



Full wwPDB NMR Structure Validation Report ⓘ

Feb 13, 2017 – 02:19 am GMT

PDB ID : 2RT5
Title : Structural insights into the recruitment of SMRT by the co-repressor SHARP under phosphorylative regulation
Authors : Mikami, S.; Kanaba, T.; Mishima, M.
Deposited on : 2013-04-22

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/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
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	trunk28760
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

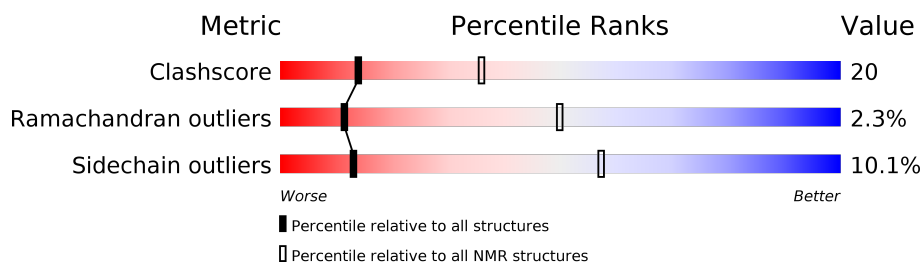
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 85%.

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	125131	11601
Ramachandran outliers	121729	10391
Sidechain outliers	121581	10367

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	169	
2	B	8	

2 Ensemble composition and analysis

This entry contains 20 models. Model 3 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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:3501-A:3539, A:3546-A:3614, A:3624-A:3664, B:2518-B:2521 (153)	0.21	3

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

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

The models can be grouped into 3 clusters and 3 single-model clusters were found.

Cluster number	Models
1	1, 2, 3, 7, 9, 10, 11, 12, 15, 18, 19, 20
2	6, 14, 17
3	4, 5
Single-model clusters	8; 13; 16

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2761 atoms, of which 1391 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Msx2-interacting protein.

Mol	Chain	Residues	Atoms						Trace
1	A	169	Total	C	H	N	O	S	0
			2634	825	1338	225	239	7	

- Molecule 2 is a protein called peptide from Silencing mediator of retinoic acid and thyroid hormone receptor.

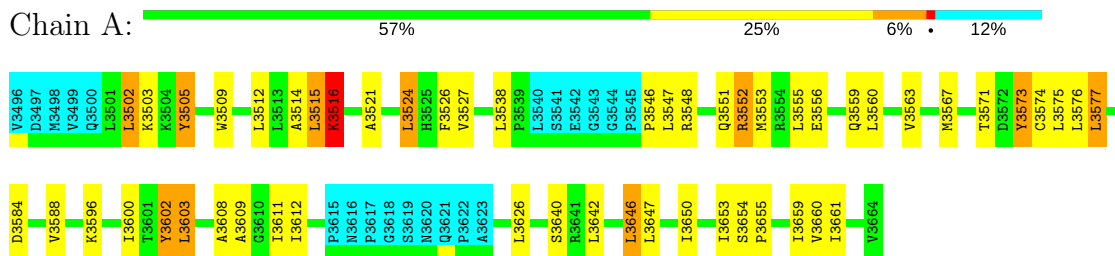
Mol	Chain	Residues	Atoms						Trace
2	B	8	Total	C	H	N	O	P	0
			127	39	53	8	25	2	

4 Residue-property plots

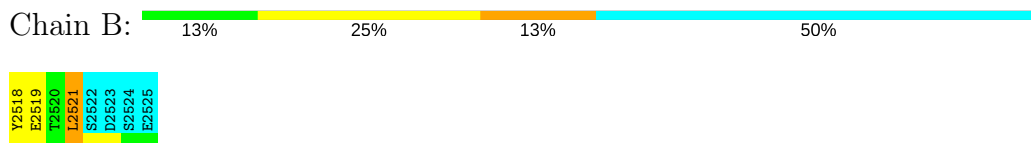
4.1 Average score per residue in the NMR ensemble

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: Msx2-interacting protein



- Molecule 2: peptide from Silencing mediator of retinoic acid and thyroid hormone receptor

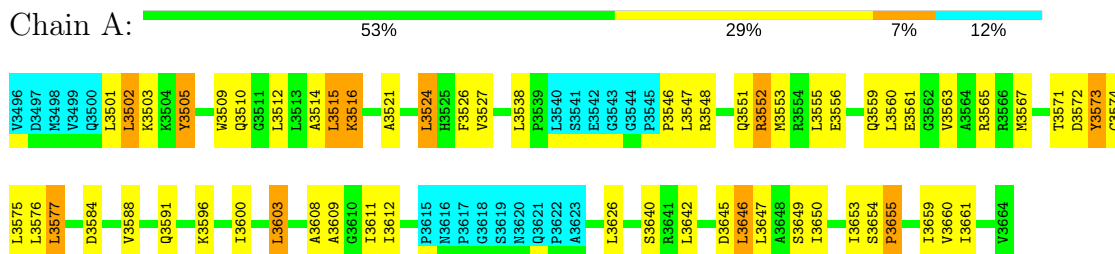


4.2 Scores per residue for each member of the ensemble


Colouring as in section 4.1 above.

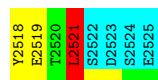
4.2.1 Score per residue for model 1

- Molecule 1: Msx2-interacting protein



- Molecule 2: peptide from Silencing mediator of retinoic acid and thyroid hormone receptor

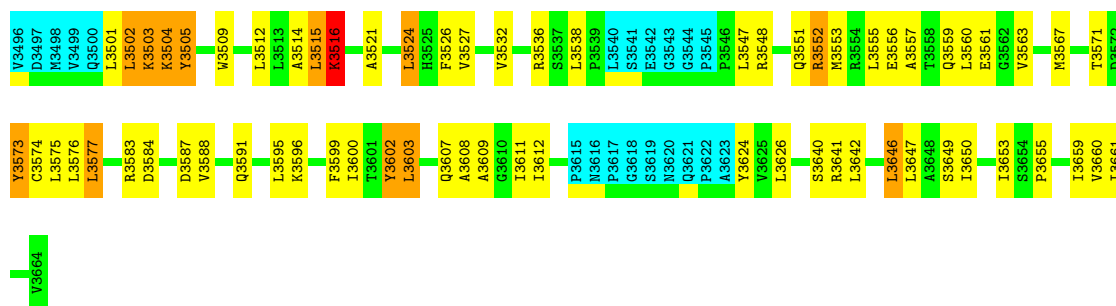
Chain B: 




4.2.2 Score per residue for model 2

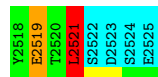
- Molecule 1: Msx2-interacting protein

Chain A: 



- Molecule 2: peptide from Silencing mediator of retinoic acid and thyroid hormone receptor

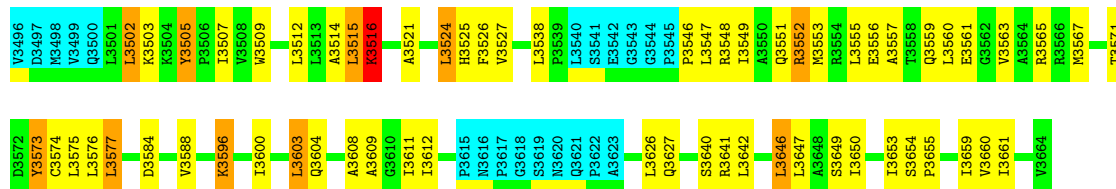
Chain B: 



4.2.3 Score per residue for model 3 (medoid)

- Molecule 1: Msx2-interacting protein

Chain A: 



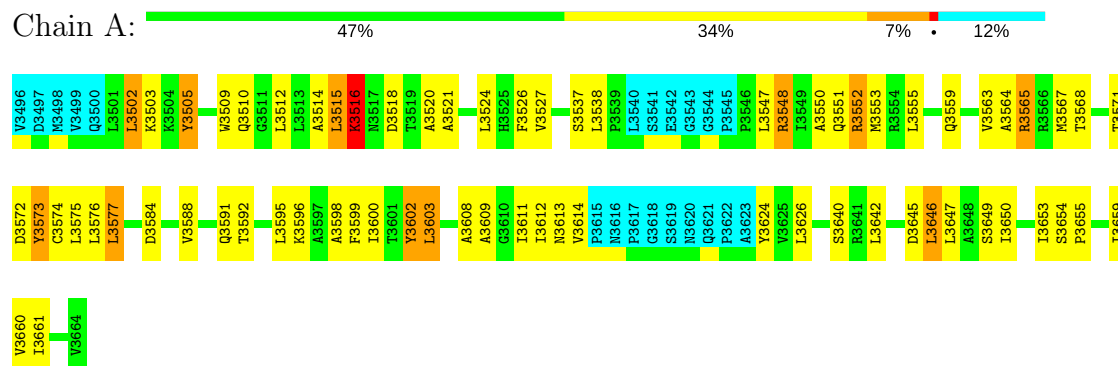
- Molecule 2: peptide from Silencing mediator of retinoic acid and thyroid hormone receptor

Chain B: 



4.2.4 Score per residue for model 4

- Molecule 1: Msx2-interacting protein

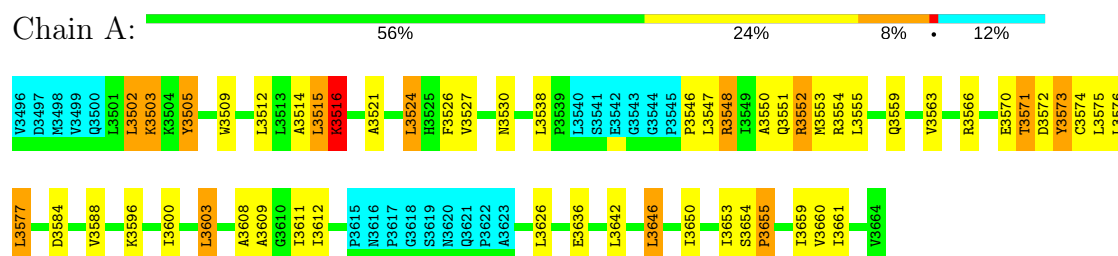


- Molecule 2: peptide from Silencing mediator of retinoic acid and thyroid hormone receptor

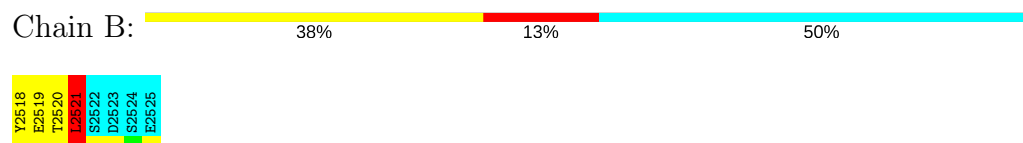


4.2.5 Score per residue for model 5

- Molecule 1: Msx2-interacting protein

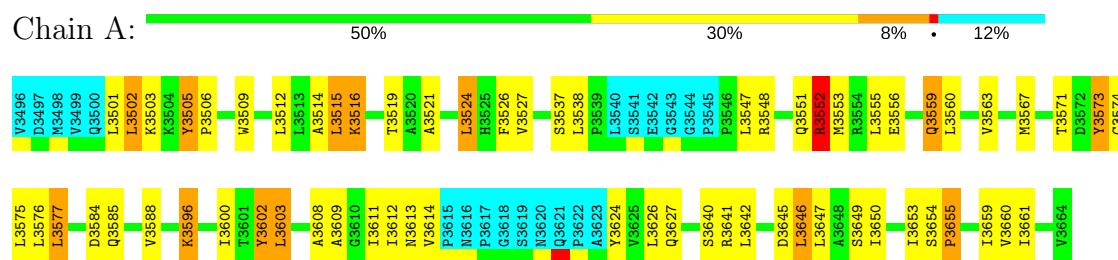


- Molecule 2: peptide from Silencing mediator of retinoic acid and thyroid hormone receptor

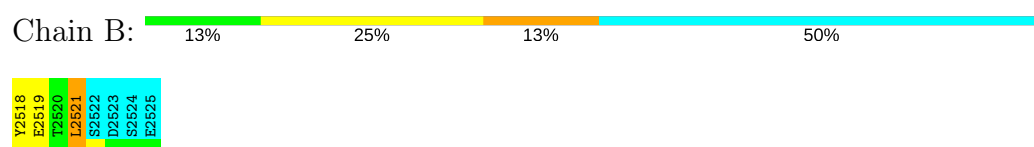


4.2.6 Score per residue for model 6

- Molecule 1: Msx2-interacting protein

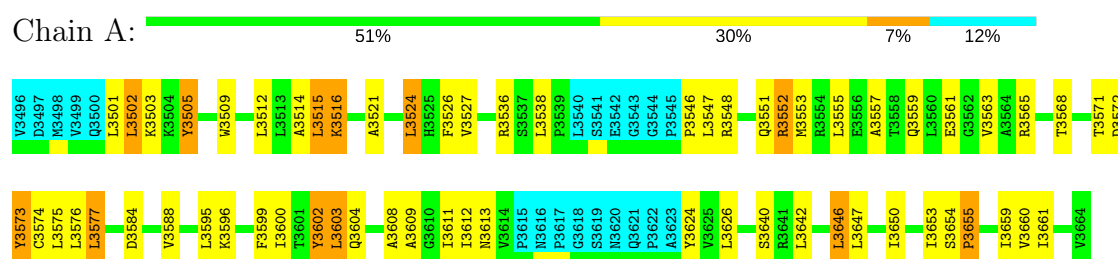


- Molecule 2: peptide from Silencing mediator of retinoic acid and thyroid hormone receptor



4.2.7 Score per residue for model 7

- Molecule 1: Msx2-interacting protein

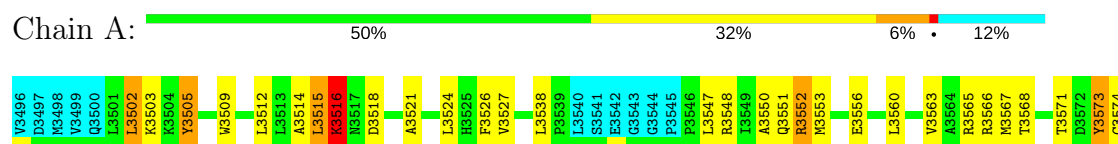


- Molecule 2: peptide from Silencing mediator of retinoic acid and thyroid hormone receptor



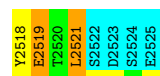
4.2.8 Score per residue for model 8

- Molecule 1: Msx2-interacting protein



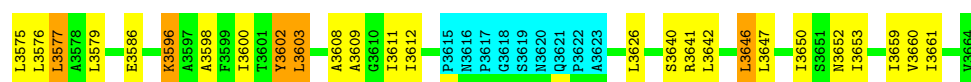
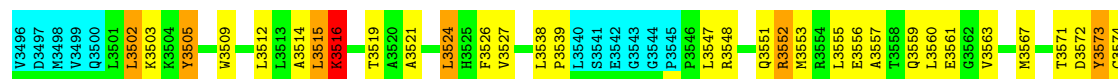


- Molecule 2: peptide from Silencing mediator of retinoic acid and thyroid hormone receptor

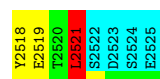
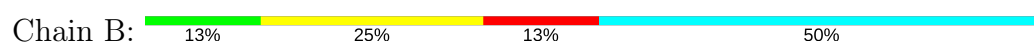


4.2.9 Score per residue for model 9

- Molecule 1: Msx2-interacting protein

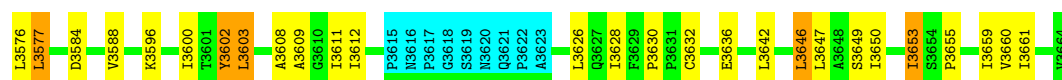
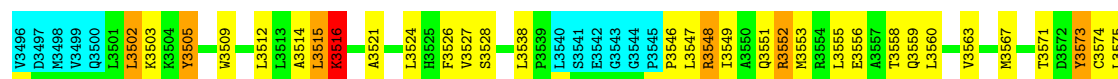
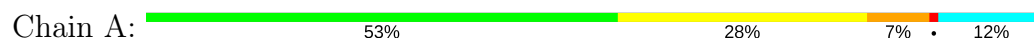


- Molecule 2: peptide from Silencing mediator of retinoic acid and thyroid hormone receptor

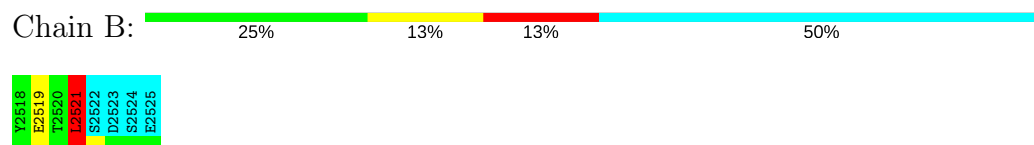


4.2.10 Score per residue for model 10

- Molecule 1: Msx2-interacting protein

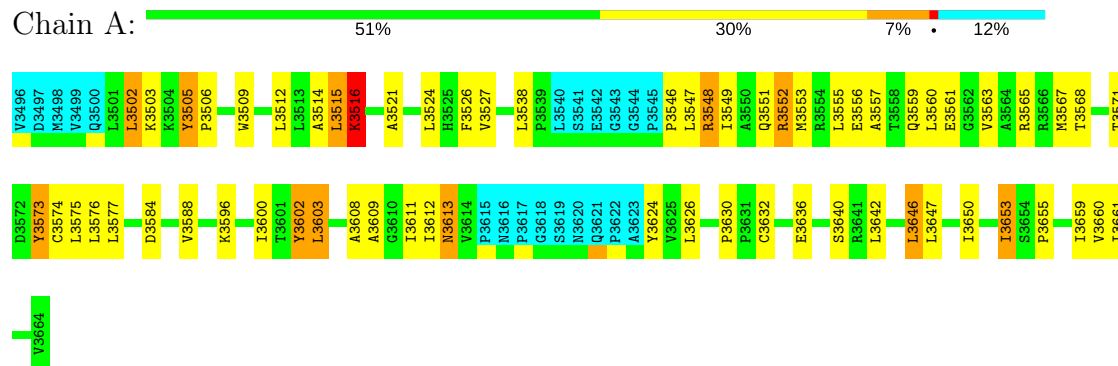


- Molecule 2: peptide from Silencing mediator of retinoic acid and thyroid hormone receptor

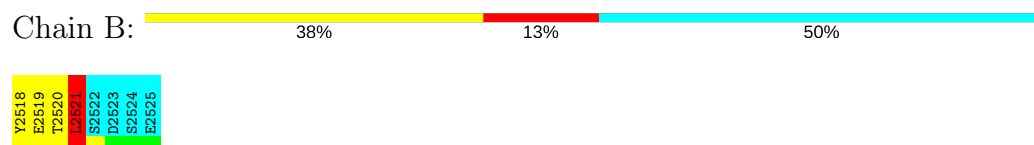


4.2.11 Score per residue for model 11

- Molecule 1: Msx2-interacting protein

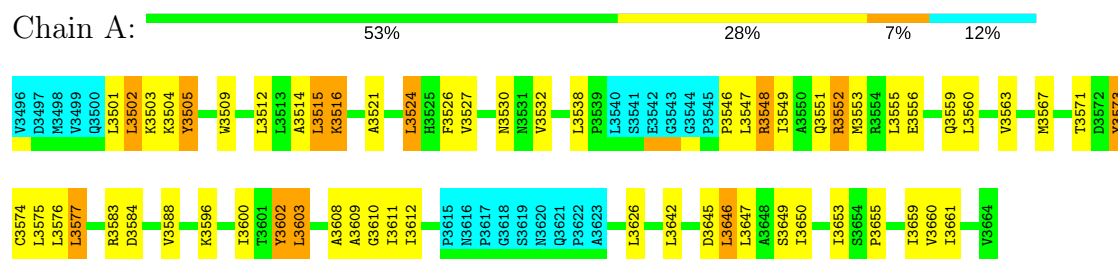


- Molecule 2: peptide from Silencing mediator of retinoic acid and thyroid hormone receptor

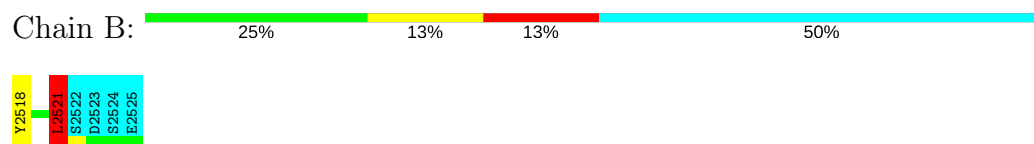


4.2.12 Score per residue for model 12

- Molecule 1: Msx2-interacting protein

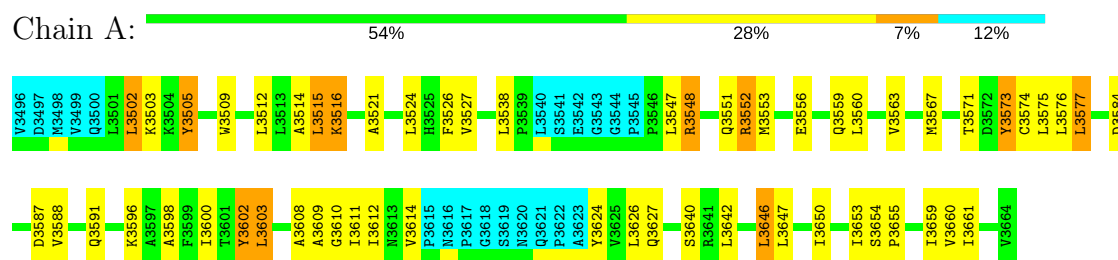


- Molecule 2: peptide from Silencing mediator of retinoic acid and thyroid hormone receptor

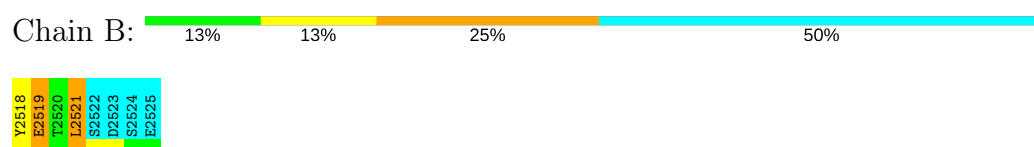


4.2.13 Score per residue for model 13

- Molecule 1: Msx2-interacting protein

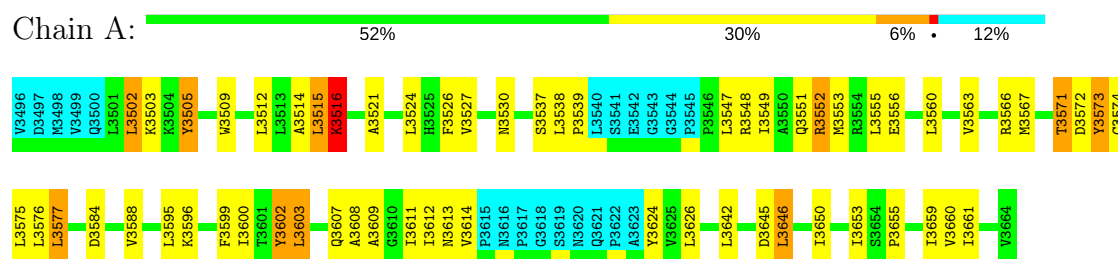


- Molecule 2: peptide from Silencing mediator of retinoic acid and thyroid hormone receptor

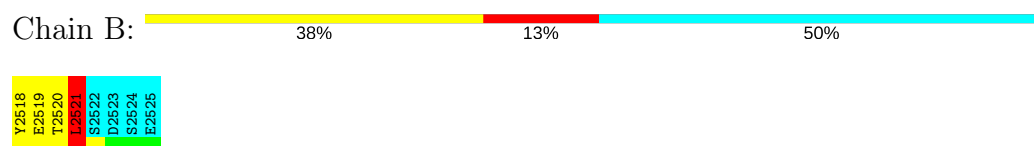


4.2.14 Score per residue for model 14

- Molecule 1: Msx2-interacting protein

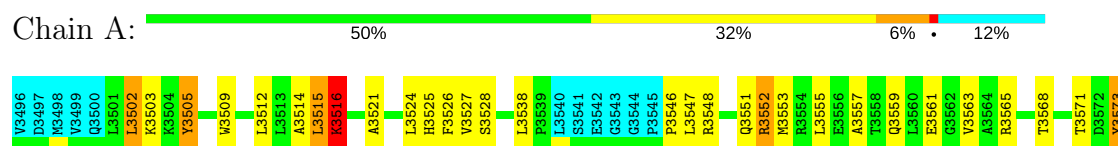


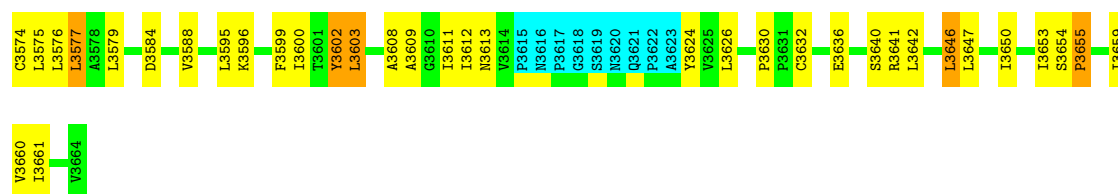
- Molecule 2: peptide from Silencing mediator of retinoic acid and thyroid hormone receptor



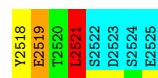
4.2.15 Score per residue for model 15

- Molecule 1: Msx2-interacting protein



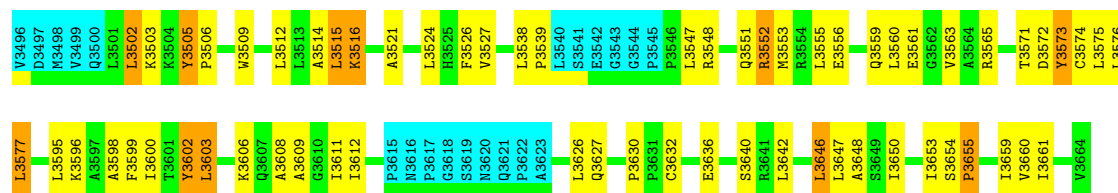


- Molecule 2: peptide from Silencing mediator of retinoic acid and thyroid hormone receptor

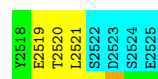


4.2.16 Score per residue for model 16

- Molecule 1: Msx2-interacting protein

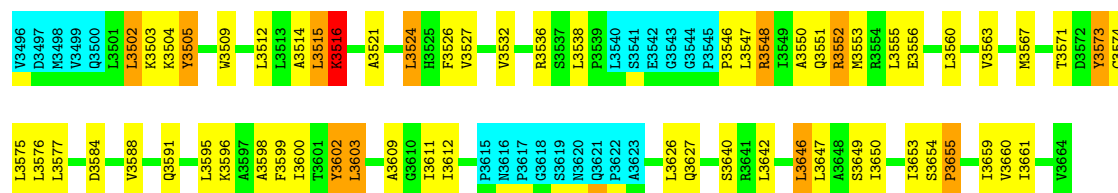


- Molecule 2: peptide from Silencing mediator of retinoic acid and thyroid hormone receptor

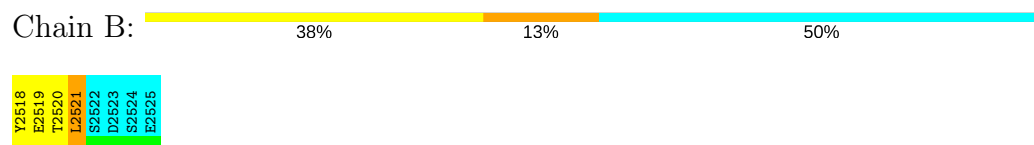


4.2.17 Score per residue for model 17

- Molecule 1: Msx2-interacting protein

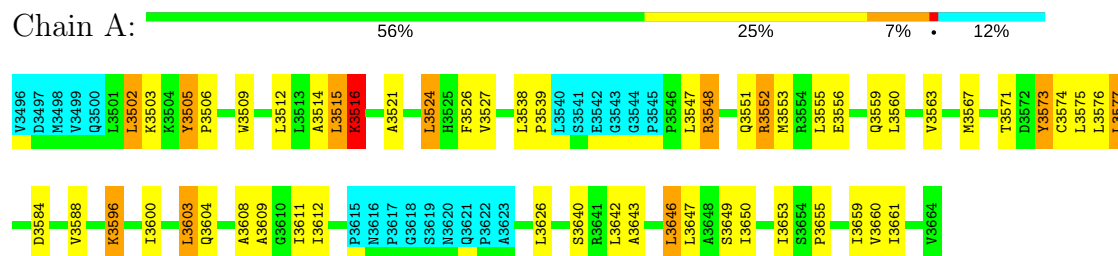


- Molecule 2: peptide from Silencing mediator of retinoic acid and thyroid hormone receptor

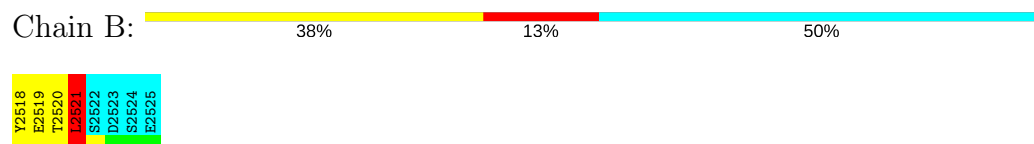


4.2.18 Score per residue for model 18

- Molecule 1: Msx2-interacting protein

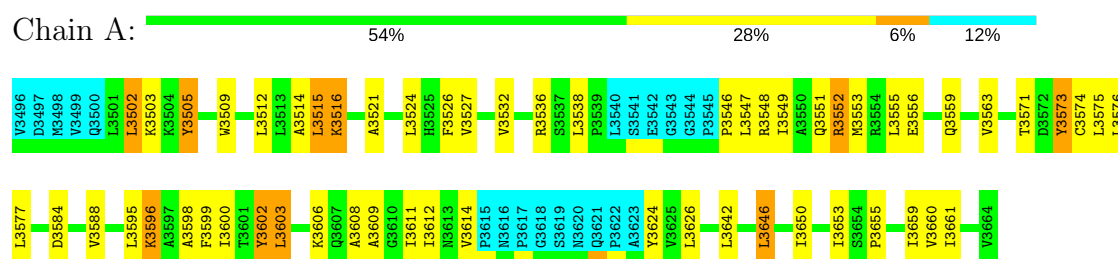


- Molecule 2: peptide from Silencing mediator of retinoic acid and thyroid hormone receptor

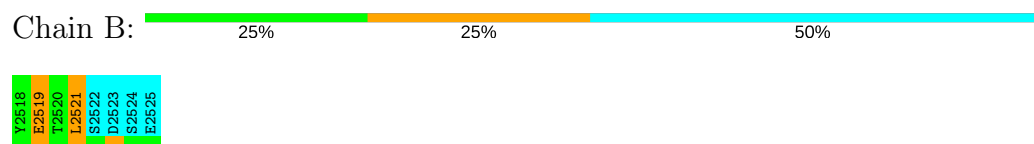


4.2.19 Score per residue for model 19

- Molecule 1: Msx2-interacting protein

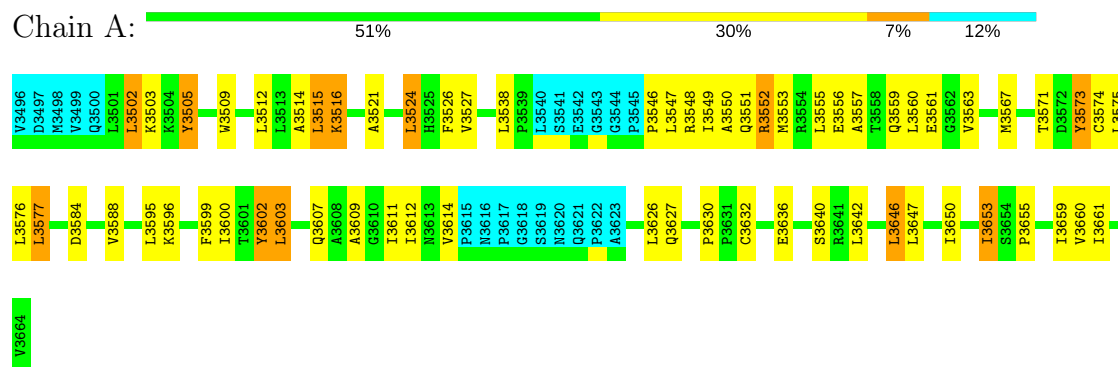


- Molecule 2: peptide from Silencing mediator of retinoic acid and thyroid hormone receptor

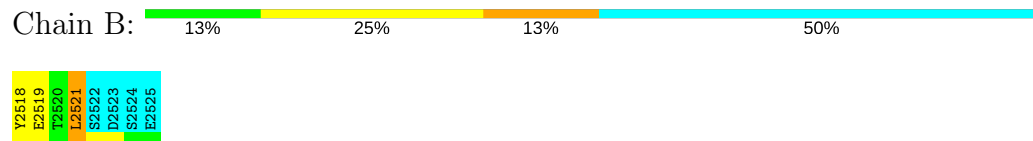


4.2.20 Score per residue for model 20

- Molecule 1: Msx2-interacting protein



- Molecule 2: peptide from Silencing mediator of retinoic acid and thyroid hormone receptor



5 Refinement protocol and experimental data overview

The models were refined using the following method: *simulated annealing*.

Of the 100 calculated structures, 20 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
CNS	refinement	

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)	2rt5_cs.str
Number of chemical shift lists	1
Total number of shifts	2023
Number of shifts mapped to atoms	2023
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	85%

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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SEP

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

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	0.1±0.2
All	All	0	1

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

All unique planar outliers are listed below.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	3552	ARG	Sidechain	1

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	1158	1208	1204	47±3
2	B	36	35	32	5±2
All	All	23880	24860	24720	961

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 20.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:3640:SER:HA	1:A:3647:LEU:HD22	0.87	1.46	15	6
1:A:3520:ALA:HB1	1:A:3591:GLN:HE22	0.78	1.39	4	1
2:B:2519:GLU:HG3	2:B:2520:THR:H	0.77	1.37	16	2
1:A:3596:LYS:HA	1:A:3600:ILE:CG1	0.73	2.13	2	20
1:A:3524:LEU:HD21	1:A:3659:ILE:HD12	0.73	1.59	6	20
1:A:3509:TRP:CD1	1:A:3524:LEU:HD12	0.70	2.20	16	1
1:A:3515:LEU:HD12	1:A:3516:LYS:CD	0.70	2.17	9	13
1:A:3552:ARG:HA	1:A:3609:ALA:O	0.69	1.87	18	20
1:A:3602:TYR:CE2	1:A:3603:LEU:HD22	0.69	2.22	10	16
1:A:3551:GLN:CB	1:A:3611:ILE:HB	0.69	2.17	4	20
1:A:3514:ALA:O	1:A:3548:ARG:HA	0.67	1.89	7	20
1:A:3559:GLN:HE21	1:A:3559:GLN:HA	0.67	1.49	6	1
1:A:3505:TYR:HB2	1:A:3526:PHE:O	0.65	1.91	1	20
2:B:2519:GLU:HG2	2:B:2520:THR:H	0.64	1.51	17	5
1:A:3575:LEU:HD22	1:A:3642:LEU:HD13	0.64	1.70	7	20
1:A:3509:TRP:CE3	1:A:3524:LEU:HD12	0.63	2.29	10	6
1:A:3650:ILE:HA	1:A:3653:ILE:HG22	0.63	1.69	10	19
1:A:3547:LEU:HB3	1:A:3612:ILE:HD13	0.62	1.72	3	20
1:A:3553:MET:HB3	1:A:3609:ALA:HB3	0.62	1.72	13	9
1:A:3552:ARG:HD3	2:B:2521:LEU:HB2	0.61	1.71	3	2
1:A:3596:LYS:HA	1:A:3600:ILE:HG12	0.61	1.72	14	10
1:A:3504:LYS:HD3	1:A:3505:TYR:CE2	0.61	2.30	12	1
1:A:3573:TYR:HD2	1:A:3660:VAL:HG13	0.60	1.56	1	20
1:A:3640:SER:HA	1:A:3647:LEU:HG	0.60	1.74	16	9
1:A:3556:GLU:O	1:A:3560:LEU:HG	0.60	1.95	1	15
1:A:3512:LEU:O	1:A:3546:PRO:HA	0.59	1.98	7	11
1:A:3504:LYS:N	1:A:3504:LYS:HD2	0.58	2.13	2	1
1:A:3509:TRP:HB2	1:A:3538:LEU:HD13	0.58	1.75	1	19
1:A:3613:ASN:HA	1:A:3624:TYR:O	0.57	1.99	4	6
1:A:3551:GLN:HB2	1:A:3611:ILE:HB	0.57	1.76	1	20
1:A:3577:LEU:HG	1:A:3646:LEU:HD11	0.57	1.76	2	15
1:A:3549:ILE:CG2	2:B:2521:LEU:HD23	0.57	2.30	3	1
1:A:3515:LEU:HD12	1:A:3516:LYS:HD3	0.56	1.77	20	12
1:A:3509:TRP:HE3	1:A:3524:LEU:HD12	0.56	1.61	1	8
1:A:3549:ILE:CG2	2:B:2521:LEU:HD22	0.56	2.31	19	2
1:A:3563:VAL:O	1:A:3567:MET:HG3	0.56	2.01	11	13
1:A:3584:ASP:O	1:A:3588:VAL:HG23	0.54	2.02	12	18
1:A:3537:SER:O	1:A:3614:VAL:HG11	0.54	2.01	4	2
1:A:3552:ARG:NH1	2:B:2521:LEU:HD23	0.54	2.16	12	3
1:A:3502:LEU:HD13	1:A:3503:LYS:N	0.54	2.16	15	20
1:A:3555:LEU:O	1:A:3555:LEU:HD12	0.54	2.03	2	4
1:A:3555:LEU:HD12	1:A:3555:LEU:O	0.54	2.02	7	14

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:3602:TYR:CD2	1:A:3603:LEU:HD22	0.54	2.38	12	10
1:A:3549:ILE:HG22	2:B:2521:LEU:HD22	0.53	1.80	19	1
1:A:3553:MET:HB2	2:B:2518:TYR:CD1	0.53	2.39	12	13
1:A:3509:TRP:CB	1:A:3538:LEU:HD13	0.53	2.32	2	20
1:A:3551:GLN:HG2	2:B:2519:GLU:O	0.53	2.04	7	13
1:A:3614:VAL:HG22	1:A:3624:TYR:HB2	0.52	1.81	6	1
1:A:3502:LEU:HB2	1:A:3506:PRO:HA	0.52	1.80	18	4
1:A:3557:ALA:O	1:A:3561:GLU:HG2	0.52	2.05	3	7
1:A:3515:LEU:CD1	2:B:2521:LEU:HD11	0.52	2.34	11	7
1:A:3576:LEU:HD11	1:A:3661:ILE:HD11	0.52	1.81	16	20
1:A:3603:LEU:HD12	1:A:3608:ALA:O	0.52	2.04	12	15
1:A:3549:ILE:CG2	2:B:2521:LEU:HD12	0.52	2.34	12	4
1:A:3551:GLN:HA	2:B:2520:THR:HA	0.51	1.83	17	2
1:A:3552:ARG:HH11	2:B:2521:LEU:HD12	0.51	1.63	17	1
1:A:3561:GLU:O	1:A:3565:ARG:HD3	0.51	2.05	1	2
1:A:3641:ARG:HA	1:A:3641:ARG:NE	0.51	2.21	3	1
1:A:3505:TYR:OH	1:A:3645:ASP:HB2	0.51	2.06	12	6
1:A:3570:GLU:O	1:A:3571:THR:HB	0.51	2.06	5	1
1:A:3552:ARG:HD2	2:B:2521:LEU:HD12	0.51	1.82	1	5
1:A:3653:ILE:O	1:A:3653:ILE:HG23	0.50	2.06	20	3
1:A:3512:LEU:HG	1:A:3521:ALA:HA	0.50	1.83	20	20
1:A:3549:ILE:HG22	2:B:2521:LEU:HD12	0.50	1.83	12	4
1:A:3505:TYR:CE1	1:A:3646:LEU:HB3	0.50	2.42	9	8
1:A:3565:ARG:O	1:A:3568:THR:HB	0.50	2.06	8	3
1:A:3553:MET:HB2	2:B:2518:TYR:CE1	0.50	2.42	12	6
1:A:3587:ASP:O	1:A:3591:GLN:HG2	0.50	2.07	8	2
1:A:3527:VAL:CG1	1:A:3575:LEU:HD23	0.50	2.37	1	20
1:A:3549:ILE:HG22	2:B:2521:LEU:HD23	0.50	1.82	3	1
1:A:3553:MET:HB2	2:B:2518:TYR:CD2	0.49	2.42	17	3
1:A:3515:LEU:HD12	1:A:3516:LYS:HD2	0.49	1.84	6	3
1:A:3598:ALA:O	1:A:3602:TYR:HB3	0.49	2.08	13	5
1:A:3503:LYS:HA	1:A:3503:LYS:HE2	0.49	1.84	13	1
1:A:3553:MET:O	1:A:3608:ALA:HA	0.49	2.06	2	7
1:A:3599:PHE:HA	1:A:3602:TYR:HD2	0.49	1.67	17	2
1:A:3515:LEU:HD12	2:B:2521:LEU:HD21	0.49	1.84	18	2
1:A:3603:LEU:HB3	1:A:3630:PRO:HB3	0.49	1.84	11	4
1:A:3553:MET:HG3	2:B:2518:TYR:CE1	0.49	2.42	5	3
1:A:3563:VAL:O	1:A:3566:ARG:HG2	0.48	2.07	8	3
1:A:3602:TYR:O	1:A:3606:LYS:HG2	0.48	2.09	19	2
1:A:3507:ILE:HG12	1:A:3525:HIS:CD2	0.48	2.44	3	1
1:A:3559:GLN:O	1:A:3563:VAL:HG23	0.48	2.08	11	15

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:3632:CYS:O	1:A:3636:GLU:HG2	0.48	2.08	20	5
1:A:3573:TYR:HE2	1:A:3575:LEU:HD13	0.48	1.68	5	3
1:A:3556:GLU:HB2	1:A:3559:GLN:HG2	0.48	1.85	1	3
1:A:3553:MET:HG3	2:B:2518:TYR:CE2	0.48	2.43	7	1
1:A:3555:LEU:HG	1:A:3607:GLN:O	0.47	2.09	2	3
1:A:3650:ILE:HA	1:A:3653:ILE:CG2	0.47	2.39	13	7
1:A:3595:LEU:HD12	1:A:3599:PHE:HB2	0.47	1.86	4	10
1:A:3552:ARG:HG2	2:B:2519:GLU:HB2	0.47	1.85	1	3
1:A:3521:ALA:H	1:A:3591:GLN:NE2	0.47	2.07	17	2
1:A:3644:PRO:HA	1:A:3647:LEU:HB3	0.47	1.87	8	1
1:A:3574:CYS:HB3	1:A:3661:ILE:HB	0.46	1.85	18	20
2:B:2519:GLU:CG	2:B:2520:THR:H	0.46	2.24	14	5
1:A:3626:LEU:HG	1:A:3661:ILE:HG12	0.46	1.87	15	20
1:A:3596:LYS:HA	1:A:3600:ILE:CB	0.46	2.40	2	4
1:A:3640:SER:CA	1:A:3647:LEU:HG	0.46	2.40	2	3
1:A:3646:LEU:HD12	1:A:3646:LEU:O	0.46	2.11	16	12
1:A:3503:LYS:HE3	1:A:3503:LYS:HA	0.46	1.86	5	2
1:A:3528:SER:OG	1:A:3642:LEU:HB3	0.46	2.11	10	2
1:A:3550:ALA:C	2:B:2521:LEU:H	0.46	2.14	4	3
1:A:3611:ILE:CD1	1:A:3627:GLN:HG2	0.46	2.40	20	4
1:A:3567:MET:HG2	1:A:3573:TYR:CE2	0.46	2.46	8	4
1:A:3646:LEU:O	1:A:3646:LEU:HD12	0.45	2.11	2	8
1:A:3602:TYR:OH	2:B:2521:LEU:HG	0.45	2.12	14	3
1:A:3532:VAL:O	1:A:3536:ARG:HG2	0.45	2.11	19	3
1:A:3567:MET:HA	1:A:3573:TYR:CE1	0.45	2.47	11	1
1:A:3596:LYS:HA	1:A:3600:ILE:HB	0.45	1.89	2	4
1:A:3629:PHE:HB2	1:A:3658:MET:HE3	0.45	1.89	8	1
1:A:3515:LEU:HD13	2:B:2521:LEU:HD21	0.45	1.88	3	2
1:A:3573:TYR:HA	1:A:3661:ILE:O	0.45	2.12	16	2
1:A:3504:LYS:HD2	1:A:3505:TYR:CD2	0.44	2.46	17	1
1:A:3530:ASN:OD1	1:A:3532:VAL:HB	0.44	2.12	12	1
1:A:3653:ILE:HG13	1:A:3653:ILE:O	0.44	2.12	7	9
1:A:3547:LEU:HB3	1:A:3612:ILE:CD1	0.44	2.42	6	9
1:A:3653:ILE:C	1:A:3655:PRO:HD2	0.44	2.32	4	1
1:A:3654:SER:N	1:A:3655:PRO:HD2	0.44	2.27	5	11
1:A:3515:LEU:CD1	2:B:2521:LEU:HD21	0.44	2.43	4	4
1:A:3565:ARG:O	1:A:3568:THR:HG22	0.43	2.13	15	2
1:A:3647:LEU:HA	1:A:3650:ILE:HG12	0.43	1.91	10	6
1:A:3548:ARG:H	1:A:3548:ARG:HD3	0.43	1.73	13	2
1:A:3530:ASN:HB2	1:A:3571:THR:HA	0.43	1.91	5	2
1:A:3579:LEU:HD21	1:A:3650:ILE:HG22	0.43	1.89	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:3596:LYS:O	1:A:3600:ILE:HB	0.43	2.14	4	4
1:A:3653:ILE:O	1:A:3653:ILE:HG13	0.43	2.14	15	3
1:A:3527:VAL:CG2	1:A:3577:LEU:HB2	0.43	2.44	10	4
1:A:3515:LEU:HD12	2:B:2521:LEU:HD11	0.43	1.91	11	2
1:A:3514:ALA:HB2	1:A:3519:THR:HG22	0.42	1.90	6	2
1:A:3550:ALA:O	1:A:3551:GLN:HG3	0.42	2.14	4	1
1:A:3503:LYS:O	1:A:3503:LYS:HD3	0.42	2.14	20	1
1:A:3647:LEU:HA	1:A:3650:ILE:CG1	0.42	2.45	2	7
1:A:3505:TYR:CZ	1:A:3643:ALA:HB1	0.42	2.50	18	1
1:A:3627:GLN:O	1:A:3659:ILE:HA	0.42	2.15	17	2
1:A:3551:GLN:HB3	1:A:3611:ILE:HB	0.42	1.88	4	1
1:A:3501:LEU:HD13	1:A:3646:LEU:HB2	0.42	1.92	1	4
1:A:3614:VAL:O	1:A:3624:TYR:HB2	0.42	2.15	13	1
1:A:3603:LEU:HD11	1:A:3610:GLY:N	0.42	2.30	12	2
1:A:3502:LEU:HA	1:A:3505:TYR:O	0.41	2.14	11	1
1:A:3576:LEU:CD1	1:A:3661:ILE:HD11	0.41	2.45	4	1
2:B:2519:GLU:HG3	2:B:2520:THR:N	0.41	2.24	4	1
1:A:3536:ARG:HD3	1:A:3624:TYR:OH	0.41	2.16	19	1
1:A:3537:SER:O	1:A:3614:VAL:HG21	0.41	2.14	6	1
1:A:3509:TRP:HB3	1:A:3524:LEU:HB2	0.41	1.92	16	1
1:A:3525:HIS:CE1	1:A:3579:LEU:HD12	0.41	2.51	15	1
1:A:3583:ARG:HG2	1:A:3587:ASP:HB2	0.41	1.92	2	1
1:A:3518:ASP:HB3	1:A:3598:ALA:HB1	0.41	1.93	4	1
1:A:3603:LEU:HG	1:A:3630:PRO:HD3	0.41	1.92	16	1
1:A:3524:LEU:HD22	1:A:3576:LEU:HD13	0.41	1.91	18	1
1:A:3514:ALA:HA	1:A:3518:ASP:O	0.41	2.16	8	1
1:A:3570:GLU:O	1:A:3571:THR:CB	0.40	2.69	5	1
1:A:3592:THR:O	1:A:3596:LYS:HG3	0.40	2.16	4	1
1:A:3628:ILE:HG12	1:A:3659:ILE:HG12	0.40	1.93	10	1
1:A:3561:GLU:O	1:A:3565:ARG:HG3	0.40	2.16	3	1
1:A:3559:GLN:HA	1:A:3559:GLN:OE1	0.40	2.15	4	1
1:A:3591:GLN:HA	1:A:3591:GLN:OE1	0.40	2.16	2	1
1:A:3603:LEU:HA	1:A:3603:LEU:HD13	0.40	1.80	9	1
1:A:3564:ALA:HA	1:A:3567:MET:HB2	0.40	1.94	4	1

6.3 Torsion angles ⓘ

6.3.1 Protein backbone ⓘ

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	148/169 (88%)	137±1 (92±1%)	9±1 (6±1%)	3±0 (2±0%)	14	57
2	B	3/8 (38%)	1±0 (32±7%)	1±1 (40±17%)	1±0 (28±16%)	0	1
All	All	3020/3540 (85%)	2756 (91%)	194 (6%)	70 (2%)	11	50

All 6 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	3571	THR	20
2	B	2521	LEU	16
1	A	3516	LYS	16
1	A	3655	PRO	16
2	B	2519	GLU	1
1	A	3539	PRO	1

6.3.2 Protein sidechains ⓘ

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	128/144 (89%)	116±2 (90±1%)	12±2 (10±1%)	14	59
2	B	4/6 (67%)	3±1 (79±16%)	1±1 (21±16%)	4	32
All	All	2640/3000 (88%)	2374 (90%)	266 (10%)	13	57

All 32 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	3552	ARG	20
1	A	3577	LEU	20
1	A	3505	TYR	20
1	A	3573	TYR	20
1	A	3603	LEU	20
1	A	3646	LEU	20
1	A	3502	LEU	20

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Mol	Chain	Res	Type	Models (Total)
1	A	3515	LEU	20
1	A	3602	TYR	16
1	A	3516	LYS	16
1	A	3524	LEU	11
2	B	2521	LEU	10
1	A	3548	ARG	8
1	A	3572	ASP	7
2	B	2519	GLU	7
1	A	3596	LYS	6
1	A	3641	ARG	4
1	A	3653	ILE	3
1	A	3604	GLN	3
1	A	3503	LYS	2
1	A	3510	GLN	2
1	A	3585	GLN	1
1	A	3636	GLU	1
1	A	3652	ASN	1
1	A	3565	ARG	1
1	A	3586	GLU	1
1	A	3504	LYS	1
1	A	3554	ARG	1
1	A	3559	GLN	1
1	A	3558	THR	1
1	A	3613	ASN	1
1	A	3583	ARG	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds for which Mogul statistics could be retrieved, the number of bonds that are observed in the model and the number of bonds that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length is the number of standard deviations the observed value is removed from the expected value. A bond length with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
2	SEP	B	2522	2	9,9,10	1.09±0.07	0±0 (0±0%)
2	SEP	B	2524	2	9,9,10	1.13±0.05	0±0 (0±0%)

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of angles that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond angle is the number of standard deviations the observed value is removed from the expected value. A bond angle with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
2	SEP	B	2522	2	9,12,14	1.29±0.07	0±0 (0±0%)
2	SEP	B	2524	2	9,12,14	1.71±0.06	0±0 (0±0%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SEP	B	2522	2	-	0±0,5,8,10	0±0,0,0,0
2	SEP	B	2524	2	-	0±0,5,8,10	0±0,0,0,0

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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

The completeness of assignment taking into account all chemical shift lists is 85% for the well-defined parts and 84% for the entire structure.

7.1 Chemical shift list 1

File name: 2rt5_cs.str

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping

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	2023
Number of shifts mapped to atoms	2023
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

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	169	-0.19 ± 0.13	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	163	0.01 ± 0.12	None needed (< 0.5 ppm)
$^{13}\text{C}'$	163	0.22 ± 0.11	None needed (< 0.5 ppm)
^{15}N	157	-0.93 ± 0.48	None needed (imprecise)

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 85%, i.e. 1621 atoms were assigned a chemical shift out of a possible 1897. 33 out of 36 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	729/749 (97%)	291/298 (98%)	296/306 (97%)	142/145 (98%)
Sidechain	836/1028 (81%)	493/599 (82%)	337/386 (87%)	6/43 (14%)

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	Total	^1H	^{13}C	^{15}N
Aromatic	56/120 (47%)	28/62 (45%)	28/49 (57%)	0/9 (0%)
Overall	1621/1897 (85%)	812/959 (85%)	661/741 (89%)	148/197 (75%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 84%, i.e. 1796 atoms were assigned a chemical shift out of a possible 2128. 35 out of 39 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	814/851 (96%)	325/338 (96%)	332/350 (95%)	157/163 (96%)
Sidechain	926/1157 (80%)	548/676 (81%)	372/434 (86%)	6/47 (13%)
Aromatic	56/120 (47%)	28/62 (45%)	28/49 (57%)	0/9 (0%)
Overall	1796/2128 (84%)	901/1076 (84%)	732/833 (88%)	163/219 (74%)

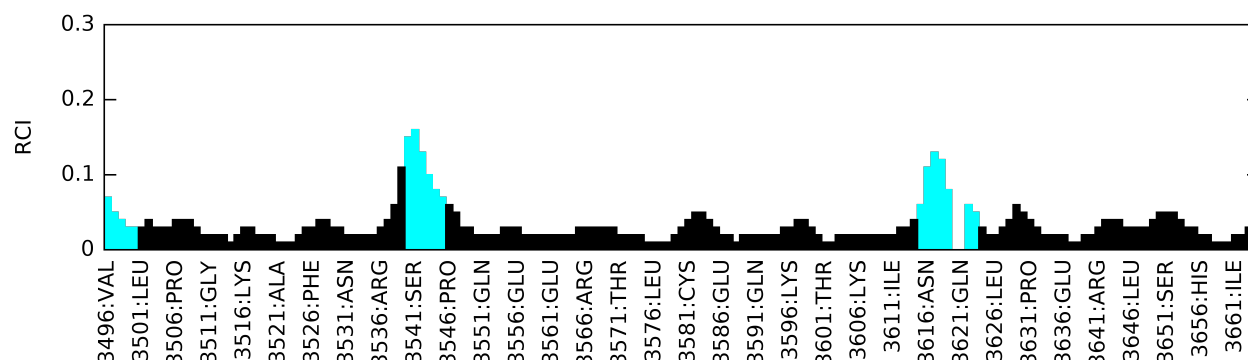
7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

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

The images below report *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:



Random coil index (RCI) for chain B:

