Full wwPDB NMR Structure Validation Report (i)

May 7, 2024 – 03:15 pm BST

PDB ID	:	2VDA
Title	:	Solution structure of the SecA-signal peptide complex
Authors	:	Gelis, I.; Bonvin, A.M.J.J.; Keramisanou, D.; Koukaki, M.; Gouridis, G.; Karamanou, S.; Economou, A.; Kalodimos, C.G.
Deposited on	:	2007-10-01

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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

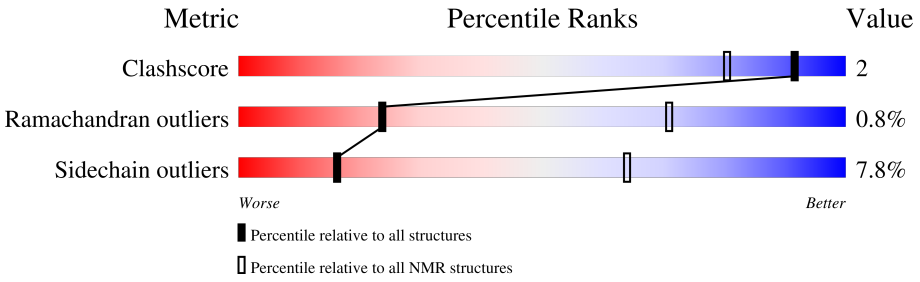
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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	828	76% • 20%
2	B	28	100%

2 Ensemble composition and analysis (i)

This entry contains 10 models. Model 2 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative.

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	**Residue range (total)**	**Backbone RMSD (Å)**	**Medoid model**
1	A:10-A:225, A:373-A:787, A:799-A:831 (664)	0.55	2

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

NmrClust was unable to cluster the ensemble.

Error message: Inconsistent models

3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 12995 atoms, of which 6195 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called TRANSLOCASE SUBUNIT SECA.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	828	12574	4128	5979	1166	1270	31	0

- Molecule 2 is a protein called MALTOPORIN.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
2	B	28	421	129	216	40	32	4	0

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: TRANSLOCASE SUBUNIT SECA

Chain A: 76% • 20%

V9 S12 R13 N14 M21 G57 H83 T104 T109 T130 M161 T178 S194 E210 V211 D212 R220 S226 G227 P228 A229 E230 D231 S232 S233 E234 M235 Y236 K237 R238 V239 N240 K241 I242 I243 P244 H245 L246 I247 R248 Q249 E250 K251 E252 D253 S254 E255

T256 F257 Q258 G259 E260 G261 H262 F263 S264 V265 D266 E267 K268 S269 R270 Q271 V272 N273 L274 T275 E276 R277 G278 L279 V280 L281 I282 E283 E284 L285 L286 V287 K288 E289 G290 I291 M292 D293 E294 G295 E296 S297 L298 Y299 S300 P301 A302 N303 I304 M305 L306 M307 H308 H309 V310 T311 A312 A313 L314 R315

A316 H317 A318 L319 F320 T321 R322 D323 V324 D325 Y326 I327 V328 K329 D330 G331 E332 V333 I334 I335 V336 D337 E338 H339 T340 G341 R342 T343 M344 Q345 G346 R347 R348 W349 S350 D351 G352 L353 H354 Q355 A356 V357 E358 A359 K360 E361 G362 V363 Q364 I365 Q366 N367 E368 N369 Q370 T371 L372 T376

T393 T396 D408 K461 R509 G510 T511 D540 S564 D580 S584 S589 L594 I597 S604 M612 K613 S673 W701 E732 E733 T734 G788 I789 H790 L791 R792 G793 Y794 A795 Q796 K797 D798 R832 M833 P834 E835 E836

• Molecule 2: MALTOPORIN

Chain B: 100%

M1 M2 I3 T4 L5 R6 K7 R8 R9 K10 L11 P12 L13 A14 V15 A16 V17 A18 A19 G20 V21 M22 S23 A24 Q25 A26 M27 A28

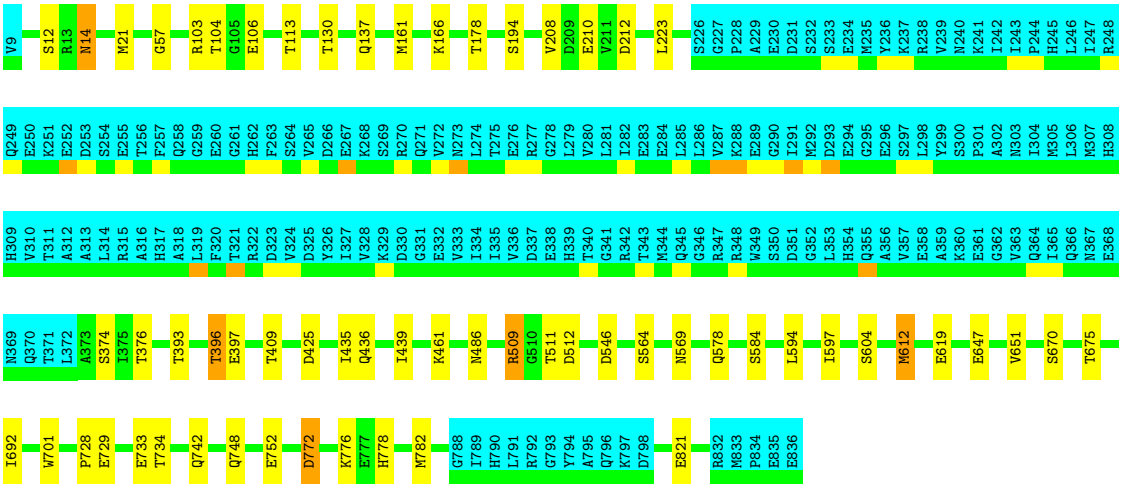
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

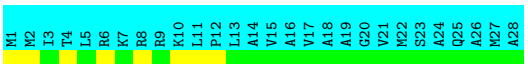
• Molecule 1: TRANSLOCASE SUBUNIT SECA

Chain A: 73% 7% • 20%



• Molecule 2: MALTOPORIN

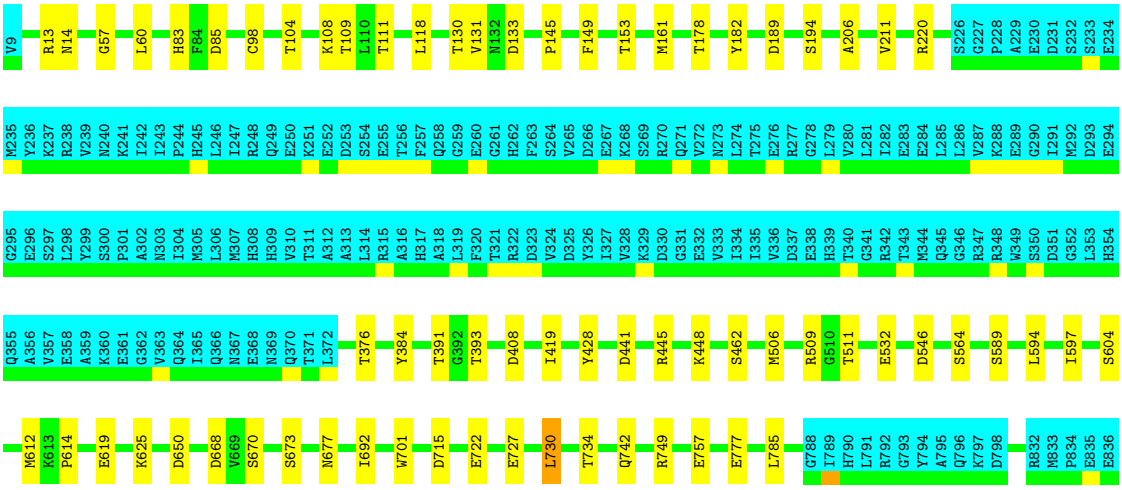
Chain B: 100%



4.2.2 Score per residue for model 2 (medoid)

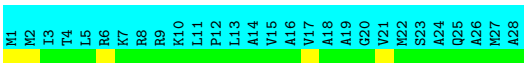
• Molecule 1: TRANSLOCASE SUBUNIT SECA

Chain A: 72% 8% 20%



• Molecule 2: MALTOPORIN

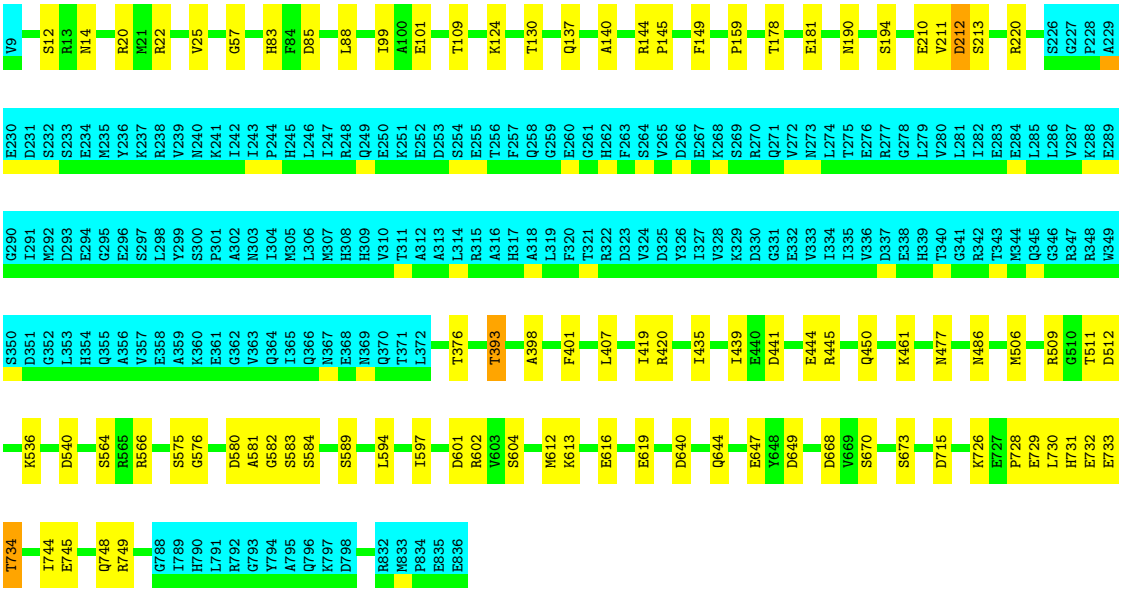
Chain B: 100%



4.2.3 Score per residue for model 3

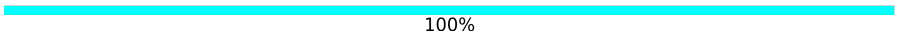
- Molecule 1: TRANSLOCASE SUBUNIT SECA

Chain A:



- Molecule 2: MALTOPORIN

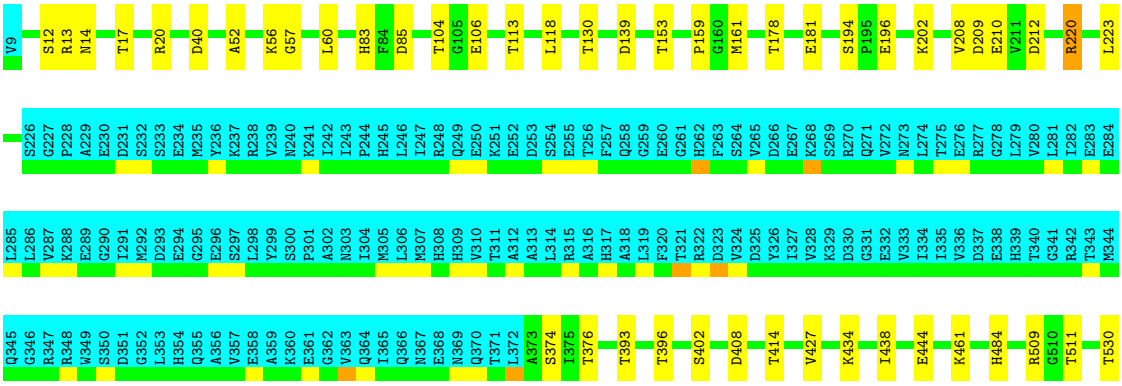
Chain B:

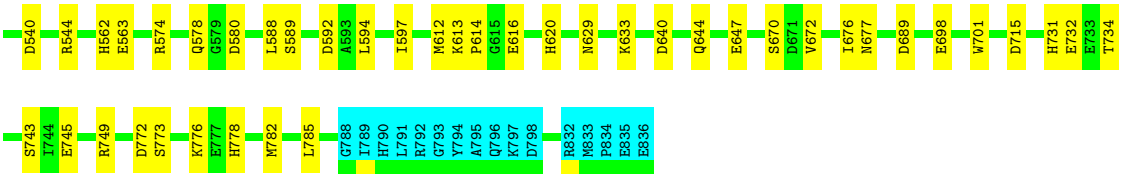


4.2.4 Score per residue for model 4

- Molecule 1: TRANSLOCASE SUBUNIT SECA

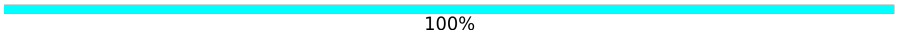
Chain A:





- Molecule 2: MALTOPORIN

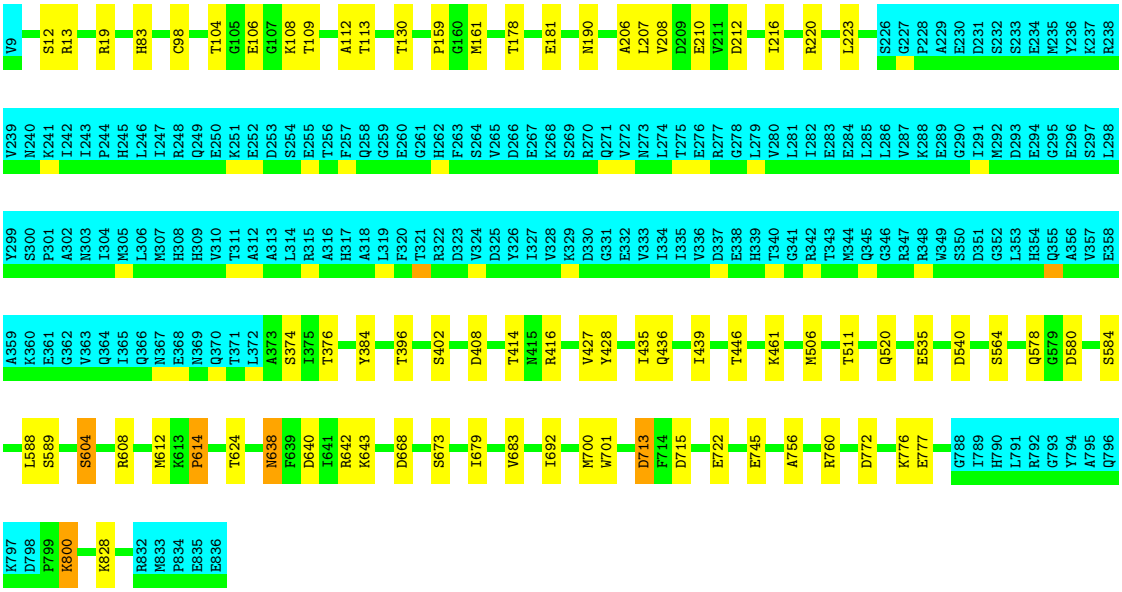
Chain B:



4.2.5 Score per residue for model 5

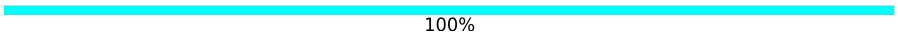
- Molecule 1: TRANSLOCASE SUBUNIT SECA

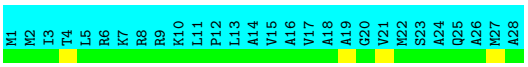
Chain A:



- Molecule 2: MALTOPORIN

Chain B:

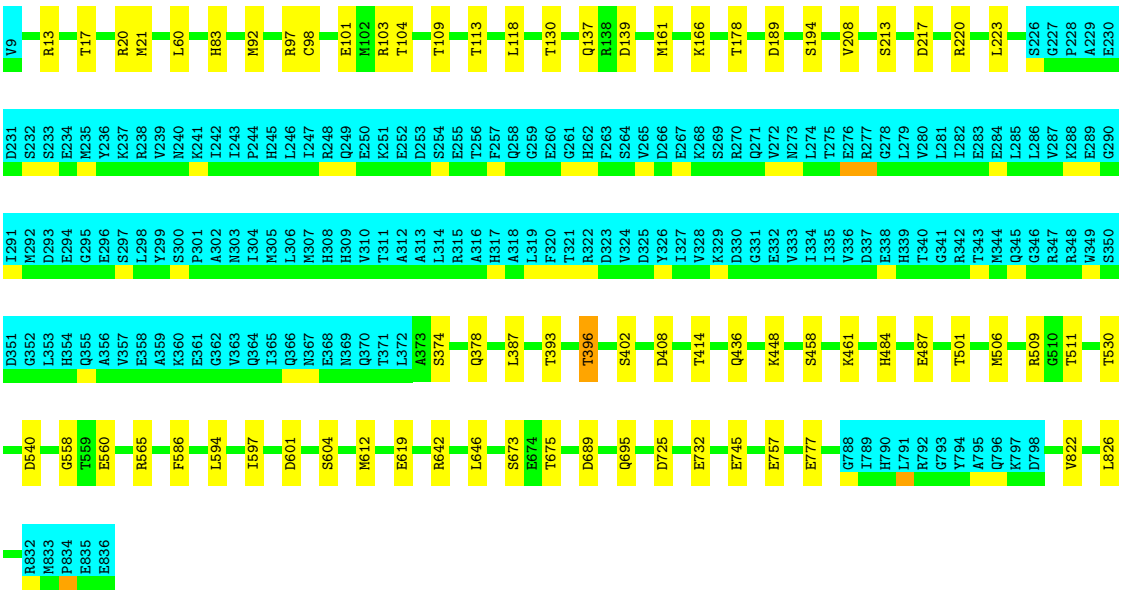




4.2.6 Score per residue for model 6

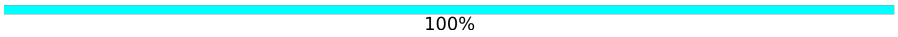
- Molecule 1: TRANSLOCASE SUBUNIT SECA

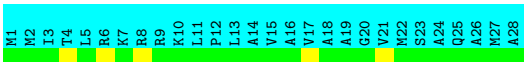
Chain A:



• Molecule 2: MALTOPORIN

Chain B:

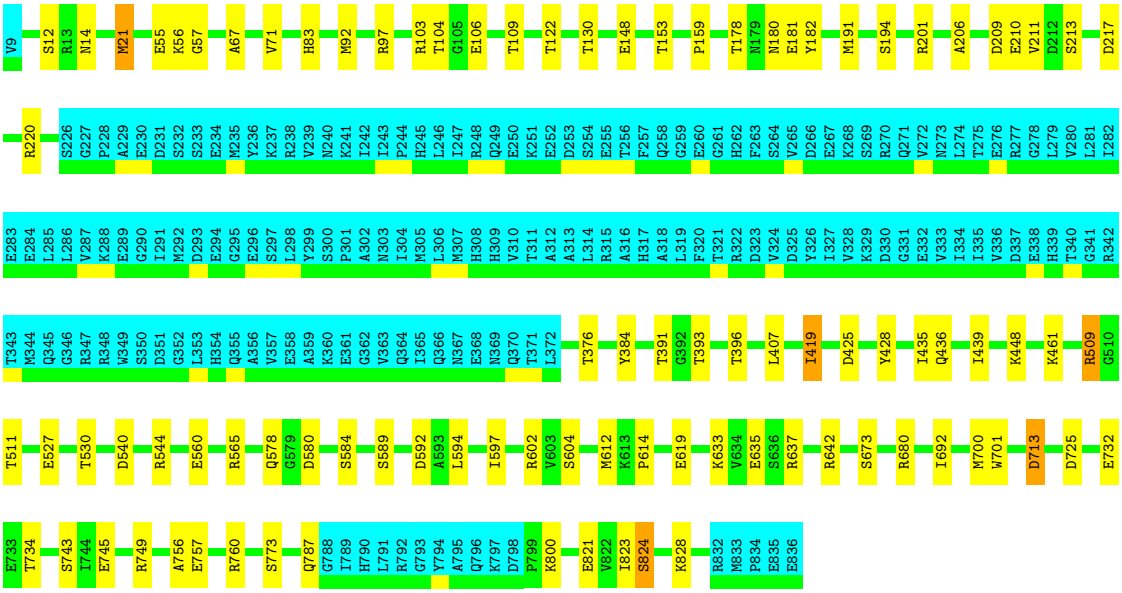




4.2.7 Score per residue for model 7

• Molecule 1: TRANSLOCASE SUBUNIT SECA

Chain A:



• Molecule 2: MALTOPORIN

Chain B: 100%

M1 M2 I3 T4 L5 R6 K7 R8 R9 K10 L11 P12 L13 A14 V15 A16 V17 A18 A19 G20 V21 M22 S23 A24 Q25 A26 M27 A28

4.2.8 Score per residue for model 8

- Molecule 1: TRANSLOCASE SUBUNIT SECA

Chain A: 70% 9% 20%

V9 S12 A52 E55 K56 G57 H83 F84 D85 I99 T104 T109 T113 T122 T130 Q137 R138 D139 M161 K166 Y182 N190 S194 R201 A206 V211 D212 S213 D217 R220 S226 G227 P228 A229 E230 D231 S232 S233

E234 M235 Y236 K237 R238 V239 N240 K241 I242 I243 P244 H245 L246 I247 R248 Q249 E250 K251 E252 D253 S254 E255 T256 F257 Q258 G259 E260 G261 H262 F263 S264 V265 D266 E267 K268 S269 R270 Q271 V272 N273 L274 T275 E276 R277 G278 L279 V280 L281 I282 E283 E284 L285 L286 V287 K288 E289 G290 I291 M292 D293

E294 G295 E296 S297 L298 Y299 S300 P301 A302 N303 I304 M305 L306 M307 H308 H309 V310 T311 A312 A313 L314 R315 A316 H317 A318 L319 F320 T321 R322 D323 V324 D325 Y326 I327 V328 K329 D330 G331 E332 V333 I334 I335 V336 D337 E338 H339 T340 G341 R342 T343 M344 Q345 G346 R347 R348 W349 S350 D351 G352 L353

H354 Q355 A356 V357 E358 A359 K360 E361 G362 V363 Q364 I365 Q366 N367 E368 N369 Q370 T371 L372 Q378 Y384 M390 T391 G392 T393 A398 F401 Y405 D422 K434 I438 D441 E444 R445 T446 T456 K461 N486 R509 G510 T511 D540 R544

R561 S564 R572 G573 R574 S575 D580 S583 S584 S589 D592 A593 L594 A599 M612 K613 R642 L646 V651 Q655 V672 T675 Q695 L706 L710 D715 D725 E729 L730 H731 E732 H761 S773 D783 Q787

G788 I789 H790 L791 R792 G793 Y794 A795 Q796 K797 D798 F799 K800 R832 M833 P834 E835 E836

- Molecule 2: MALTOPORIN

Chain B: 100%

M1 M2 I3 T4 L5 R6 K7 R8 R9 K10 L11 P12 L13 A14 V15 A16 V17 A18 A19 G20 V21 M22 S23 A24 Q25 A26 M27 A28

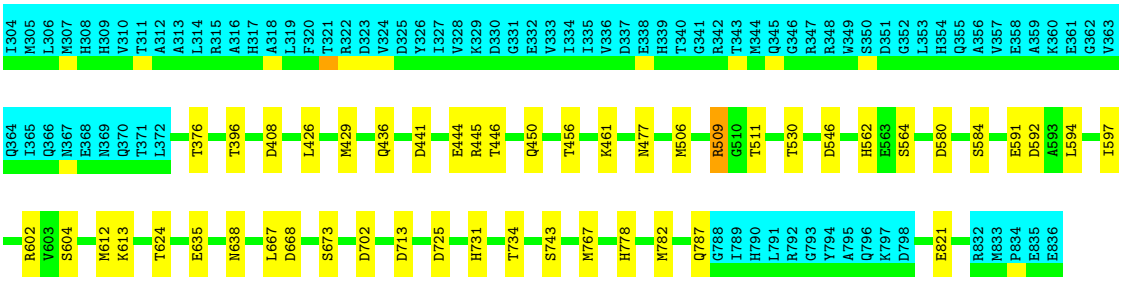
4.2.9 Score per residue for model 9

- Molecule 1: TRANSLOCASE SUBUNIT SECA

Chain A: 72% 8% 20%

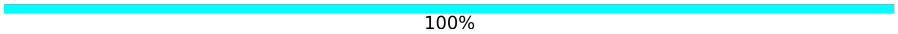
V9 S12 R13 N14 T17 L18 R19 R20 M21 E32 E36 E55 H83 M92 E101 T104 T109 Q137 T178 Y182 N190 S194 E210 V211 D212 S226 G227 P228 A229 E230 D231 S232 S233 E234 M235 Y236 K237 R238 V239 N240 K241 I242 I243

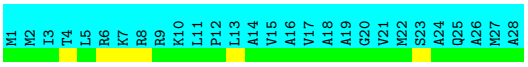
P244 H245 L246 I247 R248 Q249 E250 K251 E252 D253 S254 E255 T256 F257 Q258 G259 E260 G261 H262 F263 S264 V265 D266 E267 K268 S269 R270 Q271 V272 N273 L274 T275 E276 R277 G278 L279 V280 L281 I282 E283 E284 L285 L286 V287 K288 E289 G290 I291 M292 D293 E294 G295 E296 S297 L298 Y299 S300 P301 A302 N303



- Molecule 2: MALTOPORIN

Chain B:

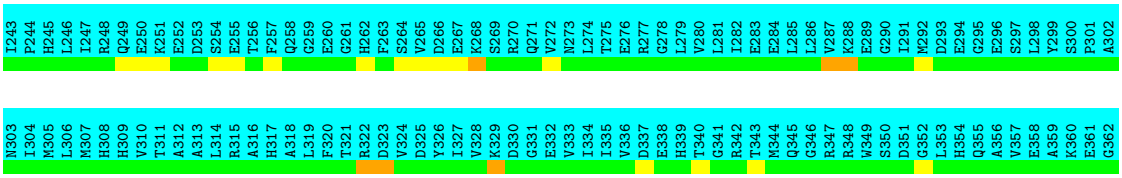


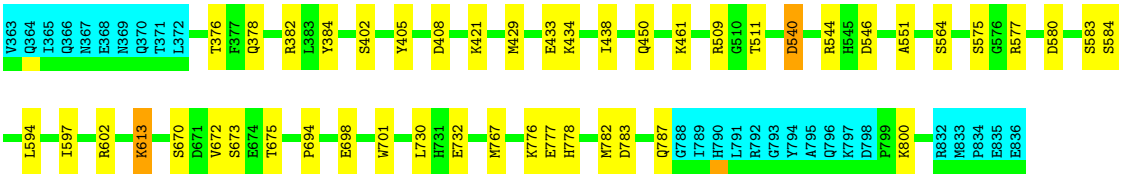


4.2.10 Score per residue for model 10

- Molecule 1: TRANSLOCASE SUBUNIT SECA

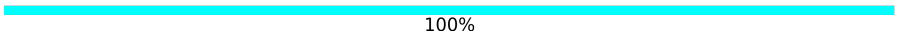
Chain A:

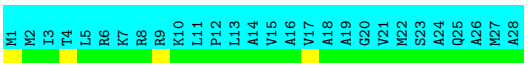




- Molecule 2: MALTOPORIN

Chain B:





5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *SEMIRIGID AND FLEXIBLE SIMULATED ANNEALING*.

Of the 200 calculated structures, 10 were deposited, based on the following criterion: *LOWEST ENERGY*.

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

Software name	**Classification**	**Version**
HADDOCK-CNS	refinement	
NMRPIPE; SPARKY; HADDOCK- CNS	structure solution	CNS

No chemical shift data was provided.

6 Model quality (i)

6.1 Standard geometry (i)

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	5286	4823	5285	16±4
2	B	0	0	0	0±0
All	All	52860	48230	52850	159

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:21:MET:HG2	1:A:92:MET:SD	0.56	2.41	9	2
1:A:713:ASP:O	1:A:828:LYS:HE3	0.56	2.00	7	1
1:A:390:MET:O	1:A:391:THR:HB	0.56	2.01	8	1
1:A:223:LEU:O	1:A:374:SER:HA	0.55	2.01	5	4
1:A:13:ARG:HD2	1:A:408:ASP:OD1	0.55	2.01	2	1
1:A:778:HIS:O	1:A:782:MET:HG2	0.55	2.02	10	4
1:A:106:GLU:OE2	1:A:578:GLN:HA	0.54	2.02	1	4
1:A:594:LEU:O	1:A:597:ILE:HG12	0.54	2.03	9	8
1:A:822:VAL:O	1:A:826:LEU:HG	0.53	2.04	6	1
1:A:640:ASP:O	1:A:644:GLN:HG2	0.51	2.05	4	2
1:A:772:ASP:O	1:A:776:LYS:HG2	0.50	2.06	4	2
1:A:441:ASP:O	1:A:445:ARG:HG2	0.50	2.07	9	4
1:A:101:GLU:CD	1:A:393:THR:HA	0.50	2.26	3	1

Continued on next page...

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:756:ALA:O	1:A:760:ARG:HG2	0.50	2.06	7	2
1:A:161:MET:O	1:A:166:LYS:HE2	0.50	2.07	1	3
1:A:396:THR:HG21	1:A:565:ARG:HB3	0.50	1.83	6	1
1:A:692:ILE:HG23	1:A:701:TRP:CD1	0.50	2.42	2	4
1:A:211:VAL:HG22	1:A:391:THR:HB	0.50	1.83	7	2
1:A:32:GLU:O	1:A:36:GLU:HG3	0.50	2.07	9	1
1:A:206:ALA:HB2	1:A:384:TYR:CD2	0.49	2.42	2	4
1:A:21:MET:HG3	1:A:92:MET:SD	0.49	2.47	7	2
1:A:642:ARG:O	1:A:646:LEU:HG	0.49	2.07	8	2
1:A:396:THR:HB	1:A:397:GLU:OE1	0.49	2.07	1	1
1:A:635:GLU:HA	1:A:638:ASN:ND2	0.49	2.23	9	1
1:A:145:PRO:O	1:A:149:PHE:HB2	0.48	2.08	3	2
1:A:575:SER:OG	1:A:582:GLY:HA3	0.48	2.07	3	1
1:A:540:ASP:O	1:A:544:ARG:HG3	0.48	2.08	4	4
1:A:435:ILE:O	1:A:439:ILE:HG12	0.48	2.08	5	4
1:A:99:ILE:HD11	1:A:407:LEU:HD13	0.48	1.85	3	1
1:A:13:ARG:HD2	1:A:408:ASP:OD2	0.48	2.08	5	2
1:A:98:CYS:SG	1:A:408:ASP:HB3	0.48	2.49	10	1
1:A:420:ARG:HA	1:A:581:ALA:O	0.47	2.09	3	1
1:A:633:LYS:O	1:A:637:ARG:HG3	0.47	2.08	7	1
1:A:103:ARG:HD2	1:A:393:THR:OG1	0.47	2.09	1	2
1:A:97:ARG:HG2	1:A:407:LEU:CD2	0.47	2.39	7	1
1:A:748:GLN:O	1:A:752:GLU:HG3	0.47	2.10	1	1
1:A:698:GLU:HA	1:A:701:TRP:CD2	0.47	2.45	10	1
1:A:99:ILE:HD12	1:A:211:VAL:HG11	0.47	1.86	8	2
1:A:220:ARG:O	1:A:220:ARG:HD3	0.46	2.11	4	1
1:A:772:ASP:O	1:A:776:LYS:HG3	0.46	2.10	5	1
1:A:97:ARG:HA	1:A:387:LEU:O	0.46	2.09	6	1
1:A:25:VAL:HG13	1:A:88:LEU:HD12	0.46	1.87	3	1
1:A:112:ALA:HB1	1:A:207:LEU:HD21	0.46	1.87	5	1
1:A:429:MET:HB2	1:A:433:GLU:OE2	0.46	2.10	10	1
1:A:576:GLY:HA2	1:A:580:ASP:O	0.46	2.10	3	1
1:A:800:LYS:HB2	1:A:800:LYS:NZ	0.46	2.26	5	1
1:A:398:ALA:HA	1:A:401:PHE:CD2	0.46	2.46	8	2
1:A:629:ASN:O	1:A:633:LYS:HG2	0.46	2.11	4	1
1:A:60:LEU:HD11	1:A:118:LEU:O	0.45	2.11	2	3
1:A:52:ALA:O	1:A:56:LYS:HG3	0.45	2.10	4	1
1:A:212:ASP:O	1:A:216:ILE:HB	0.45	2.11	5	1
1:A:445:ARG:HD2	1:A:450:GLN:OE1	0.45	2.12	9	2
1:A:159:PRO:HA	1:A:181:GLU:CD	0.45	2.33	4	3
1:A:13:ARG:HD3	1:A:408:ASP:OD2	0.45	2.12	9	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:210:GLU:HB2	1:A:509:ARG:NH2	0.45	2.27	7	3
1:A:427:VAL:HG22	1:A:588:LEU:HB3	0.45	1.89	5	1
1:A:159:PRO:HA	1:A:181:GLU:OE2	0.44	2.13	4	3
1:A:713:ASP:O	1:A:828:LYS:HE2	0.44	2.12	5	1
1:A:428:TYR:CE1	1:A:614:PRO:HA	0.44	2.47	7	2
1:A:450:GLN:HB2	1:A:551:ALA:HB1	0.44	1.90	10	1
1:A:772:ASP:O	1:A:776:LYS:HE3	0.44	2.11	1	1
1:A:604:SER:O	1:A:608:ARG:HG3	0.44	2.12	5	1
1:A:651:VAL:O	1:A:655:GLN:HG3	0.44	2.13	8	1
1:A:577:ARG:N	1:A:580:ASP:HB3	0.44	2.28	10	1
1:A:206:ALA:HB2	1:A:384:TYR:CD1	0.43	2.47	8	1
1:A:698:GLU:HA	1:A:701:TRP:CE3	0.43	2.48	4	1
1:A:679:ILE:O	1:A:683:VAL:HG23	0.43	2.14	5	1
1:A:434:LYS:O	1:A:438:ILE:HG13	0.43	2.13	4	3
1:A:727:GLU:O	1:A:730:LEU:HB2	0.43	2.14	2	1
1:A:421:LYS:O	1:A:583:SER:HA	0.43	2.13	10	1
1:A:212:ASP:OD2	1:A:566:ARG:HD3	0.43	2.14	3	1
1:A:427:VAL:HG22	1:A:588:LEU:HB2	0.43	1.91	4	1
1:A:428:TYR:CE2	1:A:614:PRO:HA	0.42	2.49	2	1
1:A:783:ASP:O	1:A:787:GLN:HG2	0.42	2.14	8	2
1:A:558:GLY:HA3	1:A:586:PHE:CD2	0.42	2.49	6	1
1:A:821:GLU:HA	1:A:824:SER:OG	0.42	2.14	7	1
1:A:378:GLN:HA	1:A:405:TYR:CE2	0.42	2.48	8	2
1:A:730:LEU:O	1:A:734:THR:HB	0.42	2.14	2	1
1:A:672:VAL:O	1:A:676:ILE:HG12	0.42	2.15	4	1
1:A:52:ALA:O	1:A:56:LYS:HG2	0.42	2.14	8	1
1:A:140:ALA:O	1:A:144:ARG:HB2	0.42	2.14	3	1
1:A:422:ASP:OD1	1:A:572:ARG:HD2	0.42	2.14	8	1
1:A:393:THR:O	1:A:569:ASN:HB3	0.42	2.14	1	1
1:A:640:ASP:O	1:A:643:LYS:HG2	0.42	2.15	5	1
1:A:733:GLU:HG2	1:A:734:THR:N	0.41	2.30	3	1
1:A:757:GLU:H	1:A:757:GLU:CD	0.41	2.18	7	1
1:A:744:ILE:O	1:A:748:GLN:HG3	0.41	2.15	3	1
1:A:638:ASN:HD21	1:A:642:ARG:NH2	0.41	2.13	5	1
1:A:647:GLU:O	1:A:651:VAL:HG23	0.41	2.15	1	1
1:A:589:SER:O	1:A:592:ASP:HB2	0.41	2.16	8	1
1:A:67:ALA:O	1:A:71:VAL:HG23	0.41	2.16	7	1
1:A:706:LEU:O	1:A:710:LEU:HG	0.41	2.16	8	1
1:A:728:PRO:HD2	1:A:729:GLU:OE1	0.40	2.16	1	1
1:A:416:ARG:HB2	1:A:578:GLN:O	0.40	2.16	5	1
1:A:131:VAL:HA	1:A:214:ILE:HD11	0.40	1.91	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:561:ARG:HB2	1:A:594:LEU:HD22	0.40	1.91	8	1
1:A:210:GLU:HB2	1:A:509:ARG:HH21	0.40	1.76	1	1
1:A:726:LYS:O	1:A:728:PRO:HD3	0.40	2.17	3	1
1:A:680:ARG:HG3	1:A:823:ILE:HD12	0.40	1.93	7	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	664/828 (80%)	628±4 (95±1%)	31±4 (5±1%)	5±2 (1±0%)	24 71
2	B	0	-	-	-	-
All	All	6640/8560 (78%)	6279 (95%)	309 (5%)	52 (1%)	24 71

All 16 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	509	ARG	9
1	A	14	ASN	6
1	A	57	GLY	6
1	A	396	THR	6
1	A	613	LYS	5
1	A	619	GLU	4
1	A	612	MET	2
1	A	212	ASP	2
1	A	419	ILE	2
1	A	614	PRO	2
1	A	731	HIS	2
1	A	672	VAL	2
1	A	393	THR	1
1	A	391	THR	1
1	A	599	ALA	1
1	A	694	PRO	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	563/705 (80%)	519±7 (92±1%)	44±7 (8±1%)	16 64
2	B	0	-	-	-
All	All	5630/7250 (78%)	5190 (92%)	440 (8%)	16 64

All 145 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	511	THR	10
1	A	130	THR	9
1	A	194	SER	9
1	A	461	LYS	9
1	A	83	HIS	9
1	A	12	SER	8
1	A	104	THR	8
1	A	178	THR	8
1	A	376	THR	8
1	A	612	MET	8
1	A	109	THR	8
1	A	220	ARG	8
1	A	564	SER	7
1	A	584	SER	7
1	A	604	SER	7
1	A	673	SER	7
1	A	589	SER	6
1	A	732	GLU	6
1	A	113	THR	5
1	A	137	GLN	5
1	A	436	GLN	5
1	A	670	SER	5
1	A	734	THR	5
1	A	182	TYR	5
1	A	506	MET	5
1	A	715	ASP	5
1	A	190	ASN	5
1	A	745	GLU	5

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Mol	Chain	Res	Type	Models (Total)
1	A	580	ASP	5
1	A	208	VAL	4
1	A	212	ASP	4
1	A	546	ASP	4
1	A	675	THR	4
1	A	85	ASP	4
1	A	153	THR	4
1	A	393	THR	4
1	A	668	ASP	4
1	A	749	ARG	4
1	A	213	SER	4
1	A	444	GLU	4
1	A	540	ASP	4
1	A	602	ARG	4
1	A	402	SER	4
1	A	530	THR	4
1	A	592	ASP	4
1	A	800	LYS	4
1	A	725	ASP	4
1	A	21	MET	3
1	A	486	ASN	3
1	A	98	CYS	3
1	A	161	MET	3
1	A	448	LYS	3
1	A	730	LEU	3
1	A	777	GLU	3
1	A	20	ARG	3
1	A	210	GLU	3
1	A	17	THR	3
1	A	139	ASP	3
1	A	209	ASP	3
1	A	414	THR	3
1	A	743	SER	3
1	A	19	ARG	3
1	A	446	THR	3
1	A	713	ASP	3
1	A	101	GLU	3
1	A	217	ASP	3
1	A	55	GLU	3
1	A	14	ASN	2
1	A	425	ASP	2
1	A	512	ASP	2

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Mol	Chain	Res	Type	Models (Total)
1	A	742	GLN	2
1	A	821	GLU	2
1	A	108	LYS	2
1	A	189	ASP	2
1	A	419	ILE	2
1	A	677	ASN	2
1	A	722	GLU	2
1	A	757	GLU	2
1	A	477	ASN	2
1	A	583	SER	2
1	A	601	ASP	2
1	A	616	GLU	2
1	A	647	GLU	2
1	A	729	GLU	2
1	A	731	HIS	2
1	A	484	HIS	2
1	A	562	HIS	2
1	A	574	ARG	2
1	A	689	ASP	2
1	A	624	THR	2
1	A	700	MET	2
1	A	378	GLN	2
1	A	560	GLU	2
1	A	695	GLN	2
1	A	122	THR	2
1	A	201	ARG	2
1	A	787	GLN	2
1	A	456	THR	2
1	A	575	SER	2
1	A	767	MET	2
1	A	409	THR	1
1	A	733	GLU	1
1	A	772	ASP	1
1	A	111	THR	1
1	A	131	VAL	1
1	A	133	ASP	1
1	A	462	SER	1
1	A	532	GLU	1
1	A	625	LYS	1
1	A	650	ASP	1
1	A	22	ARG	1
1	A	124	LYS	1

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Mol	Chain	Res	Type	Models (Total)
1	A	536	LYS	1
1	A	649	ASP	1
1	A	40	ASP	1
1	A	196	GLU	1
1	A	202	LYS	1
1	A	563	GLU	1
1	A	620	HIS	1
1	A	520	GLN	1
1	A	535	GLU	1
1	A	638	ASN	1
1	A	458	SER	1
1	A	487	GLU	1
1	A	501	THR	1
1	A	56	LYS	1
1	A	103	ARG	1
1	A	148	GLU	1
1	A	180	ASN	1
1	A	191	MET	1
1	A	527	GLU	1
1	A	565	ARG	1
1	A	619	GLU	1
1	A	635	GLU	1
1	A	642	ARG	1
1	A	824	SER	1
1	A	761	HIS	1
1	A	426	LEU	1
1	A	429	MET	1
1	A	591	GLU	1
1	A	667	LEU	1
1	A	184	PHE	1
1	A	382	ARG	1
1	A	613	LYS	1
1	A	776	LYS	1

6.3.3 RNA (i)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.5 Carbohydrates (i)

There are no monosaccharides in this entry.

6.6 Ligand geometry (i)

There are no ligands in this entry.

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