



Full wwPDB NMR Structure Validation Report ⓘ

May 29, 2020 – 01:45 am 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 ⓘ symbol.

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

Cyrange : Kirchner and Güntert (2011)
NmrClust : Kelley et al. (1996)
MolProbity : 4.02b-467
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 : 2.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

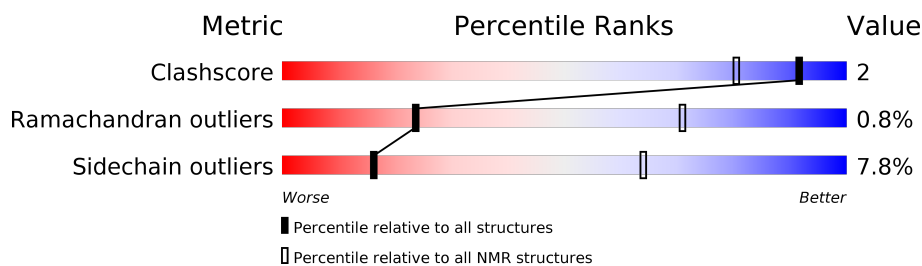
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment was not calculated.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	828	
2	B	28	

2 Ensemble composition and analysis

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)	0.32	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

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.

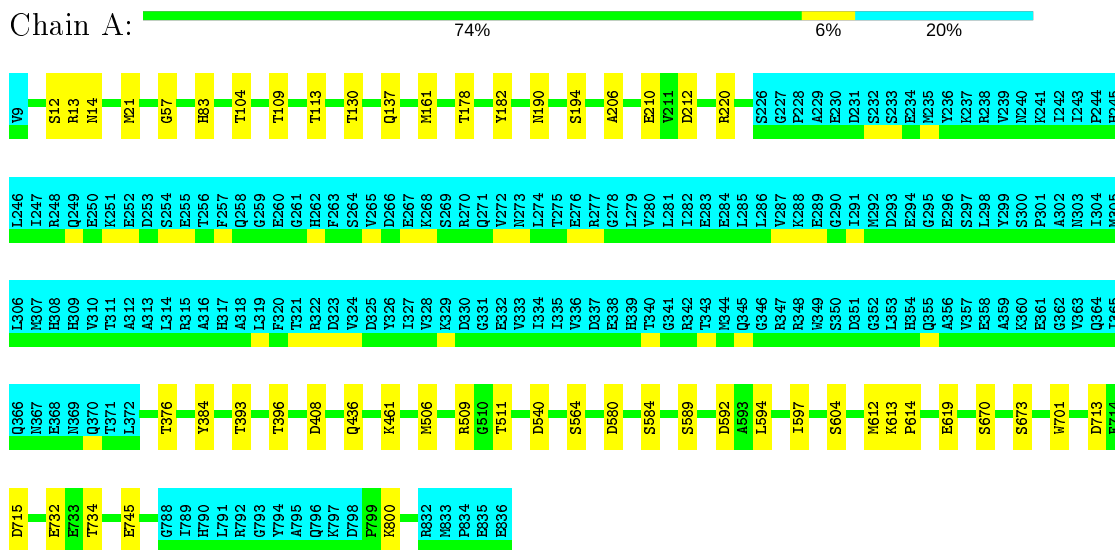
Mol	Chain	Residues	Atoms					Trace	
			Total	C	H	N	O		S
2	B	28	421	129	216	40	32	4	0

4 Residue-property plots [i](#)

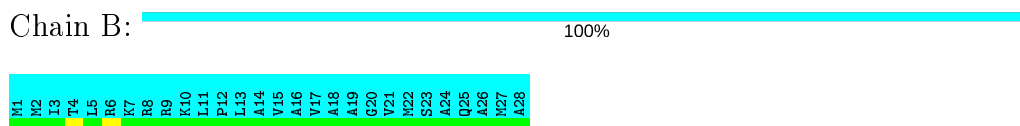
4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA 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: TRANSLOCASE SUBUNIT SECA



- Molecule 2: MALTOPORIN



4.2 Scores per residue for each member of the ensemble

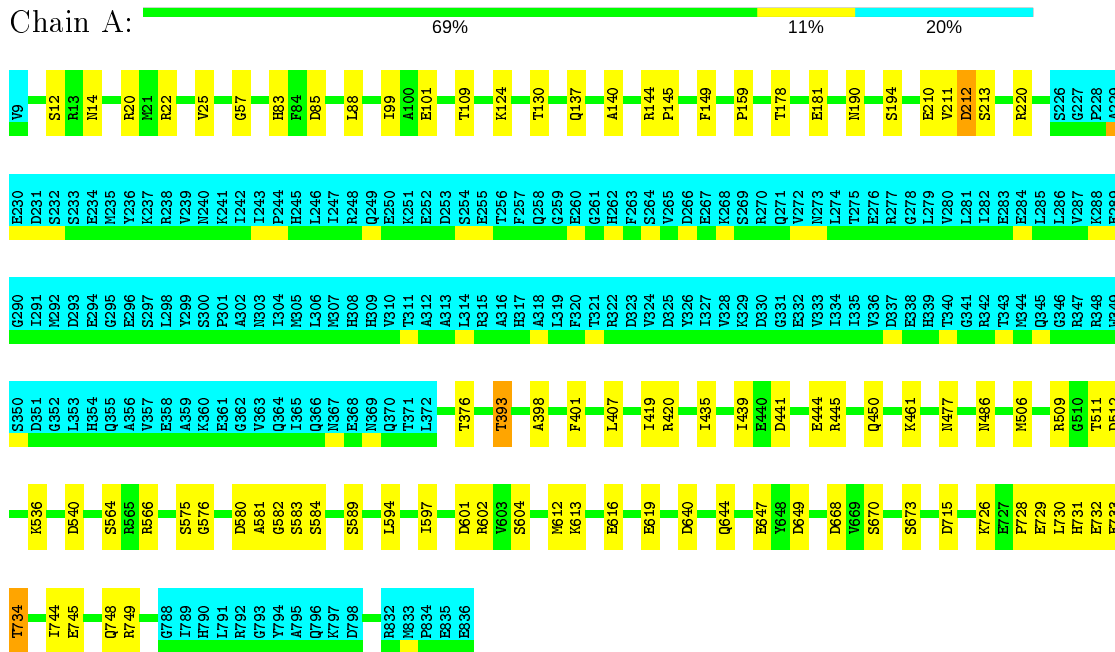
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

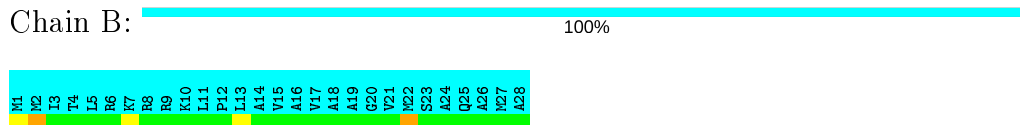
- Molecule 1: TRANSLOCASE SUBUNIT SECA

4.2.3 Score per residue for model 3

- Molecule 1: TRANSLOCASE SUBUNIT SECA

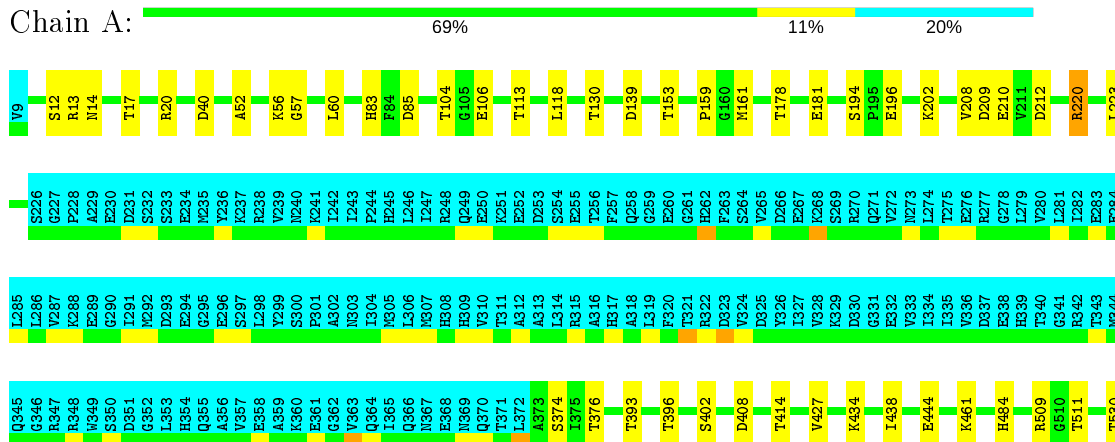


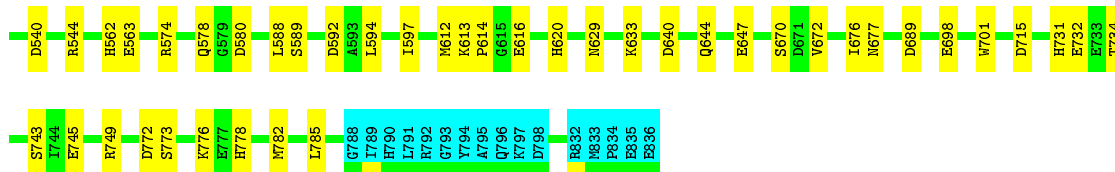
- Molecule 2: MALTOPORIN



4.2.4 Score per residue for model 4

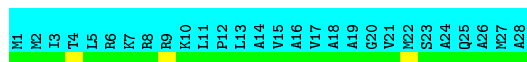
- Molecule 1: TRANSLOCASE SUBUNIT SECA





- Molecule 2: MALTOPORIN

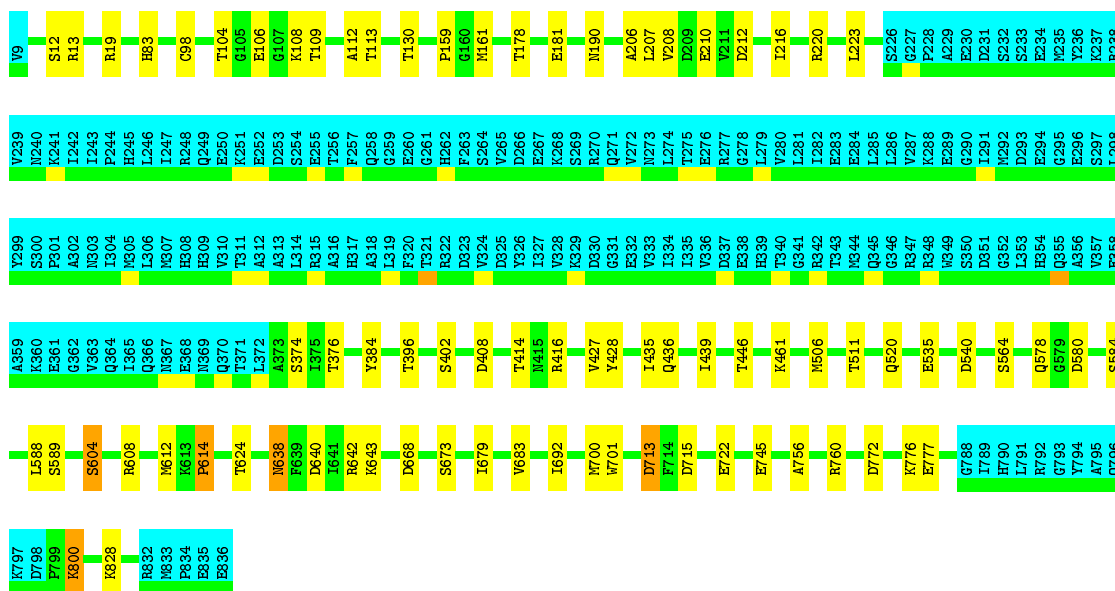
Chain B: 100%



4.2.5 Score per residue for model 5

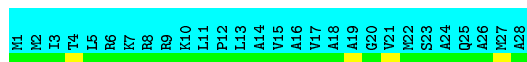
- Molecule 1: TRANSLOCASE SUBUNIT SECA

Chain A: 71% 9% 20%



- Molecule 2: MALTOPORIN

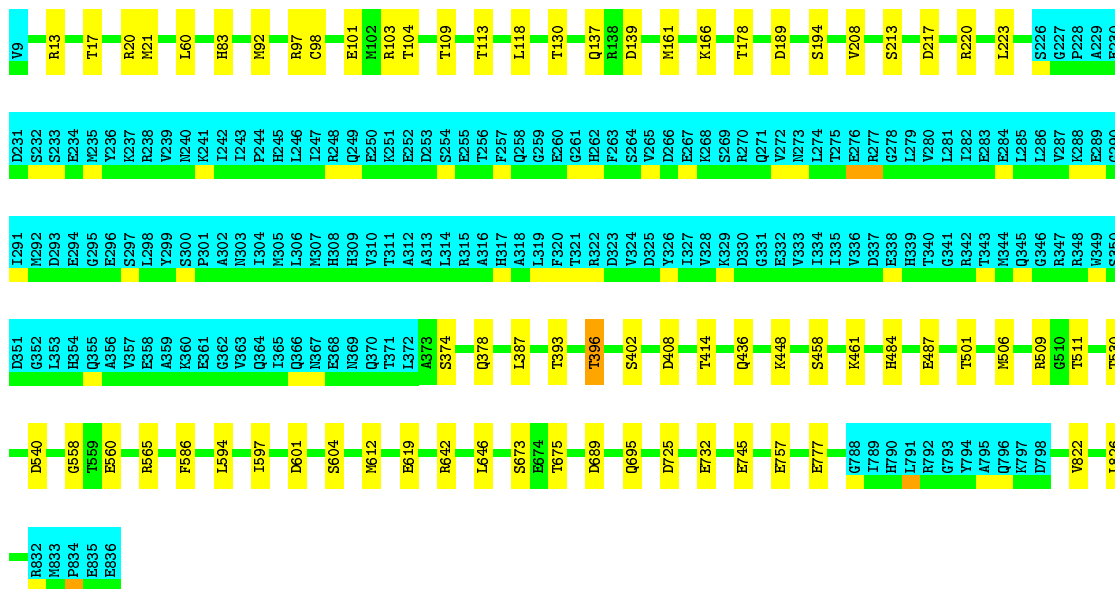
Chain B: 100%



