1
1:A:195:ALA:HB1	1:A:197:PHE:CE1	0.52	2.40	17	1
1:A:217:VAL:CG1	1:A:250:LEU:HD21	0.51	2.36	2	2
1:A:213:PHE:CE1	1:A:245:ILE:HG21	0.51	2.40	8	1
1:A:236:MET:HE3	1:A:254:ASP:OD1	0.51	2.05	12	1
1:A:118:ILE:HG23	1:A:161:VAL:HB	0.51	1.80	14	1
1:A:212:LEU:HD22	1:A:242:TYR:HA	0.51	1.82	14	1
1:A:227:GLY:HA2	1:A:255:ILE:HG21	0.51	1.81	2	1
1:A:124:ASP:OD1	1:A:212:LEU:HD21	0.51	2.06	3	1
1:A:195:ALA:HB1	1:A:219:GLU:CD	0.51	2.31	11	1
1:A:141:TRP:O	1:A:145:THR:HG22	0.51	2.06	5	5
1:A:116:TYR:OH	1:A:224:LEU:HD21	0.51	2.05	16	1
1:A:184:ALA:HB1	1:A:226:LEU:HD21	0.51	1.83	2	1
1:A:214:LEU:HD11	1:A:243:VAL:HG22	0.51	1.82	10	1
1:A:182:ALA:HB1	1:A:222:HIS:NE2	0.51	2.21	15	1
1:A:115:THR:HG23	1:A:224:LEU:HD21	0.51	1.83	19	1
1:A:214:LEU:CD2	1:A:243:VAL:HG12	0.50	2.36	18	1
1:A:234:ALA:HB2	1:A:251:SER:HB3	0.50	1.83	5	1
1:A:217:VAL:HG11	1:A:250:LEU:HD11	0.50	1.83	3	1
1:A:224:LEU:HB3	1:A:258:ILE:HG23	0.50	1.82	5	2
1:A:215:THR:HG22	1:A:219:GLU:HG3	0.50	1.82	19	1
1:A:141:TRP:CE2	1:A:220:ILE:HG21	0.50	2.40	12	1
1:A:140:VAL:HG22	1:A:250:LEU:HB3	0.50	1.84	14	1
1:A:250:LEU:HD23	1:A:255:ILE:HD13	0.50	1.82	5	1
1:A:227:GLY:HA3	1:A:236:MET:HE3	0.50	1.83	14	1
1:A:118:ILE:HG21	1:A:134:ILE:HG21	0.50	1.83	3	3
1:A:235:VAL:HG22	1:A:251:SER:HB3	0.50	1.84	7	1
1:A:214:LEU:CG	1:A:243:VAL:HG22	0.50	2.37	11	1
1:A:130:VAL:HG22	1:A:207:SER:O	0.50	2.06	4	1
1:A:255:ILE:HG23	1:A:256:ARG:HG3	0.50	1.83	20	1
1:A:250:LEU:HD22	1:A:258:ILE:HD11	0.49	1.82	2	1
1:A:146:PRO:C	1:A:147:LEU:HD12	0.49	2.32	16	1
1:A:210:THR:O	1:A:211:ASN:C	0.49	2.55	18	1
1:A:227:GLY:CA	1:A:255:ILE:HG21	0.49	2.37	2	1
1:A:214:LEU:HD11	1:A:248:PHE:CD1	0.49	2.42	1	1
1:A:249:ARG:C	1:A:250:LEU:HD23	0.49	2.31	16	1
1:A:250:LEU:HB3	1:A:255:ILE:HD11	0.49	1.85	9	1
1:A:119:ASN:C	1:A:161:VAL:HG21	0.49	2.31	16	1
1:A:144:VAL:HG11	1:A:255:ILE:HB	0.49	1.82	16	1
1:A:158:ASP:HB3	1:A:159:ILE:HD12	0.49	1.84	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:140:VAL:CG1	1:A:250:LEU:HD13	0.49	2.35	12	1
1:A:250:LEU:HD13	1:A:255:ILE:HB	0.49	1.84	8	1
1:A:187:PRO:HG3	1:A:224:LEU:HD22	0.49	1.85	9	1
1:A:162:VAL:HG13	1:A:172:HIS:HB2	0.49	1.83	11	1
1:A:141:TRP:CZ2	1:A:220:ILE:HG21	0.49	2.42	12	1
1:A:168:HIS:C	1:A:173:ALA:HB2	0.49	2.32	15	1
1:A:144:VAL:HG21	1:A:258:ILE:HA	0.49	1.84	19	1
1:A:225:GLY:HA3	1:A:258:ILE:HD12	0.49	1.83	1	1
1:A:138:PHE:CE2	1:A:159:ILE:HG21	0.49	2.42	2	1
1:A:211:ASN:C	1:A:212:LEU:HD23	0.49	2.32	7	1
1:A:250:LEU:HD12	1:A:250:LEU:O	0.48	2.08	8	1
1:A:224:LEU:HD23	1:A:258:ILE:CD1	0.48	2.36	13	1
1:A:115:THR:CG2	1:A:224:LEU:HD21	0.48	2.38	19	1
1:A:141:TRP:CD1	1:A:224:LEU:HD22	0.48	2.43	19	1
1:A:212:LEU:O	1:A:216:ALA:HB2	0.48	2.07	13	2
1:A:182:ALA:HB3	1:A:238:PRO:HA	0.48	1.84	15	1
1:A:205:THR:C	1:A:212:LEU:HD13	0.48	2.33	18	1
1:A:235:VAL:HG13	1:A:251:SER:HB2	0.48	1.84	7	1
1:A:195:ALA:HB1	1:A:219:GLU:OE1	0.48	2.08	11	1
1:A:197:PHE:CG	1:A:210:THR:HG21	0.48	2.44	14	1
1:A:223:SER:C	1:A:224:LEU:HD13	0.48	2.32	15	1
1:A:115:THR:HG22	1:A:149:PHE:C	0.48	2.33	8	1
1:A:205:THR:HG21	1:A:211:ASN:O	0.48	2.08	14	1
1:A:224:LEU:CB	1:A:258:ILE:HD11	0.48	2.39	11	1
1:A:115:THR:HG21	1:A:152:ILE:HD13	0.48	1.85	1	1
1:A:115:THR:HG22	1:A:150:SER:CB	0.48	2.39	2	1
1:A:226:LEU:HD13	1:A:228:HIS:NE2	0.48	2.24	11	1
1:A:204:THR:HG21	1:A:209:GLY:H	0.47	1.69	11	1
1:A:144:VAL:HG21	1:A:254:ASP:CB	0.47	2.38	15	1
1:A:141:TRP:CZ3	1:A:258:ILE:HG21	0.47	2.43	8	1
1:A:205:THR:CG2	1:A:212:LEU:HD23	0.47	2.38	20	1
1:A:250:LEU:HD21	1:A:255:ILE:HB	0.47	1.85	20	1
1:A:133:ALA:HB1	1:A:213:PHE:CZ	0.47	2.45	1	1
1:A:218:HIS:HA	1:A:235:VAL:HG23	0.47	1.84	2	1
1:A:217:VAL:HG11	1:A:250:LEU:HD21	0.47	1.86	17	1
1:A:250:LEU:HD22	1:A:258:ILE:HB	0.47	1.85	17	1
1:A:214:LEU:HD21	1:A:243:VAL:HG12	0.47	1.86	18	1
1:A:226:LEU:HD12	1:A:236:MET:HA	0.47	1.87	2	1
1:A:257:GLY:C	1:A:258:ILE:HD12	0.47	2.35	14	2
1:A:226:LEU:HA	1:A:258:ILE:HD13	0.47	1.87	15	1
1:A:214:LEU:HD12	1:A:243:VAL:CG1	0.47	2.40	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:181:LEU:HD11	1:A:198:ASP:CG	0.47	2.35	15	1
1:A:252:ALA:HB3	1:A:255:ILE:HB	0.47	1.85	17	1
1:A:222:HIS:HA	1:A:226:LEU:HD22	0.47	1.87	2	1
1:A:195:ALA:HB1	1:A:219:GLU:HG2	0.47	1.87	3	1
1:A:184:ALA:HB1	1:A:224:LEU:HG	0.47	1.87	5	1
1:A:205:THR:HG22	1:A:207:SER:H	0.47	1.69	19	1
1:A:184:ALA:HB3	1:A:222:HIS:CG	0.46	2.45	4	1
1:A:220:ILE:HG22	1:A:224:LEU:HD12	0.46	1.86	11	1
1:A:214:LEU:HG	1:A:243:VAL:HG12	0.46	1.86	18	1
1:A:224:LEU:HD22	1:A:258:ILE:HG22	0.46	1.85	5	1
1:A:250:LEU:N	1:A:250:LEU:CD1	0.46	2.77	5	1
1:A:250:LEU:CD2	1:A:258:ILE:HD12	0.46	2.41	17	1
1:A:114:ILE:HG21	1:A:158:ASP:CB	0.46	2.41	20	1
1:A:202:PHE:O	1:A:203:TRP:C	0.46	2.57	2	2
1:A:122:THR:HG21	1:A:209:GLY:CA	0.46	2.40	4	1
1:A:124:ASP:HB2	1:A:130:VAL:HG21	0.46	1.85	20	1
1:A:214:LEU:HD13	1:A:243:VAL:HG13	0.46	1.88	4	1
1:A:169:GLY:HA2	1:A:173:ALA:HB2	0.46	1.88	5	1
1:A:212:LEU:HD11	1:A:214:LEU:CD1	0.46	2.27	6	1
1:A:212:LEU:HD13	1:A:245:ILE:CG2	0.46	2.40	6	1
1:A:158:ASP:C	1:A:159:ILE:HD12	0.46	2.36	9	1
1:A:214:LEU:HD22	1:A:240:TYR:HB3	0.46	1.88	16	1
1:A:140:VAL:HG21	1:A:250:LEU:HD13	0.46	1.86	1	1
1:A:159:ILE:HG23	1:A:159:ILE:O	0.46	2.11	7	1
1:A:181:LEU:HD22	1:A:238:PRO:O	0.46	2.11	2	1
1:A:218:HIS:CE1	1:A:236:MET:HE3	0.45	2.45	4	1
1:A:140:VAL:C	1:A:258:ILE:HG23	0.45	2.36	17	1
1:A:217:VAL:CG1	1:A:250:LEU:HD11	0.45	2.42	3	1
1:A:235:VAL:HG22	1:A:241:LYS:HB3	0.45	1.88	15	1
1:A:214:LEU:HD13	1:A:243:VAL:CG1	0.45	2.42	4	1
1:A:213:PHE:O	1:A:216:ALA:HB3	0.45	2.12	9	1
1:A:116:TYR:CB	1:A:157:ALA:HB3	0.45	2.42	18	1
1:A:144:VAL:HG12	1:A:255:ILE:HG23	0.45	1.88	1	1
1:A:141:TRP:CE2	1:A:258:ILE:HD12	0.45	2.45	9	1
1:A:140:VAL:HG23	1:A:250:LEU:CG	0.45	2.41	5	1
1:A:234:ALA:HB2	1:A:251:SER:H	0.45	1.71	19	1
1:A:158:ASP:HB3	1:A:220:ILE:HD13	0.45	1.87	10	1
1:A:143:ASN:CG	1:A:250:LEU:HD22	0.45	2.37	18	1
1:A:243:VAL:HG21	1:A:249:ARG:CG	0.45	2.41	10	1
1:A:138:PHE:CE1	1:A:220:ILE:HG21	0.44	2.47	5	1
1:A:247:THR:O	1:A:248:PHE:C	0.44	2.59	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:141:TRP:CZ3	1:A:224:LEU:HD22	0.44	2.47	17	1
1:A:258:ILE:O	1:A:258:ILE:HG22	0.44	2.12	18	1
1:A:142:SER:HB2	1:A:147:LEU:HD21	0.44	1.89	10	1
1:A:251:SER:O	1:A:252:ALA:HB3	0.44	2.13	17	1
1:A:205:THR:HG22	1:A:209:GLY:C	0.44	2.37	15	1
1:A:116:TYR:HB3	1:A:157:ALA:HB3	0.44	1.88	18	1
1:A:159:ILE:HD13	1:A:224:LEU:HD11	0.44	1.88	13	1
1:A:158:ASP:O	1:A:159:ILE:HG23	0.44	2.12	16	1
1:A:235:VAL:O	1:A:236:MET:C	0.44	2.60	16	1
1:A:214:LEU:HD12	1:A:243:VAL:HG12	0.44	1.89	20	1
1:A:250:LEU:HD13	1:A:258:ILE:CD1	0.44	2.43	2	1
1:A:144:VAL:HG12	1:A:255:ILE:CD1	0.44	2.41	3	1
1:A:116:TYR:HB2	1:A:152:ILE:HD13	0.44	1.89	8	1
1:A:187:PRO:HG3	1:A:224:LEU:HD13	0.44	1.88	16	1
1:A:247:THR:C	1:A:248:PHE:CG	0.44	2.96	13	1
1:A:214:LEU:HD21	1:A:244:ASP:N	0.43	2.28	13	1
1:A:250:LEU:HD22	1:A:250:LEU:O	0.43	2.11	13	2
1:A:187:PRO:HD3	1:A:220:ILE:HD12	0.43	1.90	14	1
1:A:119:ASN:OD1	1:A:195:ALA:HB3	0.43	2.13	2	1
1:A:181:LEU:HD11	1:A:198:ASP:HB2	0.43	1.88	15	1
1:A:145:THR:HG21	1:A:224:LEU:HD13	0.43	1.90	2	1
1:A:141:TRP:CH2	1:A:147:LEU:HD22	0.43	2.49	14	1
1:A:214:LEU:CD2	1:A:243:VAL:HG13	0.43	2.42	14	1
1:A:118:ILE:H	1:A:118:ILE:HD13	0.43	1.73	11	1
1:A:205:THR:HG23	1:A:207:SER:H	0.43	1.73	2	1
1:A:145:THR:HG23	1:A:148:LYS:HE3	0.43	1.90	11	1
1:A:133:ALA:HB1	1:A:213:PHE:CD1	0.43	2.49	1	2
1:A:145:THR:O	1:A:147:LEU:HD23	0.43	2.13	5	1
1:A:204:THR:CG2	1:A:212:LEU:HD13	0.43	2.43	9	1
1:A:250:LEU:O	1:A:250:LEU:HD22	0.43	2.14	5	1
1:A:215:THR:HG22	1:A:219:GLU:CG	0.43	2.43	19	2
1:A:142:SER:HA	1:A:147:LEU:HD22	0.42	1.89	5	1
1:A:158:ASP:CG	1:A:159:ILE:HD13	0.42	2.39	19	1
1:A:205:THR:HG21	1:A:212:LEU:HB3	0.42	1.89	6	1
1:A:214:LEU:HD21	1:A:241:LYS:O	0.42	2.14	9	1
1:A:140:VAL:HG13	1:A:250:LEU:CD2	0.42	2.39	16	1
1:A:187:PRO:HD2	1:A:224:LEU:HD23	0.42	1.91	19	1
1:A:120:ASN:HB2	1:A:161:VAL:HG23	0.42	1.90	10	1
1:A:116:TYR:HA	1:A:159:ILE:HG23	0.42	1.91	12	1
1:A:216:ALA:O	1:A:220:ILE:HD12	0.42	2.15	8	1
1:A:235:VAL:HG13	1:A:241:LYS:CB	0.42	2.42	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:147:LEU:HD21	1:A:187:PRO:HB2	0.42	1.91	16	1
1:A:181:LEU:HD21	1:A:198:ASP:HB2	0.42	1.92	15	1
1:A:250:LEU:HD22	1:A:258:ILE:HD12	0.42	1.91	17	1
1:A:114:ILE:HG21	1:A:158:ASP:CG	0.42	2.40	18	1
1:A:220:ILE:HD13	1:A:224:LEU:HD12	0.42	1.91	1	1
1:A:234:ALA:HB1	1:A:236:MET:SD	0.42	2.54	6	1
1:A:134:ILE:HD12	1:A:158:ASP:OD1	0.42	2.14	10	1
1:A:212:LEU:HD13	1:A:242:TYR:HB3	0.42	1.91	14	1
1:A:250:LEU:HD13	1:A:258:ILE:CG1	0.42	2.44	2	1
1:A:205:THR:HG22	1:A:206:HIS:CD2	0.42	2.50	11	1
1:A:168:HIS:O	1:A:173:ALA:HB2	0.42	2.15	15	1
1:A:214:LEU:HD21	1:A:243:VAL:HB	0.42	1.90	16	1
1:A:137:ALA:HA	1:A:217:VAL:HG22	0.42	1.91	1	1
1:A:214:LEU:HD21	1:A:242:TYR:CA	0.42	2.45	3	1
1:A:140:VAL:HG22	1:A:258:ILE:HG23	0.42	1.90	19	1
1:A:144:VAL:HG11	1:A:258:ILE:HA	0.41	1.90	19	1
1:A:160:LEU:HD12	1:A:161:VAL:H	0.41	1.74	20	1
1:A:198:ASP:CB	1:A:210:THR:HG23	0.41	2.45	8	1
1:A:114:ILE:C	1:A:115:THR:CG2	0.41	2.93	11	1
1:A:258:ILE:HG23	1:A:258:ILE:O	0.41	2.15	20	1
1:A:130:VAL:HG13	1:A:212:LEU:HD23	0.41	1.93	3	1
1:A:235:VAL:HG11	1:A:254:ASP:OD2	0.41	2.14	5	1
1:A:181:LEU:HD21	1:A:240:TYR:CE1	0.41	2.50	17	1
1:A:145:THR:HG21	1:A:224:LEU:CD1	0.41	2.45	18	1
1:A:158:ASP:CB	1:A:159:ILE:HD13	0.41	2.45	19	1
1:A:223:SER:O	1:A:224:LEU:HD13	0.41	2.16	15	1
1:A:214:LEU:HD11	1:A:243:VAL:HB	0.41	1.92	16	1
