



# Full wwPDB NMR Structure Validation Report ⓘ

Mar 27, 2026 – 05:23 PM UTC

PDB ID : 2SRT / pdb\_00002srt  
Title : CATALYTIC DOMAIN OF HUMAN STROMELYSIN-1 AT PH 5.5 AND  
400C COMPLEXED WITH INHIBITOR  
Authors : Gooley, P.R.; O'Connell, J.F.  
Deposited on : 1995-03-22

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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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

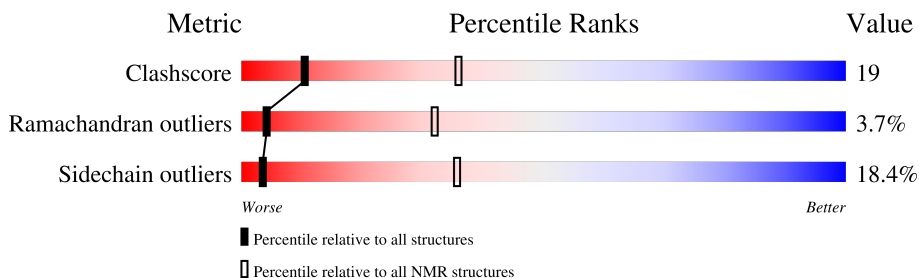
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment 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  $\geq 3$ , 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	173	

## 2 Ensemble composition and analysis i

This entry contains 30 models. Model 10 is the overall representative, medoid model (most similar to other models).

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:84-A:157, A:161-A:170, A:174-A:250 (161)	0.59	10

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 5 clusters and 1 single-model cluster was found.

Cluster number	Models
1	1, 2, 4, 5, 6, 8, 9, 10, 11, 14, 16, 18, 19, 20, 25
2	3, 7, 12, 13, 15, 22, 24, 26
3	28, 29
4	17, 23
5	27, 30
Single-model clusters	21

### 3 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 2746 atoms, of which 1333 are hydrogens and 0 are deuteriums.

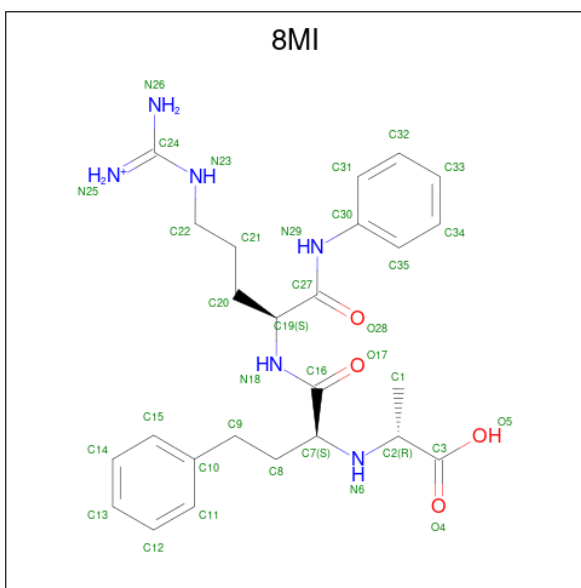
- Molecule 1 is a protein called STROMELYSIN-1.

Mol	Chain	Residues	Atoms					Trace	
			Total	C	H	N	O		S
1	A	173	2674	882	1298	228	264	2	0

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

Mol	Chain	Residues	Atoms	
			Total	Zn
2	A	2	2	2

- Molecule 3 is N-(R-CARBOXY-ETHYL)-ALPHA-(S)-(2-PHENYLETHYL)GLYCYL-L-ARGININE-N-PHENYLAMIDE (CCD ID: 8MI) (formula: C<sub>25</sub>H<sub>35</sub>N<sub>6</sub>O<sub>4</sub>).



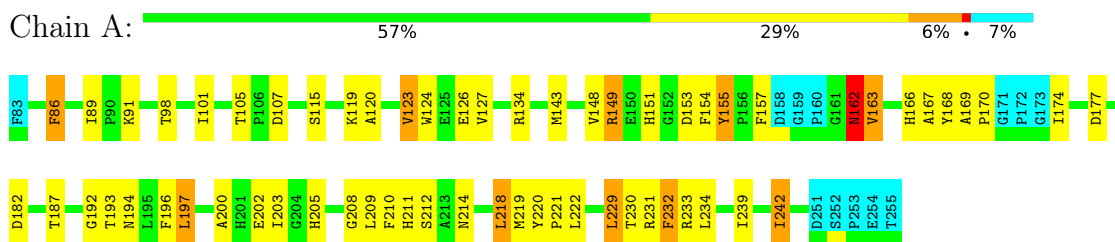
Mol	Chain	Residues	Atoms				
			Total	C	H	N	O
3	A	1	70	25	35	6	4

## 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: STROMELYSIN-1

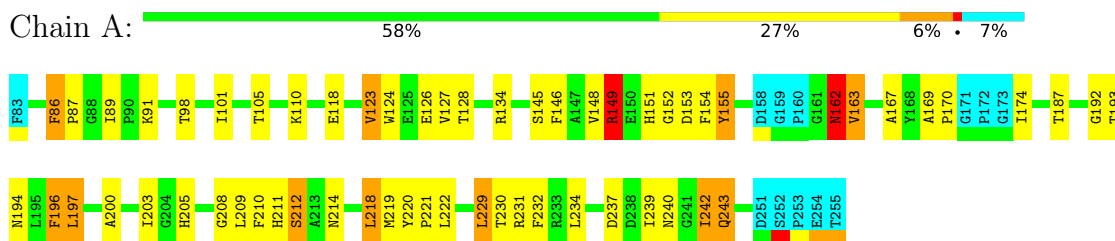


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

#### 4.2.1 Score per residue for model 1

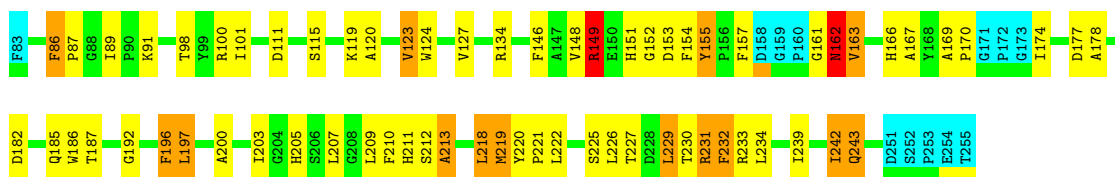
- Molecule 1: STROMELYSIN-1



#### 4.2.2 Score per residue for model 2

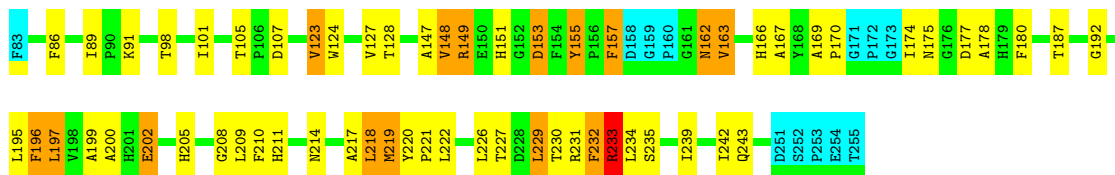
- Molecule 1: STROMELYSIN-1





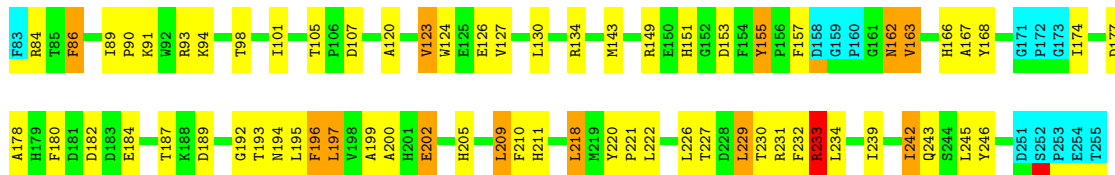
### 4.2.3 Score per residue for model 3

- Molecule 1: STROMELYSIN-1



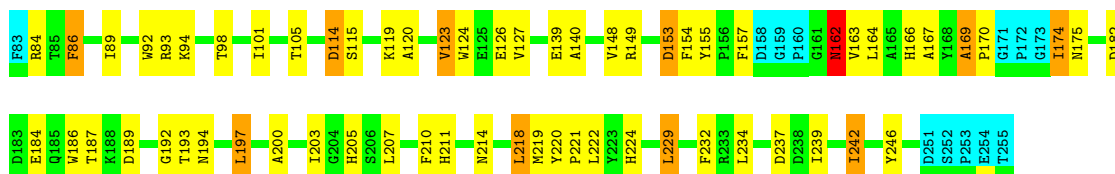
### 4.2.4 Score per residue for model 4

- Molecule 1: STROMELYSIN-1



### 4.2.5 Score per residue for model 5

- Molecule 1: STROMELYSIN-1



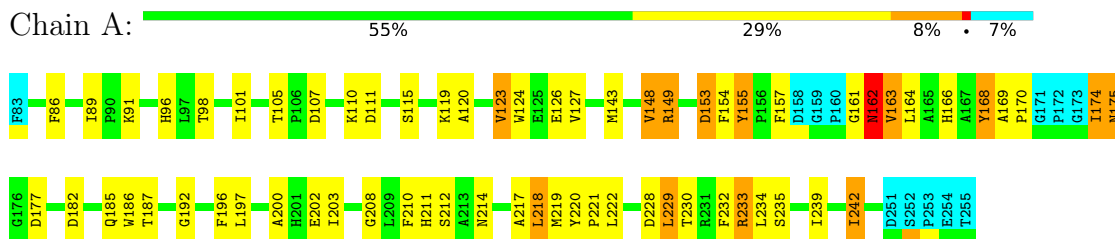
### 4.2.6 Score per residue for model 6

- Molecule 1: STROMELYSIN-1



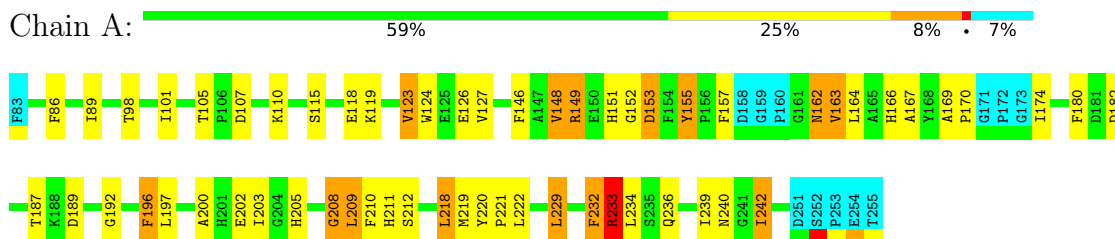
#### 4.2.7 Score per residue for model 7

- Molecule 1: STROMELYSIN-1



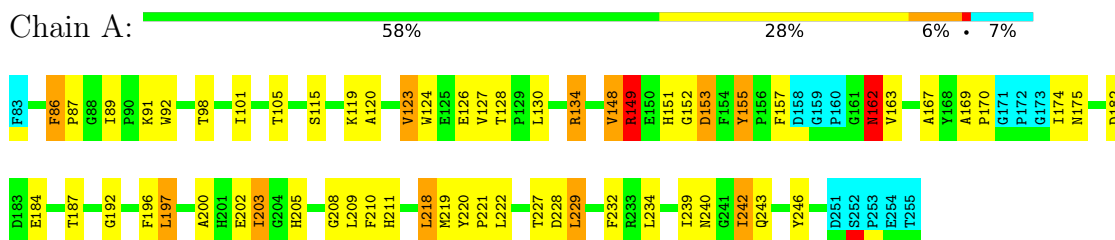
#### 4.2.8 Score per residue for model 8

- Molecule 1: STROMELYSIN-1



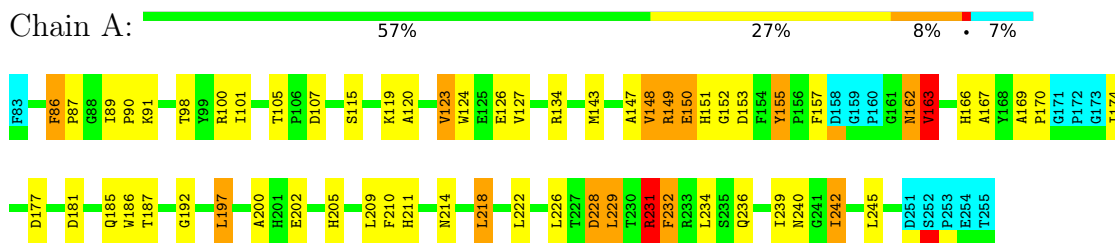
#### 4.2.9 Score per residue for model 9

- Molecule 1: STROMELYSIN-1



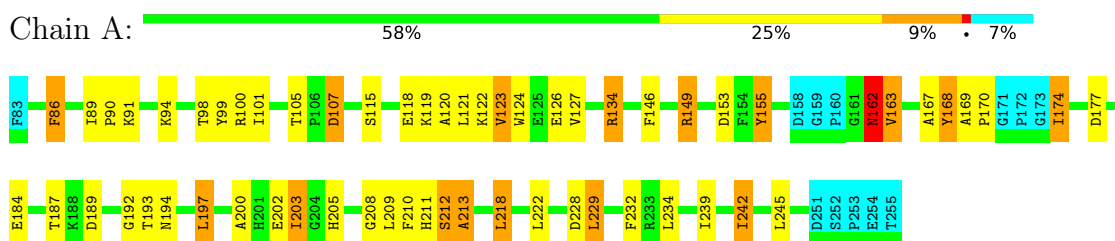
#### 4.2.10 Score per residue for model 10 (medoid)

- Molecule 1: STROMELYSIN-1



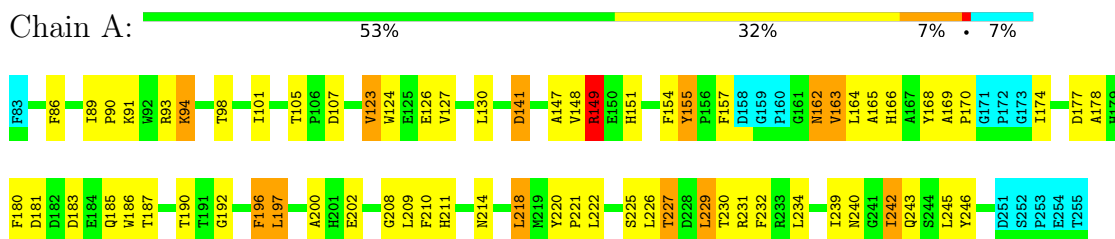
#### 4.2.11 Score per residue for model 11

- Molecule 1: STROMELYSIN-1



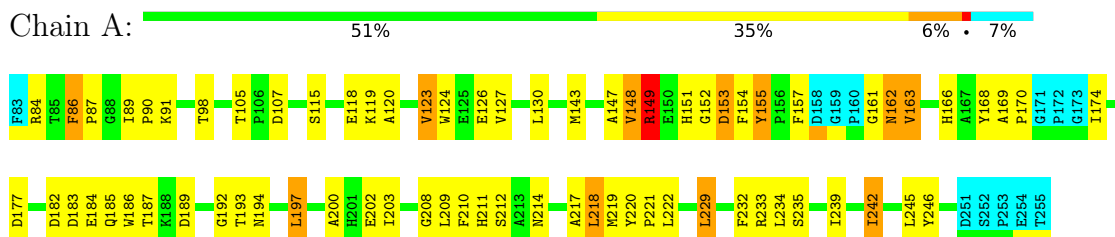
#### 4.2.12 Score per residue for model 12

- Molecule 1: STROMELYSIN-1



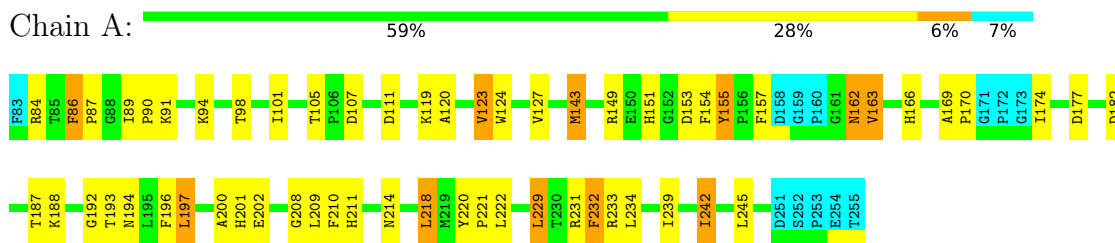
#### 4.2.13 Score per residue for model 13

- Molecule 1: STROMELYSIN-1



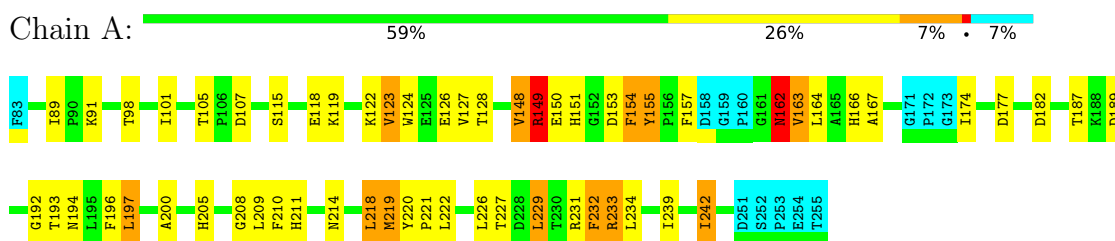
## 4.2.14 Score per residue for model 14

- Molecule 1: STROMELYSIN-1



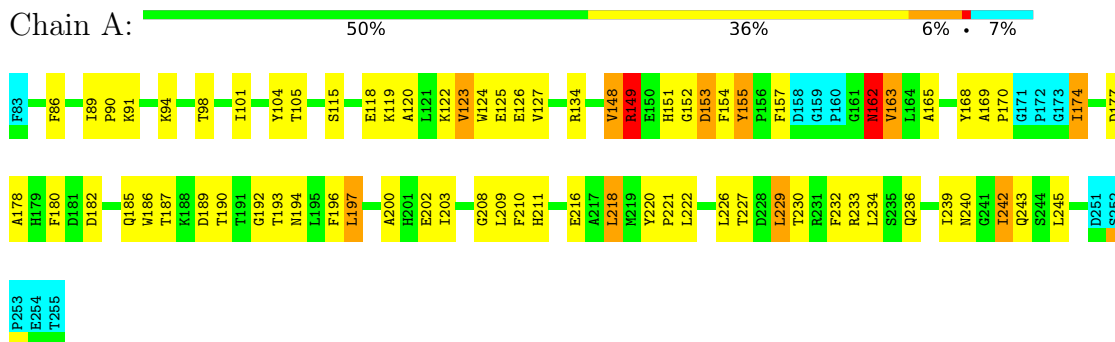
## 4.2.15 Score per residue for model 15

- Molecule 1: STROMELYSIN-1



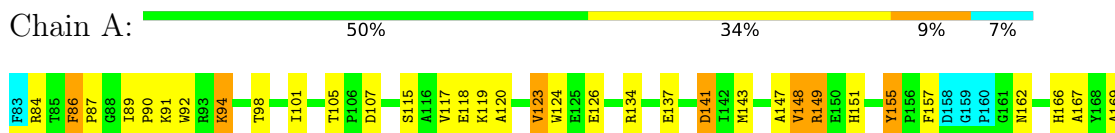
## 4.2.16 Score per residue for model 16

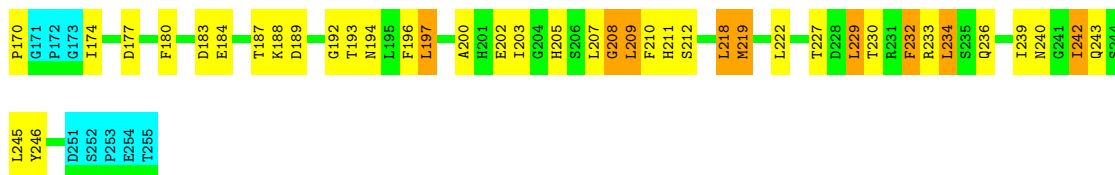
- Molecule 1: STROMELYSIN-1



## 4.2.17 Score per residue for model 17

- Molecule 1: STROMELYSIN-1

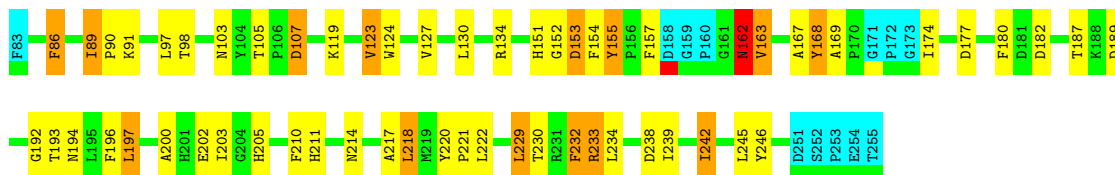




#### 4.2.18 Score per residue for model 18

- Molecule 1: STROMELYSIN-1

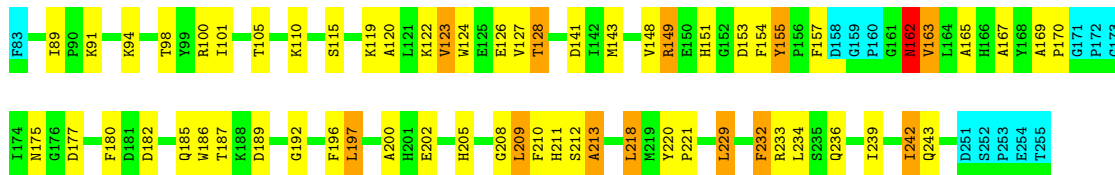
Chain A: 59% 25% 8% 7%



#### 4.2.19 Score per residue for model 19

- Molecule 1: STROMELYSIN-1

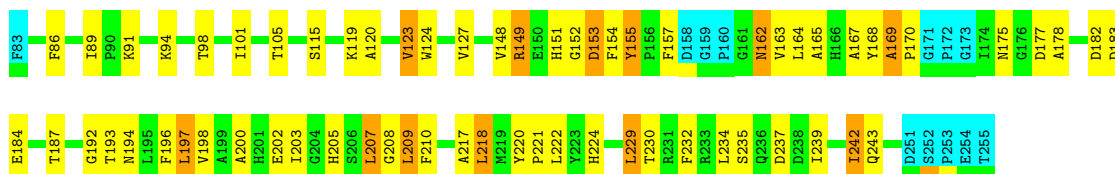
Chain A: 57% 29% 7% 7%



#### 4.2.20 Score per residue for model 20

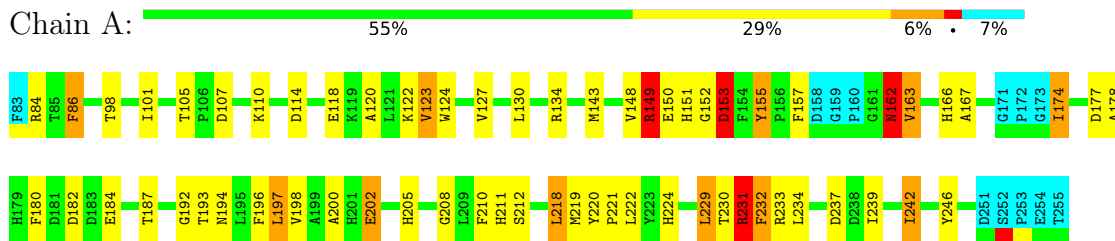
- Molecule 1: STROMELYSIN-1

Chain A: 55% 31% 7% 7%



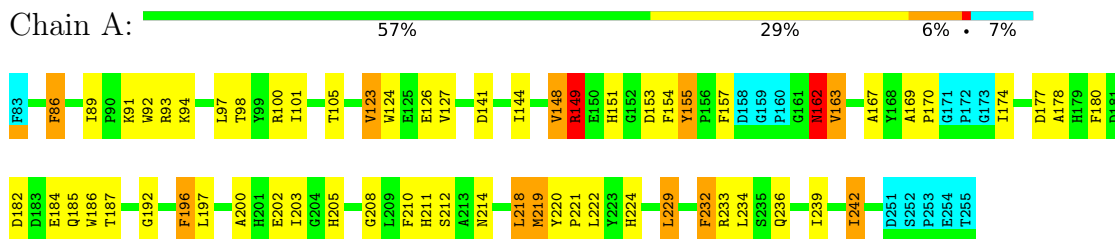
#### 4.2.21 Score per residue for model 21

- Molecule 1: STROMELYSIN-1



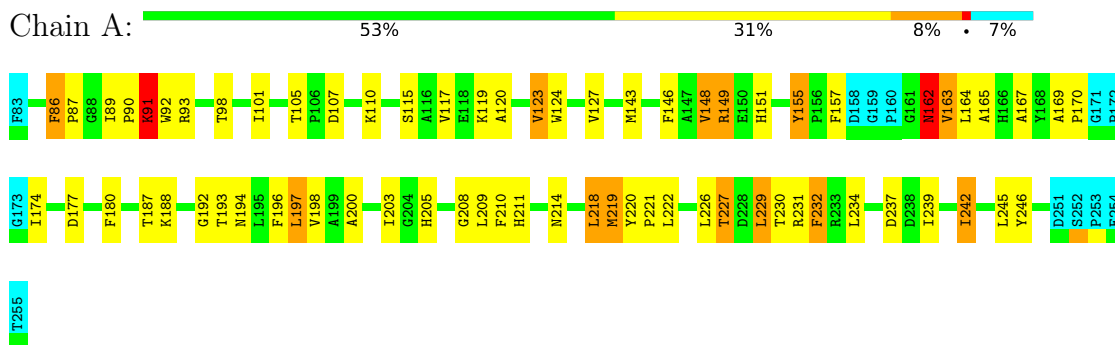
#### 4.2.22 Score per residue for model 22

- Molecule 1: STROMELYSIN-1



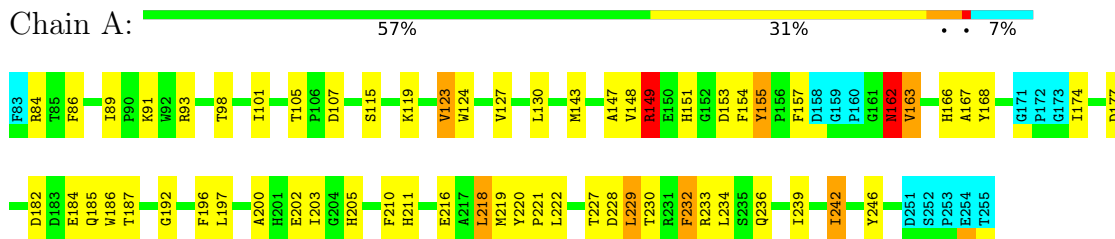
#### 4.2.23 Score per residue for model 23

- Molecule 1: STROMELYSIN-1



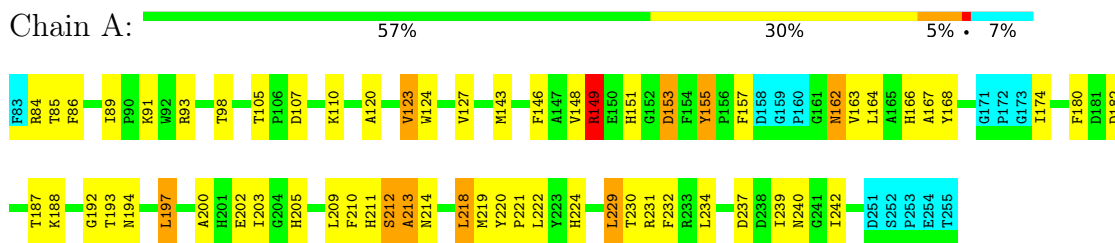
#### 4.2.24 Score per residue for model 24

- Molecule 1: STROMELYSIN-1



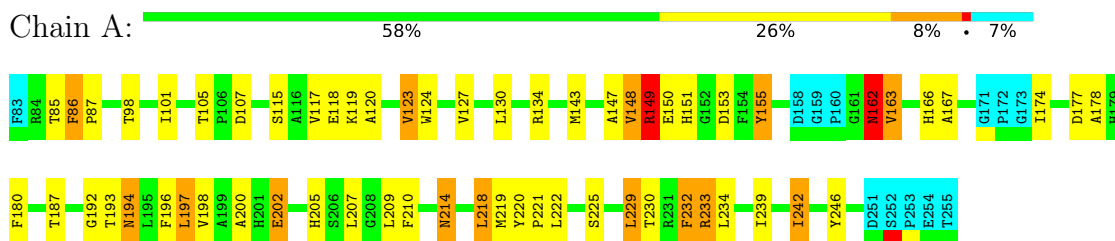
## 4.2.25 Score per residue for model 25

- Molecule 1: STROMELYSIN-1



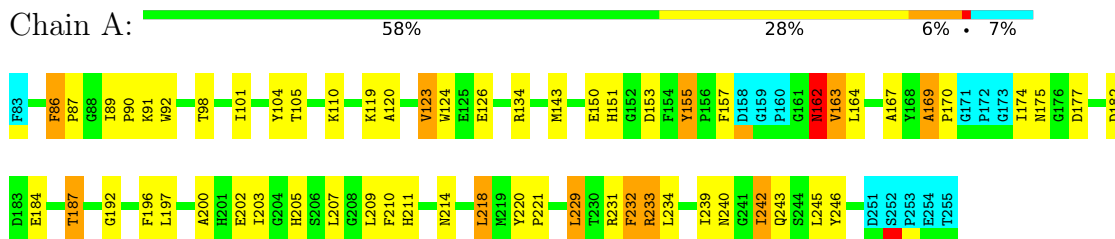
## 4.2.26 Score per residue for model 26

- Molecule 1: STROMELYSIN-1



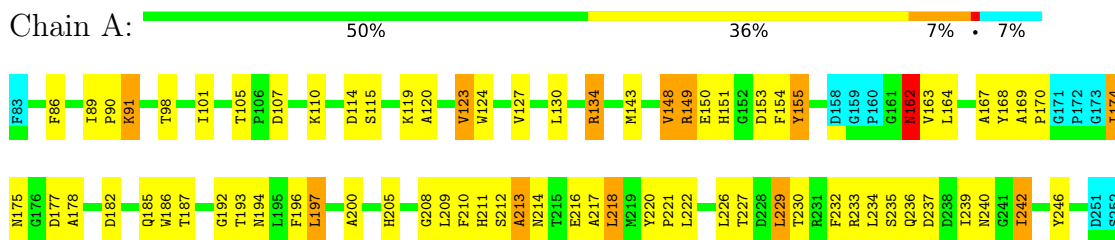
## 4.2.27 Score per residue for model 27

- Molecule 1: STROMELYSIN-1



## 4.2.28 Score per residue for model 28

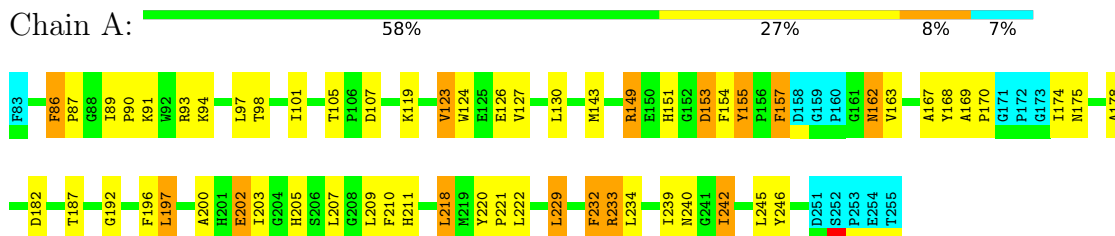
- Molecule 1: STROMELYSIN-1





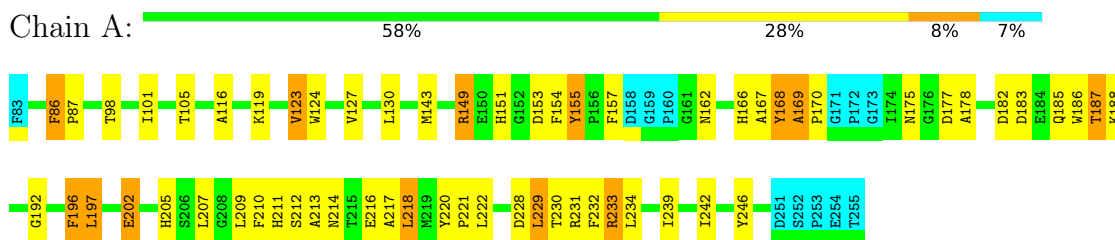
#### 4.2.29 Score per residue for model 29

- Molecule 1: STROMELYSIN-1



#### 4.2.30 Score per residue for model 30

- Molecule 1: STROMELYSIN-1



## 5 Refinement protocol and experimental data overview

Of the ? calculated structures, 30 were deposited, based on the following criterion: ?.

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

Software name	Classification	Version
DIANA	refinement	
FANTOM	refinement	

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: ZN, 8MI

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	0.80±0.00	0±0/1335 ( 0.0± 0.0%)	1.14±0.01	0±0/1825 ( 0.0± 0.0%)
All	All	0.80	0/40050 ( 0.0%)	1.14	14/54750 ( 0.0%)

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	1.9±0.9
All	All	0	57

There are no bond-length outliers.