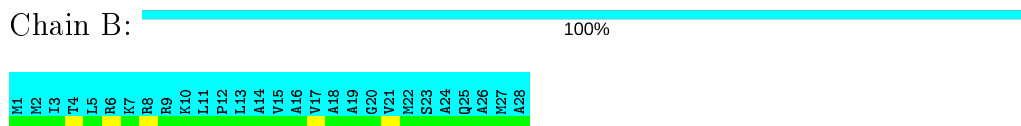
4.2.6 Score per residue for model 6

- Molecule 1: TRANSLOCASE SUBUNIT SECA

Chain A: 72% 8% 20%

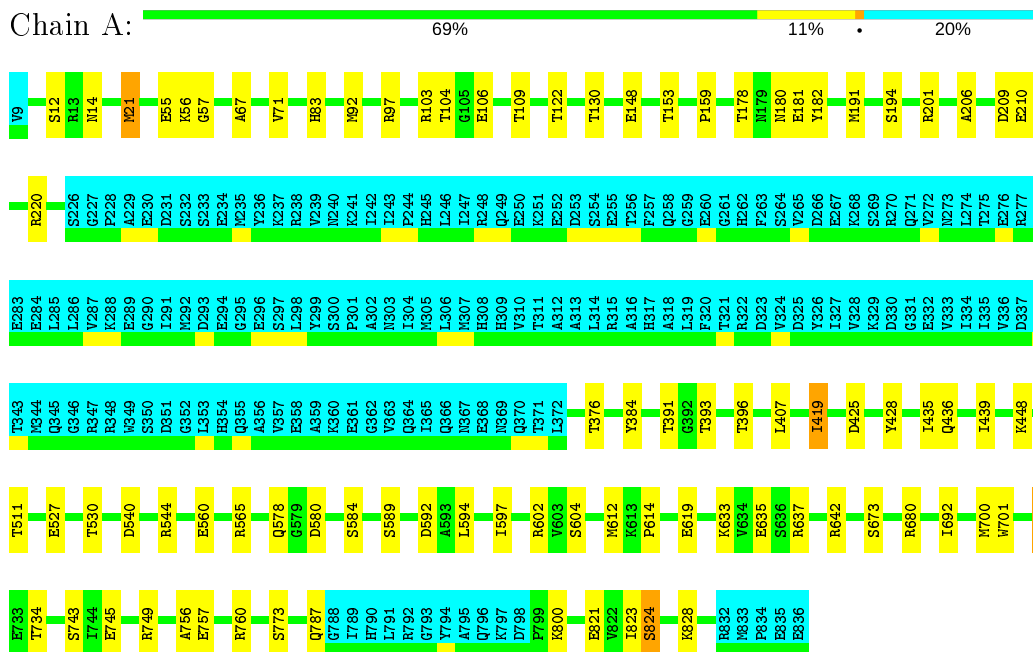


• Molecule 2: MALTOPORIN



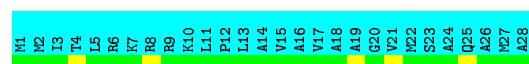
4.2.7 Score per residue for model 7

• Molecule 1: TRANSLOCASE SUBUNIT SECA



• Molecule 2: MALTOPORIN

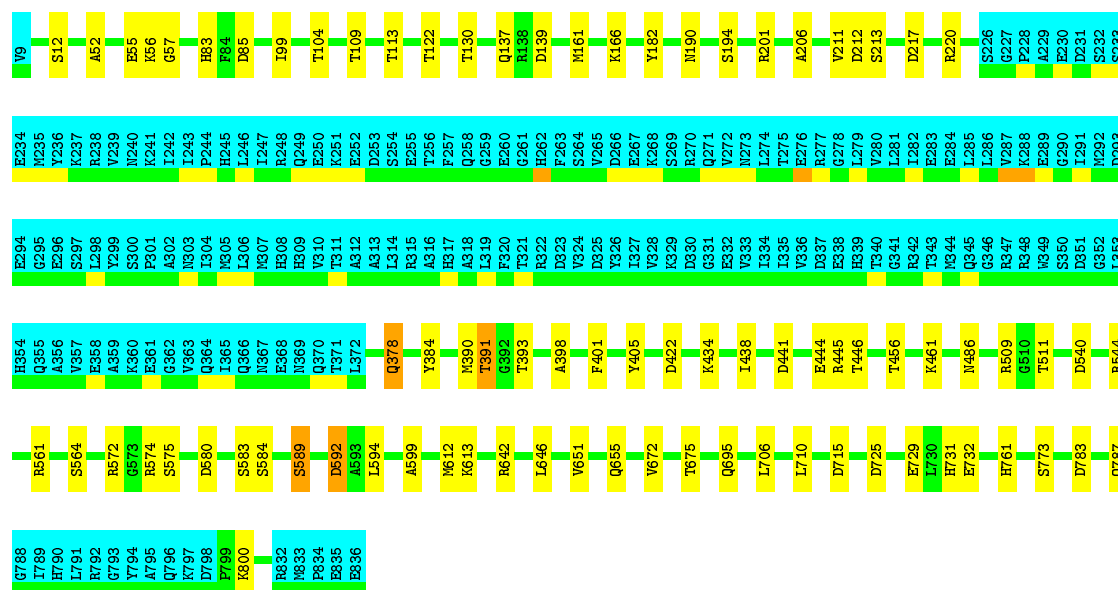
Chain B:  100%



4.2.8 Score per residue for model 8

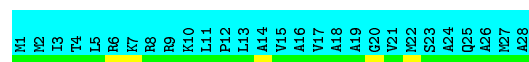
- Molecule 1: TRANSLOCASE SUBUNIT SECA

Chain A:  70%  9%  20%



- Molecule 2: MALTOPORIN

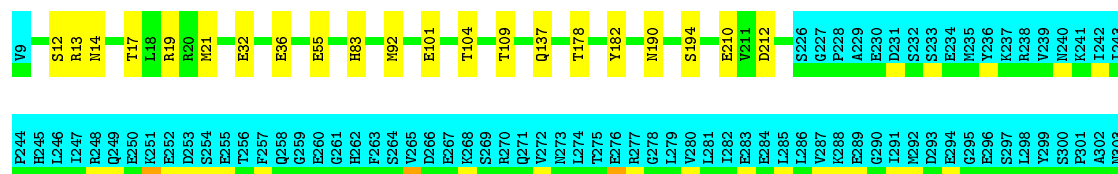
Chain B:  100%



4.2.9 Score per residue for model 9

- Molecule 1: TRANSLOCASE SUBUNIT SECA

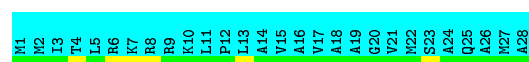
Chain A:  72%  8%  20%





- Molecule 2: MALTOPORIN

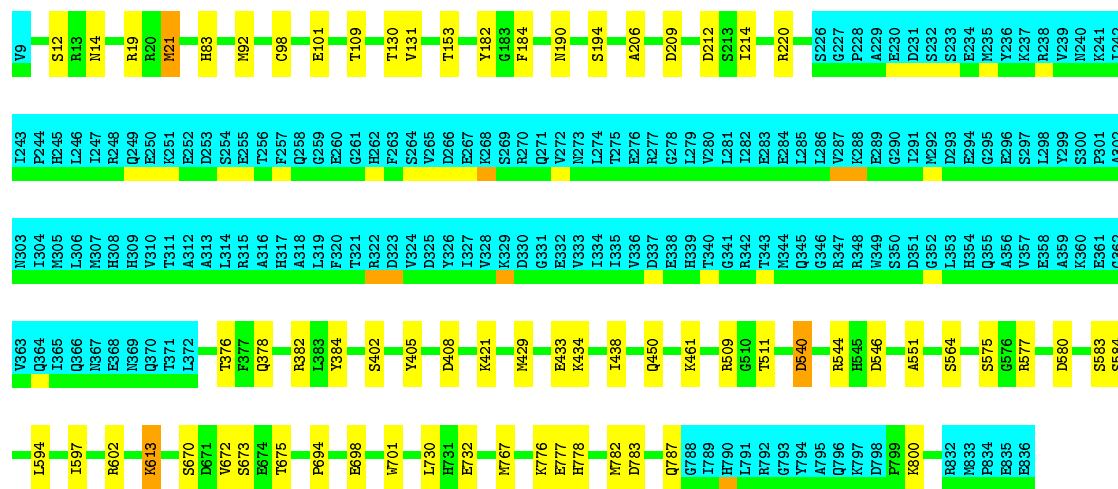
Chain B:  100%



4.2.10 Score per residue for model 10

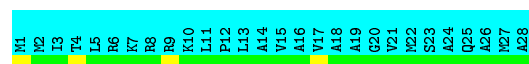
- Molecule 1: TRANSLOCASE SUBUNIT SECA

Chain A:  72% 8% 20%



- Molecule 2: MALTOPORIN

Chain B:  100%



5 Refinement protocol and experimental data overview

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. 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

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

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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:NZ	1:A:800:LYS:HB2	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	57	GLY	6
1	A	14	ASN	6
1	A	396	THR	6
1	A	613	LYS	5
1	A	619	GLU	4
1	A	672	VAL	2
1	A	614	PRO	2
1	A	731	HIS	2
1	A	612	MET	2
1	A	419	ILE	2
1	A	212	ASP	2
1	A	391	THR	1
1	A	694	PRO	1
1	A	393	THR	1
1	A	599	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	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	461	LYS	9
1	A	194	SER	9
1	A	83	HIS	9
1	A	130	THR	9
1	A	104	THR	8
1	A	220	ARG	8
1	A	109	THR	8
1	A	376	THR	8
1	A	178	THR	8
1	A	12	SER	8
1	A	612	MET	8
1	A	604	SER	7
1	A	564	SER	7
1	A	584	SER	7
1	A	673	SER	7
1	A	589	SER	6
1	A	732	GLU	6
1	A	670	SER	5
1	A	436	GLN	5
1	A	506	MET	5
1	A	734	THR	5
1	A	190	ASN	5
1	A	715	ASP	5
1	A	580	ASP	5
1	A	113	THR	5
1	A	745	GLU	5
1	A	182	TYR	5

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Mol	Chain	Res	Type	Models (Total)
1	A	137	GLN	5
1	A	725	ASP	4
1	A	208	VAL	4
1	A	749	ARG	4
1	A	402	SER	4
1	A	213	SER	4
1	A	444	GLU	4
1	A	800	LYS	4
1	A	546	ASP	4
1	A	153	THR	4
1	A	212	ASP	4
1	A	592	ASP	4
1	A	540	ASP	4
1	A	675	THR	4
1	A	602	ARG	4
1	A	393	THR	4
1	A	85	ASP	4
1	A	530	THR	4
1	A	668	ASP	4
1	A	486	ASN	3
1	A	713	ASP	3
1	A	98	CYS	3
1	A	209	ASP	3
1	A	210	GLU	3
1	A	19	ARG	3
1	A	20	ARG	3
1	A	21	MET	3
1	A	161	MET	3
1	A	446	THR	3
1	A	743	SER	3
1	A	17	THR	3
1	A	217	ASP	3
1	A	101	GLU	3
1	A	730	LEU	3
1	A	448	LYS	3
1	A	55	GLU	3
1	A	139	ASP	3
1	A	777	GLU	3
1	A	414	THR	3
1	A	695	GLN	2
1	A	700	MET	2
1	A	647	GLU	2

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Mol	Chain	Res	Type	Models (Total)
1	A	821	GLU	2
1	A	677	ASN	2
1	A	742	GLN	2
1	A	512	ASP	2
1	A	574	ARG	2
1	A	425	ASP	2
1	A	787	GLN	2
1	A	757	GLU	2
1	A	189	ASP	2
1	A	201	ARG	2
1	A	624	THR	2
1	A	729	GLU	2
1	A	484	HIS	2
1	A	689	ASP	2
1	A	601	ASP	2
1	A	378	GLN	2
1	A	575	SER	2
1	A	731	HIS	2
1	A	122	THR	2
1	A	722	GLU	2
1	A	560	GLU	2
1	A	477	ASN	2
1	A	14	ASN	2
1	A	419	ILE	2
1	A	583	SER	2
1	A	456	THR	2
1	A	767	MET	2
1	A	108	LYS	2
1	A	616	GLU	2
1	A	562	HIS	2
1	A	184	PHE	1
1	A	520	GLN	1
1	A	382	ARG	1
1	A	124	LYS	1
1	A	591	GLU	1
1	A	563	GLU	1
1	A	409	THR	1
1	A	429	MET	1
1	A	824	SER	1
1	A	56	LYS	1
1	A	191	MET	1
1	A	202	LYS	1

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Mol	Chain	Res	Type	Models (Total)
1	A	22	ARG	1
1	A	733	GLU	1
1	A	620	HIS	1
1	A	565	ARG	1
1	A	462	SER	1
1	A	103	ARG	1
1	A	649	ASP	1
1	A	535	GLU	1
1	A	131	VAL	1
1	A	426	LEU	1
1	A	536	LYS	1
1	A	613	LYS	1
1	A	111	THR	1
1	A	650	ASP	1
1	A	148	GLU	1
1	A	638	ASN	1
1	A	532	GLU	1
1	A	40	ASP	1
1	A	501	THR	1
1	A	180	ASN	1
1	A	635	GLU	1
1	A	667	LEU	1
1	A	776	LYS	1
1	A	761	HIS	1
1	A	196	GLU	1
1	A	487	GLU	1
1	A	133	ASP	1
1	A	625	LYS	1
1	A	527	GLU	1
1	A	772	ASP	1
1	A	642	ARG	1
1	A	619	GLU	1
1	A	458	SER	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 carbohydrates 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

No chemical shift data were provided