1:A:250:LEU:HD13	1:A:255:ILE:HG21	0.41	1.92	16	1
1:A:205:THR:HG22	1:A:209:GLY:N	0.41	2.31	15	1
1:A:137:ALA:HB2	1:A:216:ALA:CB	0.41	2.46	9	1
1:A:142:SER:CB	1:A:147:LEU:HD21	0.41	2.46	10	1
1:A:118:ILE:HG22	1:A:161:VAL:CG2	0.41	2.39	11	1
1:A:244:ASP:CG	1:A:247:THR:HG22	0.41	2.40	6	1
1:A:130:VAL:HG13	1:A:212:LEU:CD2	0.41	2.45	3	1
1:A:165:ARG:CD	1:A:173:ALA:HB1	0.41	2.46	5	1
1:A:165:ARG:HD2	1:A:173:ALA:HB1	0.41	1.92	5	1
1:A:214:LEU:HD12	1:A:245:ILE:CG2	0.41	2.46	8	1
1:A:122:THR:HG23	1:A:124:ASP:OD2	0.41	2.16	11	1
1:A:137:ALA:HB1	1:A:217:VAL:HG23	0.41	1.93	13	1
1:A:133:ALA:HB1	1:A:213:PHE:HB3	0.41	1.92	15	1
1:A:118:ILE:CG2	1:A:134:ILE:HD11	0.41	2.45	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:217:VAL:HG21	1:A:248:PHE:CE2	0.41	2.51	19	1
1:A:118:ILE:HA	1:A:161:VAL:HG21	0.41	1.91	1	1
1:A:206:HIS:NE2	1:A:212:LEU:HD13	0.41	2.31	1	1
1:A:222:HIS:CE1	1:A:226:LEU:HD13	0.41	2.51	2	1
1:A:217:VAL:HG21	1:A:250:LEU:CD1	0.41	2.45	4	1
1:A:141:TRP:CH2	1:A:145:THR:HG23	0.41	2.51	17	1
1:A:250:LEU:N	1:A:250:LEU:HD22	0.41	2.31	19	1
1:A:115:THR:CG2	1:A:157:ALA:HB1	0.40	2.45	7	1
1:A:115:THR:HG21	1:A:152:ILE:HB	0.40	1.93	9	1
1:A:224:LEU:O	1:A:258:ILE:HD11	0.40	2.16	11	1
1:A:159:ILE:HD13	1:A:159:ILE:N	0.40	2.31	12	1
1:A:250:LEU:HD13	1:A:255:ILE:CG2	0.40	2.46	16	1
1:A:244:ASP:O	1:A:245:ILE:C	0.40	2.63	4	1
1:A:144:VAL:HG13	1:A:255:ILE:O	0.40	2.16	6	1
1:A:206:HIS:HB2	1:A:214:LEU:HD13	0.40	1.92	8	1
1:A:142:SER:HB2	1:A:147:LEU:HD11	0.40	1.92	10	1
1:A:181:LEU:HD11	1:A:240:TYR:CE1	0.40	2.51	17	1
1:A:214:LEU:HG	1:A:243:VAL:HG22	0.40	1.93	11	1
1:A:145:THR:OG1	1:A:147:LEU:HD13	0.40	2.17	16	1
1:A:245:ILE:HD12	1:A:245:ILE:O	0.40	2.16	18	1
1:A:119:ASN:O	1:A:161:VAL:HG13	0.40	2.17	2	1
1:A:181:LEU:HD11	1:A:197:PHE:CZ	0.40	2.51	5	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	124/152 (82%)	87±4 (70±3%)	26±3 (21±3%)	12±3 (9±2%)	1	10
All	All	2480/3040 (82%)	1733 (70%)	514 (21%)	233 (9%)	1	10

All 50 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	166	GLY	20
1	A	258	ILE	11
1	A	236	MET	10
1	A	171	ASP	8
1	A	233	LYS	8
1	A	173	ALA	7
1	A	124	ASP	7
1	A	168	HIS	7
1	A	147	LEU	7
1	A	120	ASN	6
1	A	174	PHE	6
1	A	226	LEU	6
1	A	185	PHE	6
1	A	198	ASP	6
1	A	203	TRP	6
1	A	172	HIS	6
1	A	195	ALA	6
1	A	201	GLU	6
1	A	199	GLU	6
1	A	181	LEU	5
1	A	209	GLY	5
1	A	212	LEU	5
1	A	200	ASP	5
1	A	211	ASN	5
1	A	252	ALA	4
1	A	158	ASP	4
1	A	159	ILE	4
1	A	228	HIS	4
1	A	170	ASP	4
1	A	248	PHE	3
1	A	144	VAL	3
1	A	234	ALA	3
1	A	125	MET	3
1	A	202	PHE	3
1	A	245	ILE	3
1	A	146	PRO	2
1	A	210	THR	2
1	A	227	GLY	2
1	A	208	GLY	2
1	A	257	GLY	2
1	A	169	GLY	2
1	A	225	GLY	2
1	A	253	ASP	2

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Mol	Chain	Res	Type	Models (Total)
1	A	123	PRO	2
1	A	237	PHE	2
1	A	150	SER	1
1	A	205	THR	1
1	A	184	ALA	1
1	A	183	HIS	1
1	A	242	TYR	1

6.3.2 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 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	103/122 (84%)	75±4 (73±4%)	28±4 (27±4%)	1	20
All	All	2060/2440 (84%)	1494 (73%)	566 (27%)	1	20

All 84 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	125	MET	17
1	A	117	ARG	14
1	A	226	LEU	14
1	A	214	LEU	13
1	A	223	SER	13
1	A	241	LYS	13
1	A	204	THR	12
1	A	183	HIS	12
1	A	236	MET	12
1	A	126	ASN	11
1	A	237	PHE	11
1	A	207	SER	11
1	A	181	LEU	11
1	A	205	THR	11
1	A	142	SER	10
1	A	151	LYS	10
1	A	212	LEU	10
1	A	247	THR	10

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Mol	Chain	Res	Type	Models (Total)
1	A	254	ASP	10
1	A	147	LEU	10
1	A	160	LEU	10
1	A	148	LYS	10
1	A	224	LEU	9
1	A	250	LEU	9
1	A	233	LYS	9
1	A	165	ARG	9
1	A	139	GLN	8
1	A	251	SER	8
1	A	170	ASP	8
1	A	136	LYS	8
1	A	249	ARG	8
1	A	128	GLU	7
1	A	158	ASP	7
1	A	228	HIS	7
1	A	239	THR	7
1	A	210	THR	7
1	A	256	ARG	7
1	A	253	ASP	7
1	A	171	ASP	7
1	A	135	ARG	6
1	A	199	GLU	6
1	A	219	GLU	6
1	A	124	ASP	6
1	A	172	HIS	6
1	A	185	PHE	6
1	A	200	ASP	6
1	A	245	ILE	6
1	A	118	ILE	6
1	A	244	ASP	6
1	A	127	ARG	6
1	A	132	TYR	6
1	A	122	THR	5
1	A	174	PHE	5
1	A	222	HIS	5
1	A	246	ASN	5
1	A	201	GLU	5
1	A	115	THR	5
1	A	159	ILE	5
1	A	150	SER	5
1	A	198	ASP	4

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Mol	Chain	Res	Type	Models (Total)
1	A	141	TRP	4
1	A	202	PHE	4
1	A	129	ASP	4
1	A	197	PHE	4
1	A	114	ILE	4
1	A	120	ASN	3
1	A	203	TRP	3
1	A	131	ASP	3
1	A	168	HIS	3
1	A	218	HIS	3
1	A	116	TYR	3
1	A	255	ILE	3
1	A	220	ILE	3
1	A	248	PHE	2
1	A	144	VAL	2
1	A	258	ILE	2
1	A	143	ASN	2
1	A	145	THR	2
1	A	138	PHE	2
1	A	206	HIS	2
1	A	211	ASN	2
1	A	215	THR	1
1	A	119	ASN	1
1	A	134	ILE	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 oligosaccharides 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