All unique angle outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	162	ASN	CB-CA-C	-6.59	107.95	115.79	26	14

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	149	ARG	Sidechain	15
1	A	93	ARG	Sidechain	9
1	A	134	ARG	Sidechain	8
1	A	233	ARG	Sidechain	8
1	A	231	ARG	Sidechain	7
1	A	84	ARG	Sidechain	6

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Mol	Chain	Res	Type	Group	Models (Total)
1	A	100	ARG	Sidechain	4

## 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	1293	1231	1231	48±6
3	A	35	35	0	1±1
All	All	39900	37980	36930	1454

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 19.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:209:LEU:HD21	1:A:242:ILE:HD12	0.93	1.34	17	8
1:A:200:ALA:HB3	1:A:218:LEU:HD11	0.87	1.44	21	29
3:A:256:8MI:C3	3:A:256:8MI:O17	0.83	2.27	14	1
3:A:256:8MI:C1	3:A:256:8MI:C16	0.81	2.58	20	14
1:A:198:VAL:HG12	1:A:202:GLU:OE1	0.80	1.76	20	1
1:A:229:LEU:HD22	1:A:229:LEU:O	0.80	1.75	22	14
1:A:197:LEU:HD23	1:A:218:LEU:HD12	0.79	1.54	9	17
1:A:124:TRP:CE3	1:A:242:ILE:HD13	0.78	2.13	17	24
1:A:197:LEU:HD22	1:A:197:LEU:O	0.78	1.78	12	6
1:A:167:ALA:HB2	1:A:202:GLU:OE1	0.77	1.80	30	5
1:A:197:LEU:HD21	3:A:256:8MI:C13	0.76	2.10	4	5
1:A:151:HIS:CD2	1:A:155:TYR:CE1	0.76	2.74	8	14
1:A:209:LEU:CD2	1:A:242:ILE:HD12	0.75	2.12	1	5
1:A:229:LEU:C	1:A:229:LEU:HD13	0.74	2.08	26	14
1:A:151:HIS:CE1	1:A:155:TYR:CE1	0.74	2.75	21	8
1:A:209:LEU:HD22	1:A:242:ILE:HD12	0.73	1.61	1	4
1:A:86:PHE:CD2	1:A:169:ALA:HB2	0.72	2.19	28	1
1:A:169:ALA:HB1	1:A:170:PRO:HD2	0.72	1.59	7	23
1:A:124:TRP:CZ3	1:A:234:LEU:HD13	0.71	2.19	9	30
1:A:229:LEU:HD23	1:A:229:LEU:C	0.71	2.11	10	16
1:A:90:PRO:O	1:A:245:LEU:HD22	0.70	1.87	17	13

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:86:PHE:C	1:A:86:PHE:CD1	0.70	2.69	13	4
1:A:239:ILE:HG23	1:A:243:GLN:OE1	0.69	1.87	1	1
1:A:167:ALA:HB3	1:A:205:HIS:HB2	0.69	1.65	30	25
1:A:178:ALA:HB1	1:A:202:GLU:OE1	0.69	1.88	26	6
1:A:86:PHE:CE2	1:A:169:ALA:HB3	0.69	2.23	5	2
1:A:196:PHE:CD1	1:A:229:LEU:HD11	0.69	2.23	12	1
3:A:256:8MI:C1	3:A:256:8MI:C8	0.68	2.70	14	1
1:A:157:PHE:CE1	1:A:163:VAL:HG12	0.68	2.23	25	11
1:A:151:HIS:CE1	1:A:155:TYR:CD1	0.66	2.84	14	9
1:A:101:ILE:N	1:A:101:ILE:HD12	0.66	2.06	30	10
1:A:151:HIS:NE2	1:A:155:TYR:CE1	0.65	2.64	3	15
1:A:151:HIS:NE2	1:A:155:TYR:CZ	0.65	2.65	21	4
1:A:208:GLY:C	1:A:209:LEU:HD23	0.65	2.17	8	3
1:A:151:HIS:CD2	1:A:155:TYR:CZ	0.65	2.84	21	4
1:A:151:HIS:CD2	1:A:153:ASP:OD2	0.65	2.49	26	2
1:A:123:VAL:CG1	1:A:234:LEU:HD11	0.65	2.21	8	30
1:A:153:ASP:HB2	1:A:155:TYR:CE2	0.65	2.26	15	6
1:A:169:ALA:HB1	1:A:170:PRO:CD	0.64	2.23	7	19
1:A:218:LEU:HD23	1:A:219:MET:N	0.64	2.08	26	9
1:A:148:VAL:O	1:A:149:ARG:C	0.63	2.42	13	20
1:A:210:PHE:O	1:A:211:HIS:CD2	0.63	2.52	30	8
1:A:155:TYR:CD1	1:A:168:TYR:OH	0.63	2.50	16	2
1:A:217:ALA:HB2	1:A:235:SER:OG	0.62	1.93	28	5
1:A:130:LEU:HD11	1:A:246:TYR:CE2	0.62	2.29	28	6
1:A:197:LEU:HD21	3:A:256:8MI:C12	0.62	2.24	4	2
1:A:196:PHE:CD1	1:A:196:PHE:C	0.62	2.78	12	17
1:A:218:LEU:C	1:A:218:LEU:HD23	0.62	2.19	5	18
1:A:218:LEU:HD13	1:A:232:PHE:CZ	0.62	2.29	16	26
1:A:157:PHE:CE1	1:A:166:HIS:CE1	0.61	2.89	13	5
1:A:127:VAL:O	1:A:128:THR:HG23	0.61	1.96	19	3
1:A:187:THR:HG21	1:A:192:GLY:HA3	0.60	1.73	24	25
1:A:239:ILE:HA	1:A:242:ILE:HG22	0.60	1.73	27	29
1:A:123:VAL:HG13	1:A:234:LEU:HD11	0.60	1.73	17	14
1:A:198:VAL:HG22	3:A:256:8MI:C11	0.60	2.26	26	2
1:A:153:ASP:HB2	1:A:155:TYR:CE1	0.59	2.32	26	2
1:A:154:PHE:CD2	1:A:154:PHE:O	0.59	2.56	15	2
1:A:155:TYR:CD2	1:A:166:HIS:NE2	0.59	2.70	2	4
1:A:187:THR:HG21	1:A:192:GLY:N	0.58	2.14	20	13
1:A:153:ASP:CG	1:A:174:ILE:HD11	0.58	2.24	21	1
1:A:154:PHE:CG	1:A:154:PHE:O	0.58	2.57	19	8
1:A:165:ALA:HB1	1:A:202:GLU:CD	0.58	2.24	16	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:239:ILE:HG23	1:A:243:GLN:CD	0.58	2.23	1	1
1:A:219:MET:SD	1:A:219:MET:O	0.58	2.61	3	4
1:A:86:PHE:CG	1:A:87:PRO:HD2	0.57	2.34	1	9
1:A:193:THR:O	1:A:194:ASN:C	0.57	2.48	21	17
1:A:155:TYR:CD2	1:A:168:TYR:OH	0.57	2.58	4	4
1:A:180:PHE:CZ	1:A:202:GLU:OE1	0.57	2.58	16	4
1:A:86:PHE:CD2	1:A:87:PRO:HD2	0.56	2.35	13	8
1:A:155:TYR:CE1	1:A:168:TYR:CE1	0.56	2.93	11	1
1:A:217:ALA:HB1	1:A:238:ASP:OD1	0.56	2.00	18	1
1:A:157:PHE:CZ	1:A:166:HIS:CE1	0.56	2.93	12	6
1:A:153:ASP:OD2	1:A:174:ILE:CD1	0.56	2.54	5	5
1:A:152:GLY:O	1:A:155:TYR:CE1	0.56	2.59	2	5
1:A:86:PHE:CD2	1:A:169:ALA:HB3	0.56	2.35	18	2
1:A:190:THR:HG21	1:A:226:LEU:O	0.56	2.01	16	2
1:A:232:PHE:CD1	1:A:232:PHE:C	0.56	2.83	8	6
1:A:218:LEU:HD22	1:A:234:LEU:CD2	0.56	2.31	25	6
1:A:153:ASP:CB	1:A:155:TYR:CE1	0.56	2.89	26	1
1:A:147:ALA:HB1	1:A:151:HIS:CB	0.56	2.30	12	5
1:A:205:HIS:CE1	1:A:210:PHE:HA	0.56	2.36	25	10
1:A:153:ASP:OD2	1:A:155:TYR:CE1	0.56	2.58	11	1
1:A:197:LEU:CD2	1:A:218:LEU:HD12	0.55	2.31	2	6
1:A:210:PHE:O	1:A:211:HIS:C	0.55	2.50	9	19
1:A:180:PHE:CD1	1:A:202:GLU:OE2	0.55	2.59	26	4
1:A:187:THR:HG21	1:A:192:GLY:CA	0.55	2.32	2	18
1:A:153:ASP:CB	1:A:155:TYR:CZ	0.55	2.90	3	3
1:A:148:VAL:O	1:A:150:GLU:N	0.55	2.39	21	1
3:A:256:8MI:C3	3:A:256:8MI:C16	0.54	2.85	14	1
1:A:220:TYR:CD1	1:A:221:PRO:HD2	0.54	2.37	27	26
1:A:120:ALA:HB1	1:A:200:ALA:HA	0.54	1.79	21	20
1:A:197:LEU:C	1:A:197:LEU:HD13	0.54	2.27	12	3
1:A:154:PHE:O	1:A:154:PHE:CG	0.54	2.60	13	7
1:A:151:HIS:CE1	1:A:155:TYR:O	0.54	2.60	28	5
1:A:155:TYR:CD1	1:A:155:TYR:N	0.54	2.75	14	16
1:A:153:ASP:OD2	1:A:155:TYR:CE2	0.53	2.61	21	1
1:A:220:TYR:CG	1:A:221:PRO:HD2	0.53	2.38	25	8
1:A:200:ALA:CB	1:A:218:LEU:HD11	0.53	2.29	21	7
1:A:84:ARG:C	1:A:85:THR:HG23	0.53	2.29	25	1
1:A:152:GLY:O	1:A:153:ASP:CG	0.53	2.51	18	4
1:A:157:PHE:CD1	1:A:157:PHE:N	0.53	2.75	3	2
1:A:196:PHE:CD2	1:A:229:LEU:HD21	0.53	2.38	7	3
1:A:153:ASP:CB	1:A:155:TYR:CE2	0.53	2.91	13	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:177:ASP:OD1	1:A:178:ALA:N	0.53	2.42	22	7
1:A:162:ASN:O	1:A:163:VAL:C	0.52	2.51	22	28
3:A:256:8MI:C20	3:A:256:8MI:O17	0.52	2.57	25	1
1:A:218:LEU:HD13	1:A:232:PHE:HZ	0.52	1.64	10	8
1:A:232:PHE:CD1	1:A:233:ARG:N	0.52	2.77	26	13
1:A:86:PHE:CE1	1:A:210:PHE:CZ	0.52	2.97	21	6
1:A:218:LEU:HD23	1:A:218:LEU:C	0.52	2.30	26	1
1:A:196:PHE:CE2	1:A:229:LEU:HD21	0.52	2.40	21	5
1:A:187:THR:CG2	1:A:192:GLY:HA3	0.52	2.35	24	30
1:A:127:VAL:HG23	1:A:242:ILE:HG21	0.51	1.82	21	28
1:A:229:LEU:C	1:A:229:LEU:CD1	0.51	2.82	15	14
1:A:155:TYR:CD1	1:A:155:TYR:O	0.51	2.64	21	7
1:A:226:LEU:O	1:A:227:THR:C	0.51	2.54	3	8
1:A:147:ALA:HB1	1:A:151:HIS:HB3	0.51	1.83	26	6
1:A:239:ILE:O	1:A:240:ASN:C	0.51	2.53	17	3
1:A:161:GLY:C	1:A:162:ASN:CG	0.51	2.79	7	2
1:A:201:HIS:CD2	3:A:256:8MI:N6	0.51	2.79	14	1
1:A:97:LEU:HD11	1:A:130:LEU:HD13	0.51	1.82	29	2
1:A:153:ASP:OD2	1:A:174:ILE:HD11	0.51	2.05	21	1
1:A:115:SER:O	1:A:119:LYS:N	0.51	2.44	23	17
1:A:127:VAL:CG2	1:A:242:ILE:HG21	0.50	2.36	3	26
1:A:200:ALA:HB3	1:A:218:LEU:CD1	0.50	2.36	8	5
1:A:86:PHE:CD1	1:A:210:PHE:CZ	0.50	2.99	9	3
1:A:151:HIS:CG	1:A:153:ASP:OD1	0.50	2.64	15	3
1:A:124:TRP:CZ3	1:A:242:ILE:HD13	0.49	2.42	26	7
1:A:153:ASP:CG	1:A:155:TYR:CD2	0.49	2.90	13	2
1:A:124:TRP:CH2	1:A:209:LEU:HD12	0.49	2.42	16	12
1:A:209:LEU:O	1:A:210:PHE:CD2	0.49	2.66	14	4
1:A:153:ASP:OD2	1:A:155:TYR:CZ	0.49	2.65	21	1
1:A:146:PHE:N	1:A:146:PHE:CD1	0.49	2.77	11	4
1:A:146:PHE:CE1	1:A:180:PHE:CD1	0.49	3.00	8	1
1:A:207:LEU:HD13	1:A:242:ILE:HD11	0.49	1.85	17	2
1:A:229:LEU:C	1:A:229:LEU:CD2	0.49	2.83	25	13
1:A:148:VAL:O	1:A:149:ARG:O	0.49	2.31	3	9
1:A:212:SER:O	1:A:213:ALA:HB2	0.49	2.08	28	4
1:A:101:ILE:N	1:A:101:ILE:CD1	0.48	2.76	30	10
1:A:153:ASP:OD2	1:A:155:TYR:CD2	0.48	2.66	24	1
1:A:153:ASP:CG	1:A:174:ILE:CD1	0.48	2.86	28	4
1:A:210:PHE:O	1:A:219:MET:HE3	0.48	2.08	6	2
1:A:180:PHE:CE2	1:A:202:GLU:OE1	0.48	2.66	19	4
1:A:234:LEU:HB2	1:A:239:ILE:HD11	0.48	1.86	5	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:194:ASN:O	1:A:198:VAL:HG23	0.48	2.08	26	1
1:A:214:ASN:O	1:A:220:TYR:CD1	0.48	2.66	1	5
1:A:153:ASP:HB3	1:A:155:TYR:CE2	0.48	2.43	22	6
1:A:165:ALA:HB3	1:A:202:GLU:CD	0.48	2.34	20	1
1:A:155:TYR:CE2	1:A:168:TYR:CE1	0.47	3.01	18	2
1:A:119:LYS:HB3	1:A:196:PHE:CE1	0.47	2.44	18	8
1:A:209:LEU:HD21	1:A:242:ILE:CD1	0.47	2.31	19	3
1:A:166:HIS:CD2	1:A:166:HIS:C	0.47	2.93	3	5
1:A:180:PHE:CD1	1:A:202:GLU:OE1	0.47	2.68	22	1
1:A:148:VAL:HA	1:A:157:PHE:HB2	0.47	1.85	7	6
1:A:155:TYR:CG	1:A:168:TYR:OH	0.47	2.64	4	1
1:A:86:PHE:CE2	1:A:169:ALA:HB2	0.47	2.45	28	1
1:A:164:LEU:HD11	3:A:256:8MI:C31	0.47	2.39	23	1
1:A:165:ALA:CB	1:A:202:GLU:CD	0.46	2.88	20	1
1:A:153:ASP:OD1	1:A:174:ILE:CD1	0.46	2.63	28	3
1:A:169:ALA:O	1:A:175:ASN:HB3	0.46	2.10	29	8
1:A:174:ILE:HD13	1:A:174:ILE:O	0.46	2.10	16	1
1:A:209:LEU:O	1:A:210:PHE:CD1	0.46	2.68	25	1
1:A:153:ASP:HB3	1:A:155:TYR:CZ	0.46	2.44	3	2
1:A:148:VAL:HG23	1:A:149:ARG:CG	0.46	2.41	21	1
1:A:148:VAL:HG23	1:A:149:ARG:HG3	0.46	1.87	12	1
1:A:124:TRP:CE3	1:A:234:LEU:HD13	0.46	2.46	12	2
1:A:153:ASP:HB2	1:A:155:TYR:CZ	0.46	2.45	3	1
1:A:149:ARG:NH1	1:A:150:GLU:O	0.46	2.49	10	2
1:A:157:PHE:CD2	1:A:181:ASP:HA	0.45	2.46	12	2
1:A:180:PHE:CE1	1:A:202:GLU:OE1	0.45	2.69	22	3
1:A:185:GLN:HG3	1:A:186:TRP:N	0.45	2.27	10	5
1:A:151:HIS:CD2	1:A:155:TYR:OH	0.45	2.68	21	1
1:A:194:ASN:ND2	1:A:229:LEU:HD13	0.45	2.27	1	1
1:A:196:PHE:CE1	1:A:229:LEU:HD11	0.45	2.45	12	1
1:A:130:LEU:HD11	1:A:246:TYR:CZ	0.45	2.46	24	1
1:A:166:HIS:O	1:A:202:GLU:OE1	0.45	2.34	21	4
1:A:197:LEU:CD2	3:A:256:8MI:C12	0.45	2.94	4	1
3:A:256:8MI:C1	3:A:256:8MI:N18	0.45	2.79	25	1
1:A:166:HIS:HA	3:A:256:8MI:O5	0.45	2.12	10	1
1:A:155:TYR:CE1	1:A:168:TYR:CZ	0.45	3.05	16	1
1:A:90:PRO:O	1:A:91:LYS:CB	0.45	2.64	28	1
1:A:124:TRP:CH2	1:A:209:LEU:CD1	0.45	3.00	9	3
1:A:196:PHE:CD2	1:A:229:LEU:HD11	0.45	2.47	28	4
1:A:86:PHE:CB	1:A:87:PRO:CD	0.45	2.95	23	4
1:A:155:TYR:CZ	1:A:168:TYR:CE1	0.45	3.05	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:196:PHE:CD1	1:A:196:PHE:O	0.45	2.70	26	6
3:A:256:8MI:C16	3:A:256:8MI:C1	0.45	2.94	10	1
1:A:127:VAL:HG11	1:A:239:ILE:CG1	0.45	2.42	20	1
1:A:151:HIS:NE2	1:A:153:ASP:OD2	0.44	2.50	13	1
1:A:197:LEU:HD22	3:A:256:8MI:C13	0.44	2.42	26	3
1:A:218:LEU:C	1:A:218:LEU:CD2	0.44	2.88	5	4
1:A:157:PHE:N	1:A:157:PHE:CD1	0.44	2.85	22	3
1:A:197:LEU:HD22	1:A:218:LEU:HD12	0.44	1.88	12	2
1:A:231:ARG:O	1:A:232:PHE:C	0.44	2.59	10	3
1:A:130:LEU:HD21	1:A:246:TYR:CZ	0.44	2.48	21	2
1:A:84:ARG:C	1:A:85:THR:CG2	0.44	2.90	25	1
1:A:86:PHE:CD1	1:A:210:PHE:CE1	0.44	3.06	21	1
1:A:212:SER:OG	1:A:213:ALA:N	0.43	2.51	19	1
1:A:146:PHE:CD2	1:A:180:PHE:HB2	0.43	2.48	23	2
1:A:151:HIS:CD2	1:A:153:ASP:OD1	0.43	2.71	15	2
1:A:152:GLY:O	1:A:153:ASP:C	0.43	2.61	8	3
1:A:148:VAL:HA	1:A:157:PHE:CB	0.43	2.43	15	2
1:A:168:TYR:CD1	1:A:168:TYR:N	0.43	2.85	7	1
1:A:229:LEU:O	1:A:232:PHE:HB3	0.43	2.13	30	14
1:A:169:ALA:CB	1:A:170:PRO:CD	0.43	2.92	7	7
1:A:180:PHE:CZ	1:A:202:GLU:HG3	0.43	2.48	18	2
1:A:185:GLN:CG	1:A:186:TRP:N	0.43	2.82	12	6
1:A:210:PHE:C	1:A:219:MET:SD	0.43	3.02	22	2
1:A:151:HIS:NE2	1:A:155:TYR:CD1	0.43	2.87	8	1
1:A:91:LYS:NZ	1:A:245:LEU:O	0.43	2.52	23	1
1:A:94:LYS:NZ	1:A:141:ASP:OD2	0.43	2.48	12	3
1:A:217:ALA:HB1	1:A:238:ASP:CG	0.43	2.38	18	1
1:A:195:LEU:O	1:A:199:ALA:N	0.43	2.50	3	2
1:A:92:TRP:N	1:A:246:TYR:OH	0.43	2.52	27	5
1:A:207:LEU:CD1	1:A:242:ILE:HD11	0.43	2.44	17	1
1:A:164:LEU:HD11	3:A:256:8MI:C35	0.43	2.44	5	1
1:A:120:ALA:HB1	1:A:200:ALA:CA	0.43	2.43	25	2
1:A:164:LEU:HD12	3:A:256:8MI:C9	0.43	2.44	25	1
1:A:153:ASP:N	1:A:153:ASP:OD1	0.43	2.50	21	1
1:A:209:LEU:HB3	1:A:219:MET:SD	0.42	2.54	26	1
1:A:155:TYR:CD1	1:A:155:TYR:C	0.42	2.97	3	3
1:A:228:ASP:OD2	1:A:231:ARG:NH1	0.42	2.52	10	1
1:A:232:PHE:C	1:A:232:PHE:CD1	0.42	2.96	10	1
1:A:155:TYR:CG	1:A:166:HIS:CE1	0.42	3.08	10	1
1:A:143:MET:O	1:A:177:ASP:CG	0.42	2.62	14	1
1:A:165:ALA:HB1	1:A:202:GLU:OE1	0.42	2.13	16	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:90:PRO:O	1:A:91:LYS:HB3	0.42	2.14	28	1
1:A:153:ASP:OD1	1:A:155:TYR:CD2	0.42	2.72	13	1
3:A:256:8MI:O17	3:A:256:8MI:C20	0.42	2.67	14	1
1:A:196:PHE:CD1	1:A:197:LEU:N	0.42	2.87	12	1
1:A:89:ILE:HG23	1:A:245:LEU:HD23	0.42	1.90	18	1
1:A:243:GLN:CD	1:A:243:GLN:C	0.42	2.88	2	1
1:A:124:TRP:O	1:A:128:THR:OG1	0.42	2.37	19	1
1:A:151:HIS:CG	1:A:153:ASP:OD2	0.42	2.72	26	1
1:A:128:THR:CG2	1:A:242:ILE:HG12	0.42	2.44	3	1
1:A:167:ALA:CB	1:A:202:GLU:O	0.42	2.67	11	1
1:A:153:ASP:CG	1:A:155:TYR:CD1	0.42	2.97	26	1
1:A:154:PHE:CD1	1:A:154:PHE:N	0.42	2.88	2	1
1:A:153:ASP:OD1	1:A:155:TYR:N	0.42	2.53	16	1
1:A:180:PHE:CG	1:A:202:GLU:OE1	0.42	2.73	22	1
3:A:256:8MI:N18	3:A:256:8MI:C9	0.42	2.81	25	1
1:A:169:ALA:O	1:A:175:ASN:CB	0.41	2.68	29	2
1:A:197:LEU:HD22	1:A:197:LEU:C	0.41	2.37	12	1
1:A:92:TRP:CB	1:A:97:LEU:HD21	0.41	2.45	22	1
1:A:218:LEU:HD13	1:A:232:PHE:CE1	0.41	2.50	26	2
1:A:153:ASP:HB3	1:A:155:TYR:CE1	0.41	2.50	28	1
1:A:229:LEU:C	1:A:231:ARG:N	0.41	2.78	3	5
1:A:161:GLY:O	1:A:162:ASN:C	0.41	2.62	13	1
1:A:101:ILE:HD13	1:A:114:ASP:OD1	0.41	2.15	5	1
1:A:184:GLU:O	1:A:186:TRP:CD1	0.41	2.72	5	1
1:A:130:LEU:HD21	1:A:246:TYR:CE1	0.41	2.51	26	2
1:A:153:ASP:OD1	1:A:174:ILE:HD13	0.41	2.15	7	1
1:A:84:ARG:O	1:A:85:THR:CG2	0.41	2.68	25	1
1:A:202:GLU:CD	1:A:203:ILE:N	0.41	2.78	9	2
1:A:178:ALA:HB1	1:A:202:GLU:CD	0.41	2.40	29	1
1:A:229:LEU:C	1:A:231:ARG:H	0.41	2.24	12	1
1:A:152:GLY:O	1:A:153:ASP:O	0.41	2.38	18	1
1:A:209:LEU:CD2	1:A:242:ILE:CD1	0.41	2.93	1	1
1:A:197:LEU:CD2	3:A:256:8MI:C13	0.41	2.94	4	1
1:A:167:ALA:HB3	1:A:205:HIS:CB	0.41	2.43	30	1
1:A:86:PHE:CG	1:A:87:PRO:CD	0.41	3.04	1	1
1:A:209:LEU:HD23	1:A:209:LEU:HA	0.41	1.72	4	1
1:A:119:LYS:HB3	1:A:196:PHE:CD1	0.41	2.51	7	1
1:A:218:LEU:HD22	1:A:234:LEU:HD22	0.41	1.92	15	1
1:A:209:LEU:C	1:A:210:PHE:CD2	0.41	2.99	16	1
1:A:165:ALA:HB3	1:A:198:VAL:CG1	0.41	2.46	23	1
1:A:126:GLU:OE1	1:A:233:ARG:NH2	0.40	2.54	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:155:TYR:CD1	1:A:166:HIS:CE1	0.40	3.09	12	1
1:A:116:ALA:HB1	1:A:196:PHE:HA	0.40	1.91	30	1
1:A:168:TYR:C	1:A:169:ALA:O	0.40	2.64	20	1
1:A:100:ARG:O	1:A:144:ILE:N	0.40	2.55	22	1
1:A:209:LEU:HD23	1:A:209:LEU:N	0.40	2.32	1	1
1:A:139:GLU:O	1:A:140:ALA:C	0.40	2.64	5	1
1:A:167:ALA:HB3	1:A:202:GLU:O	0.40	2.17	8	1
1:A:99:TYR:CD1	1:A:121:LEU:CD1	0.40	3.05	11	1
1:A:229:LEU:HD13	1:A:229:LEU:O	0.40	2.16	27	1
1:A:127:VAL:C	1:A:128:THR:CG2	0.40	2.95	1	1
1:A:103:ASN:OD1	1:A:103:ASN:N	0.40	2.55	18	1
1:A:85:THR:OG1	1:A:86:PHE:N	0.40	2.53	26	1

## 6.3 Torsion angles [i](#)

### 6.3.1 Protein backbone [i](#)

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	161/173 (93%)	137±2 (85±1%)	18±3 (11±2%)	6±1 (4±1%)	4	32
All	All	4830/5190 (93%)	4106 (85%)	545 (11%)	179 (4%)	4	32

All 17 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	89	ILE	27
1	A	149	ARG	27
1	A	91	LYS	25
1	A	163	VAL	21
1	A	107	ASP	20
1	A	208	GLY	17
1	A	153	ASP	10
1	A	207	LEU	8
1	A	213	ALA	6
1	A	162	ASN	4

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Mol	Chain	Res	Type	Models (Total)
1	A	169	ALA	4
1	A	232	PHE	3
1	A	212	SER	3
1	A	157	PHE	1
1	A	152	GLY	1
1	A	194	ASN	1
1	A	217	ALA	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	138/147 (94%)	113±3 (82±2%)	25±3 (18±2%)	3	36
All	All	4140/4410 (94%)	3379 (82%)	761 (18%)	3	36

All 71 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	98	THR	30
1	A	123	VAL	30
1	A	155	TYR	30
1	A	162	ASN	30
1	A	218	LEU	30
1	A	229	LEU	30
1	A	105	THR	29
1	A	222	LEU	28
1	A	86	PHE	27
1	A	174	ILE	27
1	A	197	LEU	27
1	A	242	ILE	27
1	A	182	ASP	22
1	A	203	ILE	18
1	A	126	GLU	17
1	A	230	THR	17
1	A	101	ILE	17
1	A	148	VAL	17

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Mol	Chain	Res	Type	Models (Total)
1	A	143	MET	17
1	A	177	ASP	16
1	A	232	PHE	14
1	A	214	ASN	13
1	A	202	GLU	12
1	A	243	GLN	11
1	A	233	ARG	11
1	A	94	LYS	10
1	A	184	GLU	10
1	A	189	ASP	10
1	A	110	LYS	9
1	A	118	GLU	9
1	A	219	MET	9
1	A	134	ARG	9
1	A	149	ARG	8
1	A	196	PHE	8
1	A	236	GLN	8
1	A	240	ASN	8
1	A	237	ASP	7
1	A	228	ASP	7
1	A	164	LEU	7
1	A	168	TYR	7
1	A	153	ASP	6
1	A	224	HIS	6
1	A	122	LYS	6
1	A	188	LYS	6
1	A	209	LEU	5
1	A	216	GLU	5
1	A	227	THR	5
1	A	183	ASP	5
1	A	150	GLU	4
1	A	111	ASP	3
1	A	225	SER	3
1	A	114	ASP	3
1	A	141	ASP	3
1	A	157	PHE	3
1	A	117	VAL	3
1	A	154	PHE	2
1	A	175	ASN	2
1	A	231	ARG	2
1	A	107	ASP	2
1	A	104	TYR	2

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Mol	Chain	Res	Type	Models (Total)
1	A	187	THR	2
1	A	145	SER	1
1	A	212	SER	1
1	A	96	HIS	1
1	A	163	VAL	1
1	A	226	LEU	1
1	A	125	GLU	1
1	A	137	GLU	1
1	A	234	LEU	1
1	A	128	THR	1
1	A	91	LYS	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 3 ligands modelled in this entry, 2 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
3	8MI	A	256	2	36,36,36	1.18±0.00	4±0 (12±1%)

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
3	8MI	A	256	2	43,46,46	0.80±0.00	1±0 (2±0%)

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
3	8MI	A	256	2	-	0±0,36,36,36	0±0,2,2,2

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
3	A	256	8MI	C19-N18	2.86	1.51	1.45	4	30
3	A	256	8MI	C2-C3	2.62	1.56	1.52	18	30
3	A	256	8MI	O5-C3	2.50	1.22	1.30	26	30
3	A	256	8MI	C22-N23	2.32	1.51	1.46	10	30
3	A	256	8MI	C30-N29	2.06	1.37	1.41	18	10

All unique angle outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
3	A	256	8MI	C30-N29-C27	3.04	120.43	127.37	16	30

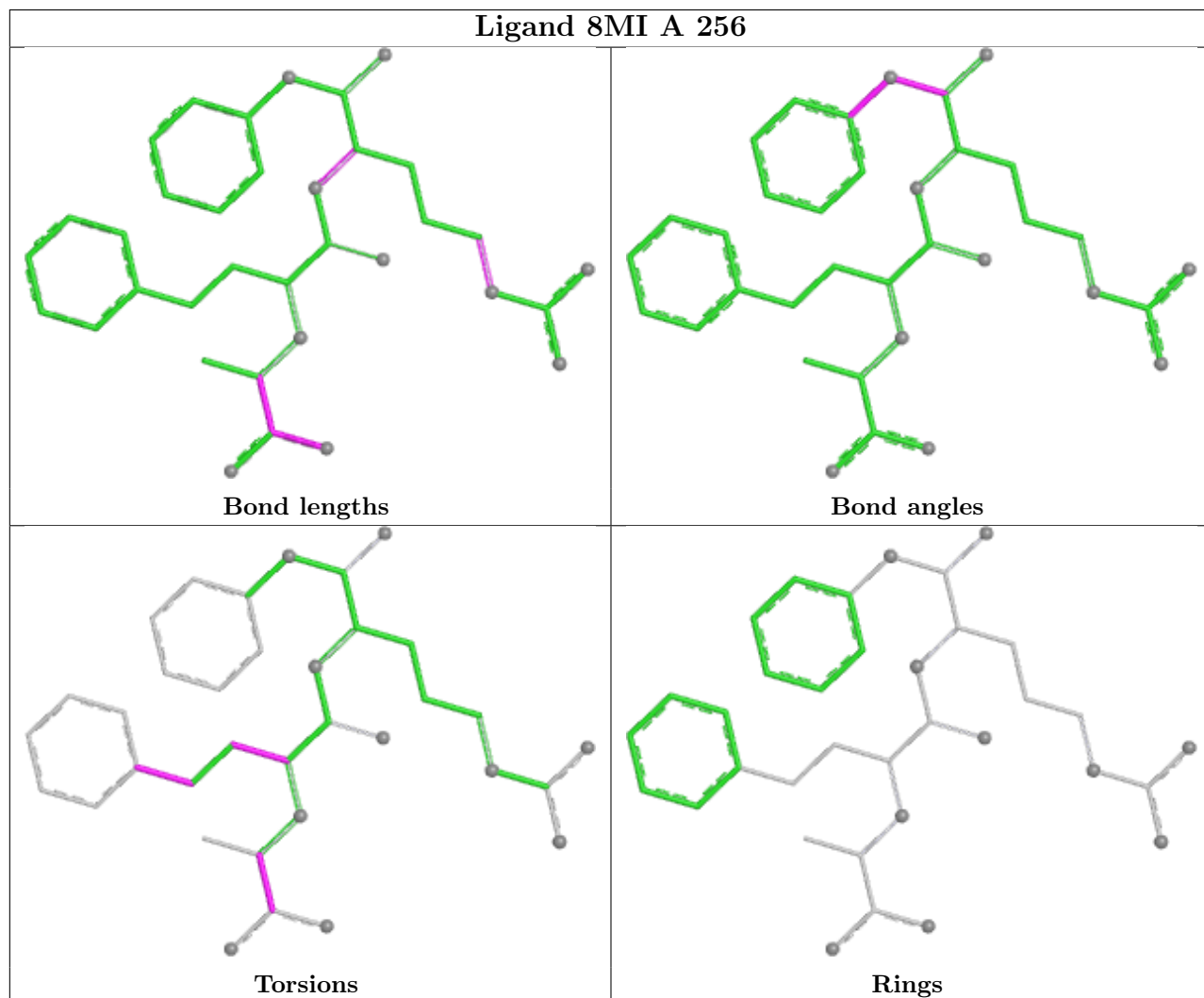
There are no chirality outliers.

There are no torsion outliers.

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

No chemical shift data were provided