



# Full wwPDB NMR Structure Validation Report ⓘ

Nov 23, 2019 – 03:56 PM EST

PDB ID : 6CLZ  
Title : MT1-MMP HPX domain with Blade 4 Loop Bound to Nanodiscs  
Authors : Marcink, T.C.; Van Doren, S.R.  
Deposited on : 2018-03-02

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.

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

Cyrange : **FAILED**  
NmrClust : **FAILED**  
MolProbity : **FAILED**  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
RCI : v\_1n\_11\_5\_13\_A (Berjanski et al., 2005)  
PANAV : Wang et al. (2010)  
ShiftChecker : 2.4  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.4

## 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 3%.

There are no overall percentile quality scores available for this entry.

The sequence quality summary graphics cannot be shown.

## 2 Ensemble composition and analysis ⓘ

This entry contains 15 models. The atoms present in the NMR models are not consistent. Some calculations may have failed as a result. All residues are included in the validation scores.

Cyrange was unable to find well-defined residues.

Error message: Cyrange did not run

NmrClust was unable to cluster the ensemble.

Error message: NmrClust did not run

### 3 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 35924 atoms, of which 20751 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Matrix metalloproteinase-14.

Mol	Chain	Residues	Atoms						Trace
1	A	196	Total	C	H	N	O	S	0
			3202	1067	1565	277	284	9	

- Molecule 2 is a protein called Apolipoprotein A-I.

Mol	Chain	Residues	Atoms						Trace
2	B	211	Total	C	H	N	O	S	0
			3498	1101	1745	308	340	4	
2	C	211	Total	C	H	N	O	S	0
			3498	1101	1745	308	340	4	

There are 44 discrepancies between the modelled and reference sequences:

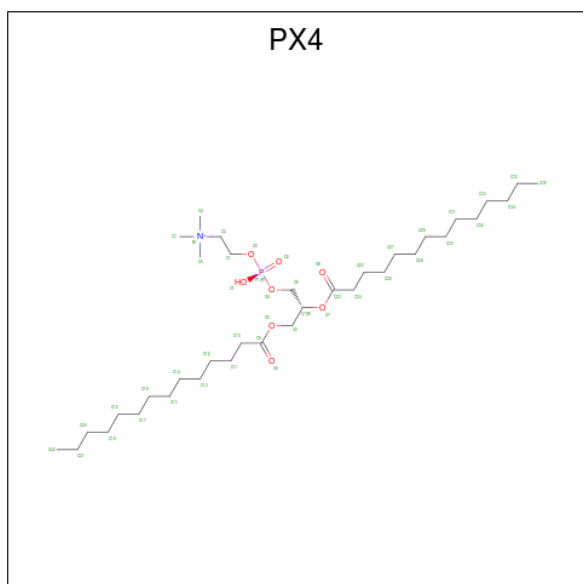
Chain	Residue	Modelled	Actual	Comment	Reference
B	99	PRO	-	insertion	UNP P02647
B	100	TYR	-	insertion	UNP P02647
B	101	LEU	-	insertion	UNP P02647
B	102	ASP	-	insertion	UNP P02647
B	103	ASP	-	insertion	UNP P02647
B	104	PHE	-	insertion	UNP P02647
B	105	GLN	-	insertion	UNP P02647
B	106	LYS	-	insertion	UNP P02647
B	107	LYS	-	insertion	UNP P02647
B	108	TRP	-	insertion	UNP P02647
B	109	GLN	-	insertion	UNP P02647
B	110	GLU	-	insertion	UNP P02647
B	111	GLU	-	insertion	UNP P02647
B	112	MET	-	insertion	UNP P02647
B	113	GLU	-	insertion	UNP P02647
B	114	LEU	-	insertion	UNP P02647
B	115	TYR	-	insertion	UNP P02647
B	116	ARG	-	insertion	UNP P02647
B	117	GLN	-	insertion	UNP P02647
B	118	LYS	-	insertion	UNP P02647
B	119	VAL	-	insertion	UNP P02647
B	120	GLU	-	insertion	UNP P02647
C	99	PRO	-	insertion	UNP P02647

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Chain	Residue	Modelled	Actual	Comment	Reference
C	100	TYR	-	insertion	UNP P02647
C	101	LEU	-	insertion	UNP P02647
C	102	ASP	-	insertion	UNP P02647
C	103	ASP	-	insertion	UNP P02647
C	104	PHE	-	insertion	UNP P02647
C	105	GLN	-	insertion	UNP P02647
C	106	LYS	-	insertion	UNP P02647
C	107	LYS	-	insertion	UNP P02647
C	108	TRP	-	insertion	UNP P02647
C	109	GLN	-	insertion	UNP P02647
C	110	GLU	-	insertion	UNP P02647
C	111	GLU	-	insertion	UNP P02647
C	112	MET	-	insertion	UNP P02647
C	113	GLU	-	insertion	UNP P02647
C	114	LEU	-	insertion	UNP P02647
C	115	TYR	-	insertion	UNP P02647
C	116	ARG	-	insertion	UNP P02647
C	117	GLN	-	insertion	UNP P02647
C	118	LYS	-	insertion	UNP P02647
C	119	VAL	-	insertion	UNP P02647
C	120	GLU	-	insertion	UNP P02647

- Molecule 3 is 1,2-DIMYRISTOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PX4) (formula: C<sub>36</sub>H<sub>73</sub>NO<sub>8</sub>P).



[illegible]

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[illegible]

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[illegible]

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[illegible]

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[illegible]

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[illegible]

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[illegible]

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[illegible]

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[illegible]

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[illegible]

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Mol	Chain	Residues	Atoms					
3	C	1	Total	C	H	N	O	P
			118	36	72	1	8	1
3	C	1	Total	C	H	N	O	P
			118	36	72	1	8	1
3	C	1	Total	C	H	N	O	P
			118	36	72	1	8	1
3	C	1	Total	C	H	N	O	P
			118	36	72	1	8	1
3	C	1	Total	C	H	N	O	P
			118	36	72	1	8	1
3	C	1	Total	C	H	N	O	P
			118	36	72	1	8	1

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	
4	A	1	Total	Na
			1	1

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	
5	A	1	Total	Cl
			1	1

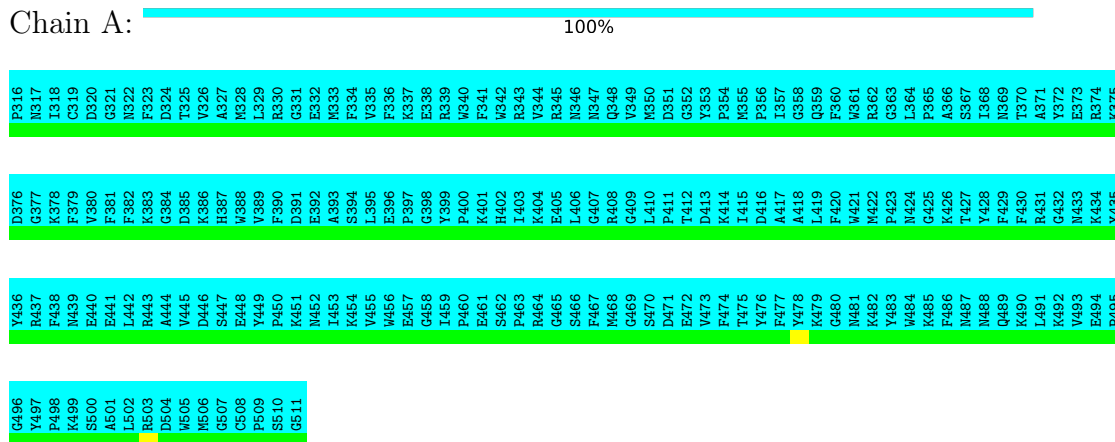


## 4 Residue-property plots

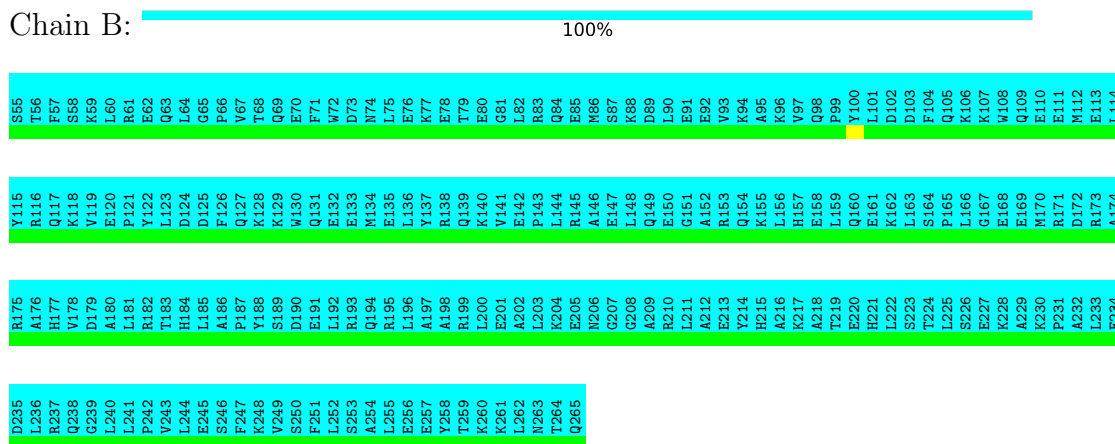
### 4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA and DNA chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

- Molecule 1: Matrix metalloproteinase-14



- Molecule 2: Apolipoprotein A-I



- Molecule 2: Apolipoprotein A-I



S55	Y115	R175	D285
T56	R116	A176	L286
F57	K117	H177	R237
S58	K118	V178	Q238
K59	V119	D179	G239
L60	E120	A180	L240
R61	P121	L181	L241
E62	Y122	R182	P242
Q63	L123	L183	V243
L64	D124	H184	L244
G65	D125	L185	E245
P66	F126	A186	S246
V67	Q127	P187	F247
T68	K128	Y188	K248
Q69	K129	S189	V249
E70	W130	D190	S250
F71	Q131	E191	F251
W72	E132	L192	L252
D73	E133	R193	S253
N74	M134	Q194	A254
L75	E135	R195	L255
E76	L136	L196	E256
K77	Y137	A197	E257
E78	R138	A198	Y258
T79	Q139	R199	T259
E80	K140	L200	K260
G81	V141	E201	K261
L82	A142	A202	L262
R83	P143	L203	N263
Q84	L144	K204	T264
R85	R145	E205	Q265
H86	A146	N206	
S87	E147	G207	
K88	L148	G208	
D89	Q149	A209	
L90	E150	R210	
E91	G151	L211	
E92	A152	A212	
V93	R153	E213	
K94	Q154	Y214	
A95	K155	H215	
K96	L156	A216	
V97	H157	K217	
Q98	E158	A218	
P99	L159	T219	
Y100	Q160	E220	
L101	E161	H221	
D102	K162	L222	
D103	L163	S223	
F104	S164	T224	
Q105	P165	L225	
K106	L166	S226	
K107	G167	E227	
W108	E168	K228	
Q109	E169	A229	
E110	M170	K230	
E111	R171	P231	
M112	D172	A232	
E113	R173	L233	
L114	A174	E234	

## 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-14

Chain A: 100%

P316	D376	V436	G496
N317	G377	R437	Y497
I318	K378	F438	P498
C319	F379	N439	K499
D320	V380	E440	S500
G321	F381	E441	A501
N322	F382	L442	L502
F323	K383	R443	R503
D324	G384	A444	D504
T325	D385	V445	W505
V326	K386	D446	M506
A327	H387	S447	G507
K328	V388	F448	C508
L329	V389	Y449	P509
R330	F390	P450	S510
G331	D391	K451	G511
E332	E392	N452	
N333	A393	L453	
F334	S394	K454	
V335	L395	V455	
F336	E396	W456	
K337	P397	E457	
E338	G398	G458	
R339	Y399	L459	
V340	P400	P460	
F341	K401	E461	
V342	H402	S462	
K343	L403	P463	
V344	K404	R464	
E345	E405	G465	
N346	L406	S466	
K347	G407	F467	
Q348	R408	N468	
V349	G409	G469	
N350	L410	S470	
D351	P411	D471	
G352	T412	E472	
V353	D413	V473	
F354	K414	F474	
N355	I415	T475	
P356	D416	V476	
I357	A417	F477	
G358	A418	Y478	
Q359	L419	K479	
F360	F420	G480	
W361	W421	N481	
R362	M422	K482	
G363	P423	Y483	
L364	N424	W484	
P365	G425	K485	
A366	K426	F486	
S367	T427	N487	
I368	Y428	N488	
N369	F429	Q489	
T370	F430	K490	
A371	R431	L491	
V372	G432	K492	
E373	N433	V493	
K374	K434	E494	
K375	Y435	P495	

- Molecule 2: Apolipoprotein A-I

Chain B: 100%

S55	Y115	R175	S55
T56	R116	A176	T56
F57	K117	H177	F57
S58	K118	V178	S58
K59	V119	D179	K59
L60	E120	A180	L60
R61	P121	L181	R61
E62	Y122	R182	E62
Q63	L123	L183	Q63
L64	D124	H184	L64
G65	D125	L185	G65
P66	F126	A186	P66
V67	Q127	P187	V67
T68	K128	Y188	T68
Q69	K129	S189	Q69
E70	W130	D190	E70
F71	Q131	E191	F71
W72	E132	L192	W72
D73	E133	R193	D73
N74	M134	Q194	N74
L75	E135	R195	L75
E76	L136	L196	E76
K77	Y137	A197	K77
E78	R138	A198	E78
T79	Q139	R199	T79
E80	K140	L200	E80
G81	V141	E201	G81
L82	A142	A202	L82
R83	P143	L203	R83
Q84	L144	K204	Q84
E85	R145	E205	E85
H86	A146	N206	H86
S87	E147	G207	S87
K88	L148	G208	K88
D89	Q149	A209	D89
L90	E150	R210	L90
E91	G151	L211	E91
E92	A152	A212	E92
V93	R153	E213	V93
K94	Q154	Y214	K94
A95	K155	H215	A95
K96	L156	A216	K96
V97	H157	K217	V97
Q98	E158	A218	Q98
P99	L159	T219	P99
Y100	Q160	E220	Y100
L101	E161	H221	L101
D102	K162	L222	D102
D103	L163	S223	D103
F104	S164	T224	F104
Q105	P165	L225	Q105
K106	L166	S226	K106
K107	G167	E227	K107
W108	E168	K228	W108
Q109	E169	A229	Q109
E110	M170	K230	E110
E111	R171	P231	E111
M112	D172	A232	M112
E113	R173	L233	E113
L114	A174	E234	L114

D235
L236
F57
Q237
Q238
Q239
K59
L240
L241
L242
P243
V243
L244
E245
E246
S246
F247
K248
V249
S250
E251
F251
L252
S253
A254
L255
E256
E257
E257
Y258
T259
K260
L261
L262
N263
Q265

## • Molecule 2: Apolipoprotein A-I

Chain C:

100%

S55
T56
F57
S58
K59
L60
L61
P62
Q63
L64
L64
G65
P66
F67
T68
Q69
E70
F71
Q72
L73
D73
N74
L75
E76
K77
Y137
R138
E78
T79
E80
G81
L82
R83
P83
Q84
E85
E86
S87
L88
D89
L90
E91
E92
Y93
Q94
A95
K96
Y97
Q98
P99
Y100
L101
D102
D103
F104
Q105
K106
K107
W108
E109
Q109
M110
E111
M112
E113
L114

Y115
R116
K117
V118
D119
A120
P121
Y122
L123
L124
D125
F126
Q127
K128
K129
W130
E131
Q132
E133
E134
E135
L136
E137
A138
Q139
K140
E141
E142
P143
L144
E145
E146
E147
L148
Q149
E150
E151
A152
R153
Q154
K155
A156
L157
E158
L159
Y160
E161
K162
L163
S164
P165
L166
G167
E168
E169
M170
R171
D172
L173
A174

R175
A176
H177
D178
D179
A180
L181
R182
T183
H184
L185
A186
P187
Y188
S189
D190
E191
L192
E193
Q194
R195
L196
A197
Y198
T199
K200
E201
A202
L203
K204
E205
N206
G207
G208
A209
R210
L211
A212
E213
Y214
H215
A216
K217
A218
T219
E220
H221
L222
S223
T224
L225
S226
E227
K228
A229
K230
P231
A232
L233
E234

## 4.2.2 Score per residue for model 2

## • Molecule 1: Matrix metalloproteinase-14

Chain A:

100%

P316
N317
C318
D320
G321
N322
F323
D324
T325
V326
A327
M328
L329
R330
D331
E332
M333
F334
V335
F336
K337
E338
R339
W340
F341
K342
R343
V344
R345
K346
K347
Q348
G349
M350
D351
G352
Y353
P354
M355
P356
I357
G358
Q359
F360
K361
G362
G363
L364
P365
A366
S367
I368
N369
T370
A371
Y372
E373
R374
K375

Y376
R377
K378
F379
V380
E381
L382
K383
G384
V385
D386
K387
H388
Y389
F390
D391
E392
A393
S394
L395
E396
P397
G398
Y399
P400
K401
H402
L403
K404
E405
L406
G407
R408
G409
L410
P411
T412
D413
K414
L415
D416
Y417
F418
L419
F420
N421
N422
P423
N424
G425
K426
Y427
Y428
F429
F430
R431
G432
N433
K434
Y435

## • Molecule 2: Apolipoprotein A-I

Chain B:

100%

S55
T56
F57
S58
K59
L60
L61
P62
Q63
L64
L64
G65
P66
F67
T68
Q69
E70
F71
Q72
L73
D73
N74
L75
E76
K77
Y137
R138
E78
T79
E80
G81
L82
R83
P83
Q84
E85
E86
S87
L88
D89
L90
E91
E92
Y93
Q94
A95
K96
Y97
Q98
P99
Y100
L101
D102
D103
F104
Q105
K106
K107
W108
E109
Q109
M110
E111
M112
E113
L114

Y115
R116
K117
V118
D119
A120
P121
Y122
L123
L124
D125
F126
Q127
K128
K129
W130
E131
Q132
E133
E134
E135
L136
E137
A138
Q139
K140
E141
E142
P143
L144
E145
E146
E147
L148
Q149
E150
E151
A152
R153
Q154
K155
A156
L157
E158
L159
Y160
E161
K162
L163
S164
P165
L166
G167
E168
E169
M170
R171
D172
L173
A174

D235
L236
R237
Q238
Q239
L240
L241
P242
V243
L244
E245
S246
F247
K248
V249
S250
F251
L252
S253
A254
E256
E257
T258
T259
K260
L261
L262
N263
T264
Q265

## • Molecule 2: Apolipoprotein A-I

Chain C:

100%

S55
T56
F57
S58
K59
L60
L61
E62
Q63
L64
E65
P66
F67
T68
Q69
E70
F71
Q72
L73
D74
L75
E76
K77
E78
R79
Q80
G81
L82
L83
P84
K85
E86
S87
K88
Q89
L90
L91
E92
F93
Y94
K95
A96
K97
H98
Q99
F100
L101
E102
D103
F104
Q105
L106
K107
E108
Q109
M110
E111
M112
E113
L114

D235
L236
R237
Q238
Q239
L240
L241
P242
V243
L244
E245
S246
F247
K248
V249
S250
F251
L252
S253
A254
E256
E257
T258
T259
K260
L261
N263
T264
Q265

### 4.2.3 Score per residue for model 3

## • Molecule 1: Matrix metalloproteinase-14

Chain A:

100%

P316
N317
L318
F319
D320
G321
N322
F323
D324
T325
V326
A327
M328
L329
R330
D331
E332
M333
F334
V335
F336
K337
E338
R339
W340
F341
K342
L343
V344
R345
K346
N347
Q348
G349
M350
D351
G352
Y353
P354
M355
P356
I357
G358
Q359
F360
K361
R362
G363
L364
P365
A366
S367
I368
N369
T370
A371
Y372
E373
R374
K375

Y436
R437
F438
N439
S440
E441
L442
R443
A444
V445
D446
S447
E448
Y449
P450
K451
N452
L453
K454
V455
W456
E457
G458
I459
P460
E461
S462
P463
R464
G465
S466
F467
M468
G469
S470
D471
E472
W473
F474
T475
Y476
F477
Y478
K479
G480
N481
K482
Y483
W484
K485
F486
N487
N488
Q489
R490
L491
K492
Y493
E494
P495

## • Molecule 2: Apolipoprotein A-I

Chain B:

100%

S55
T56
F57
S58
K59
L60
L61
E62
Q63
L64
E65
P66
F67
T68
Q69
E70
F71
Q72
L73
D74
L75
E76
K77
E78
R79
Q80
G81
L82
L83
P84
K85
E86
S87
K88
Q89
L90
L91
E92
F93
Y94
K95
A96
K97
H98
Q99
F100
L101
D102
D103
F104
Q105
L106
K107
E108
Q109
M110
E111
M112
E113
L114

R175
A176
H177
V178
D179
A180
L181
R182
Q183
L184
L185
F186
P187
Y188
S189
D190
E191
L192
E193
Q194
R195
L196
A197
R198
Q199
L200
E201
A202
L203
K204
E205
N206
G207
L208
Q209
R210
L211
A212
E213
Q214
K215
A216
K217
H218
L219
E220
L221
L222
D223
T224
L225
S226
E227
K228
E229
Q230
P231
A232
L233
E234

D235
L236
F237
Q238
Q239
L240
L241
L242
P243
V244
L245
E246
S247
F248
K249
V250
E251
L252
S253
A254
E255
E256
E257
Y258
T259
K260
L261
L262
N263
Q265

## • Molecule 2: Apolipoprotein A-I

Chain C:

100%

S55
T56
F57
S58
K59
L60
L61
P62
Q63
L64
L65
G66
P67
T68
Q69
E70
F71
L72
W73
D74
E75
L76
E77
Y78
R79
Q80
L81
L82
R83
P84
L85
Q86
E87
S88
H89
K90
L91
L92
E93
E94
A95
K96
Y97
Q98
P99
Y100
L101
D102
D103
L104
F105
Q106
K107
W108
E109
Q110
E111
M112
L113
L114

Y115
R116
K117
K118
V119
L120
P121
Y122
L123
L124
D125
E126
F127
K128
K129
W130
E131
Q132
E133
E134
E135
L136
Y137
E138
R139
Q140
E141
E142
P143
L144
Q145
E146
E147
E148
K149
E150
L151
A152
R153
Q154
K155
A156
L157
E158
L159
E160
E161
K162
L163
S164
P165
L166
G167
E168
E169
M170
R171
D172
L173
A174

R175
A176
H177
V178
D179
A180
L181
R182
T183
H184
L185
A186
P187
Y188
S189
D190
E191
L192
E193
Q194
R195
L196
A197
Y198
T199
K200
E201
A202
L203
K204
E205
N206
G207
K208
A209
R210
L211
A212
E213
Y214
H215
A216
K217
A218
T219
E220
H221
L222
S223
T224
L225
S226
E227
K228
A229
K230
P231
A232
L233
E234

### 4.2.4 Score per residue for model 4

## • Molecule 1: Matrix metalloproteinase-14

Chain A:

100%

P316
N317
L318
C319
D320
G321
N322
F323
D324
T325
V326
A327
M328
L329
R330
D331
E332
M333
F334
V335
F336
K337
E338
R339
W340
F341
W342
L343
V344
R345
K346
N347
Q348
G349
M350
D351
G352
Y353
P354
M355
P356
I357
G358
A359
F360
W361
R362
G363
L364
P365
A366
S367
I368
N369
T370
A371
Y372
E373
R374
K375

D376
G377
K378
F379
V380
F381
N382
K383
D384
K385
D386
V387
H388
Y389
F390
D391
E392
A393
S394
L395
E396
P397
G398
Y399
P400
K401
H402
L403
K404
E405
L406
G407
R408
G409
L410
P411
T412
D413
K414
L415
D416
A417
A418
L419
F420
N421
N422
P423
N424
G425
K426
T427
Y428
F429
F430
R431
K432
N433
K434
Y435

## • Molecule 2: Apolipoprotein A-I

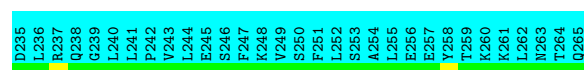
Chain B:

100%

S55
T56
F57
S58
K59
L60
L61
P62
Q63
L64
L65
G66
P67
T68
Q69
E70
F71
L72
W73
D74
E75
L76
E77
Y78
R79
Q80
L81
L82
R83
Q84
E85
H86
S87
K88
D89
L90
L91
E92
E93
Y94
K95
A96
Y97
Q98
P99
Y100
L101
D102
D103
F104
Q105
K106
K107
W108
Q109
E110
E111
M112
L113
L114

Y115
R116
K117
K118
V119
L120
P121
Y122
L123
L124
D125
E126
F127
K128
K129
W130
E131
Q132
E133
E134
E135
L136
Y137
E138
R139
Q140
E141
E142
P143
L144
Q145
E146
E147
E148
K149
E150
L151
A152
R153
Q154
K155
A156
L157
E158
L159
E160
E161
K162
L163
S164
P165
L166
G167
E168
E169
M170
R171
D172
L173
A174

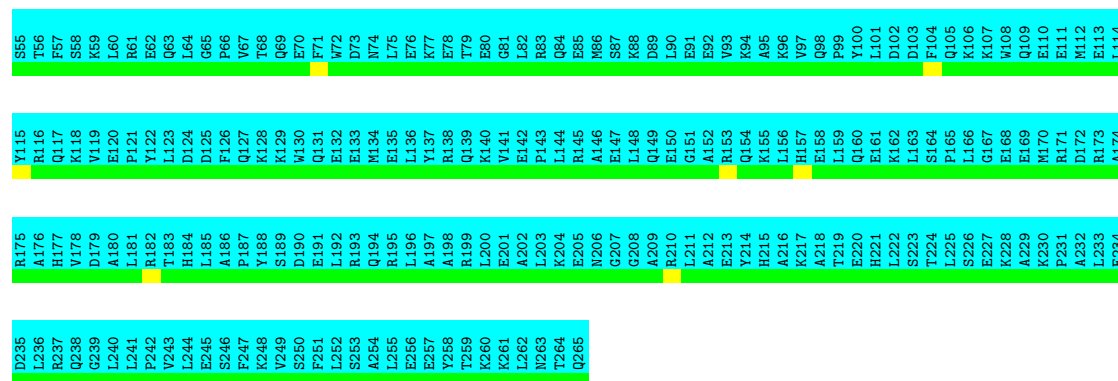
R175
A176
H177
V178
D179
A180
L181
R182
T183
H184
L185
A186
P187
Y188
S189
D190
E191
L192
E193
Q194
R195
L196
A197
Y198
T199
K200
E201
A202
L203
K204
E205
N206
G207
K208
A209
R210
L211
A212
E213
Y214
H215
A216
K217
A218
T219
E220
H221
L222
S223
T224
L225
S226
E227
K228
A229
K230
P231
A232
L233
E234



### • Molecule 2: Apolipoprotein A-I

Chain C:

100%

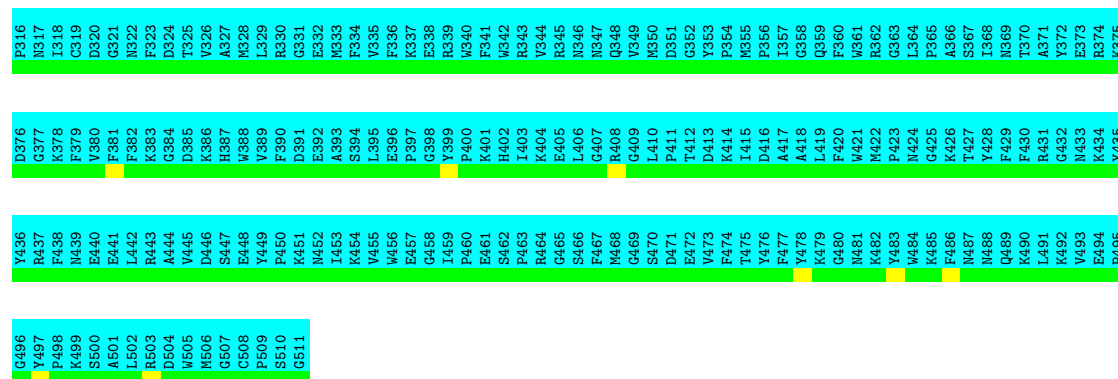


### 4.2.5 Score per residue for model 5

### • Molecule 1: Matrix metalloproteinase-14

Chain A:

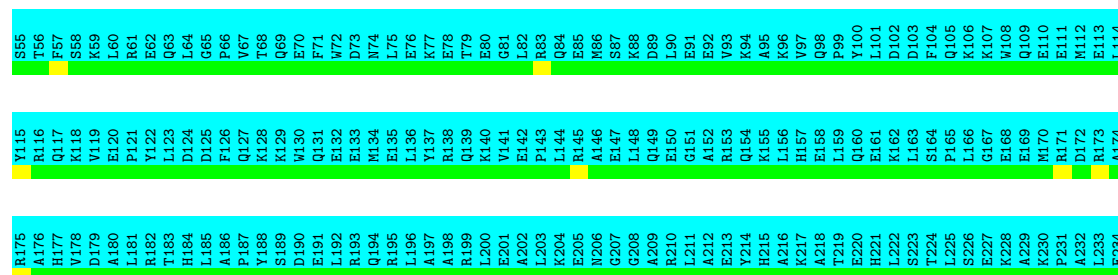
100%



### • Molecule 2: Apolipoprotein A-I

Chain B:

100%



D235
L236
R237
Q238
Q239
L240
L241
L242
P243
V244
L245
E246
S247
F248
K249
V250
E251
F252
L253
S254
A255
E256
E257
E258
T259
K260
L261
L262
N263
T264
Q265

## • Molecule 2: Apolipoprotein A-I

Chain C:

100%

S55
T56
F57
S58
K59
L60
L61
P62
Q63
L64
L65
G66
P67
T68
Q69
E70
F71
L72
W73
D74
N75
L76
E77
K78
T79
E80
G81
L82
R83
L84
K85
E86
H87
L88
E89
L90
E91
E92
Y93
K94
A95
K96
V97
Q98
P99
Y100
L101
D102
L103
F104
Q105
L106
K107
W108
E109
M110
E111
M112
E113
L114

D235
L236
R237
Q238
Q239
L240
L241
P242
V243
L244
E245
S246
F247
K248
V249
E250
F251
L252
S253
A254
E255
E256
E257
Y258
T259
K260
L261
N263
T264
Q265

## 4.2.6 Score per residue for model 6

## • Molecule 1: Matrix metalloproteinase-14

Chain A:

100%

P316
N317
L318
F319
D320
G321
N322
F323
D324
T325
V326
A327
M328
L329
R330
G331
E332
M333
F334
V335
F336
K337
E338
R339
W340
F341
W342
L343
V344
R345
K346
N347
Q348
G349
M350
D351
G352
Y353
P354
M355
P356
I357
G358
A359
F360
W361
R362
G363
L364
P365
A366
S367
L368
N369
T370
A371
Y372
E373
R374
E375
Y436
R437
F438
N439
E440
E441
L442
R443
A444
V445
D446
S447
E448
Y449
P450
K451
E452
L453
K454
V455
W456
E457
G458
I459
P460
E461
S462
L463
R464
G465
S466
F467
M468
G469
S470
D471
E472
W473
F474
T475
Y476
F477
Y478
K479
G480
N481
K482
Y483
W484
K485
F486
N487
N488
Q489
F490
R491
K492
V493
E494
P495
D376
G377
K378
F379
V380
F381
F382
K383
D384
D385
K386
H387
W388
V389
F390
D391
E392
A393
S394
L395
E396
P397
G398
Y399
P400
K401
H402
L403
K404
E405
L406
G407
R408
G409
L410
P411
T412
D413
K414
L415
D416
A417
A418
L419
F420
W421
N422
P423
N424
G425
K426
T427
Y428
F429
F430
R431
K432
N433
K434
Y435
G496
Y497
P498
K499
S500
A501
L502
R503
D504
W505
M506
G507
C508
P509
S510
G511

## • Molecule 2: Apolipoprotein A-I

Chain B:

100%

S55
T56
F57
S58
K59
L60
L61
P62
Q63
L64
G65
P66
V67
T68
Q69
E70
F71
L72
W73
D74
N75
L76
E77
K78
T79
E80
G81
L82
R83
L84
K85
E86
H87
L88
E89
L90
E91
E92
Y93
K94
A95
K96
V97
Q98
P99
Y100
L101
D102
L103
F104
Q105
L106
K107
W108
E109
M110
E111
M112
E113
L114

R175
A176
H177
V178
D179
A180
L181
R182
Q183
L184
L185
P186
F187
Y188
K189
W190
E191
L192
E193
Q194
R195
L196
Y197
R198
E199
L200
E201
A202
L203
K204
E205
N206
G207
L208
A209
E210
L211
A212
E213
Y214
H215
A216
K217
E218
L219
E220
H221
L222
S223
T224
L225
S226
E227
K228
E129
K230
P231
A232
L233
E234

D235
L236
R237
Q238
Q239
L240
L241
L242
P243
Q243
L244
E245
E246
S246
F247
K248
V249
S250
F251
L252
S253
A254
E256
E257
E257
Y258
T259
K260
L261
L262
N263
Q265

### • Molecule 2: Apolipoprotein A-I

Chain C:

100%

S55
T56
F57
S58
K59
L60
L61
E62
Q63
L64
D125
G65
P66
F126
Q127
K128
K129
W130
E70
F71
Q131
W72
L132
E133
D73
N74
L75
E76
K77
Y137
R138
T79
Q139
K140
G81
L82
L83
P143
R83
Q84
L144
R145
E85
H86
S87
K88
Q149
D89
L90
E150
G151
E91
E92
Y93
Q154
K94
K155
A95
K96
Y97
H157
Q98
F99
Y100
L101
E161
D102
D103
L163
F104
S165
Q105
L106
G107
K108
E168
Q109
M170
E111
E112
L113
L114

D235
L236
Q238
Q239
L240
L241
P242
P243
L244
E245
S246
F247
K248
V249
F251
L252
S253
A254
E256
E257
Y258
T259
K260
L261
N263
T264
Q265

### 4.2.7 Score per residue for model 7

### • Molecule 1: Matrix metalloproteinase-14

Chain A:

100%

P316
N317
L318
C319
D320
G321
N322
F323
D324
T325
V326
A327
K328
L329
R330
D331
E332
M333
F334
V335
F336
K337
E338
R339
W340
F341
K342
R343
V344
R345
K346
N347
Q348
G349
M350
D351
G352
Y353
P354
M355
P356
I357
G358
Q359
F360
W361
R362
G363
L364
P365
A366
S367
I368
N369
T370
A371
Y372
E373
R374
K375

Y436
R437
F438
N439
E440
E441
L442
R443
A444
V445
D446
S447
E448
Y449
P450
K451
N452
I453
K454
V455
W456
E457
G458
I459
P460
E461
S462
P463
R464
G465
S466
F467
M468
G469
S470
D471
E472
W473
F474
T475
Y476
F477
Y478
K479
G480
N481
K482
Y483
W484
K485
F486
N487
N488
Q489
K490
L491
K492
V493
E494
P495

### • Molecule 2: Apolipoprotein A-I

Chain B:

100%

S55
T56
F57
S58
K59
L60
L61
E62
Q63
L64
D125
G65
P66
F126
Q127
K128
K129
W130
E70
F71
Q131
W72
L132
E133
D73
N74
L75
E76
K77
Y137
R138
T79
Q139
K140
G81
L82
L83
P143
R83
Q84
L144
R145
E85
H86
S87
K88
Q149
D89
L90
E150
G151
E91
E92
Y93
Q154
K94
K155
A95
K96
Y97
H157
Q98
F99
Y100
L101
D102
D103
L163
F104
S165
Q105
L106
G107
K108
E168
Q109
M170
E111
E112
L113
L114

R175
A176
H177
V178
D179
A180
L181
L182
Q183
L184
L185
F186
A186
P187
Y188
S189
D190
E191
L192
E193
Q194
L195
L196
A197
R198
Q199
L200
E201
A202
L203
K204
E205
N206
G208
A209
R210
L211
A212
E213
Y214
H215
A216
K217
A218
T219
E220
H221
L222
S223
T224
L225
S226
E227
K228
E169
Q230
P231
A232
L233
E234



D235
L236
R237
Q238
Q239
L240
L241
L242
P243
V243
L244
E245
E246
S246
F247
K248
V249
S250
F251
L252
S253
A254
E256
E257
E257
Y258
T259
K260
L261
L262
N263
Q265

## • Molecule 2: Apolipoprotein A-I

Chain C:

100%

S55
T56
R116
H117
K118
V119
K59
L60
E120
P121
Y122
L123
L123
L124
L124
L125
G65
P66
F126
Q127
K128
T68
Q69
E70
F71
Q131
L132
E132
D73
D73
N74
L75
E76
L136
Y137
E77
R138
E78
Y258
T79
E80
G81
L82
E142
P143
R83
L144
Q84
E85
E85
H86
E147
S87
K88
Q148
Q149
E150
L90
E91
G151
A152
E92
Y93
Q154
K94
K155
A95
K96
L156
H157
Q98
E158
L159
P99
Y100
L101
E161
K162
D102
D102
L163
D103
F104
S164
P165
L166
G167
K107
E168
W108
E169
Q109
M170
R171
E111
M112
E113
L114

D235
L236
Q238
Q239
L240
L241
P242
V243
L244
E245
S246
F247
K248
V249
S250
F251
L252
S253
A254
E256
E257
Y258
T259
K260
L261
L262
N263
T264
Q265

## 4.2.8 Score per residue for model 8

## • Molecule 1: Matrix metalloproteinase-14

Chain A:

100%

P316
N317
L318
C319
D320
V380
G321
N322
F323
D324
T325
V326
A327
M328
L329
R330
D331
E332
M333
F334
V335
F336
K337
E338
R339
W340
F341
W342
R343
V344
R345
R346
N347
Q348
G409
M350
D351
G352
Y353
P354
M355
P356
I357
G358
Q359
F360
W361
R362
G363
L364
P365
A366
S367
I368
N369
T370
R371
Y372
E373
R374
K375

Y436
R437
P438
K439
S500
A501
L502
R503
A443
D504
W505
M506
S447
G507
C508
P509
S510
G511

## • Molecule 2: Apolipoprotein A-I

Chain B:

100%

S55
T56
F57
S58
K59
L60
E61
S62
Q63
L64
L64
G65
P66
V67
T68
Q69
F71
Q131
L132
D73
D73
N74
L75
E76
L136
Y137
E77
R138
E78
T79
E80
G81
L82
E142
P143
R83
L144
Q84
E85
E85
H86
E147
S87
K88
Q148
Q149
E150
L90
E91
G151
A152
E92
Y93
Q154
K94
K155
A95
K96
L156
H157
Q98
E158
L159
P99
Y100
L101
E161
K162
D102
D102
L163
D103
F104
S164
P165
L166
G167
K107
E168
W108
E169
Q109
M170
R171
E111
M112
E113
L114

R175
A176
H177
V178
D179
A180
L181
L182
L183
L183
L184
L185
L185
F186
A186
Q187
K188
S189
D190
E191
L192
R193
Q194
L195
L196
A197
R198
A198
Q139
K140
E201
A202
L203
K204
E205
N206
G208
A209
R210
L211
A212
E213
Y214
H215
A216
K217
A218
T219
E220
H221
L222
L222
S223
T224
L225
S226
E227
K228
E169
Q109
K230
P231
A232
L233
E234

D235
L236
R237
Q238
Q239
L240
L241
L242
P243
V244
L245
E246
S247
K248
V249
S250
F251
L252
S253
A254
E256
E257
E258
T259
K260
L261
L262
N263
Q265

## • Molecule 2: Apolipoprotein A-I

Chain C:

100%

S55	Y115	R175
T56	R116	A176
F57	H117	H177
S58	K118	V178
K59	V119	D179
L60	E120	A180
L61	P121	L181
S62	Y122	R182
Q63	L123	T183
L64	D124	H184
E65	D125	L185
P66	F126	A186
V67	Q127	P187
T68	K128	Y188
Q69	K129	S189
E70	W130	D190
F71	Q131	E191
L72	E132	L192
W73	E133	R193
D74	M134	Q194
L75	E135	R195
E76	L136	L196
K77	Y137	A197
E78	R138	A198
T79	Q139	R199
E80	K140	L200
G81	V141	E201
L82	E142	A202
R83	P143	L203
Q84	L144	K204
E85	R145	E205
H86	A146	N206
S87	E147	G207
K88	L148	G208
D89	Q149	A209
L90	E150	R210
E91	G151	L211
E92	A152	A212
Y93	R153	E213
K94	Q154	Y214
A95	K155	H215
K96	L156	A216
V97	H157	K217
Q98	E158	A218
P99	L159	T219
Y100	Q160	E220
L101	E161	H221
D102	K162	L222
D103	L163	S223
F104	S164	T224
Q105	P165	L225
K106	L166	S226
K107	G167	E227
W108	E168	K228
Q109	E169	A229
M170	M170	K230
E111	R171	P231
M112	D172	A232
E113	R173	L233
L114	A174	E234

D235
L236
R237
Q238
Q239
L240
L241
P242
V243
L244
E245
S246
F247
K248
V249
S250
F251
L252
S253
A254
E256
E257
E258
T259
K260
L261
L262
N263
T264
Q265

### 4.2.9 Score per residue for model 9

## • Molecule 1: Matrix metalloproteinase-14

Chain A:

100%

P316	D376	Y436
N317	G377	R437
L318	K378	F438
C319	F379	N439
D320	V380	E440
G321	F381	A441
N322	F382	L442
F323	K383	R443
D324	G384	A444
T325	D385	V445
V326	K386	D446
A327	H387	S447
M328	V388	E448
L329	V389	Y449
R330	F390	P450
D331	K391	K451
E332	E392	L452
M333	A393	N453
F334	S394	K454
V335	L395	V455
F336	E396	W456
K337	P397	E457
E338	G398	G458
R339	Y399	I459
W340	P400	P460
F341	K401	E461
W342	H402	S462
L343	L403	P463
V344	K404	R464
R345	E405	G465
K346	L406	S466
N347	G407	F467
Q348	R408	M468
V349	G409	G469
M350	L410	S470
D351	P411	D471
G352	T412	E472
Y353	D413	W473
P354	K414	F474
M355	L415	T475
P356	D416	Y476
I357	A417	F477
G358	A418	Y478
Q359	L419	K479
F360	F420	G480
K361	W421	N481
R362	N422	K482
G363	P423	Y483
L364	N424	W484
P365	G425	K485
A366	K426	F486
S367	T427	N487
I368	Y428	N488
N369	F429	Q489
T370	F430	K490
A371	R431	L491
Y372	G432	K492
E373	N433	V493
L233	K434	E494
E234	Y435	P495

G496
Y497
P498
K499
S500
A501
L502
R503
D504
W505
M506
G507
C508
P509
S510
G511

## • Molecule 2: Apolipoprotein A-I

Chain B:

100%

S55	Y115	R175
T56	R116	A176
F57	Q117	H177
S58	K118	V178
K59	V119	D179
L60	E120	A180
L61	P121	L181
S62	Y122	R182
Q63	L123	T183
L64	D124	H184
E65	D125	L185
P66	F126	A186
V67	Q127	P187
T68	K128	Y188
Q69	K129	S189
E70	W130	D190
F71	Q131	E191
L72	E132	L192
W73	E133	R193
D74	M134	Q194
L75	E135	R195
E76	L136	L196
K77	Y137	A197
E78	R138	A198
T79	Q139	R199
E80	K140	L200
G81	V141	E201
L82	E142	A202
R83	P143	L203
Q84	L144	K204
E85	R145	E205
H86	A146	N206
S87	E147	G207
K88	L148	G208
D89	Q149	A209
L90	E150	R210
E91	G151	L211
E92	A152	A212
Y93	R153	E213
K94	Q154	Y214
A95	K155	H215
K96	L156	A216
V97	H157	K217
Q98	E158	A218
P99	L159	T219
Y100	Q160	E220
L101	E161	H221
D102	K162	L222
D103	L163	S223
F104	S164	T224
Q105	P165	L225
K106	L166	S226
K107	G167	E227
W108	E168	K228
Q109	E169	A229
M170	M170	K230
E111	R171	P231
M112	D172	A232
E113	R173	L233
L114	A174	E234

D235
L236
L237
Q238
Q239
L240
L241
P242
V243
L244
E245
E246
F247
K248
V249
S250
F251
L252
S253
A254
E256
E257
Y258
T259
K260
L261
L262
N263
T264
Q265

## • Molecule 2: Apolipoprotein A-I

Chain C:

100%

S55
T56
F57
S58
K59
L60
L61
P62
Q63
L64
G65
E66
F67
T68
Q69
E70
F71
L72
D73
N74
L75
E76
E77
Y78
E79
K80
L81
L82
R83
K84
E85
E86
S87
K88
D89
L90
E91
E92
Y93
K94
A95
K96
Y97
Q98
P99
Y100
L101
D102
D103
F104
Q105
K106
K107
W108
E109
M110
E111
M112
E113
L114

Y115
R116
Q117
K118
V119
L120
P121
Y122
L123
L124
D125
F126
Q127
K128
K129
W130
Q131
E132
E133
M134
E135
L136
Y137
A138
Q139
K140
E141
A142
P143
K144
E145
E146
E147
L148
Q149
E150
G151
A152
R153
Q154
K155
L156
H157
E158
L159
Q160
E161
K162
L163
S164
P165
L166
G167
E168
E169
M170
R171
D172
R173
A174

R175
A176
H177
V178
D179
A180
L181
R182
T183
H184
L185
A186
P187
Y188
S189
D190
E191
L192
R193
Q194
E195
L196
A197
A198
R199
L200
E201
A202
L203
K204
E205
N206
G207
G208
A209
R210
L211
A212
E213
Y214
H215
A216
K217
A218
T219
E220
H221
L222
S223
T224
L225
S226
E227
K228
A229
K230
P231
A232
L233
E234

D235
L236
Q237
Q238
G239
L240
L241
P242
V243
L244
E245
S246
F247
K248
V249
F250
L251
L252
S253
A254
E256
E257
Y258
T259
K260
L261
N263
T264
Q265

## 4.2.10 Score per residue for model 10

## • Molecule 1: Matrix metalloproteinase-14

Chain A:

100%

P316
N317
L318
C319
D320
G321
N322
F323
D324
T325
V326
A327
M328
L329
R330
D331
E332
M333
F334
V335
F336
K337
E338
R339
W340
F341
K342
R343
V344
R345
K346
N347
Q348
G349
M350
D351
G352
Y353
P354
M355
P356
I357
G358
Q359
F360
K361
G362
G363
L364
P365
A366
S367
I368
N369
T370
R371
Y372
E373
R374
K375

D376
G377
K378
F379
V380
F381
N382
K383
G384
D385
K386
A387
H388
W389
F390
D391
E392
A393
S394
L395
E396
K397
G398
Y399
P400
K401
H402
L403
K404
E405
L406
G407
R408
G409
L410
D411
T412
D413
K414
L415
D416
A417
A418
L419
F420
N421
N422
P423
N424
G425
K426
T427
N428
F429
F430
R431
G432
N433
K434
Y435

Y436
R437
P438
N439
E440
A441
L442
R443
A444
V445
D446
S447
E448
Y449
P450
K451
N452
L453
K454
V455
W456
E457
G458
I459
R460
E461
S462
P463
R464
E465
S466
F467
M468
G469
S470
D471
E472
W473
F474
T475
Y476
F477
Y478
K479
G480
N481
K482
Y483
W484
K485
F486
N487
N488
Q489
K490
L491
K492
V493
E494
P495

G496
Y497
P498
K499
S500
A501
L502
R503
D504
W505
M506
G507
C508
P509
S510
G511

## • Molecule 2: Apolipoprotein A-I

Chain B:

100%

S55
T56
F57
S58
K59
L60
L61
P62
Q63
L64
G65
E66
F67
T68
Q69
E70
F71
L72
D73
N74
L75
E76
E77
Y78
E79
K80
L81
L82
R83
K84
E85
E86
S87
K88
D89
L90
E91
E92
Y93
K94
A95
K96
Y97
Q98
P99
Y100
L101
D102
D103
F104
Q105
K106
K107
W108
E109
M110
E111
M112
E113
L114

Y115
R116
Q117
K118
V119
L120
P121
Y122
L123
L124
D125
F126
Q127
K128
K129
W130
Q131
E132
E133
M134
E135
L136
Y137
A138
Q139
K140
E141
A142
P143
K144
E145
E146
E147
L148
Q149
E150
G151
A152
R153
Q154
K155
L156
H157
E158
L159
Q160
E161
K162
L163
S164
P165
L166
G167
E168
E169
M170
R171
D172
R173
A174

R175
A176
H177
V178
D179
A180
L181
R182
T183
H184
L185
A186
P187
Y188
S189
D190
E191
L192
R193
Q194
E195
L196
A197
A198
R199
L200
E201
A202
L203
K204
E205
N206
G207
G208
A209
R210
L211
A212
E213
Y214
H215
A216
K217
A218
T219
E220
H221
L222
S223
T224
L225
S226
E227
K228
A229
K230
P231
A232
L233
E234

D235
L236
L237
Q238
Q239
L240
L241
L242
P243
V243
L244
E245
S246
F247
K248
V249
S250
F251
L252
S253
A254
E256
E257
E258
T259
K260
L261
L262
N263
Q265

## • Molecule 2: Apolipoprotein A-I

Chain C:

100%

S55
T56
F57
S58
K59
L60
L61
S62
Q63
L64
L65
G66
P66
F67
T68
Q69
E70
F71
L72
W72
D73
W74
L75
E76
K77
Y137
R138
T79
E80
G81
L82
R83
P143
Q84
R85
E86
A146
E147
L148
Q149
E150
L90
E91
E92
Y93
Q94
A95
K155
L156
Y97
H157
Q98
P99
Y100
L101
E161
D102
D103
L163
F104
Q105
L106
K107
E108
E169
Q109
M170
R171
D172
R173
L114

D235
L236
L237
Q238
Q239
L240
L241
L242
P243
V243
L244
E245
S246
F247
K248
V249
S250
F251
L252
S253
A254
E256
E257
E258
T259
K260
L261
L262
N263
T264
Q265

## 4.2.11 Score per residue for model 11

## • Molecule 1: Matrix metalloproteinase-14

Chain A:

100%

P316
N317
C318
C319
D320
G321
N322
F323
P324
D324
T325
V326
A327
K328
L329
R330
G331
E332
M333
F334
V335
F336
K337
E338
R339
W340
F341
W342
L343
V344
R345
K346
N347
Q348
G349
M350
D351
G352
Y353
P354
M355
P356
I357
G358
Q359
F360
W361
R362
G363
L364
P365
A366
S367
I368
N369
T370
A371
Y372
E373
R374
K375

D376
G377
K378
F379
N380
V381
F382
K383
D384
D385
K386
A387
W388
V389
F390
K391
E392
A393
S394
L395
E396
P397
G398
Y399
P400
K401
H402
L403
K404
E405
L406
G407
M408
G409
L410
P411
T412
D413
K414
M415
D416
Y417
A418
L419
F420
N421
M422
P423
N424
G425
K426
T427
N428
Y429
F430
R431
G432
M433
K434
Y435

Y436
R437
P438
N439
S440
E441
L442
R443
D444
V445
D446
S447
E448
Y449
P450
K451
N452
I453
K454
V455
W456
E457
G458
I459
P460
E461
S462
L463
K464
G465
S466
F467
M468
G469
S470
D471
E472
W473
F474
T475
Y476
F477
Y478
K479
G480
N481
K482
Y483
W484
K485
F486
N487
N488
Q489
K490
L491
K492
V493
E494
P495

G496
Y497
P498
K499
S500
A501
L502
R503
D504
W505
M506
G507
C508
P509
S510
G511

## • Molecule 2: Apolipoprotein A-I

Chain B:

100%

S55
T56
F57
S58
K59
L60
L61
S62
Q63
L64
G65
P66
F67
T68
Q69
E70
F71
L72
W72
D73
W74
L75
E76
K77
E78
T79
E80
G81
L82
R83
P143
Q84
R85
E86
A146
E147
L148
Q149
E150
L90
E91
E92
Y93
Q94
A95
K96
Y97
H157
Q98
P99
Y100
L101
D102
D103
F104
Q105
L106
K107
E108
Q109
E110
E111
M112
L113
L114

Y115
R116
Q117
K118
V119
E120
P121
Y122
Q123
L124
D125
G126
F126
Q127
K128
K129
W130
D131
E132
E133
M134
E135
L136
Y137
R138
Q139
K140
V141
A202
L203
K204
L144
E205
E206
G207
L148
Q208
A209
R210
L211
A212
E213
Q154
K155
A216
L156
E157
E158
L159
Q160
E161
K162
L163
S164
P165
L166
E227
L228
E168
E169
Q170
R171
D172
R173
A174

R175
A176
H177
V178
D179
A180
L181
R182
Q183
H184
L185
F186
A187
Y188
E189
D190
E191
L192
R193
Q194
R195
L196
A197
A198
R199
L200
E201
A202
L203
K204
E205
E206
G207
L208
Q209
R210
L211
A212
E213
Q154
H215
A216
K217
E158
T219
E220
H221
L222
S223
T224
L225
S226
E227
K228
E169
Q230
P231
A232
L233
E234

D235
L236
R237
Q238
Q239
L240
L241
P242
V243
L244
E245
E246
S247
K248
V249
S250
F251
L252
S253
A254
E256
E257
T258
T259
K260
L261
L262
N263
Q265

## • Molecule 2: Apolipoprotein A-I

Chain C:

100%

S55
T56
F57
S58
K59
L60
L61
E62
Q63
L64
L65
G66
P66
F67
T68
Q69
E70
F71
L72
W72
D73
N74
L75
E76
K77
Y137
R138
T79
Q139
K140
G81
L82
L83
R83
Q84
E85
H86
S87
K88
D89
Q149
E150
L90
E91
F91
E92
Y93
Q94
A95
K96
Y97
H157
Q98
P99
Y100
L101
E161
D102
D103
L163
F104
Q105
K106
G107
W108
E169
Q109
M170
R171
D172
E113
L114
Y115
R116
H117
K118
V119
L120
P121
Y122
L123
L124
D125
E126
F126
Q127
K128
K129
W130
E131
Q131
E132
E133
M134
E135
L136
E137
A138
Q139
L200
E201
A202
L203
K204
E205
N206
G207
G208
A209
R210
L211
A212
E213
Y214
H215
A216
K217
A218
T219
E220
H221
L222
S223
T224
L225
S226
E227
K228
A229
K230
P231
A232
L233
E234
R176
V177
V178
D179
A180
L181
R182
T183
H184
L185
A186
P187
Y188
S189
D190
E191
L192
R193
Q194
R195
L196
A197
Y198
T199
L200
E201
A202
L203
K204
E205
N206
G207
G208
A209
R210
L211
A212
E213
Y214
H215
A216
K217
A218
T219
E220
H221
L222
S223
T224
L225
S226
E227
K228
A229
K230
P231
A232
L233
E234
D235
L236
R237
Q238
Q239
L240
L241
P242
V243
L244
E245
S246
F247
K248
V249
S250
F251
L252
S253
A254
E256
E257
T258
T259
K260
L261
N263
T264
Q265

## 4.2.12 Score per residue for model 12

## • Molecule 1: Matrix metalloproteinase-14

Chain A:

100%

P316
N317
L318
C319
D320
G321
N322
F323
P324
T325
V326
A327
M328
L329
R330
G331
E332
M333
F334
V335
F336
K337
E338
R339
W340
F341
W342
L343
V344
R345
K346
N347
Q348
V349
M350
D351
G352
Y353
P354
M355
P356
I357
G358
A418
L419
F360
R361
R362
G363
L364
P365
A366
S367
I368
N369
T370
A371
Y372
E373
K374
K375
D376
G377
K378
F379
N380
V381
E441
L442
F382
K383
G384
A444
D385
K386
V446
S447
H387
V388
Y449
F390
D391
E392
A393
S394
L395
E396
P397
G398
Y399
P400
K401
H402
L403
K404
E405
L406
G407
R408
G409
L410
D411
T412
D413
K414
L415
D416
A417
A418
L419
F420
N421
N422
P423
N424
G425
K426
T427
Y428
F429
F430
R431
K432
N433
E434
Y435
Y436
R437
F438
N439
E440
A501
L502
R503
D504
W505
M506
G507
C508
P509
S510
G511
Y436
R437
F438
N439
E440
A501
L502
R503
D504
W505
M506
G507
C508
P509
S510
G511
Y436
R437
F438
N439
E440
A501
L502
R503
D504
W505
M506
G507
C508
P509
S510
G511
Y436
R437
F438
N439
E440
A501
L502
R503
D504
W505
M506
G507
C508
P509
S510
G511

## • Molecule 2: Apolipoprotein A-I

Chain B:

100%

S55
T56
F57
S58
K59
L60
L61
E62
Q63
L64
G65
P66
F67
T68
Q69
E70
F71
L72
W72
D73
N74
L75
E76
K77
Y137
R138
T79
Q139
K140
G81
L82
L83
R83
Q84
E85
H86
S87
K88
D89
Q149
E150
L90
E91
F91
E92
Y93
Q94
A95
K96
Y97
H157
Q98
P99
Y100
L101
D102
D103
L163
F104
Q105
K106
G107
W108
E169
Q109
M170
R171
D172
E113
L114
Y115
R116
H117
K118
V119
L120
P121
Y122
L123
L124
D125
E126
F126
Q127
K128
K129
W130
E131
Q131
E132
E133
M134
E135
L136
E137
A138
Q139
L200
E201
A202
L203
K204
E205
N206
G207
G208
A209
R210
L211
A212
E213
Y214
H215
A216
K217
A218
T219
E220
H221
L222
S223
T224
L225
S226
E227
K228
A229
K230
P231
A232
L233
E234
R176
V177
V178
D179
A180
L181
R182
T183
H184
L185
A186
P187
Y188
S189
D190
E191
L192
R193
Q194
R195
L196
A197
Y198
T199
L200
E201
A202
L203
K204
E205
N206
G207
G208
A209
R210
L211
A212
E213
Y214
H215
A216
K217
A218
T219
E220
H221
L222
S223
T224
L225
S226
E227
K228
A229
K230
P231
A232
L233
E234
D235
L236
R237
Q238
Q239
L240
L241
P242
V243
L244
E245
S246
F247
K248
V249
S250
F251
L252
S253
A254
E256
E257
T258
T259
K260
L261
N263
T264
Q265

D235
L236
R237
F57
Q238
K239
L240
L241
L242
P243
Q243
L244
E245
E246
S246
F247
K248
V249
S250
E250
F251
L252
W252
S253
A254
L256
E256
E257
E257
Y258
T259
K260
L261
L262
N263
Q265

## • Molecule 2: Apolipoprotein A-I

Chain C:

100%

S55
T56
F57
S58
K59
L60
L61
S62
Q63
L64
L64
E65
E66
P66
F67
T68
Q69
E70
F71
Q72
W72
D73
D73
N74
L75
E76
E77
Y137
R138
E78
Y258
T79
E80
G81
L82
L82
R83
P143
P143
Q84
Q84
E85
E86
A146
E147
E147
L148
Q149
D89
E150
L90
E91
E92
Y93
Q94
A95
K155
L156
K96
Y97
H157
Q98
P99
Y100
L101
D102
D102
L103
F104
S164
P165
L166
K106
G107
E108
E169
Q109
M170
E111
E112
E113
L114

Y115
R116
Q117
K118
V119
L120
P121
Y122
L123
L124
D125
L185
F126
Q127
K128
K129
W130
Q131
E132
E133
M134
E135
L136
E137
R138
Q139
K140
E141
E142
P143
K144
E145
E205
N206
G207
G208
A209
E210
L211
A152
R153
Q154
K155
L156
K217
A218
T219
E220
H221
L222
L163
S223
T224
L225
S226
E227
K228
A229
K230
P231
A232
L233
E234

R175
A176
H177
V178
D179
A180
L181
R182
T183
H184
L185
A186
P187
Y188
S189
D190
E191
L192
R193
Q194
R195
L196
A197
A198
Q199
L200
E201
A202
L203
K204
E205
N206
G207
G208
A209
E210
L211
A212
E213
Y214
H215
A216
K217
A218
T219
E220
H221
L222
L163
S223
T224
L225
S226
E227
K228
A229
K230
P231
A232
L233
E234

D235
L236
R237
F57
Q238
K239
L240
L241
L242
P243
Q243
L244
E245
E246
S246
F247
K248
V249
S250
E250
F251
L252
W252
S253
A254
L256
E256
E257
E257
Y258
T259
K260
L261
L262
N263
T264
Q265

## 4.2.13 Score per residue for model 13

## • Molecule 1: Matrix metalloproteinase-14

Chain A:

100%

P316
N317
C318
C319
D320
G321
N322
F323
P243
D324
T325
V326
A327
M328
L329
R330
D331
E332
M333
F334
V335
F336
K337
E338
R339
W340
F341
W342
L343
V344
R345
E346
N347
Q348
G409
M350
D351
G352
Y353
P354
M355
P356
I357
G358
Q359
F360
W361
R362
G363
L364
P365
A366
S367
I368
N369
T370
A371
Y372
E373
R374
K375

D376
G377
K378
F379
V380
F381
F382
K383
D384
D385
K386
A387
H388
V389
F390
D391
E392
A393
S394
L395
E396
P397
G398
Y399
P400
K401
H402
L403
K404
E405
L406
G407
R408
G409
L410
P411
T412
D413
K414
M415
D416
A417
A418
L419
F420
N421
M422
P423
N424
G425
K426
T427
Y428
F429
F430
R431
K432
M433
K434
Y435

Y436
R437
F438
N439
E440
E441
L442
R443
A444
V445
D446
S447
E448
Y449
P450
K451
N452
L453
K454
V455
W456
E457
G458
I459
P460
E461
S462
P463
R464
E465
S466
E467
M468
G469
S470
D471
E472
W473
F474
T475
Y476
F477
Y478
K479
G480
N481
K482
M483
W484
K485
F486
N487
N488
Q489
F490
R491
K492
V493
E494
P495

G496
Y497
P498
K499
S500
A501
L502
R503
D504
W505
M506
G507
C508
P509
S510
G511

## • Molecule 2: Apolipoprotein A-I

Chain B:

100%

S55
T56
F57
S58
K59
L60
L61
S62
Q63
L64
E65
E66
P66
F67
T68
Q69
E70
F71
Q72
W72
D73
D73
N74
L75
E76
E77
Y137
R138
E78
Y258
T79
E80
G81
L82
L82
R83
P143
P143
Q84
Q84
E85
E86
A146
E147
E147
L148
Q149
D89
E150
L90
E91
E92
Y93
Q94
A95
K155
L156
K96
Y97
H157
Q98
P99
Y100
L101
D102
D102
L103
F104
S164
P165
L166
K106
G107
E108
E169
Q109
M170
E111
E112
E113
L114

Y115
R116
Q117
K118
V119
L120
P121
Y122
L123
L124
D125
L185
F126
Q127
K128
K129
W130
Q131
E132
E133
M134
E135
L136
E137
R138
Q139
K140
E141
E142
P143
K144
E145
E205
N206
G207
G208
A209
E210
L211
A152
R153
Q154
K155
L156
K217
A218
T219
E220
H221
L222
L163
S223
T224
L225
S226
E227
K228
A229
K230
P231
A232
L233
E234

R175
A176
H177
V178
D179
A180
L181
R182
T183
H184
L185
A186
P187
Y188
S189
D190
E191
L192
R193
Q194
R195
L196
A197
A198
Q199
L200
E201
A202
L203
K204
E205
N206
G207
G208
A209
E210
L211
A212
E213
Y214
H215
A216
K217
A218
T219
E220
H221
L222
L163
S223
T224
L225
S226
E227
K228
A229
K230
P231
A232
L233
E234

D235
L236
Q237
Q238
Q239
L240
L241
L242
P243
V243
L244
E245
E246
S246
F247
K248
V249
S250
E250
F251
L252
S253
A254
E256
E257
E257
Y258
T259
K260
L261
L262
N263
Q265

## • Molecule 2: Apolipoprotein A-I

Chain C:

100%

S55
T56
F57
S58
K59
L60
L61
S62
Q63
L64
D65
E66
F66
F67
T68
Q69
E70
S71
F71
L72
W72
D73
D73
N74
L75
E76
E77
Y137
R138
T79
Q139
K140
G81
L82
R83
P143
K84
L144
E85
E85
H86
S87
K88
Q149
E150
L90
E91
E92
Y93
Q94
A95
K96
L156
H157
Q98
P99
Y100
L101
D102
D103
F104
Q105
K106
K107
W108
E169
Q109
M170
R171
D172
L173
L114

D235
L236
Q237
Q238
L240
L241
P243
V243
L244
E245
S246
F247
K248
V249
F251
L252
S253
A254
E256
E257
Y258
T259
K260
L261
N263
T264
Q265

### 4.2.14 Score per residue for model 14

## • Molecule 1: Matrix metalloproteinase-14

Chain A:

100%

P316
N317
C318
C319
D320
G321
N322
F323
D324
T325
V326
A327
M328
L329
R330
G331
E332
M333
F334
V335
F336
K337
E338
R339
W340
F341
W342
L343
V344
R345
K346
N347
Q348
V349
M350
D351
G352
Y353
P354
M355
P356
I357
G358
Q359
F360
W361
R362
G363
L364
P365
A366
S367
I368
N369
T370
A371
Y372
E373
R374
K375

D376
G377
K378
F379
V380
F381
L382
K383
G384
V385
D386
K386
H387
V388
V389
F390
D391
E392
A393
S394
L395
E396
K397
G398
Y399
P400
K401
H402
L403
K404
E405
L406
G407
R408
G409
L410
D411
T412
D413
K414
L415
D416
A417
A418
L419
F420
W421
N422
P423
N424
G425
K426
T427
N428
F429
F430
R431
G432
N433
E434
Y435

Y436
R437
F438
N439
S440
E441
L442
R443
A444
V445
D446
S447
E448
Y449
P450
K451
N452
L453
K454
V455
W456
E457
G458
I459
R460
E461
S462
P463
R464
E465
S466
F467
M468
G469
S470
D471
E472
W473
F474
T475
Y476
F477
Y478
K479
G480
N481
K482
Y483
W484
K485
F486
N487
N488
Q489
K490
L491
K492
V493
E494
P495

## • Molecule 2: Apolipoprotein A-I

Chain B:

100%

S55
T56
F57
S58
K59
L60
L61
S62
Q63
L64
D65
E66
F66
F67
T68
Q69
E70
S71
F71
L72
W72
D73
D73
N74
L75
E76
E77
Y137
R138
T79
Q139
K140
G81
L82
R83
P143
K84
L144
E85
E85
H86
S87
K88
Q149
E150
L90
E91
E92
Y93
Q94
A95
K96
L156
H157
Q98
P99
Y100
L101
D102
D103
F104
Q105
K106
K107
W108
E169
Q109
M170
R171
D172
L173
L114

R175
A176
H177
V178
D179
A180
L181
R182
Q183
L184
H185
D186
F186
A186
P187
Y188
S189
D190
E191
L192
E193
Q194
R195
L196
A197
R198
Q199
L200
E201
A202
L203
K204
E205
N206
G207
L148
A209
R210
L211
A212
E213
Q154
K155
A216
K217
A218
T219
E220
H221
L222
S223
T224
L225
S226
E227
K228
E169
Q230
P231
A232
L233
E234

D235
L236
R237
Q238
Q239
L240
L241
P242
V243
L244
E245
E246
F247
K248
V249
S250
F251
L252
S253
A254
E256
E257
Y258
T259
K260
L261
L262
N263
Q265

### • Molecule 2: Apolipoprotein A-I

Chain C:

100%

S55
T56
F57
S58
K59
L60
L61
E62
Q63
L64
E65
E66
F67
T68
Q69
E70
F71
L72
W73
D74
N75
L76
E77
E78
Y79
E80
G81
L82
R83
Q84
E85
E86
S87
K88
D89
L90
E91
E92
Y93
K94
A95
K96
Y97
Q98
F99
Y100
L101
D102
D103
F104
Q105
K106
K107
W108
Q109
M110
E111
M112
E113
L114

D235
L236
R237
Q238
Q239
L240
L241
P242
V243
L244
E245
E246
F247
K248
V249
S250
F251
L252
S253
A254
E256
E257
Y258
T259
K260
L261
L262
N263
T264
Q265

### 4.2.15 Score per residue for model 15

### • Molecule 1: Matrix metalloproteinase-14

Chain A:

100%

P316
N317
I318
C319
D320
G321
N322
F323
D324
T325
V326
A327
M328
L329
R330
D331
E332
M333
F334
V335
F336
K337
E338
R339
W340
F341
W342
L343
V344
R345
K346
N347
Q348
G349
M350
D351
G352
Y353
P354
M355
P356
I357
G358
Q359
F360
W361
R362
G363
L364
P365
A366
S367
I368
N369
T370
A371
Y372
E373
L374
E375

Y436
R437
P438
N439
E440
E441
L442
R443
A444
V445
D446
S447
E448
Y449
P450
K451
N452
I453
K454
V455
W456
E457
G458
I459
P460
E461
S462
L463
K464
G465
S466
F467
M468
G469
S470
D471
E472
W473
F474
T475
Y476
F477
Y478
K479
G480
N481
K482
Y483
W484
K485
F486
N487
N488
Q489
K490
L491
K492
V493
E494
P495

### • Molecule 2: Apolipoprotein A-I

Chain B:

100%

S55
T56
F57
S58
K59
L60
L61
E62
Q63
L64
E65
E66
F67
T68
Q69
E70
F71
L72
W73
D74
N75
L76
E77
E78
Y79
E80
G81
L82
R83
Q84
E85
E86
S87
K88
D89
L90
E91
E92
Y93
K94
A95
K96
Y97
Q98
F99
Y100
L101
D102
D103
F104
Q105
K106
K107
W108
Q109
M110
E111
M112
E113
L114

Y115
R116
Q117
K118
V119
E120
P121
Y122
Q123
L124
D125
E126
F127
K128
M129
W130
E131
L132
E133
M134
E135
L136
Y137
E138
R139
Q140
V141
E142
P143
K144
E145
N206
G208
A209
R210
L211
A212
E213
Q154
K155
A216
K217
E158
L159
Q160
E161
K162
L163
S164
P165
L166
G167
E168
E169
M170
R171
D172
R173
A174

R175
A176
H177
V178
D179
A180
L181
R182
Q183
H184
L185
E186
F187
Y188
D189
E190
E191
L192
R193
Q194
R195
L196
A197
A198
R199
L200
E201
A202
L203
K204
E205
N206
G208
A209
R210
L211
A212
E213
Q154
K155
A216
K217
E158
L159
Q160
E161
K162
L163
S164
P165
L166
G167
E168
E169
M170
R171
D172
R173
A174



D235	L236	R237	Q238	G239	L240	L241	P242	V243	L244	E245	S246	F247	K248	V249	S250	F251	L252	S253	A254	L255	E256	E257	Y258	T259	K260	L261	L262	N263	T264	Q265
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------

● Molecule 2: Apolipoprotein A-I

Chain C: 

100%

S55	T56	F57	S58	K59	L60	P61	E62	Q63	L64	G65	P66	V67	T68	Q69	E70	F71	L72	D73	N74	L75	E76	K77	E78	T79	E80	G81	L82	R83	Q84	F85	R86	S87	K88	D89	L90	E91	E92	V93	K94	A95	K96	V97	Q98	P99	Y100	L101	D102	D103	F104	Q105	L106	K107	W108	Q109	E110	E111	M112	E113	L114
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Y115	R116	Q117	K118	V119	E120	P121	Y122	L123	D124	L125	F126	Q127	K128	K129	W130	Q131	E132	E133	M134	E135	L136	Y137	R138	Q139	K140	V141	E142	P143	L144	R145	A146	E147	L148	Q149	E150	G151	A152	R153	Q154	K155	L156	H157	E158	L159	Q160	E161	K162	L163	S164	P165	L166	G167	E168	E169	M170	R171	D172	R173	A174
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R175	A176	H177	V178	D179	A180	L181	R182	T183	H184	L185	A186	P187	Y188	S189	D190	E191	L192	R193	Q194	R195	L196	A197	A198	R199	L200	E201	A202	L203	K204	E205	N206	G207	G208	A209	R210	L211	A212	E213	Y214	H215	A216	K217	A218	T219	E220	H221	L222	S223	T224	L225	S226	E227	K228	A229	K230	P231	A232	L233	E234
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D235	L236	R237	Q238	G239	L240	L241	P242	V243	L244	E245	S246	F247	K248	V249	S250	F251	L252	S253	A254	L255	E256	E257	Y258	T259	K260	L261	L262	N263	T264	Q265
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## 5 Refinement protocol and experimental data overview

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

Of the 500 calculated structures, 15 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
HADDOCK	structure calculation	HADDOCK2.1
NAMD	structure calculation	NAMD2.1 with CUDA GPU processing
NAMD	refinement	NAMD2.1 with CUDA GPU processing

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)	6clz_cs.cif
Number of chemical shift lists	1
Total number of shifts	324
Number of shifts mapped to atoms	324
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	3%

No validations of the models with respect to experimental NMR restraints is performed at this time.

## 6 Model quality [i](#)

### 6.1 Standard geometry [i](#)

MolProbity failed to run properly - this section will have to be empty.

### 6.2 Too-close contacts [i](#)

MolProbity failed to run properly - this section will have to be empty.

### 6.3 Torsion angles [i](#)

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

MolProbity failed to run properly - this section will have to be empty.

#### 6.3.2 Protein sidechains [i](#)

MolProbity failed to run properly - this section will have to be empty.

#### 6.3.3 RNA [i](#)

MolProbity failed to run properly - this section will have to be empty.

### 6.4 Non-standard residues in protein, DNA, RNA chains [i](#)

MolProbity failed to run properly - this section will have to be empty.

### 6.5 Carbohydrates [i](#)

MolProbity failed to run properly - this section will have to be empty.

### 6.6 Ligand geometry [i](#)

MolProbity failed to run properly - this section will have to be empty.

### 6.7 Other polymers [i](#)

MolProbity failed to run properly - this section will have to be empty.

## 6.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 7 Chemical shift validation [i](#)

The completeness of assignment taking into account all chemical shift lists is 3% for the well-defined parts and 3% for the entire structure.

### 7.1 Chemical shift list 1

File name: 6clz\_cs.cif

Chemical shift list name: *showstar5.txt*

#### 7.1.1 Bookkeeping [i](#)

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	324
Number of shifts mapped to atoms	324
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

#### 7.1.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	0	—	None (insufficient data)
$^{13}\text{C}_\beta$	0	—	None (insufficient data)
$^{13}\text{C}'$	0	—	None (insufficient data)
$^{15}\text{N}$	92	$1.11 \pm 0.58$	None needed (imprecise)

#### 7.1.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 3%, i.e. 262 atoms were assigned a chemical shift out of a possible 8156. 0 out of 99 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	184/3030 (6%)	92/1206 (8%)	0/1236 (0%)	92/588 (16%)
Sidechain	78/4413 (2%)	35/2615 (1%)	43/1561 (3%)	0/237 (0%)

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	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Aromatic	0/713 (0%)	0/377 (0%)	0/310 (0%)	0/26 (0%)
Overall	262/8156 (3%)	127/4198 (3%)	43/3107 (1%)	92/851 (11%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 3%, i.e. 262 atoms were assigned a chemical shift out of a possible 8156. 0 out of 99 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Backbone	184/3030 (6%)	92/1206 (8%)	0/1236 (0%)	92/588 (16%)
Sidechain	78/4413 (2%)	35/2615 (1%)	43/1561 (3%)	0/237 (0%)
Aromatic	0/713 (0%)	0/377 (0%)	0/310 (0%)	0/26 (0%)
Overall	262/8156 (3%)	127/4198 (3%)	43/3107 (1%)	92/851 (11%)

#### 7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

#### 7.1.5 Random Coil Index (RCI) plots [i](#)

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.

Random coil index (RCI) for chain A:

