Full wwPDB NMR Structure Validation Report (i)

Sep 22, 2021 – 02:09 PM EDT

PDB ID	:	2SRT
Title	:	CATALYTIC DOMAIN OF HUMAN STROMELYSIN-1 AT PH 5.5 AND 40OC 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*
A user guide is available at
https://www.wwpdb.org/validation/2017/NMRValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

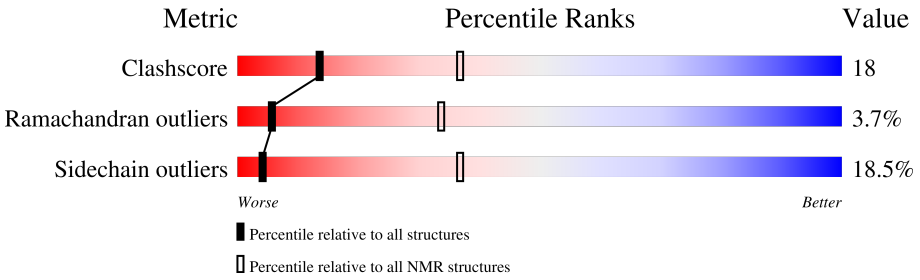
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.23.1
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.1

1 Overall quality at a glance (i)

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	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	173	61% 25% 7% 7%

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)	0.34	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.

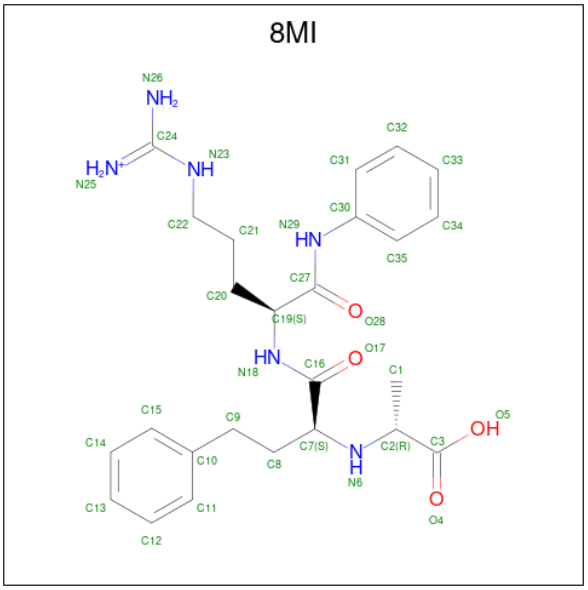
- Molecule 1 is a protein called STROMELYSIN-1.

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 (three-letter code: 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 (three-letter code: 8MI) (formula: $C_{25}H_{35}N_6O_4$).



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

Chain A: 61% 25% 7% 7%

F83 F86 I89 P90 K91 T98 T105 P106 D107 S115 K119 A120 V123 W124 V127 R134 M143 V148 R149 E150 H151 G152 D153 F154 Y155 P156 F157 D158 G159 P160 G161 N162 V163 H166 A167 Y168 A169 P170 G171 P172 G173 I174 D177 D182 T187

G192 F196 L197 A200 H201 E202 H205 G208 L209 F210 H211 S212 A213 N214 L218 M219 Y220 P221 L222 L229 T230 R231 F232 R233 L234 I239 I242 D251 S252 P253 E254 T255

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

Chain A: 59% 27% 7% • 7%

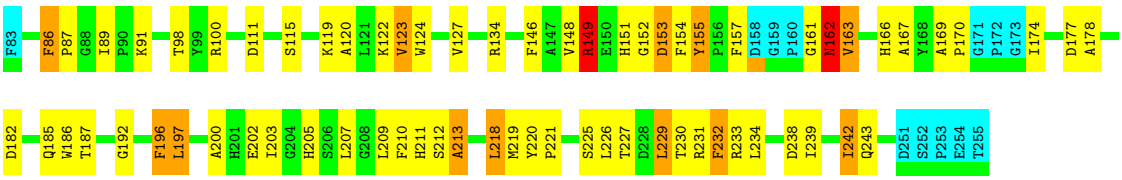
F83 F86 P87 G88 I89 P90 K91 T98 I101 T105 K110 S115 E118 V123 W124 V127 R134 F146 R149 E150 H151 G152 D153 F154 Y155 D158 G159 P160 G161 N162 V163 H166 A167 Y168 A169 P170 G171 P172 G173 I174 T187 G192 T193 N194

L195 F196 L197 A200 H201 E202 I203 G204 H205 G208 L209 F210 H211 S212 A213 N214 L218 M219 Y220 P221 L222 L229 T230 R231 F232 R233 L234 D237 D238 I239 N240 G241 I242 Q243 D251 S252 P253 E254 T255

4.2.2 Score per residue for model 2

• Molecule 1: STROMELYSIN-1

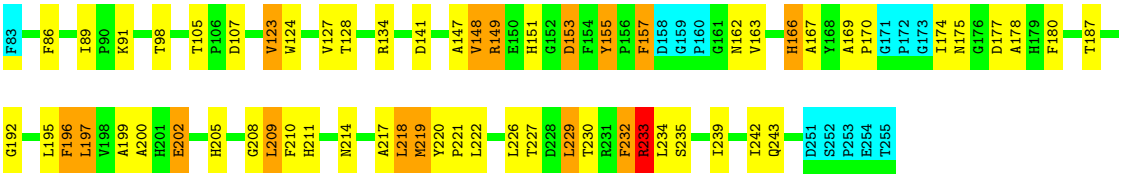
Chain A: 54% 31% 7% • 7%



4.2.3 Score per residue for model 3

- Molecule 1: STROMELYSIN-1

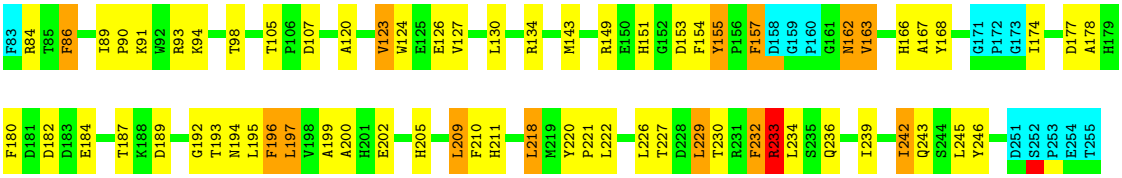
Chain A: 58% 26% 9% • 7%



4.2.4 Score per residue for model 4

- Molecule 1: STROMELYSIN-1

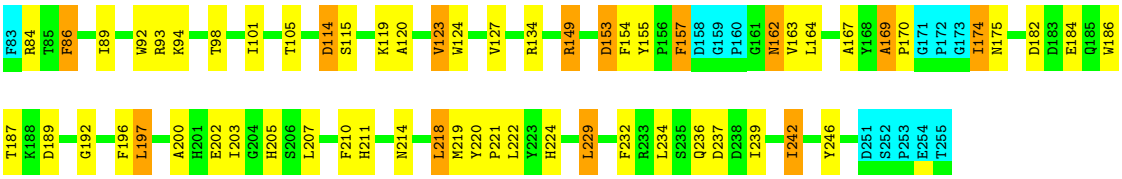
Chain A: 54% 31% 8% • 7%



4.2.5 Score per residue for model 5

- Molecule 1: STROMELYSIN-1

Chain A: 58% 27% 8% 7%



4.2.6 Score per residue for model 6

- Molecule 1: STROMELYSIN-1

Chain A: 64% 24% 5% 7%

F83 F86 I89 P90 K91 W92 R93 T98 T105 P106 D107 A120 L121 K122 V123 W124 V127 R134 M143 R149 E150 H151 Y155 P156 F157 D158 G159 P160 G161 N162 V163 H166 A167 Y168 A169 P170 G171 P172 G173 I174 D177 D182 T187 G192 T193

N194 L197 A200 H205 S206 L207 F210 E216 A217 L218 M219 Y220 P221 L222 Y223 H224 D228 L229 F232 R233 L234 I239 I242 L245 D251 S252 P253 E254 T255

4.2.7 Score per residue for model 7

- Molecule 1: STROMELYSIN-1

Chain A: 55% 29% 8% • 7%

F83 F86 I89 P90 K91 H96 L97 T98 T105 P106 D107 K110 D111 S115 K119 A120 V123 W124 E125 E126 V127 M143 V148 R149 D153 F154 Y155 P156 F157 D158 G159 P160 G161 N162 V163 L164 A165 H166 A167 Y168 A169 P170 G171 P172 G173 I174 N175 G176 D177

D182 Q185 W186 T187 G192 F196 L197 A200 H201 E202 G208 L209 F210 H211 S212 A213 N214 T215 E216 A217 L218 M219 Y220 P221 L222 D228 L229 T230 R231 F232 R233 L234 S235 Q236 I239 I242 D251 S252 P253 E254 T255

4.2.8 Score per residue for model 8

- Molecule 1: STROMELYSIN-1

Chain A: 61% 24% 8% • 7%

F83 F86 I89 R93 T98 T105 P106 D107 D111 S115 K119 V123 W124 E125 E126 V127 M143 F146 R149 E150 H151 G152 D153 F154 Y155 P156 F157 D158 G159 P160 G161 N162 V163 A167 Y168 A169 P170 G171 P172 G173 I174 F180 D181 D182 T187

K188 D189 G192 F196 L197 A200 H201 E202 I203 G204 H205 G208 L209 F210 H211 S212 L218 M219 Y220 P221 L222 L229 F232 R233 L234 S235 Q236 I239 N240 G241 I242 D251 S252 P253 E254 T255

4.2.9 Score per residue for model 9

- Molecule 1: STROMELYSIN-1

Chain A: 58% 28% 6% • 7%

F83 F86 P87 G88 I89 P90 K91 W92 T98 T105 D111 D114 S115 K119 A120 V123 W124 V127 T128 P129 L130 R134 R149 E150 H151 G152 D153 F154 Y155 P156 F157 D158 G159 P160 G161 N162 V163 A167 Y168 A169 P170 G171 P172 G173 I174 N175 D182 D183

E184 T187 G192 F196 L197 A200 H201 E202 I203 G204 H205 G208 L209 F210 H211 L218 M219 Y220 P221 L222 T227 D228 L229 F232 R233 L234 I239 N240 G241 I242 Q243 Y246 D251 S252 P253 E254 T255

4.2.10 Score per residue for model 10 (medoid)

- Molecule 1: STROMELYSIN-1

Chain A: 58% 25% 8% • 7%

F83 F86 P87 G88 I89 P90 K91 T98 Y99 R100 I101 T105 P106 D107 K110 S115 K119 A120 V123 W124 V127 R134 M143 A147 V148 R149 E150 H151 G152 D153 F154 Y155 P156 F157 D158 G159 P160 G161 N162 V163 H166 A167 Y168 A169 P170 G171 P172 G173

I174 D177 D181 Q185 W186 T187 G192 F196 L197 A200 H201 E202 H205 L209 F210 H211 L218 D228 L229 T230 R231 F232 R233 L234 S235 Q236 I239 N240 G241 I242 L245 D251 S252 P253 E254 T255

4.2.11 Score per residue for model 11

- Molecule 1: STROMELYSIN-1

Chain A: 58% 25% 9% 7%

F83 F86 I89 P90 K91 K94 T98 Y99 R100 I101 T105 P106 D107 S115 E118 K119 A120 L121 K122 V123 W124 V127 R134 F146 R149 D153 F154 Y155 P156 F157 D158 G159 P160 G161 N162 V163 H166 A167 Y168 A169 P170 G171 P172 G173 I174 D177

D182 D183 E184 T187 K188 D189 G192 F196 L197 A200 H201 E202 I203 G204 H205 G208 L209 F210 H211 S212 A213 L218 L222 L229 F232 R233 L234 I239 I242 L245 D251 S252 P253 E254 T255

4.2.12 Score per residue for model 12

- Molecule 1: STROMELYSIN-1

Chain A: 55% 30% 7% • 7%

F83 F86 I89 P90 K91 W92 R93 K94 T98 I101 T105 P106 D107 V123 W124 V127 L130 D141 I142 M143 A147 V148 R149 E150 H151 F154 Y155 P156 F157 D158 G159 P160 G161 N162 V163 L164 A165 H166 A167 Y168 A169 P170 G171 P172 G173 I174 D177 A178

H179 F180 D181 D182 D183 E184 Q185 W186 T187 T190 T191 G192 F196 L197 A200 H201 E202 G208 L209 F210 N214 L218 M219 Y220 P221 L222 S225 L226 L229 T230 R231 F232 R233 L234 I239 N240 G241 I242 L245 Y246 D251 S252 P253 E254 T255

4.2.13 Score per residue for model 13

- Molecule 1: STROMELYSIN-1

Chain A: 54% 32% 6% • 7%

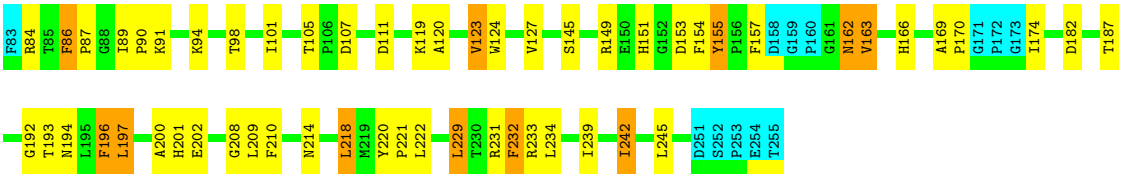
F83 R84 T85 F86 P87 G88 I89 P90 K91 T98 T105 P106 D107 S115 K119 A120 V123 W124 V127 L130 M143 A147 V148 R149 E150 H151 G152 D153 F154 Y155 P156 F157 D158 G159 P160 G161 N162 V163 H166 A167 Y168 A169 P170 G171 P172 G173 I174 D177

D182 D183 E184 Q185 W186 T187 K188 D189 G192 L197 A200 H201 E202 I203 G208 L209 F210 H211 S212 A213 N214 A217 L218 M219 Y220 P221 L222 L229 F232 R233 L234 S235 I239 I242 L245 Y246 D251 S252 P253 E254 T255

4.2.14 Score per residue for model 14

- Molecule 1: STROMELYSIN-1

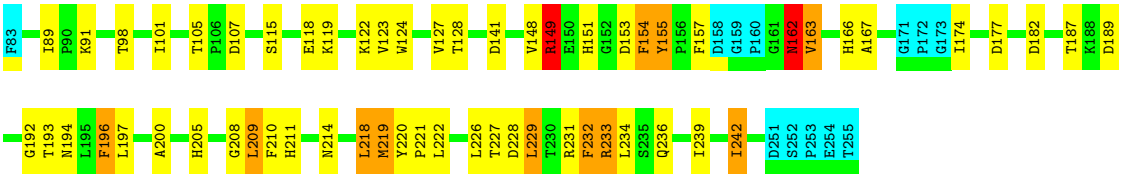
Chain A: 61% 26% 6% 7%



4.2.15 Score per residue for model 15

- Molecule 1: STROMELYSIN-1

Chain A: 59% 27% 6% • 7%



4.2.16 Score per residue for model 16

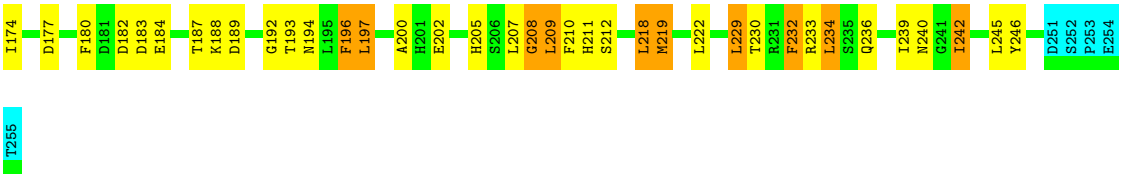
- Molecule 1: STROMELYSIN-1

Chain A: 52% 36% 5% • 7%

4.2.17 Score per residue for model 17

- Molecule 1: STROMELYSIN-1

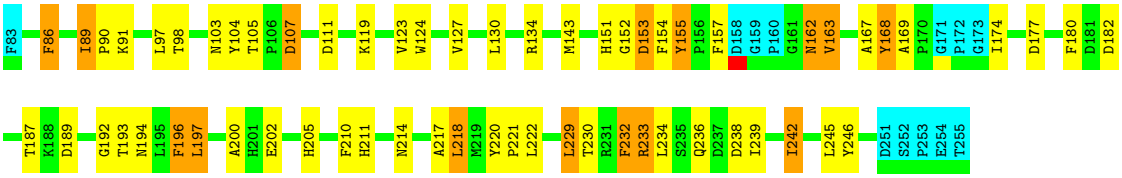
Chain A: 53% 30% 9% • 7%



4.2.18 Score per residue for model 18

- Molecule 1: STROMELYSIN-1

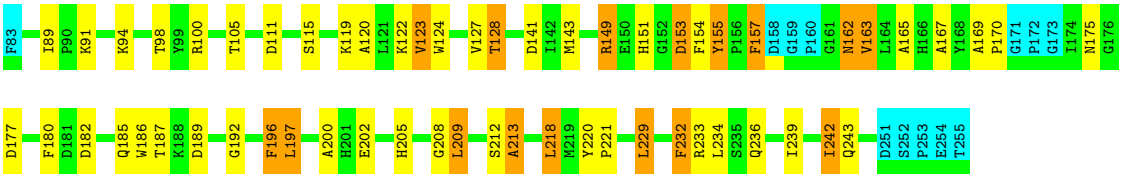
Chain A: 57% 27% 9% 7%



4.2.19 Score per residue for model 19

- Molecule 1: STROMELYSIN-1

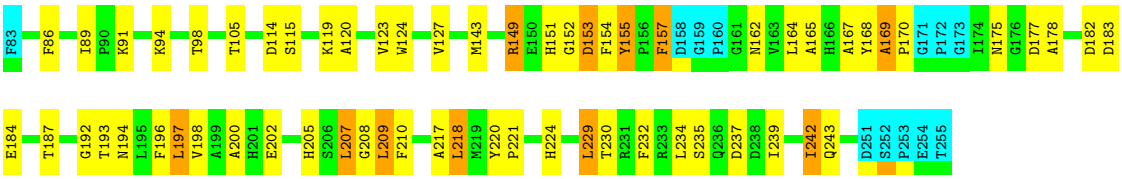
Chain A: 60% 24% 9% 7%



4.2.20 Score per residue for model 20

- Molecule 1: STROMELYSIN-1

Chain A: 57% 29% 6% 7%



4.2.21 Score per residue for model 21

- Molecule 1: STROMELYSIN-1

Chain A: 57% 28% 6% • 7%

F83 R84 T85 F86 T98 T105 P106 D107 K110 D114 E118 K119 A120 L121 K122 V123 W124 V127 L130 R134 M143 V148 R149 E150 H151 G152 D153 F154 Y155 P156 F157 D158 G159 P160 G161 N162 V163 H166 A167 G171 P172 G173 I174 D177 A178 H179 F180

D181 D182 D183 E184 T187 G192 T193 N194 L195 F196 L197 V198 A199 A200 H201 E202 H205 G208 L209 F210 H211 S212 L218 M219 Y220 P221 L222 Y223 H224 L229 T230 R231 F232 R233 L234 D237 D238 I239 I242 Y246 D251 S252 P253 E254 T255

4.2.22 Score per residue for model 22

- Molecule 1: STROMELYSIN-1

Chain A: 56% 30% 6% • 7%

F83 F86 I89 P90 K91 W92 R93 K94 L97 T98 Y99 R100 I101 T105 K122 V123 W124 E125 E126 V127 D141 I144 V148 R149 E150 H151 G152 D153 F154 Y155 P156 F157 D158 G159 P160 G161 N162 V163 H166 A167 Y168 A169 P170 G171 P172 G173 I174 D177 A178 H179

F180 D181 D182 D183 E184 Q185 W186 T187 G192 F196 L197 A200 H201 E202 H205 G208 L209 F210 H211 S212 A213 N214 L218 M219 Y220 P221 L222 Y223 H224 L229 F232 R233 L234 S235 Q236 I239 I242 D251 S252 P253 E254 T255

4.2.23 Score per residue for model 23

- Molecule 1: STROMELYSIN-1

Chain A: 53% 32% 8% • 7%

F83 F86 P87 G88 I89 P90 K91 W92 R93 T98 T105 P106 D107 K110 S115 K119 A120 V123 W124 V127 D141 I142 M143 F146 R149 E150 H151 Y155 P156 F157 D158 G159 P160 G161 N162 V163 L164 A165 H166 A167 Y168 A169 P170 G171 P172 G173 I174

D177 F180 D181 D182 T187 K188 G192 T193 N194 L195 F196 L197 V198 A199 A200 H201 E202 I203 G204 H205 G208 L209 F210 H211 N214 T215 E216 A217 L218 M219 Y220 P221 L222 L229 T230 R231 F232 R233 L234 D237 D238 I239 I242 L245 Y246 D251 S252 P253 E254 T255

4.2.24 Score per residue for model 24

- Molecule 1: STROMELYSIN-1

Chain A: 58% 29% 5% • 7%

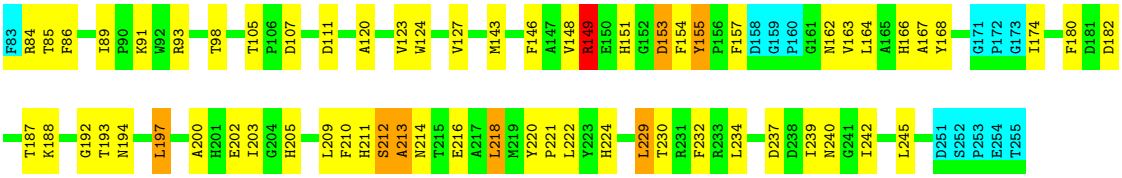
F83 R84 T85 F86 I89 P90 K91 W92 R93 T98 I101 T105 P106 D107 S115 K119 V123 W124 V127 L130 M143 A147 V148 R149 E150 H151 G152 D153 F154 Y155 P156 F157 D158 G159 P160 G161 N162 V163 H166 A167 Y168 G171 P172 G173 I174 D177

D182 D183 E184 Q185 W186 T187 G192 F196 L197 A200 H201 E202 I203 G204 H205 F210 H211 E216 A217 L218 M219 Y220 P221 L222 T227 D228 L229 T230 R231 F232 R233 L234 S235 Q236 I239 I242 Y246 D251 S252 P253 E254 T255

4.2.25 Score per residue for model 25

- Molecule 1: STROMELYSIN-1

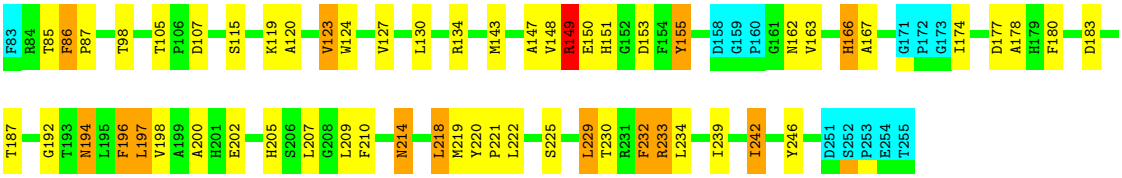
Chain A: 57% 32% • • 7%



4.2.26 Score per residue for model 26

- Molecule 1: STROMELYSIN-1

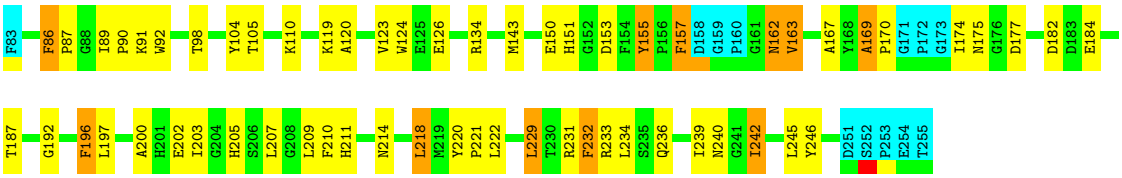
Chain A: 60% 25% 8% • 7%



4.2.27 Score per residue for model 27

- Molecule 1: STROMELYSIN-1

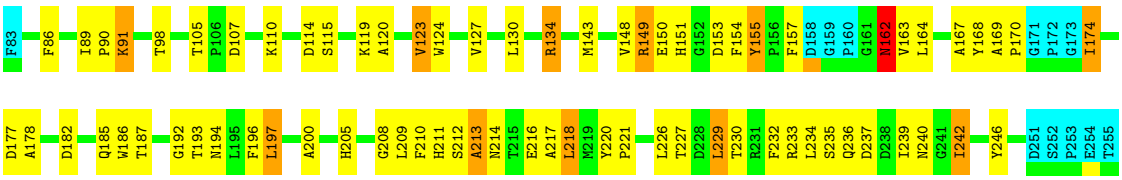
Chain A: 58% 28% 6% 7%



4.2.28 Score per residue for model 28

- Molecule 1: STROMELYSIN-1

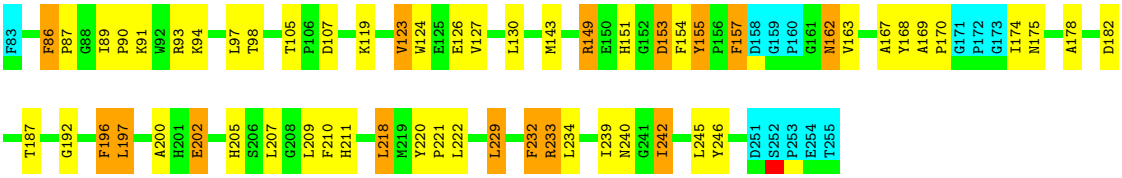
Chain A: 51% 35% 6% • 7%



4.2.29 Score per residue for model 29

- Molecule 1: STROMELYSIN-1

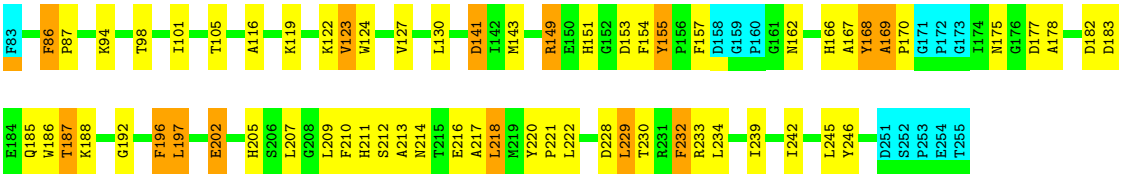
Chain A: 60% 25% 9% 7%



4.2.30 Score per residue for model 30

- Molecule 1: STROMELYSIN-1

Chain A: 56% 29% 8% 7%



5 Refinement protocol and experimental data overview (i)

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

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

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.

There are no bond-angle outliers.

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
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	45±5
3	A	35	35	0	1±1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes
All	All	39900	37980	36930	1377

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 18.

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: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:90:PRO:O	1:A:245:LEU:HD22	0.70	1.87	17	13
1:A:239:ILE:HG23	1:A:243:GLN:OE1	0.69	1.87	1	1
1:A:229:LEU:C	1:A:229:LEU:HD13	0.69	2.08	26	14
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:229:LEU:HD23	1:A:229:LEU:C	0.66	2.11	10	16
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:151:HIS:CD2	1:A:155:TYR:CZ	0.65	2.84	21	4
1:A:86:PHE:C	1:A:86:PHE:CD1	0.65	2.69	13	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:155:TYR:CD1	1:A:168:TYR:OH	0.64	2.50	16	2
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:210:PHE:O	1:A:211:HIS:CD2	0.63	2.52	30	8
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: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:208:GLY:C	1:A:209:LEU:HD23	0.60	2.17	8	3
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:148:VAL:O	1:A:149:ARG:C	0.58	2.42	13	14
1:A:187:THR:HG21	1:A:192:GLY:N	0.58	2.14	20	13
1:A:154:PHE:CG	1:A:154:PHE:O	0.58	2.57	19	9
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:196:PHE:CD1	1:A:196:PHE:C	0.57	2.78	12	16
1:A:155:TYR:CD2	1:A:168:TYR:OH	0.57	2.58	4	4
1:A:218:LEU:C	1:A:218:LEU:HD23	0.57	2.19	5	13
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: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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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: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:154:PHE:O	1:A:154:PHE:CG	0.54	2.60	13	6
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:CG	1:A:174:ILE:HD11	0.53	2.24	21	1
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:157:PHE:CD1	1:A:157:PHE:N	0.53	2.75	3	2
1:A:165:ALA:HB1	1:A:202:GLU:CD	0.53	2.24	16	2
1:A:239:ILE:HG23	1:A:243:GLN:CD	0.53	2.23	1	1
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
1:A:177:ASP:OD1	1:A:178:ALA:N	0.53	2.42	22	7
1:A:193:THR:O	1:A:194:ASN:C	0.52	2.48	21	13
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: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:155:TYR:CD1	1:A:155:TYR:O	0.51	2.64	21	7
1:A:232:PHE:CD1	1:A:232:PHE:C	0.51	2.83	8	5
1:A:147:ALA:HB1	1:A:151:HIS:HB3	0.51	1.83	26	6
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:210:PHE:O	1:A:211:HIS:C	0.51	2.50	9	14
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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:124:TRP:CH2	1:A:209:LEU:HD12	0.49	2.42	16	12
1:A:197:LEU:C	1:A:197:LEU:HD13	0.49	2.27	12	2
1:A:218:LEU:HD23	1:A:218:LEU:C	0.49	2.28	3	4
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:155:TYR:CE2	1:A:168:TYR:OH	0.49	2.63	20	1
1:A:152:GLY:O	1:A:153:ASP:CG	0.49	2.51	18	4
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:180:PHE:CE2	1:A:202:GLU:OE1	0.48	2.66	19	4
1:A:84:ARG:C	1:A:85:THR:HG23	0.48	2.29	25	1
1:A:234:LEU:HB2	1:A:239:ILE:HD11	0.48	1.86	5	2
1:A:194:ASN:O	1:A:198:VAL:HG23	0.48	2.08	26	1
1:A:162:ASN:O	1:A:163:VAL:C	0.48	2.51	22	22
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: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:180:PHE:CD1	1:A:202:GLU:OE1	0.47	2.68	22	1
1:A:229:LEU:C	1:A:229:LEU:CD1	0.47	2.82	15	11
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:226:LEU:O	1:A:227:THR:C	0.46	2.54	3	6
1:A:153:ASP:OD1	1:A:174:ILE:CD1	0.46	2.63	28	3
1:A:239:ILE:O	1:A:240:ASN:C	0.46	2.53	17	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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:185:GLN:HG3	1:A:186:TRP:N	0.46	2.26	19	5
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: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:153:ASP:CG	1:A:155:TYR:CD2	0.45	2.90	13	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:229:LEU:C	1:A:229:LEU:CD2	0.45	2.85	2	6
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
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: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:153:ASP:CG	1:A:174:ILE:CD1	0.44	2.86	28	4
1:A:130:LEU:HD21	1:A:246:TYR:CZ	0.44	2.48	21	2
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: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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:185:GLN:CG	1:A:186:TRP:N	0.43	2.82	12	6
1:A:151:HIS:NE2	1:A:155:TYR:CD1	0.43	2.87	8	1
1:A:94:LYS:NZ	1:A:141:ASP:OD2	0.43	2.51	17	4
1:A:91:LYS:NZ	1:A:245:LEU:O	0.43	2.52	23	1
1:A:165:ALA:HB3	1:A:202:GLU:CD	0.43	2.34	20	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:153:ASP:N	1:A:153:ASP:OD1	0.43	2.50	21	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:209:LEU:HB3	1:A:219:MET:SD	0.42	2.54	26	1
1:A:228:ASP:OD2	1:A:231:ARG:NH1	0.42	2.52	10	1
1:A:155:TYR:CG	1:A:166:HIS:CE1	0.42	3.08	10	1
1:A:166:HIS:CD2	1:A:166:HIS:C	0.42	2.93	3	2
1:A:165:ALA:HB1	1:A:202:GLU:OE1	0.42	2.13	16	2
1:A:90:PRO:O	1:A:91:LYS:HB3	0.42	2.14	28	1
1:A:155:TYR:CE1	1:A:168:TYR:OH	0.42	2.66	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: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: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:165:ALA:CB	1:A:202:GLU:CD	0.42	2.88	20	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: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:161:GLY:C	1:A:162:ASN:CG	0.41	2.79	7	2
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:148:VAL:HG23	1:A:149:ARG:N	0.41	2.31	26	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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: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: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
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: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: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:O	1:A:229:LEU:HD13	0.40	2.16	27	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%)	6	34
All	All	4830/5190 (93%)	4106 (85%)	545 (11%)	179 (4%)	6	34

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

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Mol	Chain	Res	Type	Models (Total)
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
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%)	112±3 (82±2%)	26±3 (18±2%)	4 37
All	All	4140/4410 (94%)	3375 (82%)	765 (18%)	4 37

All 73 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	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	86	PHE	27
1	A	174	ILE	27
1	A	242	ILE	26

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Mol	Chain	Res	Type	Models (Total)
1	A	182	ASP	26
1	A	197	LEU	25
1	A	222	LEU	25
1	A	196	PHE	24
1	A	143	MET	21
1	A	123	VAL	20
1	A	232	PHE	19
1	A	230	THR	16
1	A	177	ASP	16
1	A	202	GLU	15
1	A	236	GLN	14
1	A	157	PHE	13
1	A	214	ASN	12
1	A	203	ILE	11
1	A	134	ARG	11
1	A	149	ARG	10
1	A	166	HIS	10
1	A	94	LYS	10
1	A	184	GLU	10
1	A	189	ASP	10
1	A	122	LYS	9
1	A	153	ASP	9
1	A	243	GLN	8
1	A	111	ASP	8
1	A	219	MET	8
1	A	141	ASP	8
1	A	233	ARG	8
1	A	216	GLU	8
1	A	240	ASN	8
1	A	110	LYS	7
1	A	237	ASP	7
1	A	209	LEU	7
1	A	126	GLU	7
1	A	228	ASP	7
1	A	168	TYR	7
1	A	224	HIS	6
1	A	183	ASP	6
1	A	118	GLU	5
1	A	154	PHE	5
1	A	114	ASP	5
1	A	115	SER	4
1	A	164	LEU	4

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Mol	Chain	Res	Type	Models (Total)
1	A	188	LYS	4
1	A	225	SER	3
1	A	150	GLU	3
1	A	107	ASP	3
1	A	104	TYR	3
1	A	238	ASP	2
1	A	227	THR	2
1	A	231	ARG	2
1	A	245	LEU	2
1	A	212	SER	1
1	A	148	VAL	1
1	A	84	ARG	1
1	A	96	HIS	1
1	A	175	ASN	1
1	A	93	ARG	1
1	A	145	SER	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
1	A	187	THR	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 monosaccharides 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	33,36,36	1.03±0.00	2±0 (6±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	41,46,46	0.77±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±0,32,36,36	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	2.83	1.51	1.45	4	30
3	A	256	8MI	C22-N23	2.28	1.51	1.46	10	30
3	A	256	8MI	C30-N29	2.05	1.37	1.41	18	9

All unique angle outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	A	256	8MI	C30-N29-C27	2.91	120.43	127.40	16	30

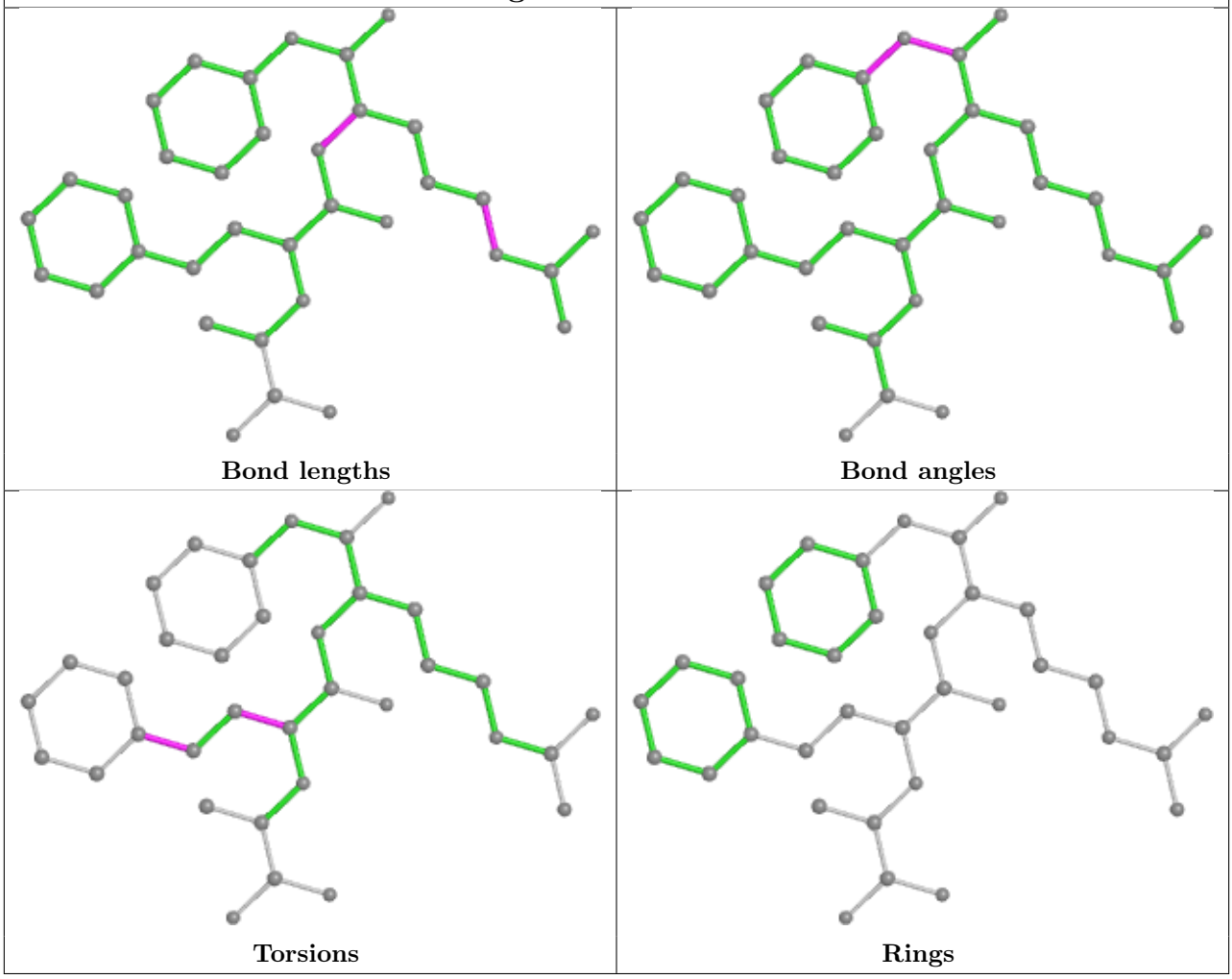
There are no chirality outliers.

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 then 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.

Ligand 8MI A 256



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 (i)

No chemical shift data were provided