



Full wwPDB NMR Structure Validation Report ⓘ

Mar 6, 2026 – 11:33 PM UTC

PDB ID : 2JNP / pdb_00002jnp
BMRB ID : 15120
Title : Solution structure of matrix metalloproteinase 3 (MMP-3) in the presence of
N-isobutyl-N-[4-methoxyphenylsulfonyl]glycyl hydroxamic acid (NNGH)
Authors : Alcaraz, L.A.; Banci, L.; Bertini, I.; Cantini, F.; Donaire, A.; Gonnelli, L.
Deposited on : 2007-01-30

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
Mogul : 2022.3.0, CSD as543be (2022)
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
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

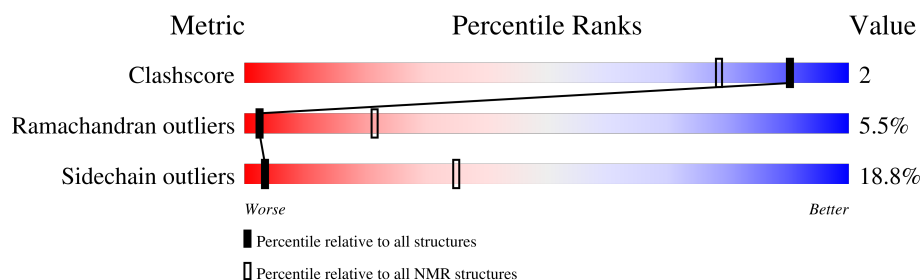
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 64%.

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	161	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA and RNA chains that are outliers for geometric criteria:

Mol	Chain	Compound	Res	Total models with violations	
				Chirality	Geometry
4	A	NGH	253	9	-

2 Ensemble composition and analysis

This entry contains 25 models. Model 14 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:89-A:247 (159)	1.05	14

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 2 clusters and 1 single-model cluster was found.

Cluster number	Models
1	1, 2, 3, 4, 5, 6, 7, 9, 10, 11, 12, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 25
2	8, 13
Single-model clusters	24

3 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 2533 atoms, of which 1230 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Matrix metalloproteinase-3.

Mol	Chain	Residues	Atoms						Trace
1	A	161	Total	C	H	N	O	S	0
			2489	818	1211	213	245	2	

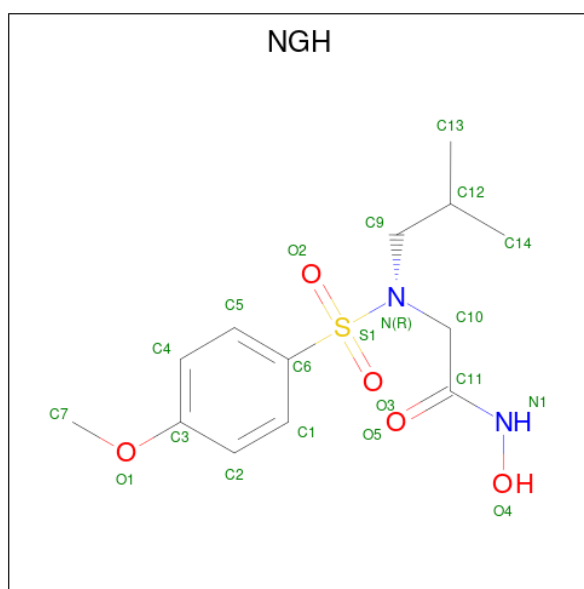
- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	
2	A	2	Total	Zn
			2	2

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	
3	A	2	Total	Ca
			2	2

- Molecule 4 is N-ISOBUTYL-N-[4-METHOXYPHENYLSULFONYL]GLYCYL HYDROX-AMIC ACID (CCD ID: NGH) (formula: C₁₃H₂₀N₂O₅S).



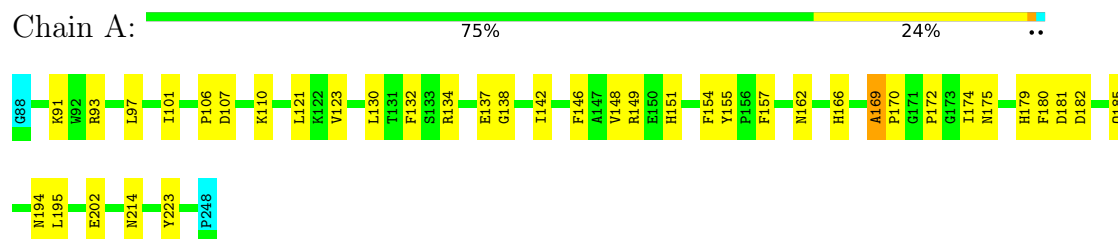
Mol	Chain	Residues	Atoms					
4	A	1	Total	C	H	N	O	S
			40	13	19	2	5	1

4 Residue-property plots [i](#)

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: Matrix metalloproteinase-3

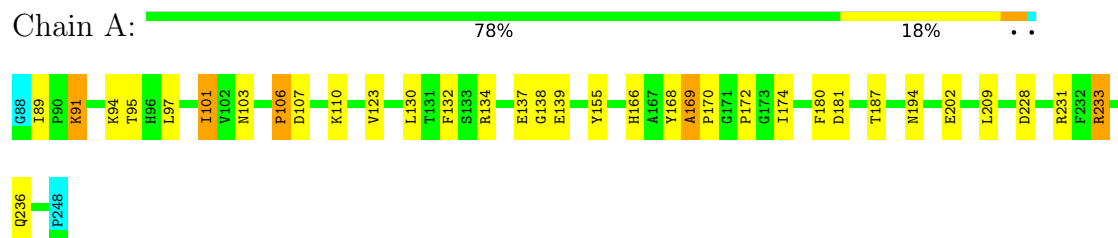


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

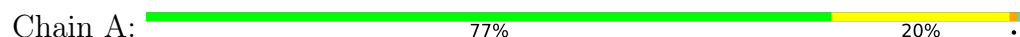
4.2.1 Score per residue for model 1

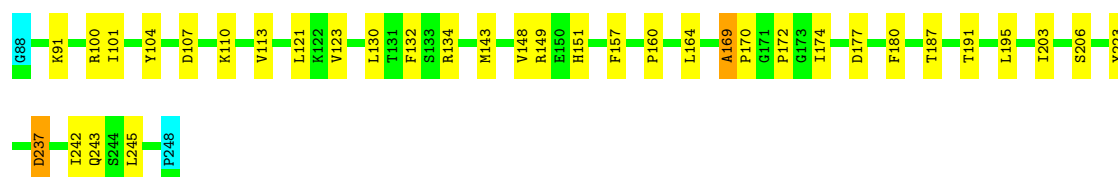
- Molecule 1: Matrix metalloproteinase-3



4.2.2 Score per residue for model 2

- Molecule 1: Matrix metalloproteinase-3

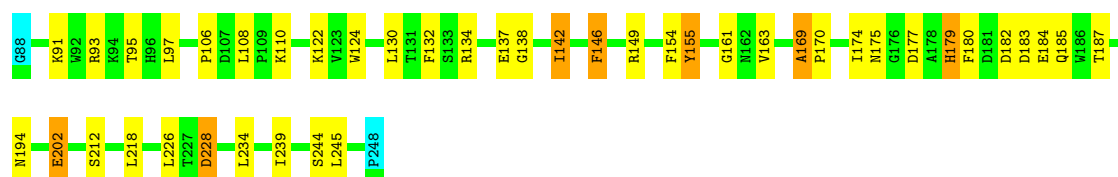




4.2.3 Score per residue for model 3

- Molecule 1: Matrix metalloproteinase-3

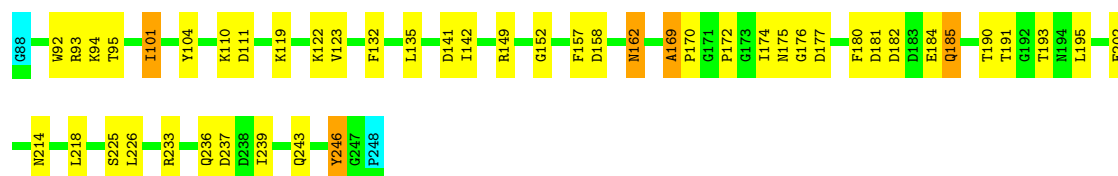
Chain A: 72% 22%



4.2.4 Score per residue for model 4

- Molecule 1: Matrix metalloproteinase-3

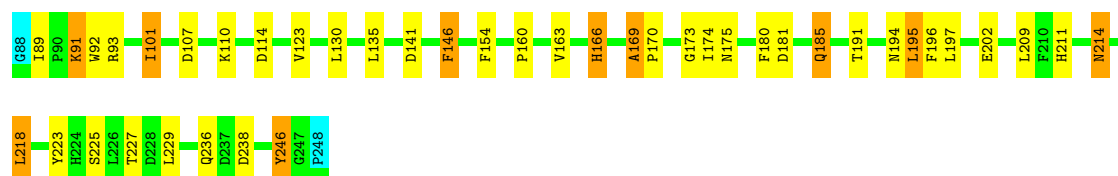
Chain A: 70% 26%



4.2.5 Score per residue for model 5

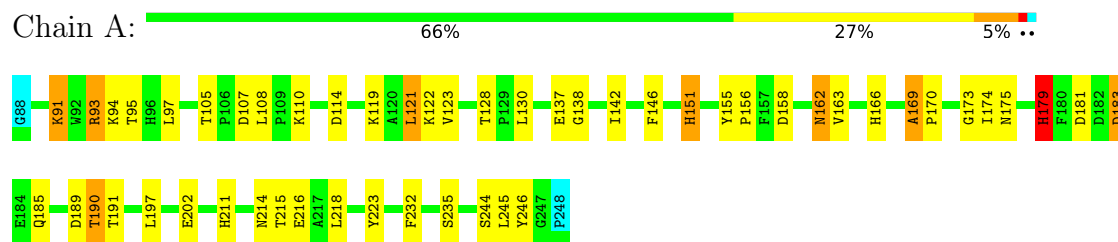
- Molecule 1: Matrix metalloproteinase-3

Chain A: 73% 20% 6%



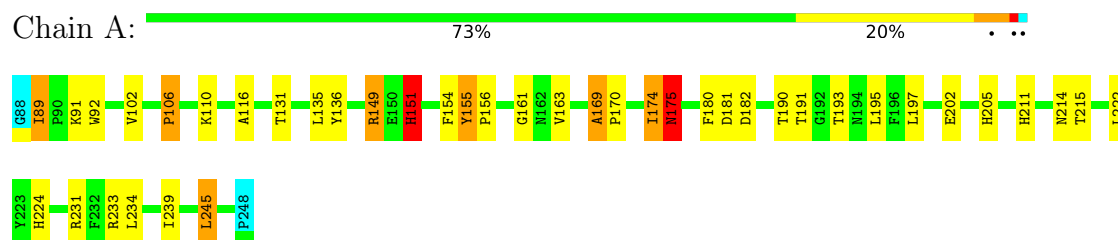
4.2.6 Score per residue for model 6

- Molecule 1: Matrix metalloproteinase-3



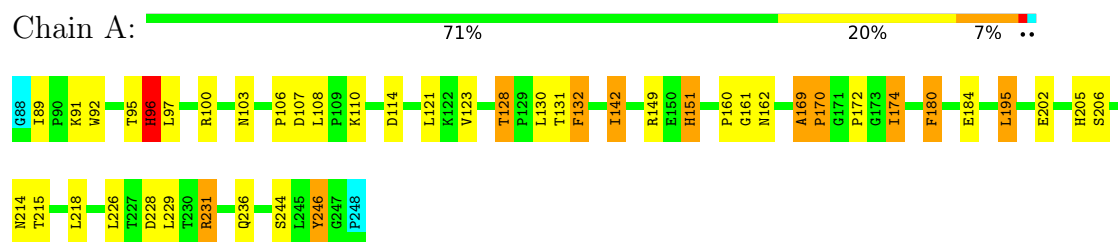
4.2.7 Score per residue for model 7

- Molecule 1: Matrix metalloproteinase-3



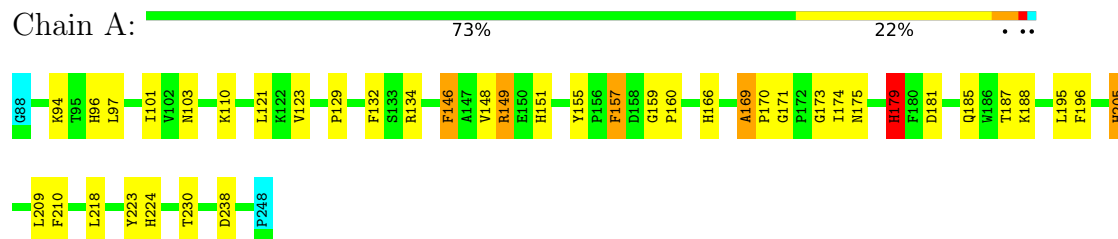
4.2.8 Score per residue for model 8

- Molecule 1: Matrix metalloproteinase-3



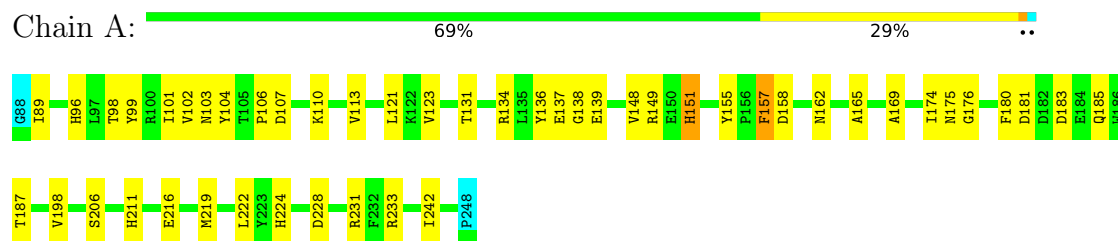
4.2.9 Score per residue for model 9

- Molecule 1: Matrix metalloproteinase-3



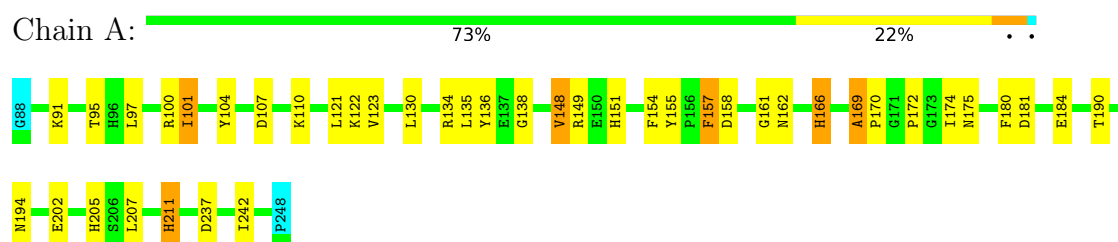
4.2.10 Score per residue for model 10

- Molecule 1: Matrix metalloproteinase-3



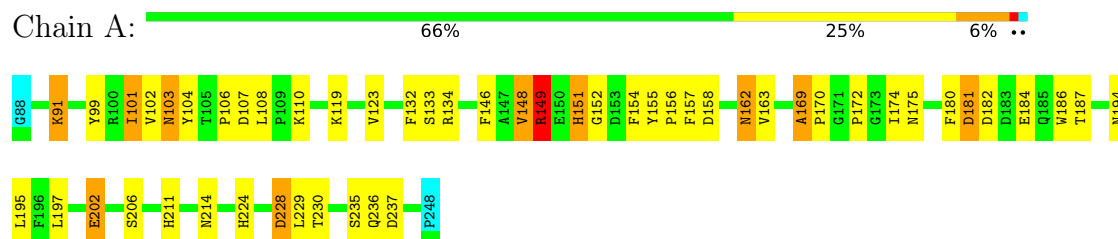
4.2.11 Score per residue for model 11

- Molecule 1: Matrix metalloproteinase-3



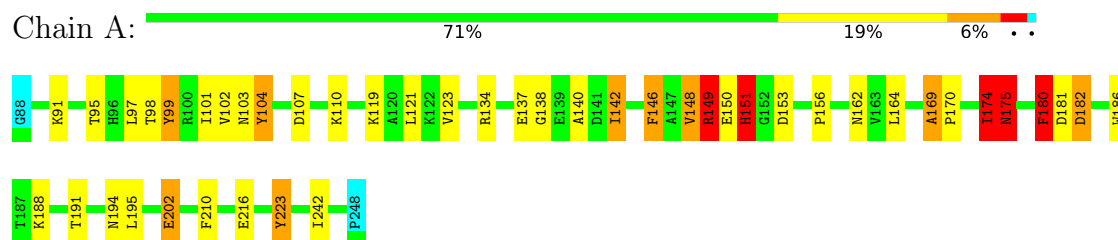
4.2.12 Score per residue for model 12

- Molecule 1: Matrix metalloproteinase-3



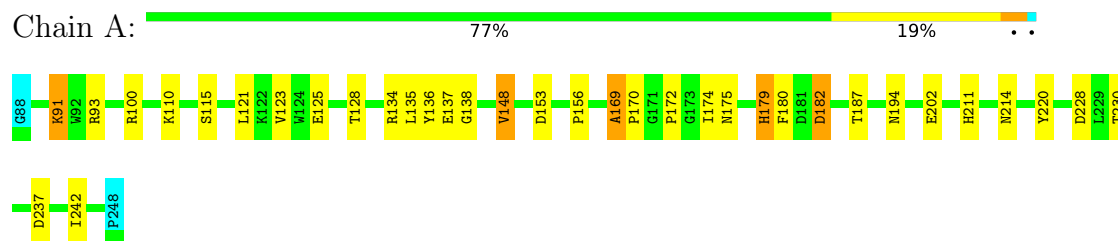
4.2.13 Score per residue for model 13

- Molecule 1: Matrix metalloproteinase-3



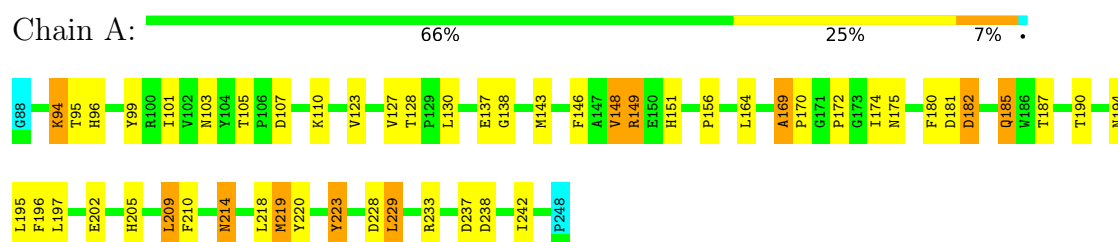
4.2.14 Score per residue for model 14 (medoid)

- Molecule 1: Matrix metalloproteinase-3



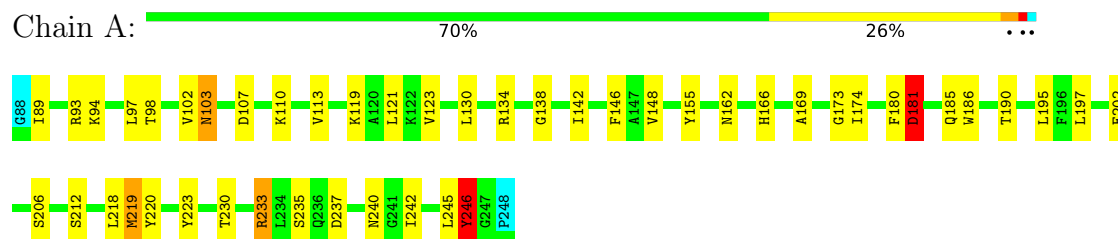
4.2.15 Score per residue for model 15

- Molecule 1: Matrix metalloproteinase-3



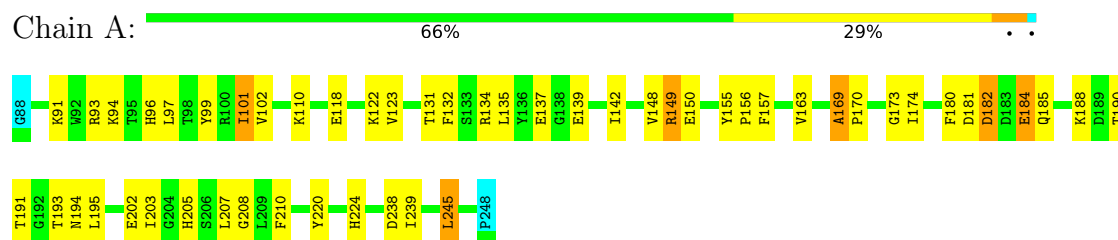
4.2.16 Score per residue for model 16

- Molecule 1: Matrix metalloproteinase-3



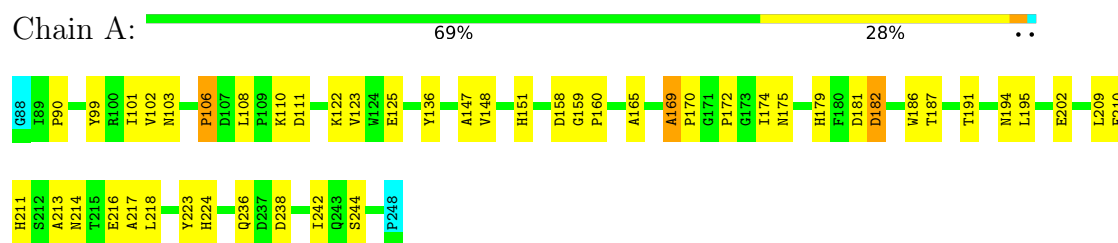
4.2.17 Score per residue for model 17

- Molecule 1: Matrix metalloproteinase-3



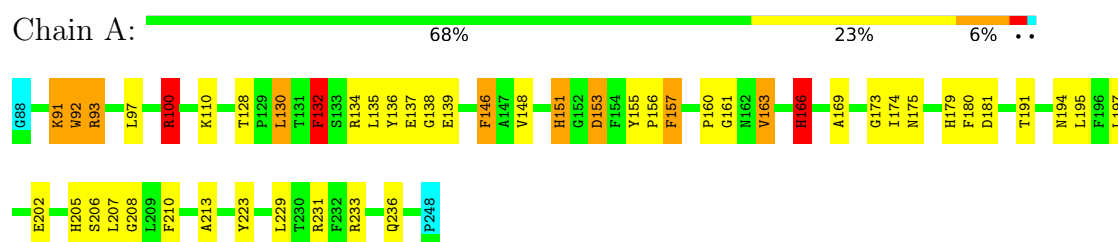
4.2.18 Score per residue for model 18

- Molecule 1: Matrix metalloproteinase-3



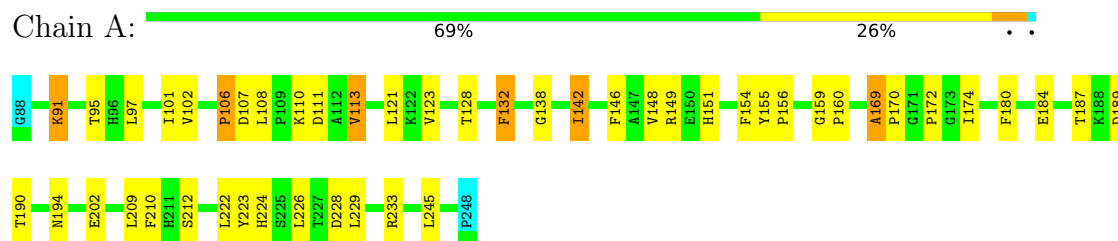
4.2.19 Score per residue for model 19

- Molecule 1: Matrix metalloproteinase-3



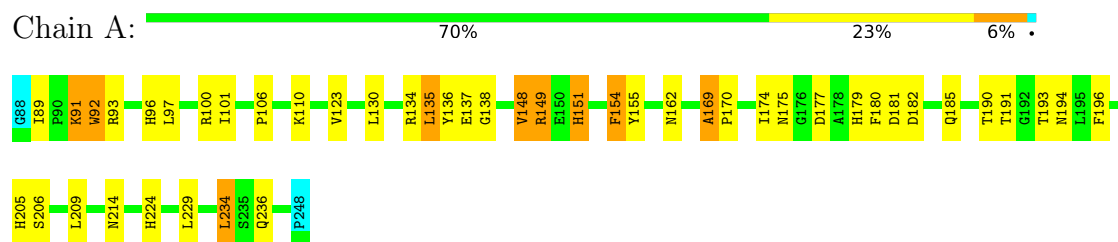
4.2.20 Score per residue for model 20

- Molecule 1: Matrix metalloproteinase-3



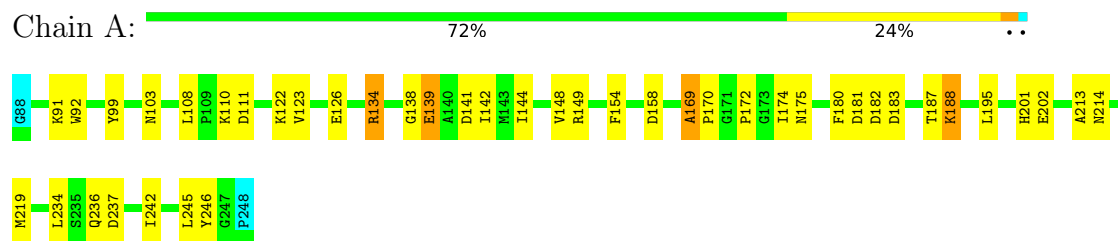
4.2.21 Score per residue for model 21

- Molecule 1: Matrix metalloproteinase-3



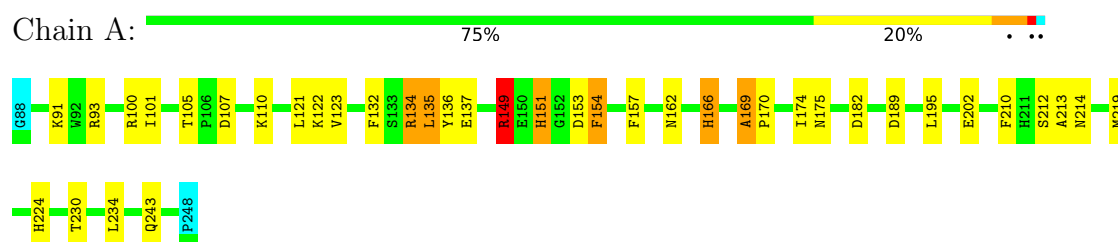
4.2.22 Score per residue for model 22

- Molecule 1: Matrix metalloproteinase-3



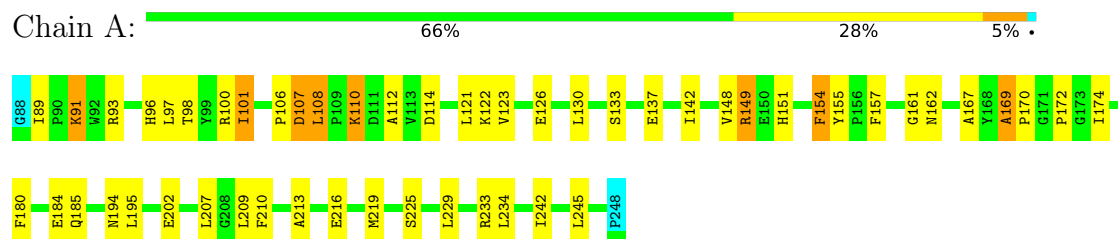
4.2.23 Score per residue for model 23

- Molecule 1: Matrix metalloproteinase-3



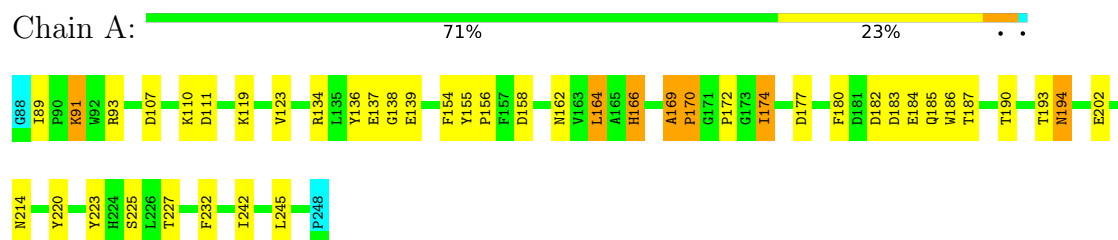
4.2.24 Score per residue for model 24

- Molecule 1: Matrix metalloproteinase-3



4.2.25 Score per residue for model 25

- Molecule 1: Matrix metalloproteinase-3



5 Refinement protocol and experimental data overview

The models were refined using the following method: *molecular dynamics*.

Of the 400 calculated structures, 25 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	
Amber	refinement	8
CSI	structure solution	2.0

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	1374
Number of shifts mapped to atoms	1374
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	64%

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: NGH, ZN, CA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the (average) root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.96±0.02	1±1/1305 (0.1± 0.0%)	1.60±0.04	12±4/1783 (0.7± 0.3%)
All	All	0.96	23/32625 (0.1%)	1.60	303/44575 (0.7%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	2.7±1.6
All	All	0	67

All unique bond outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	153	ASP	N-CA	6.08	1.53	1.46	13	1
1	A	228	ASP	CA-CB	5.89	1.61	1.52	1	1
1	A	202	GLU	CD-OE2	5.63	1.36	1.25	19	19
1	A	228	ASP	CA-C	5.59	1.59	1.53	14	1
1	A	158	ASP	CA-C	5.20	1.59	1.52	11	1

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	170	PRO	N-CA-CB	13.91	112.23	102.35	8	2
1	A	181	ASP	CA-CB-CG	9.89	122.49	112.60	17	14
1	A	180	PHE	CA-CB-CG	9.49	123.29	113.80	16	18

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	151	HIS	CB-CG-CD2	-9.01	119.49	131.20	13	8
1	A	153	ASP	CA-CB-CG	8.60	121.20	112.60	13	4
1	A	182	ASP	CA-CB-CG	8.54	121.14	112.60	23	9
1	A	185	GLN	OE1-CD-NE2	-8.50	114.10	122.60	4	5
1	A	157	PHE	CA-CB-CG	8.22	122.02	113.80	11	3
1	A	132	PHE	CA-CB-CG	8.09	121.89	113.80	20	5
1	A	175	ASN	CA-CB-CG	7.75	120.35	112.60	13	2
1	A	107	ASP	CA-CB-CG	7.66	120.26	112.60	23	7
1	A	196	PHE	CA-CB-CG	7.54	121.34	113.80	21	4
1	A	146	PHE	CA-CB-CG	7.48	121.28	113.80	5	6
1	A	161	GLY	O-C-N	7.27	129.16	122.77	3	2
1	A	184	GLU	N-CA-C	7.14	114.63	108.78	12	1
1	A	160	PRO	CA-C-N	7.11	126.74	119.92	8	4
1	A	160	PRO	C-N-CA	7.11	126.74	119.92	8	4
1	A	211	HIS	CA-CB-CG	-7.10	106.70	113.80	7	1
1	A	160	PRO	N-CA-CB	6.98	110.58	103.25	18	1
1	A	166	HIS	CA-CB-CG	6.96	120.76	113.80	9	4
1	A	183	ASP	CA-C-N	6.90	131.18	120.75	3	1
1	A	183	ASP	C-N-CA	6.90	131.18	120.75	3	1
1	A	160	PRO	N-CD-CG	6.89	113.54	103.20	9	1
1	A	162	ASN	CA-CB-CG	6.85	119.45	112.60	6	2
1	A	154	PHE	CA-C-N	6.74	128.21	122.28	5	1
1	A	154	PHE	C-N-CA	6.74	128.21	122.28	5	1
1	A	149	ARG	CA-C-N	6.72	132.73	122.37	7	3
1	A	149	ARG	C-N-CA	6.72	132.73	122.37	7	3
1	A	103	ASN	CA-CB-CG	6.71	119.31	112.60	15	6
1	A	174	ILE	N-CA-CB	6.57	117.80	110.51	13	1
1	A	114	ASP	CA-CB-CG	6.56	119.16	112.60	8	3
1	A	92	TRP	CA-C-N	6.54	134.03	121.54	21	3
1	A	92	TRP	C-N-CA	6.54	134.03	121.54	21	3
1	A	214	ASN	N-CA-CB	-6.54	102.54	112.28	18	1
1	A	211	HIS	CB-CG-CD2	-6.52	122.73	131.20	11	5
1	A	159	GLY	CA-C-O	-6.49	112.23	121.52	20	2
1	A	236	GLN	OE1-CD-NE2	-6.44	116.16	122.60	5	3
1	A	174	ILE	CA-CB-CG1	6.38	121.25	110.40	25	1
1	A	161	GLY	CA-C-N	6.34	130.84	120.63	8	4
1	A	161	GLY	C-N-CA	6.34	130.84	120.63	8	4
1	A	231	ARG	CD-NE-CZ	6.34	133.28	124.40	8	3
1	A	151	HIS	CA-CB-CG	6.34	120.14	113.80	15	2
1	A	96	HIS	CA-CB-CG	6.32	120.12	113.80	21	3
1	A	214	ASN	CA-C-N	6.31	129.37	120.28	21	4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	214	ASN	C-N-CA	6.31	129.37	120.28	21	4
1	A	184	GLU	CB-CG-CD	6.23	123.20	112.60	17	1
1	A	181	ASP	N-CA-C	6.21	119.31	107.75	4	4
1	A	136	TYR	CA-C-N	6.20	128.91	120.54	23	2
1	A	136	TYR	C-N-CA	6.20	128.91	120.54	23	2
1	A	157	PHE	N-CA-C	6.15	119.18	110.50	23	1
1	A	179	HIS	CA-CB-CG	6.15	119.95	113.80	3	2
1	A	111	ASP	CA-CB-CG	6.11	118.71	112.60	25	1
1	A	237	ASP	CA-CB-CG	6.06	118.66	112.60	4	4
1	A	194	ASN	CA-C-N	6.05	129.90	120.82	13	9
1	A	194	ASN	C-N-CA	6.05	129.90	120.82	13	9
1	A	238	ASP	CA-CB-CG	6.03	118.63	112.60	5	2
1	A	142	ILE	CA-CB-CG1	5.98	120.57	110.40	3	4
1	A	235	SER	CA-C-N	5.94	128.83	120.28	12	1
1	A	235	SER	C-N-CA	5.94	128.83	120.28	12	1
1	A	106	PRO	CA-C-N	5.82	128.33	120.65	24	6
1	A	106	PRO	C-N-CA	5.82	128.33	120.65	24	6
1	A	141	ASP	N-CA-C	-5.81	104.63	110.97	4	2
1	A	154	PHE	CA-CB-CG	5.81	119.61	113.80	24	2
1	A	209	LEU	CB-CA-C	5.78	120.10	109.46	15	1
1	A	211	HIS	CA-C-O	-5.76	114.42	120.58	7	1
1	A	148	VAL	N-CA-C	5.71	112.32	106.21	19	1
1	A	195	LEU	CA-C-N	5.70	128.19	120.44	5	1
1	A	195	LEU	C-N-CA	5.70	128.19	120.44	5	1
1	A	214	ASN	N-CA-C	5.67	119.51	112.47	18	1
1	A	139	GLU	CB-CG-CD	5.65	122.21	112.60	17	1
1	A	179	HIS	CB-CG-CD2	-5.65	123.85	131.20	6	4
1	A	214	ASN	CA-CB-CG	5.63	118.23	112.60	15	1
1	A	157	PHE	CA-C-N	5.60	127.72	120.44	9	1
1	A	157	PHE	C-N-CA	5.60	127.72	120.44	9	1
1	A	190	THR	CA-C-N	5.60	132.24	121.54	7	2
1	A	190	THR	C-N-CA	5.60	132.24	121.54	7	2
1	A	182	ASP	N-CA-C	5.59	120.59	111.37	17	1
1	A	162	ASN	N-CA-C	5.55	117.01	111.07	16	2
1	A	174	ILE	CB-CG1-CD1	-5.55	102.14	113.80	25	1
1	A	155	TYR	CA-C-N	5.55	126.78	119.84	7	1
1	A	155	TYR	C-N-CA	5.55	126.78	119.84	7	1
1	A	128	THR	CA-C-N	5.53	126.75	119.84	14	1
1	A	128	THR	C-N-CA	5.53	126.75	119.84	14	1
1	A	177	ASP	CB-CA-C	5.51	118.84	109.80	4	1
1	A	159	GLY	CA-C-N	5.50	126.72	119.84	18	2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	159	GLY	C-N-CA	5.50	126.72	119.84	18	2
1	A	205	HIS	CB-CG-CD2	-5.49	124.07	131.20	9	2
1	A	189	ASP	CA-CB-CG	5.47	118.07	112.60	23	1
1	A	151	HIS	CB-CG-ND1	5.47	130.90	122.70	10	2
1	A	246	TYR	CA-CB-CG	5.46	123.73	113.90	16	1
1	A	196	PHE	N-CA-CB	-5.43	102.19	110.07	5	1
1	A	228	ASP	CA-CB-CG	-5.36	107.24	112.60	3	2
1	A	186	TRP	CA-C-N	5.34	129.72	122.19	12	1
1	A	186	TRP	C-N-CA	5.34	129.72	122.19	12	1
1	A	89	ILE	N-CA-CB	5.34	118.69	111.21	7	1
1	A	194	ASN	CA-CB-CG	-5.32	107.28	112.60	3	1
1	A	210	PHE	CA-CB-CG	5.30	119.10	113.80	18	1
1	A	162	ASN	CA-C-N	5.28	131.47	121.97	12	1
1	A	162	ASN	C-N-CA	5.28	131.47	121.97	12	1
1	A	113	VAL	CA-CB-CG1	5.27	119.36	110.40	20	1
1	A	224	HIS	CB-CG-CD2	-5.26	124.37	131.20	23	1
1	A	110	LYS	CA-C-N	5.26	128.06	120.38	24	1
1	A	110	LYS	C-N-CA	5.26	128.06	120.38	24	1
1	A	166	HIS	CB-CG-CD2	-5.25	124.38	131.20	19	2
1	A	177	ASP	CA-CB-CG	5.23	117.83	112.60	21	1
1	A	243	GLN	OE1-CD-NE2	-5.23	117.37	122.60	2	1
1	A	231	ARG	NE-CZ-NH1	5.20	126.70	121.50	8	1
1	A	183	ASP	CB-CA-C	5.19	119.79	110.81	6	1
1	A	170	PRO	CA-N-CD	-5.18	104.75	112.00	8	1
1	A	177	ASP	N-CA-C	5.17	117.16	108.73	2	1
1	A	121	LEU	CB-CA-C	5.17	119.37	110.79	6	1
1	A	153	ASP	N-CA-C	-5.17	107.11	113.41	13	1
1	A	237	ASP	CA-C-N	5.17	127.16	120.44	15	1
1	A	237	ASP	C-N-CA	5.17	127.16	120.44	15	1
1	A	91	LYS	CB-CG-CD	5.14	123.12	111.30	19	1
1	A	185	GLN	CA-C-N	5.12	131.32	121.54	25	1
1	A	185	GLN	C-N-CA	5.12	131.32	121.54	25	1
1	A	229	LEU	N-CA-C	5.07	118.56	112.38	15	1
1	A	206	SER	CA-C-N	5.05	128.68	120.60	21	1
1	A	206	SER	C-N-CA	5.05	128.68	120.60	21	1
1	A	118	GLU	CA-C-N	5.04	127.35	120.54	17	1
1	A	118	GLU	C-N-CA	5.04	127.35	120.54	17	1
1	A	167	ALA	N-CA-C	5.04	115.95	108.60	24	1
1	A	171	GLY	CA-C-N	5.03	126.03	120.45	9	1
1	A	171	GLY	C-N-CA	5.03	126.03	120.45	9	1
1	A	139	GLU	N-CA-CB	5.02	118.98	110.49	22	1

There are no chirality outliers.

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

Mol	Chain	Res	Type	Group	Models (Total)
1	A	223	TYR	Sidechain	7
1	A	134	ARG	Sidechain	7
1	A	100	ARG	Sidechain	6
1	A	155	TYR	Sidechain	6
1	A	233	ARG	Sidechain	5
1	A	93	ARG	Sidechain	5
1	A	246	TYR	Sidechain	4
1	A	151	HIS	Sidechain	4
1	A	149	ARG	Sidechain	4
1	A	104	TYR	Sidechain	3
1	A	99	TYR	Sidechain	3
1	A	231	ARG	Sidechain	2
1	A	179	HIS	Sidechain	2
1	A	232	PHE	Sidechain	2
1	A	211	HIS	Sidechain	2
1	A	168	TYR	Sidechain	1
1	A	180	PHE	Sidechain	1
1	A	181	ASP	Sidechain	1
1	A	220	TYR	Sidechain	1
1	A	166	HIS	Sidechain	1

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	1266	1199	1198	4±2
4	A	21	19	20	0±0
All	All	32275	30450	30447	108

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 2.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:169:ALA:HB3	1:A:170:PRO:HD3	0.59	1.74	9	20
1:A:219:MET:HE2	1:A:220:TYR:N	0.57	2.14	16	2
1:A:165:ALA:HB1	1:A:202:GLU:CD	0.56	2.25	18	1
1:A:91:LYS:HE2	1:A:169:ALA:HB1	0.56	1.77	20	3
1:A:100:ARG:NH2	1:A:135:LEU:HD12	0.56	2.14	21	1
1:A:91:LYS:CE	1:A:169:ALA:HB1	0.56	2.31	20	2
1:A:176:GLY:HA2	1:A:206:SER:HB2	0.53	1.80	10	1
1:A:169:ALA:HB3	1:A:170:PRO:CD	0.53	2.34	14	11
1:A:164:LEU:HD21	1:A:193:THR:HG23	0.53	1.81	25	1
1:A:130:LEU:HD21	1:A:132:PHE:CD2	0.52	2.39	19	1
1:A:146:PHE:CZ	1:A:180:PHE:CD2	0.52	2.97	13	1
1:A:148:VAL:HG22	1:A:149:ARG:H	0.51	1.66	11	5
1:A:234:LEU:HD23	1:A:234:LEU:H	0.51	1.66	23	1
1:A:101:ILE:HD12	1:A:101:ILE:H	0.50	1.66	4	7
1:A:134:ARG:C	1:A:135:LEU:HD23	0.49	2.32	23	1
1:A:100:ARG:HH21	1:A:135:LEU:C	0.49	2.15	21	1
1:A:209:LEU:HD11	1:A:238:ASP:HA	0.47	1.85	9	1
1:A:100:ARG:HH22	1:A:135:LEU:HD12	0.47	1.69	21	1
1:A:212:SER:OG	1:A:219:MET:HE3	0.47	2.09	16	1
1:A:146:PHE:CD1	1:A:180:PHE:HB2	0.47	2.45	13	1
1:A:216:GLU:CD	1:A:216:GLU:H	0.46	2.18	24	1
1:A:108:LEU:HD13	1:A:112:ALA:CB	0.46	2.40	24	1
1:A:104:TYR:HA	1:A:113:VAL:HG11	0.46	1.88	2	2
1:A:128:THR:HB	1:A:246:TYR:CE1	0.46	2.46	8	1
1:A:116:ALA:HB2	1:A:195:LEU:HD13	0.46	1.88	7	1
1:A:208:GLY:HA3	1:A:245:LEU:HD11	0.46	1.88	17	1
4:A:253:NGH:H133	4:A:253:NGH:H102	0.46	1.88	20	1
1:A:174:ILE:O	1:A:175:ASN:C	0.46	2.58	13	2
1:A:216:GLU:N	1:A:216:GLU:CD	0.45	2.75	6	1
1:A:100:ARG:HH21	1:A:139:GLU:C	0.45	2.19	19	1
1:A:99:TYR:CE2	1:A:121:LEU:HD22	0.44	2.48	13	1
1:A:146:PHE:CD2	1:A:186:TRP:CH2	0.44	3.06	13	1
1:A:107:ASP:CG	1:A:185:GLN:HE21	0.44	2.21	24	1
1:A:234:LEU:H	1:A:234:LEU:CD2	0.44	2.26	24	1
1:A:94:LYS:HE3	1:A:96:HIS:O	0.43	2.13	15	1
1:A:116:ALA:HB2	1:A:195:LEU:CD1	0.43	2.44	7	1
1:A:213:ALA:HA	1:A:217:ALA:HB3	0.43	1.90	18	1
1:A:103:ASN:HB2	1:A:146:PHE:CD1	0.43	2.48	16	1
1:A:101:ILE:HD12	1:A:101:ILE:N	0.43	2.29	17	1
1:A:146:PHE:CE1	1:A:180:PHE:CG	0.42	3.06	13	1
1:A:103:ASN:HB2	1:A:146:PHE:CD2	0.42	2.49	12	1
1:A:169:ALA:HB2	1:A:205:HIS:O	0.42	2.14	17	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:169:ALA:CB	1:A:170:PRO:CD	0.42	2.98	23	3
1:A:234:LEU:H	1:A:234:LEU:HD22	0.42	1.74	21	1
1:A:197:LEU:CD2	4:A:253:NGH:H71	0.42	2.44	6	1
1:A:98:THR:HG22	1:A:133:SER:HB3	0.42	1.92	24	1
1:A:165:ALA:HB3	1:A:198:VAL:CG1	0.42	2.44	10	1
1:A:188:LYS:HA	1:A:188:LYS:HE2	0.42	1.90	22	1
1:A:101:ILE:H	1:A:101:ILE:HD12	0.42	1.74	24	1
1:A:211:HIS:CD2	1:A:211:HIS:N	0.41	2.88	18	1
1:A:101:ILE:N	1:A:101:ILE:HD12	0.41	2.31	11	1
1:A:91:LYS:HE3	1:A:169:ALA:C	0.41	2.41	23	1
1:A:147:ALA:HB1	1:A:151:HIS:CG	0.41	2.51	18	1
1:A:108:LEU:HD12	1:A:195:LEU:CD2	0.41	2.46	8	1
1:A:103:ASN:HB2	1:A:146:PHE:CG	0.40	2.52	13	1
1:A:197:LEU:HD23	1:A:197:LEU:C	0.40	2.41	15	1
1:A:96:HIS:HA	1:A:131:THR:O	0.40	2.17	8	1
1:A:169:ALA:HB2	1:A:206:SER:HA	0.40	1.94	8	1
1:A:99:TYR:CE2	1:A:132:PHE:CG	0.40	3.09	12	1
1:A:142:ILE:HG23	1:A:176:GLY:O	0.40	2.16	4	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	159/161 (99%)	126±4 (79±3%)	24±4 (15±3%)	9±2 (6±1%)	2	21
All	All	3975/4025 (99%)	3146 (79%)	609 (15%)	220 (6%)	2	21

All 45 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	169	ALA	25
1	A	175	ASN	16
1	A	149	ARG	15
1	A	91	LYS	14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	138	GLY	14
1	A	148	VAL	14
1	A	172	PRO	13
1	A	156	PRO	10
1	A	154	PHE	9
1	A	106	PRO	8
1	A	190	THR	7
1	A	137	GLU	6
1	A	162	ASN	6
1	A	173	GLY	6
1	A	163	VAL	5
1	A	139	GLU	4
1	A	213	ALA	4
1	A	245	LEU	3
1	A	93	ARG	3
1	A	89	ILE	3
1	A	228	ASP	3
1	A	224	HIS	3
1	A	194	ASN	3
1	A	152	GLY	2
1	A	225	SER	2
1	A	229	LEU	2
1	A	210	PHE	2
1	A	218	LEU	1
1	A	191	THR	1
1	A	174	ILE	1
1	A	129	PRO	1
1	A	157	PHE	1
1	A	195	LEU	1
1	A	140	ALA	1
1	A	182	ASP	1
1	A	185	GLN	1
1	A	90	PRO	1
1	A	216	GLU	1
1	A	160	PRO	1
1	A	208	GLY	1
1	A	223	TYR	1
1	A	212	SER	1
1	A	219	MET	1
1	A	183	ASP	1
1	A	186	TRP	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	134/135 (99%)	109±4 (81±3%)	25±4 (19±3%)	3	35
All	All	3350/3375 (99%)	2719 (81%)	631 (19%)	3	35

All 116 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	110	LYS	25
1	A	174	ILE	25
1	A	123	VAL	22
1	A	195	LEU	14
1	A	97	LEU	13
1	A	101	ILE	13
1	A	151	HIS	13
1	A	130	LEU	12
1	A	187	THR	12
1	A	121	LEU	11
1	A	242	ILE	11
1	A	91	LYS	10
1	A	134	ARG	10
1	A	155	TYR	10
1	A	95	THR	9
1	A	191	THR	9
1	A	122	LYS	9
1	A	142	ILE	9
1	A	218	LEU	9
1	A	135	LEU	9
1	A	214	ASN	9
1	A	132	PHE	8
1	A	166	HIS	8
1	A	107	ASP	8
1	A	157	PHE	8
1	A	245	LEU	8
1	A	184	GLU	8
1	A	102	VAL	8
1	A	94	LYS	7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	209	LEU	7
1	A	108	LEU	7
1	A	137	GLU	7
1	A	182	ASP	7
1	A	158	ASP	7
1	A	185	GLN	7
1	A	136	TYR	7
1	A	89	ILE	6
1	A	233	ARG	6
1	A	236	GLN	6
1	A	146	PHE	6
1	A	119	LYS	6
1	A	92	TRP	6
1	A	93	ARG	6
1	A	229	LEU	6
1	A	210	PHE	6
1	A	223	TYR	5
1	A	179	HIS	5
1	A	246	TYR	5
1	A	197	LEU	5
1	A	128	THR	5
1	A	205	HIS	5
1	A	224	HIS	5
1	A	180	PHE	5
1	A	230	THR	5
1	A	219	MET	5
1	A	164	LEU	4
1	A	206	SER	4
1	A	237	ASP	4
1	A	202	GLU	4
1	A	226	LEU	4
1	A	234	LEU	4
1	A	239	ILE	4
1	A	244	SER	4
1	A	111	ASP	4
1	A	162	ASN	4
1	A	193	THR	4
1	A	181	ASP	4
1	A	96	HIS	4
1	A	188	LYS	4
1	A	207	LEU	4
1	A	103	ASN	3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	163	VAL	3
1	A	228	ASP	3
1	A	105	THR	3
1	A	183	ASP	3
1	A	215	THR	3
1	A	131	THR	3
1	A	222	LEU	3
1	A	98	THR	3
1	A	99	TYR	3
1	A	194	ASN	3
1	A	143	MET	2
1	A	203	ILE	2
1	A	177	ASP	2
1	A	212	SER	2
1	A	104	TYR	2
1	A	190	THR	2
1	A	243	GLN	2
1	A	225	SER	2
1	A	227	THR	2
1	A	189	ASP	2
1	A	235	SER	2
1	A	154	PHE	2
1	A	216	GLU	2
1	A	150	GLU	2
1	A	100	ARG	2
1	A	125	GLU	2
1	A	148	VAL	2
1	A	220	TYR	2
1	A	113	VAL	2
1	A	186	TRP	2
1	A	238	ASP	2
1	A	126	GLU	2
1	A	149	ARG	2
1	A	124	TRP	1
1	A	175	ASN	1
1	A	114	ASP	1
1	A	231	ARG	1
1	A	133	SER	1
1	A	115	SER	1
1	A	127	VAL	1
1	A	240	ASN	1
1	A	153	ASP	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	141	ASP	1
1	A	144	ILE	1
1	A	201	HIS	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 5 ligands modelled in this entry, 4 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds for which Mogul statistics could be retrieved, the number of bonds that are observed in the model and the number of bonds that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length is the number of standard deviations the observed value is removed from the expected value. A bond length with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
4	NGH	A	253	2	21,21,21	1.73±0.09	4±1 (21±3%)

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of angles that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond angle is the number of standard deviations the observed value is removed from the expected value. A bond angle with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
4	NGH	A	253	2	29,29,29	1.42±0.23	5±2 (16±6%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NGH	A	253	2	1±0,1,5,5	0±0,24,24,24	0±0,1,1,1

All unique bond outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
4	A	253	NGH	O4-N1	5.30	1.27	1.40	9	25
4	A	253	NGH	C11-N1	3.81	1.36	1.32	23	21
4	A	253	NGH	O3-S1	3.79	1.47	1.43	4	21
4	A	253	NGH	O2-S1	3.63	1.47	1.43	24	23
4	A	253	NGH	C6-S1	3.55	1.81	1.76	21	21

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	253	NGH	C6-S1-N	6.97	115.69	107.28	5	17
4	A	253	NGH	O5-C11-N1	5.33	116.72	123.27	19	5
4	A	253	NGH	C12-C9-N	4.65	117.80	112.41	20	8
4	A	253	NGH	O2-S1-C6	4.22	102.86	108.10	20	13
4	A	253	NGH	O3-S1-O2	4.04	113.28	119.59	13	9
4	A	253	NGH	O3-S1-C6	3.84	103.33	108.10	16	17
4	A	253	NGH	O3-S1-N	3.70	103.20	106.69	5	7
4	A	253	NGH	C1-C6-S1	3.26	122.97	119.73	9	4
4	A	253	NGH	O2-S1-N	3.22	103.65	106.69	25	7
4	A	253	NGH	O4-N1-C11	3.12	124.41	119.79	21	10
4	A	253	NGH	C7-O1-C3	3.07	124.09	117.50	9	16
4	A	253	NGH	C10-C11-N1	2.75	122.29	115.64	11	1
4	A	253	NGH	C9-N-S1	2.65	123.10	117.32	17	5
4	A	253	NGH	O5-C11-C10	2.48	116.68	121.02	11	1
4	A	253	NGH	C5-C6-S1	2.22	117.53	119.73	9	1
4	A	253	NGH	C10-N-C9	2.16	111.28	116.35	16	1

All unique chiral outliers are listed below.

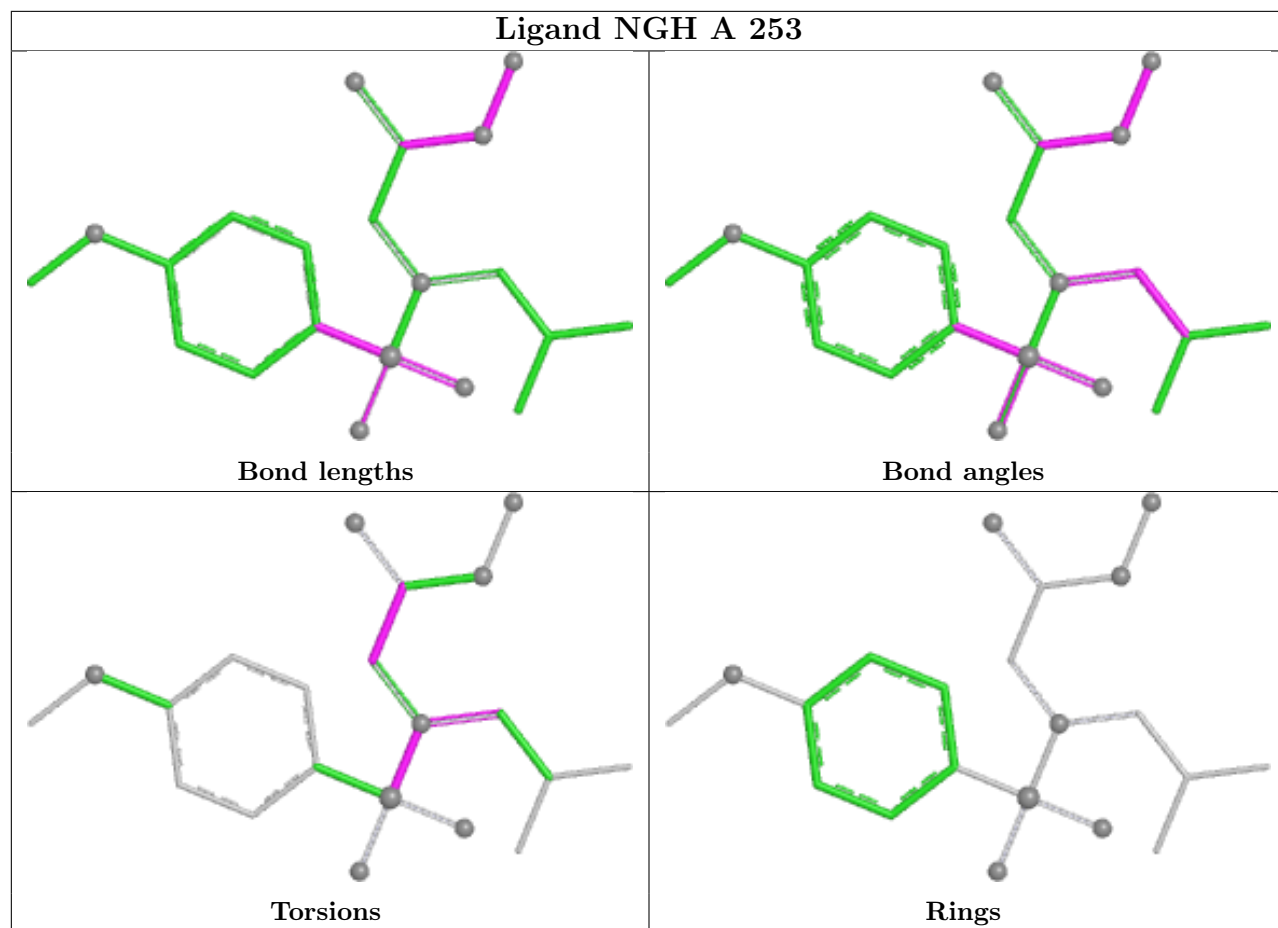
Mol	Chain	Res	Type	Atoms	Models (Total)
4	A	253	NGH	N	9

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

Mol	Chain	Res	Type	Atoms	Models (Total)
4	A	253	NGH	C10-C11-N1-O4	1
4	A	253	NGH	O5-C11-N1-O4	1

There are no ring outliers.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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

The completeness of assignment taking into account all chemical shift lists is 64% for the well-defined parts and 64% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	1374
Number of shifts mapped to atoms	1374
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	14

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	121	2.57 ± 0.20	Should be applied
$^{13}\text{C}_\beta$	110	2.78 ± 0.17	Should be applied
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	146	0.17 ± 0.36	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 64%, i.e. 1372 atoms were assigned a chemical shift out of a possible 2132. 0 out of 24 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	570/789 (72%)	303/321 (94%)	121/318 (38%)	146/150 (97%)
Sidechain	765/1099 (70%)	544/717 (76%)	215/349 (62%)	6/33 (18%)

Continued on next page...

Continued from previous page...

	Total	¹ H	¹³ C	¹⁵ N
Aromatic	37/244 (15%)	34/122 (28%)	0/111 (0%)	3/11 (27%)
Overall	1372/2132 (64%)	881/1160 (76%)	336/778 (43%)	155/194 (80%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 64%, i.e. 1374 atoms were assigned a chemical shift out of a possible 2150. 0 out of 24 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	571/798 (72%)	304/325 (94%)	121/322 (38%)	146/151 (97%)
Sidechain	766/1108 (69%)	545/723 (75%)	215/352 (61%)	6/33 (18%)
Aromatic	37/244 (15%)	34/122 (28%)	0/111 (0%)	3/11 (27%)
Overall	1374/2150 (64%)	883/1170 (75%)	336/785 (43%)	155/195 (79%)

7.1.4 Statistically unusual chemical shifts ⓘ

The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	208	GLY	CA	55.80	38.93 – 51.79	8.1
1	A	105	THR	HB	1.94	2.57 – 5.77	-7.0
1	A	93	ARG	CD	37.30	38.57 – 47.75	-6.4
1	A	152	GLY	CA	53.30	38.93 – 51.79	6.2
1	A	91	LYS	CE	47.07	37.57 – 46.21	6.0
1	A	94	LYS	CG	18.85	19.35 – 30.45	-5.5
1	A	119	LYS	CD	23.17	23.50 – 34.42	-5.3
1	A	91	LYS	CG	19.06	19.35 – 30.45	-5.3
1	A	202	GLU	HB2	0.96	1.00 – 3.05	-5.2
1	A	193	THR	HG21	0.05	0.08 – 2.19	-5.1
1	A	193	THR	HG22	0.05	0.08 – 2.19	-5.1
1	A	193	THR	HG23	0.05	0.08 – 2.19	-5.1
1	A	122	LYS	CE	37.48	37.57 – 46.21	-5.1
1	A	218	LEU	H	11.40	5.09 – 11.34	5.1

7.1.5 Random Coil Index (RCI) plots ⓘ

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble

composition. If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A:

