



Full wwPDB NMR Structure Validation Report ⓘ

Apr 26, 2016 – 06:28 PM BST

PDB ID : 1XC5
Title : Solution Structure of the SMRT Deacetylase Activation Domain
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Deposited on : 2004-09-01

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
<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 : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : rb-20027457
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027457

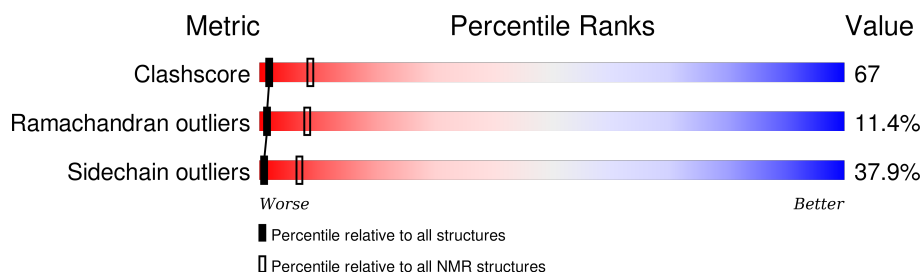
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 49%.

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	114402	11133
Ramachandran outliers	111179	9975
Sidechain outliers	111093	9958

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	71	

2 Ensemble composition and analysis

This entry contains 28 models. Model 12 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:421-A:471 (51)	0.26	12

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 6 clusters. No single-model clusters were found.

Cluster number	Models
1	3, 4, 7, 8, 18, 22, 23, 24, 28
2	10, 14, 17, 19, 21, 26
3	5, 9, 11, 15, 20
4	6, 12, 16
5	1, 2, 13
6	25, 27

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1158 atoms, of which 577 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Nuclear receptor corepressor 2.

Mol	Chain	Residues	Atoms						Trace
1	A	68	Total	C	H	N	O	S	0
			1158	373	577	97	105	6	

There are 2 discrepancies between the modelled and reference sequences:

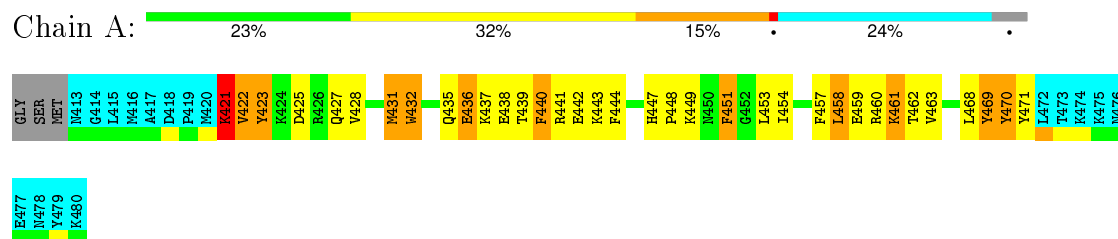
Chain	Residue	Modelled	Actual	Comment	Reference
A	410	GLY	-	CLONING ARTIFACT	UNP Q9Y618
A	411	SER	-	CLONING ARTIFACT	UNP Q9Y618

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: Nuclear receptor corepressor 2

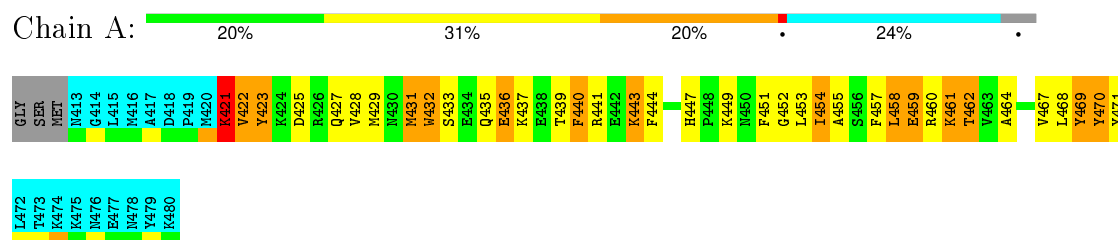


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

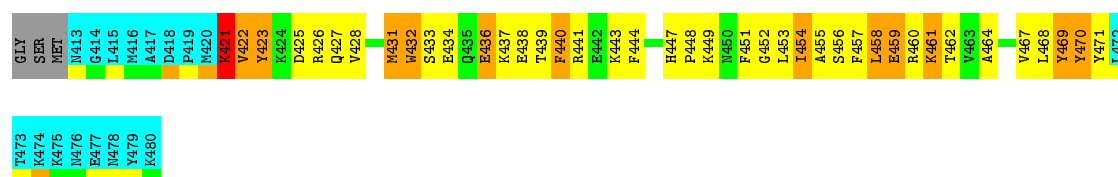
- Molecule 1: Nuclear receptor corepressor 2



4.2.2 Score per residue for model 2

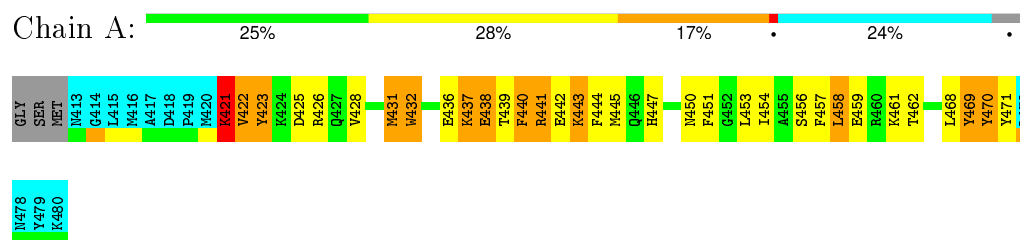
- Molecule 1: Nuclear receptor corepressor 2





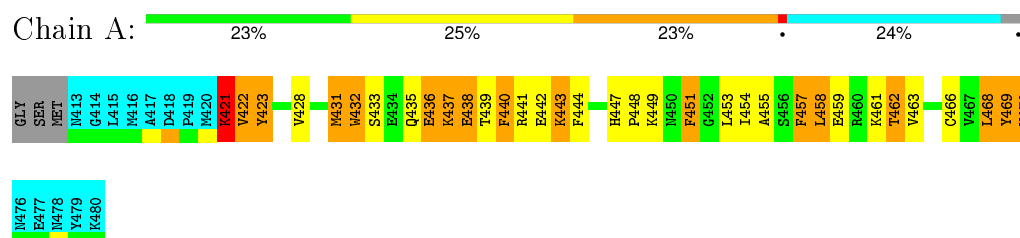
4.2.3 Score per residue for model 3

- Molecule 1: Nuclear receptor corepressor 2



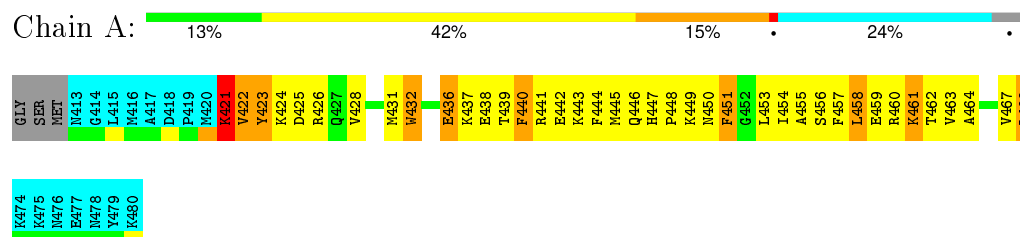
4.2.4 Score per residue for model 4

- Molecule 1: Nuclear receptor corepressor 2



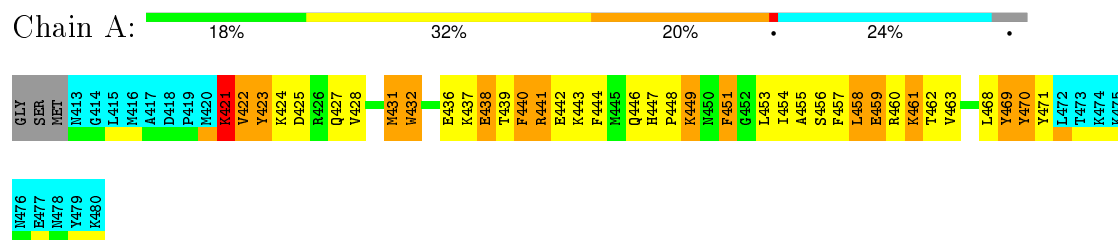
4.2.5 Score per residue for model 5

- Molecule 1: Nuclear receptor corepressor 2



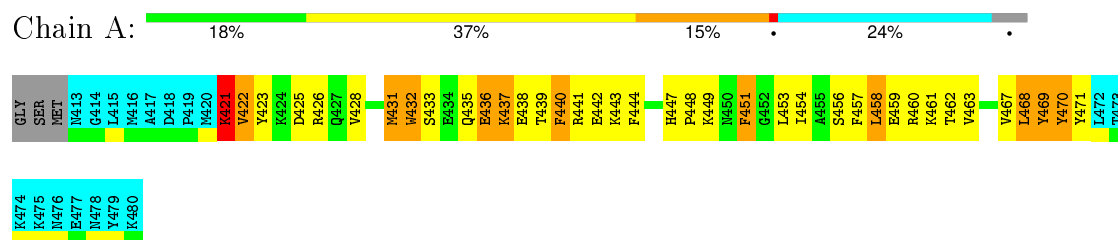
4.2.6 Score per residue for model 6

- Molecule 1: Nuclear receptor corepressor 2



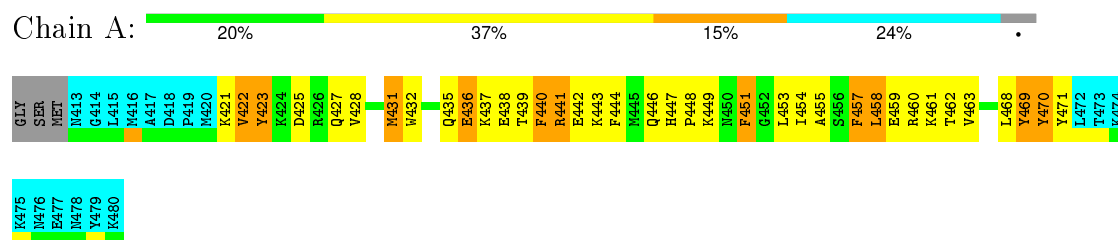
4.2.7 Score per residue for model 7

- Molecule 1: Nuclear receptor corepressor 2



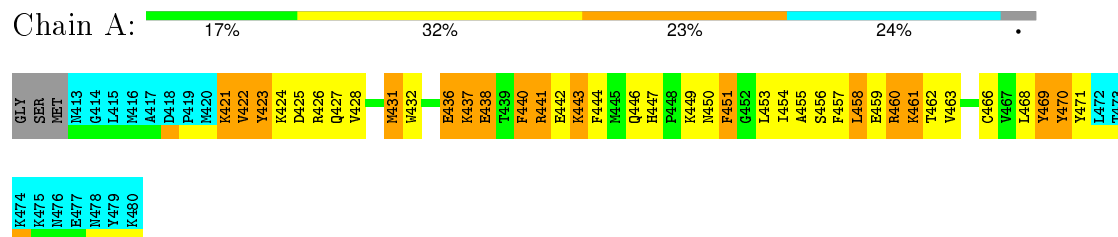
4.2.8 Score per residue for model 8

- Molecule 1: Nuclear receptor corepressor 2



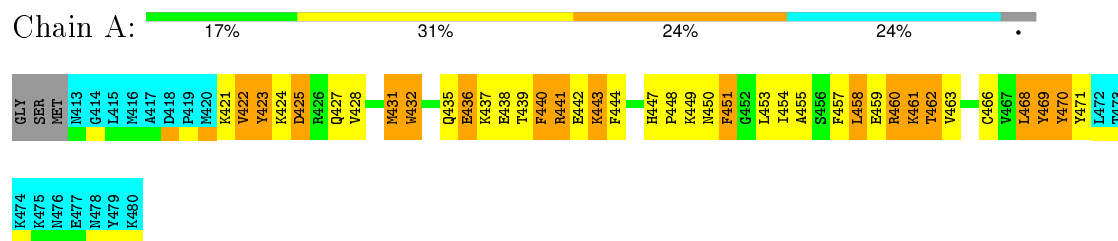
4.2.9 Score per residue for model 9

- Molecule 1: Nuclear receptor corepressor 2



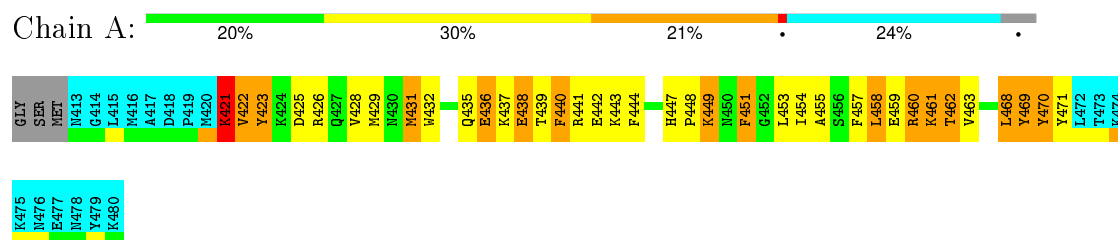
4.2.10 Score per residue for model 10

- Molecule 1: Nuclear receptor corepressor 2



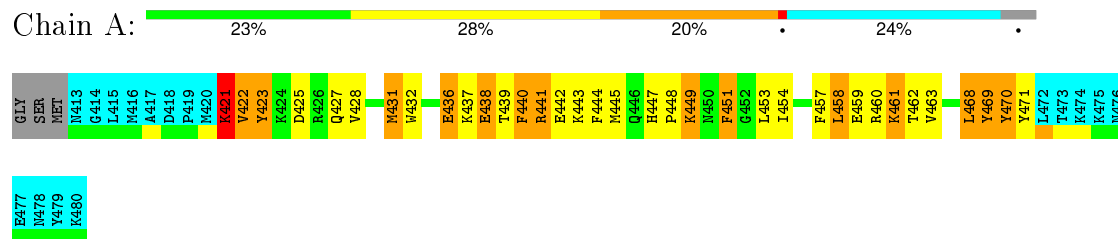
4.2.11 Score per residue for model 11

- Molecule 1: Nuclear receptor corepressor 2



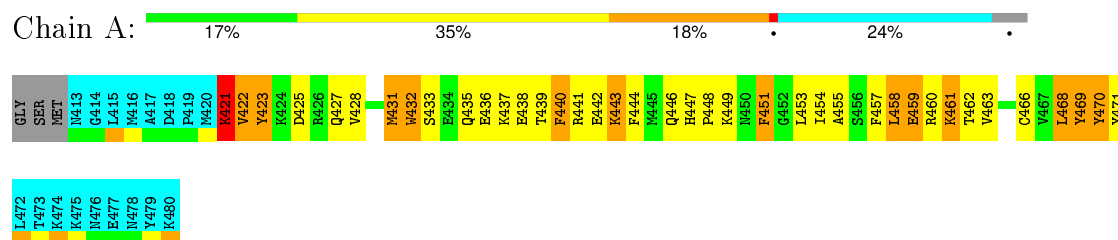
4.2.12 Score per residue for model 12 (medoid)

- Molecule 1: Nuclear receptor corepressor 2



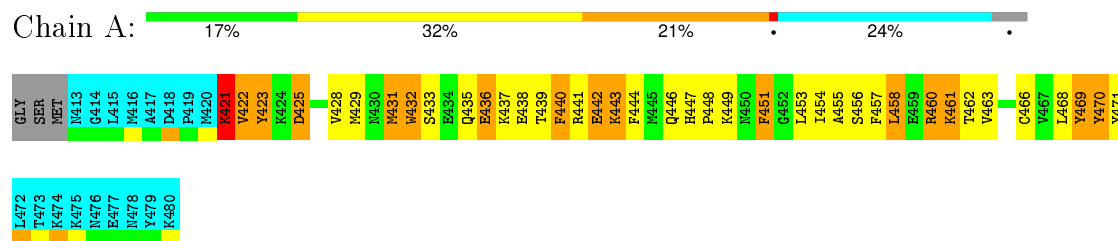
4.2.13 Score per residue for model 13

- Molecule 1: Nuclear receptor corepressor 2



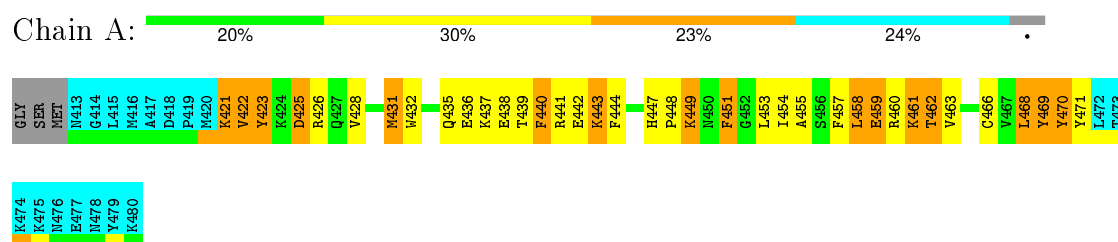
4.2.14 Score per residue for model 14

- Molecule 1: Nuclear receptor corepressor 2



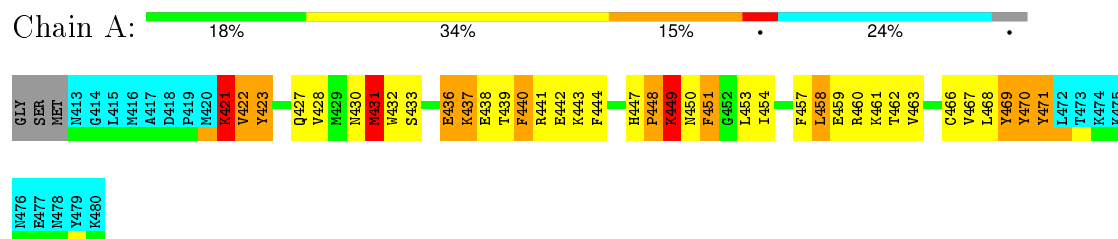
4.2.15 Score per residue for model 15

- Molecule 1: Nuclear receptor corepressor 2



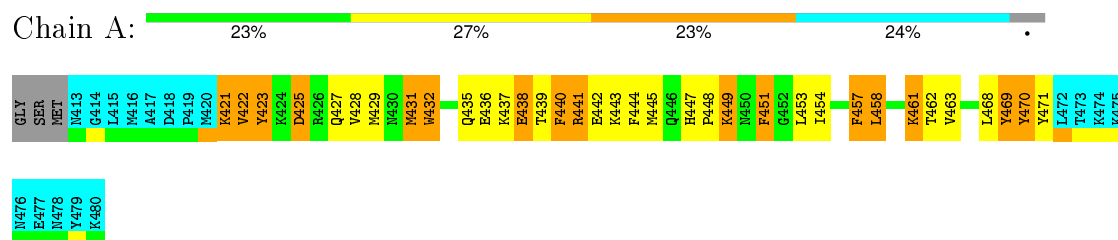
4.2.16 Score per residue for model 16

- Molecule 1: Nuclear receptor corepressor 2



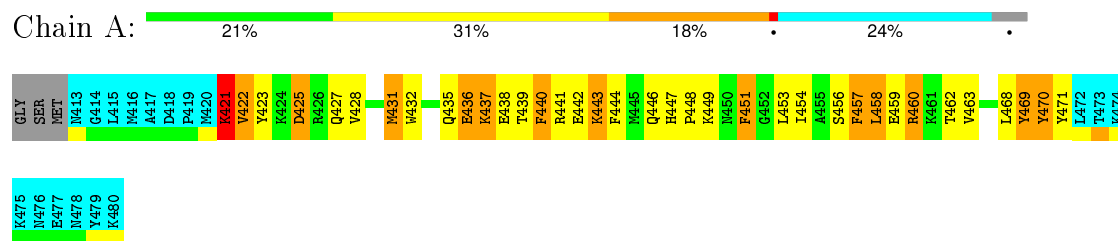
4.2.17 Score per residue for model 17

- Molecule 1: Nuclear receptor corepressor 2



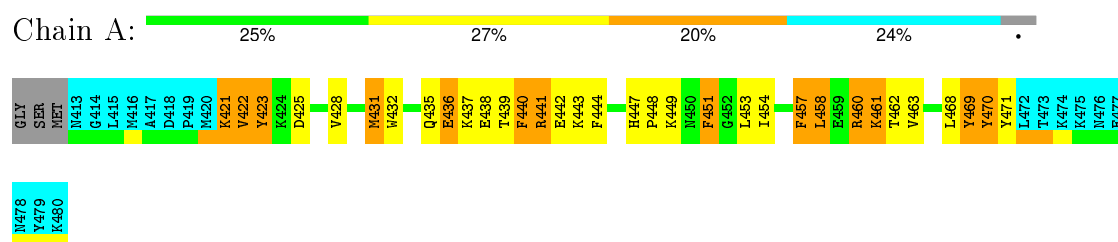
4.2.18 Score per residue for model 18

- Molecule 1: Nuclear receptor corepressor 2



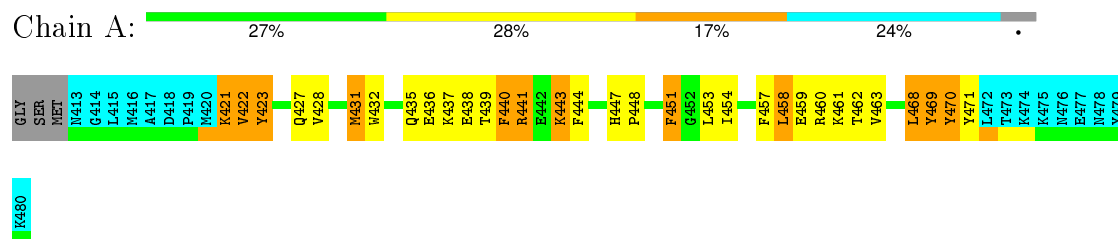
4.2.19 Score per residue for model 19

- Molecule 1: Nuclear receptor corepressor 2



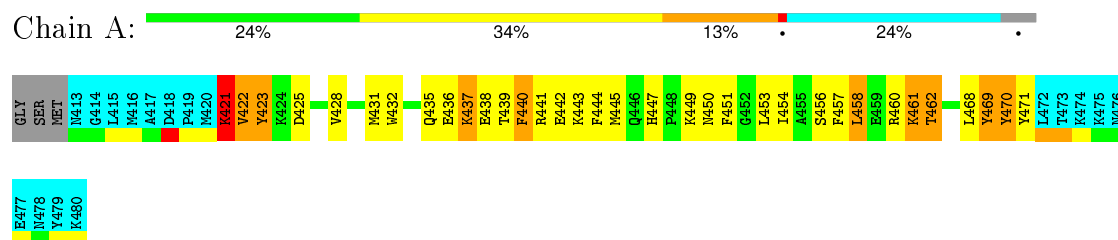
4.2.20 Score per residue for model 20

- Molecule 1: Nuclear receptor corepressor 2



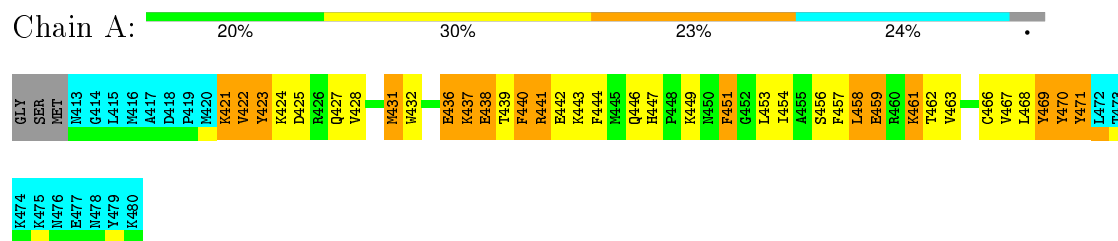
4.2.21 Score per residue for model 21

- Molecule 1: Nuclear receptor corepressor 2



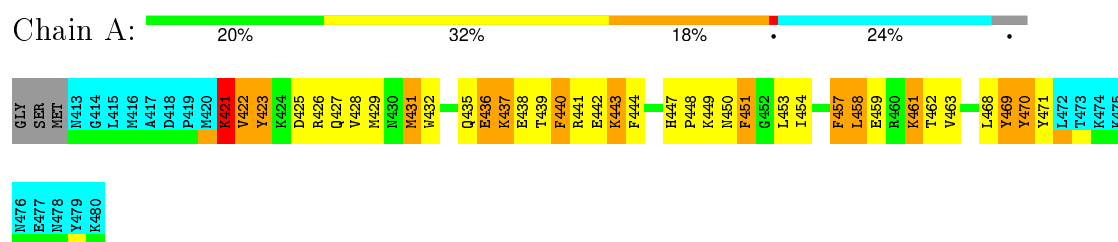
4.2.22 Score per residue for model 22

- Molecule 1: Nuclear receptor corepressor 2



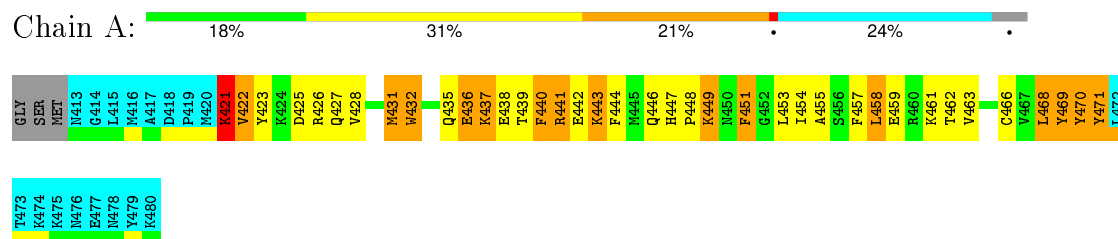
4.2.23 Score per residue for model 23

- Molecule 1: Nuclear receptor corepressor 2



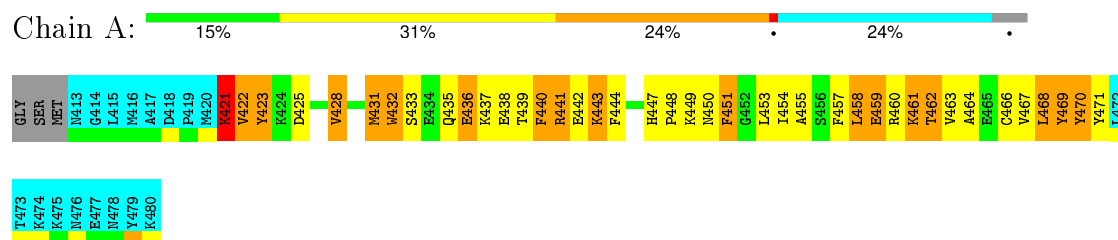
4.2.24 Score per residue for model 24

- Molecule 1: Nuclear receptor corepressor 2



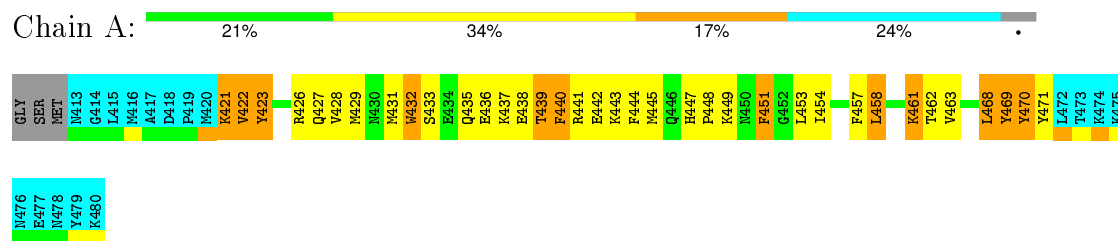
4.2.25 Score per residue for model 25

- Molecule 1: Nuclear receptor corepressor 2



4.2.26 Score per residue for model 26

- Molecule 1: Nuclear receptor corepressor 2



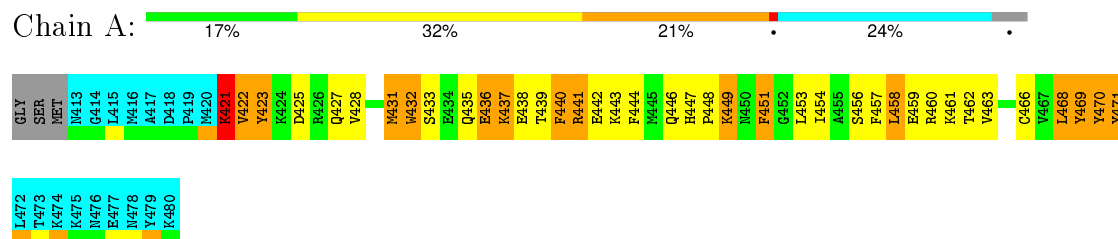
4.2.27 Score per residue for model 27

- Molecule 1: Nuclear receptor corepressor 2



4.2.28 Score per residue for model 28

- Molecule 1: Nuclear receptor corepressor 2



5 Refinement protocol and experimental data overview

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

Of the 50 calculated structures, 28 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	structure solution	1.1
CNS	refinement	1.1

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)	BMRB entry 6286
Number of chemical shift lists	1
Total number of shifts	476
Number of shifts mapped to atoms	476
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	49%

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

6 Model quality ⓘ

6.1 Standard geometry ⓘ

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 ⓘ

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	445	439	438	59±5
All	All	12460	12292	12264	1649

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 67.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:447:HIS:CE1	1:A:453:LEU:HD13	0.87	2.05	23	28
1:A:428:VAL:HG11	1:A:440:PHE:CZ	0.85	2.07	1	6
1:A:428:VAL:HG13	1:A:432:TRP:HA	0.83	1.50	27	28
1:A:447:HIS:CD2	1:A:453:LEU:HD22	0.82	2.10	1	28
1:A:451:PHE:O	1:A:463:VAL:HG22	0.80	1.77	14	15
1:A:439:THR:HG22	1:A:457:PHE:CZ	0.79	2.12	4	18
1:A:440:PHE:CD1	1:A:458:LEU:HD23	0.79	2.12	11	25
1:A:437:LYS:HA	1:A:440:PHE:CD2	0.78	2.14	26	28
1:A:432:TRP:CE2	1:A:469:TYR:HB3	0.78	2.14	23	26
1:A:428:VAL:HG13	1:A:432:TRP:CA	0.77	2.09	27	28
1:A:428:VAL:HG21	1:A:436:GLU:HG2	0.77	1.56	2	8
1:A:451:PHE:CB	1:A:463:VAL:HG13	0.75	2.11	23	6
1:A:428:VAL:HG21	1:A:436:GLU:HG3	0.75	1.57	25	1
1:A:421:LYS:HG2	1:A:439:THR:HG21	0.75	1.59	12	11

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:444:PHE:N	1:A:454:ILE:HD11	0.72	1.98	10	26
1:A:451:PHE:HB3	1:A:463:VAL:HG13	0.72	1.60	28	20
1:A:421:LYS:HG3	1:A:439:THR:HG21	0.71	1.59	24	7
1:A:432:TRP:CD2	1:A:469:TYR:HB2	0.70	2.21	14	27
1:A:437:LYS:HA	1:A:440:PHE:CE2	0.69	2.22	27	28
1:A:458:LEU:HD13	1:A:461:LYS:HB2	0.69	1.65	1	7
1:A:421:LYS:CE	1:A:439:THR:HG21	0.67	2.20	2	2
1:A:422:VAL:HG22	1:A:460:ARG:HG3	0.67	1.67	18	1
1:A:441:ARG:HA	1:A:469:TYR:OH	0.66	1.90	2	26
1:A:428:VAL:HG21	1:A:436:GLU:CG	0.66	2.20	5	5
1:A:422:VAL:HG12	1:A:423:TYR:CE1	0.65	2.27	10	1
1:A:423:TYR:CD1	1:A:423:TYR:N	0.65	2.64	1	19
1:A:428:VAL:HG13	1:A:432:TRP:CB	0.64	2.22	27	6
1:A:469:TYR:CD1	1:A:469:TYR:C	0.63	2.72	14	14
1:A:421:LYS:HE2	1:A:439:THR:HG21	0.63	1.71	26	2
1:A:428:VAL:HG22	1:A:432:TRP:HA	0.62	1.69	25	2
1:A:454:ILE:HG22	1:A:458:LEU:HD11	0.62	1.71	19	8
1:A:458:LEU:HD13	1:A:461:LYS:HG2	0.62	1.70	27	6
1:A:432:TRP:HE3	1:A:440:PHE:CE2	0.62	2.13	25	23
1:A:468:LEU:HA	1:A:471:TYR:CZ	0.62	2.29	16	4
1:A:469:TYR:C	1:A:469:TYR:CD1	0.62	2.73	15	14
1:A:464:ALA:O	1:A:467:VAL:HG12	0.61	1.95	5	4
1:A:428:VAL:HG21	1:A:436:GLU:CB	0.61	2.25	13	1
1:A:454:ILE:O	1:A:458:LEU:HD11	0.61	1.95	25	10
1:A:440:PHE:CD1	1:A:458:LEU:CD2	0.60	2.85	20	24
1:A:451:PHE:O	1:A:463:VAL:HG13	0.60	1.96	6	1
1:A:439:THR:HG22	1:A:440:PHE:CD1	0.60	2.31	26	1
1:A:423:TYR:N	1:A:423:TYR:CD1	0.60	2.64	17	9
1:A:422:VAL:HG22	1:A:460:ARG:CG	0.60	2.27	18	1
1:A:432:TRP:CE2	1:A:469:TYR:CB	0.59	2.85	9	27
1:A:422:VAL:HG23	1:A:458:LEU:C	0.59	2.18	11	2
1:A:428:VAL:HG22	1:A:436:GLU:OE1	0.59	1.97	26	1
1:A:454:ILE:HA	1:A:457:PHE:CD2	0.59	2.33	8	25
1:A:455:ALA:HA	1:A:458:LEU:HD11	0.59	1.74	1	7
1:A:421:LYS:CG	1:A:439:THR:HG21	0.59	2.27	1	5
1:A:443:LYS:C	1:A:454:ILE:HD11	0.59	2.19	27	26
1:A:432:TRP:CD2	1:A:469:TYR:CB	0.58	2.86	3	25
1:A:440:PHE:HD1	1:A:458:LEU:HD23	0.58	1.58	10	23
1:A:428:VAL:HG22	1:A:436:GLU:CD	0.58	2.18	26	1
1:A:432:TRP:CZ2	1:A:469:TYR:HB3	0.58	2.32	3	24
1:A:454:ILE:O	1:A:458:LEU:CD1	0.58	2.51	13	28

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:428:VAL:CG1	1:A:432:TRP:HA	0.58	2.25	27	2
1:A:458:LEU:HD13	1:A:461:LYS:CG	0.58	2.29	25	10
1:A:447:HIS:NE2	1:A:453:LEU:HD13	0.58	2.12	23	15
1:A:438:GLU:O	1:A:442:GLU:HB2	0.57	1.99	10	7
1:A:437:LYS:O	1:A:441:ARG:CB	0.57	2.52	6	28
1:A:458:LEU:HD13	1:A:461:LYS:CB	0.57	2.29	2	7
1:A:422:VAL:HG22	1:A:460:ARG:HG2	0.57	1.76	8	1
1:A:444:PHE:HB2	1:A:454:ILE:HD12	0.57	1.76	2	2
1:A:428:VAL:HG12	1:A:432:TRP:CD2	0.57	2.35	4	21
1:A:451:PHE:CE2	1:A:467:VAL:HG22	0.57	2.35	22	1
1:A:447:HIS:CE1	1:A:453:LEU:CD1	0.56	2.89	3	26
1:A:461:LYS:O	1:A:462:THR:HG23	0.56	2.00	25	1
1:A:421:LYS:CD	1:A:439:THR:HG21	0.56	2.30	2	1
1:A:439:THR:HG23	1:A:443:LYS:HE2	0.56	1.78	25	1
1:A:421:LYS:O	1:A:422:VAL:HB	0.55	2.01	10	10
1:A:436:GLU:C	1:A:440:PHE:CZ	0.55	2.79	16	28
1:A:436:GLU:C	1:A:440:PHE:CE2	0.55	2.79	1	25
1:A:458:LEU:HD22	1:A:461:LYS:HG3	0.55	1.77	2	4
1:A:453:LEU:HD23	1:A:454:ILE:N	0.55	2.16	25	14
1:A:455:ALA:HB1	1:A:462:THR:HA	0.55	1.78	10	1
1:A:432:TRP:CE2	1:A:469:TYR:HB2	0.55	2.36	1	3
1:A:428:VAL:CG1	1:A:432:TRP:CE3	0.54	2.89	13	28
1:A:455:ALA:HB1	1:A:462:THR:C	0.54	2.22	25	4
1:A:428:VAL:HG13	1:A:432:TRP:CG	0.54	2.38	27	5
1:A:428:VAL:HG21	1:A:436:GLU:HB3	0.54	1.77	13	1
1:A:443:LYS:O	1:A:447:HIS:CD2	0.54	2.61	22	26
1:A:454:ILE:HG23	1:A:458:LEU:HD21	0.54	1.78	26	9
1:A:436:GLU:HB3	1:A:440:PHE:HZ	0.53	1.63	15	14
1:A:421:LYS:O	1:A:422:VAL:CB	0.53	2.55	10	1
1:A:432:TRP:HE3	1:A:440:PHE:CD2	0.53	2.22	1	7
1:A:458:LEU:O	1:A:460:ARG:N	0.53	2.42	13	9
1:A:440:PHE:HB3	1:A:458:LEU:HD21	0.53	1.80	23	12
1:A:468:LEU:HA	1:A:471:TYR:CE2	0.53	2.39	8	3
1:A:444:PHE:CA	1:A:454:ILE:HD11	0.53	2.34	23	19
1:A:437:LYS:O	1:A:441:ARG:HB2	0.52	2.04	25	1
1:A:437:LYS:CA	1:A:440:PHE:CE2	0.52	2.93	26	22
1:A:423:TYR:HD1	1:A:423:TYR:H	0.52	1.48	25	6
1:A:425:ASP:OD1	1:A:428:VAL:HG21	0.52	2.04	19	2
1:A:447:HIS:NE2	1:A:453:LEU:HD22	0.52	2.20	23	11
1:A:470:TYR:CD1	1:A:470:TYR:C	0.52	2.83	8	2
1:A:461:LYS:HD2	1:A:461:LYS:N	0.52	2.20	27	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:454:ILE:CG2	1:A:458:LEU:HD21	0.51	2.35	26	3
1:A:447:HIS:CD2	1:A:453:LEU:CD2	0.51	2.93	3	4
1:A:439:THR:HG23	1:A:457:PHE:CZ	0.51	2.40	26	1
1:A:422:VAL:CG1	1:A:423:TYR:CE1	0.50	2.93	10	1
1:A:432:TRP:CD2	1:A:469:TYR:HB3	0.50	2.42	23	1
1:A:422:VAL:CG1	1:A:423:TYR:N	0.50	2.75	17	27
1:A:468:LEU:HD13	1:A:471:TYR:CE2	0.50	2.42	10	1
1:A:422:VAL:O	1:A:425:ASP:N	0.50	2.45	21	10
1:A:422:VAL:HG23	1:A:458:LEU:CA	0.50	2.37	11	2
1:A:436:GLU:HB3	1:A:440:PHE:CZ	0.50	2.42	15	21
1:A:453:LEU:HD23	1:A:453:LEU:C	0.49	2.27	1	2
1:A:423:TYR:H	1:A:423:TYR:HD1	0.49	1.51	2	5
1:A:425:ASP:CB	1:A:436:GLU:HG2	0.49	2.38	27	1
1:A:428:VAL:HG21	1:A:436:GLU:OE1	0.49	2.08	15	1
1:A:470:TYR:CD1	1:A:471:TYR:N	0.48	2.81	26	25
1:A:467:VAL:HG13	1:A:470:TYR:CD2	0.48	2.43	7	1
1:A:432:TRP:CE3	1:A:440:PHE:CE2	0.48	3.00	27	2
1:A:439:THR:HG22	1:A:457:PHE:HZ	0.48	1.64	4	1
1:A:447:HIS:O	1:A:449:LYS:N	0.48	2.46	23	2
1:A:422:VAL:HG22	1:A:460:ARG:HD3	0.48	1.85	14	1
1:A:437:LYS:N	1:A:440:PHE:CE2	0.48	2.81	1	4
1:A:451:PHE:HB3	1:A:463:VAL:HG22	0.48	1.85	18	2
1:A:421:LYS:CB	1:A:439:THR:HG21	0.48	2.39	11	1
1:A:447:HIS:ND1	1:A:453:LEU:HD13	0.48	2.24	3	3
1:A:457:PHE:CD1	1:A:457:PHE:C	0.48	2.86	13	13
1:A:425:ASP:CB	1:A:436:GLU:HG3	0.48	2.39	25	1
1:A:455:ALA:HB3	1:A:463:VAL:HG22	0.48	1.85	13	3
1:A:428:VAL:CG1	1:A:432:TRP:CD2	0.47	2.97	22	25
1:A:428:VAL:HG12	1:A:432:TRP:CE3	0.47	2.44	7	10
1:A:451:PHE:O	1:A:455:ALA:HB3	0.47	2.09	8	2
1:A:451:PHE:CE1	1:A:466:CYS:CB	0.47	2.96	28	1
1:A:438:GLU:O	1:A:442:GLU:CB	0.47	2.62	25	18
1:A:453:LEU:C	1:A:453:LEU:HD23	0.47	2.29	2	13
1:A:432:TRP:N	1:A:432:TRP:CD1	0.47	2.82	27	16
1:A:421:LYS:HE3	1:A:439:THR:HG21	0.47	1.86	2	1
1:A:451:PHE:CE1	1:A:466:CYS:HB3	0.47	2.45	22	4
1:A:440:PHE:HD2	1:A:469:TYR:CD2	0.47	2.28	27	1
1:A:469:TYR:CD1	1:A:470:TYR:N	0.47	2.83	27	2
1:A:447:HIS:CG	1:A:453:LEU:HD13	0.47	2.44	3	3
1:A:428:VAL:HG11	1:A:440:PHE:CE2	0.47	2.44	3	1
1:A:451:PHE:HE2	1:A:467:VAL:HG22	0.47	1.70	22	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:440:PHE:CD1	1:A:440:PHE:N	0.46	2.83	3	4
1:A:428:VAL:CG2	1:A:432:TRP:HA	0.46	2.40	25	1
1:A:440:PHE:HB2	1:A:469:TYR:CE2	0.46	2.45	22	13
1:A:457:PHE:CD1	1:A:458:LEU:N	0.46	2.83	10	1
1:A:432:TRP:CG	1:A:469:TYR:HB2	0.46	2.45	26	16
1:A:439:THR:CG2	1:A:440:PHE:CD1	0.46	2.98	26	1
1:A:428:VAL:CG2	1:A:436:GLU:HG2	0.46	2.41	9	5
1:A:421:LYS:HB3	1:A:457:PHE:CD1	0.46	2.44	24	3
1:A:468:LEU:HD12	1:A:471:TYR:OH	0.46	2.11	16	2
1:A:421:LYS:HD3	1:A:439:THR:HG21	0.46	1.86	10	1
1:A:422:VAL:HG22	1:A:422:VAL:O	0.46	2.11	10	1
1:A:432:TRP:CD1	1:A:432:TRP:N	0.46	2.84	25	10
1:A:436:GLU:O	1:A:440:PHE:CZ	0.46	2.69	20	24
1:A:432:TRP:CE3	1:A:469:TYR:HB2	0.45	2.45	1	1
1:A:425:ASP:HA	1:A:428:VAL:HG23	0.45	1.88	12	5
1:A:457:PHE:C	1:A:457:PHE:CD1	0.45	2.89	25	12
1:A:421:LYS:HG2	1:A:439:THR:CG2	0.45	2.41	1	2
1:A:439:THR:HG23	1:A:457:PHE:CE1	0.45	2.46	26	1
1:A:437:LYS:HG3	1:A:469:TYR:CD2	0.45	2.47	25	1
1:A:454:ILE:HA	1:A:457:PHE:CE2	0.45	2.46	24	10
1:A:458:LEU:HD13	1:A:461:LYS:HG3	0.45	1.87	25	3
1:A:461:LYS:N	1:A:461:LYS:HD2	0.45	2.27	14	2
1:A:443:LYS:CD	1:A:457:PHE:CE2	0.45	3.00	1	1
1:A:432:TRP:CB	1:A:437:LYS:CG	0.45	2.94	8	1
1:A:470:TYR:CG	1:A:471:TYR:N	0.45	2.84	1	2
1:A:432:TRP:HB2	1:A:437:LYS:CG	0.45	2.42	8	1
1:A:421:LYS:CD	1:A:421:LYS:C	0.45	2.84	7	3
1:A:422:VAL:HG23	1:A:458:LEU:HA	0.45	1.89	11	2
1:A:439:THR:HG22	1:A:440:PHE:CE1	0.45	2.47	26	1
1:A:422:VAL:HG22	1:A:460:ARG:HD2	0.44	1.89	11	2
1:A:451:PHE:CE2	1:A:467:VAL:HG23	0.44	2.47	16	1
1:A:432:TRP:CH2	1:A:461:LYS:HD3	0.44	2.47	25	1
1:A:460:ARG:HB2	1:A:461:LYS:HD2	0.44	1.87	27	1
1:A:468:LEU:HD13	1:A:471:TYR:HE2	0.44	1.72	10	1
1:A:443:LYS:O	1:A:447:HIS:N	0.44	2.48	10	12
1:A:444:PHE:HA	1:A:454:ILE:HD11	0.44	1.90	20	1
1:A:437:LYS:HG2	1:A:469:TYR:CE2	0.44	2.48	25	3
1:A:444:PHE:HA	1:A:454:ILE:CD1	0.44	2.42	20	3
1:A:454:ILE:HG23	1:A:455:ALA:N	0.44	2.28	1	2
1:A:458:LEU:O	1:A:459:GLU:C	0.44	2.56	2	6
1:A:432:TRP:CE3	1:A:469:TYR:CD2	0.44	3.06	3	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:425:ASP:O	1:A:428:VAL:HB	0.44	2.13	5	1
1:A:455:ALA:HA	1:A:458:LEU:CD1	0.43	2.44	24	5
1:A:458:LEU:CD1	1:A:458:LEU:O	0.43	2.67	23	2
1:A:454:ILE:O	1:A:458:LEU:CG	0.43	2.67	15	3
1:A:425:ASP:HB2	1:A:428:VAL:HG21	0.43	1.89	17	1
1:A:422:VAL:HG22	1:A:460:ARG:CD	0.43	2.44	14	1
1:A:454:ILE:O	1:A:458:LEU:HG	0.43	2.13	15	9
1:A:425:ASP:OD2	1:A:440:PHE:CE1	0.43	2.72	8	3
1:A:422:VAL:HG23	1:A:460:ARG:H	0.43	1.73	10	1
1:A:451:PHE:CZ	1:A:466:CYS:HB3	0.42	2.49	14	4
1:A:425:ASP:O	1:A:428:VAL:N	0.42	2.51	28	1
1:A:458:LEU:O	1:A:458:LEU:CD1	0.42	2.67	22	5
1:A:461:LYS:CD	1:A:461:LYS:N	0.42	2.82	27	3
1:A:421:LYS:C	1:A:421:LYS:HD3	0.42	2.35	14	1
1:A:425:ASP:OD2	1:A:428:VAL:HG21	0.42	2.14	27	1
1:A:447:HIS:CD2	1:A:453:LEU:HD13	0.42	2.50	22	1
1:A:448:PRO:O	1:A:449:LYS:O	0.42	2.37	16	1
1:A:432:TRP:HE1	1:A:468:LEU:HD23	0.42	1.75	28	1
1:A:462:THR:O	1:A:466:CYS:N	0.42	2.51	10	3
1:A:441:ARG:CD	1:A:441:ARG:O	0.42	2.68	25	1
1:A:443:LYS:CD	1:A:457:PHE:CD2	0.42	3.03	9	1
1:A:436:GLU:CB	1:A:440:PHE:HZ	0.42	2.28	1	1
1:A:432:TRP:HB3	1:A:440:PHE:CE2	0.42	2.50	2	3
1:A:443:LYS:CB	1:A:454:ILE:HG13	0.42	2.45	26	3
1:A:429:MET:O	1:A:468:LEU:HD23	0.41	2.15	14	1
1:A:450:ASN:N	1:A:450:ASN:OD1	0.41	2.53	25	3
1:A:421:LYS:HB3	1:A:457:PHE:CE1	0.41	2.51	10	1
1:A:437:LYS:HG2	1:A:469:TYR:CD2	0.41	2.50	15	2
1:A:443:LYS:HD2	1:A:457:PHE:CD2	0.41	2.50	9	1
1:A:441:ARG:CB	1:A:469:TYR:OH	0.41	2.68	1	1
1:A:450:ASN:OD1	1:A:450:ASN:N	0.41	2.53	5	2
1:A:436:GLU:CB	1:A:440:PHE:CZ	0.41	3.04	1	1
1:A:425:ASP:OD1	1:A:440:PHE:CE1	0.41	2.73	24	2
1:A:428:VAL:CG2	1:A:436:GLU:CG	0.41	2.98	18	2
1:A:425:ASP:OD1	1:A:440:PHE:CZ	0.41	2.73	5	1
1:A:444:PHE:CA	1:A:454:ILE:CD1	0.41	2.98	22	8
1:A:439:THR:HG22	1:A:457:PHE:CE1	0.41	2.51	2	1
1:A:440:PHE:N	1:A:440:PHE:CD1	0.41	2.89	16	1
1:A:437:LYS:CG	1:A:469:TYR:CD2	0.41	3.04	18	1
1:A:451:PHE:CE2	1:A:463:VAL:O	0.41	2.74	16	2
1:A:421:LYS:HD2	1:A:439:THR:HG21	0.41	1.93	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:470:TYR:C	1:A:470:TYR:CD1	0.41	2.94	11	2
1:A:425:ASP:O	1:A:428:VAL:HG23	0.41	2.15	10	1
1:A:430:ASN:C	1:A:431:MET:CG	0.41	2.90	16	1
1:A:421:LYS:HA	1:A:423:TYR:CE1	0.41	2.51	7	1
1:A:422:VAL:HG21	1:A:460:ARG:CB	0.41	2.46	25	1
1:A:437:LYS:O	1:A:441:ARG:N	0.41	2.50	6	1
1:A:421:LYS:HG2	1:A:457:PHE:CE1	0.41	2.50	26	1
1:A:467:VAL:HG13	1:A:470:TYR:CE2	0.41	2.51	7	1
1:A:422:VAL:CG1	1:A:423:TYR:CZ	0.40	3.04	10	1
1:A:425:ASP:O	1:A:461:LYS:NZ	0.40	2.53	9	1
1:A:439:THR:CG2	1:A:457:PHE:CZ	0.40	2.98	4	1
1:A:448:PRO:O	1:A:450:ASN:N	0.40	2.53	27	1
1:A:422:VAL:CG2	1:A:460:ARG:HB3	0.40	2.46	25	1
1:A:425:ASP:HA	1:A:428:VAL:CG2	0.40	2.46	11	1
1:A:468:LEU:O	1:A:471:TYR:CE1	0.40	2.74	16	1
1:A:471:TYR:CD1	1:A:471:TYR:C	0.40	2.95	14	1
1:A:454:ILE:CG2	1:A:455:ALA:N	0.40	2.85	1	1
1:A:421:LYS:CG	1:A:439:THR:CG2	0.40	3.00	1	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	51/71 (72%)	38±1 (74±3%)	7±1 (15±3%)	6±1 (11±1%)	1	8
All	All	1428/1988 (72%)	1056 (74%)	209 (15%)	163 (11%)	1	8

All 9 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	431	MET	28
1	A	422	VAL	28
1	A	421	LYS	27
1	A	449	LYS	24

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Mol	Chain	Res	Type	Models (Total)
1	A	448	PRO	23
1	A	459	GLU	22
1	A	462	THR	6
1	A	450	ASN	3
1	A	452	GLY	2

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	48/65 (74%)	30±2 (62±5%)	18±2 (38±5%)	1 7
All	All	1344/1820 (74%)	835 (62%)	509 (38%)	1 7

All 40 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	470	TYR	28
1	A	469	TYR	28
1	A	440	PHE	28
1	A	458	LEU	28
1	A	451	PHE	28
1	A	461	LYS	27
1	A	431	MET	25
1	A	423	TYR	25
1	A	462	THR	23
1	A	421	LYS	19
1	A	436	GLU	19
1	A	435	GLN	19
1	A	427	GLN	18
1	A	432	TRP	16
1	A	468	LEU	14
1	A	441	ARG	14
1	A	443	LYS	14
1	A	460	ARG	13
1	A	456	SER	12
1	A	437	LYS	12

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Mol	Chain	Res	Type	Models (Total)
1	A	433	SER	11
1	A	426	ARG	11
1	A	438	GLU	11
1	A	449	LYS	10
1	A	446	GLN	10
1	A	429	MET	6
1	A	445	MET	6
1	A	425	ASP	6
1	A	457	PHE	6
1	A	424	LYS	5
1	A	471	TYR	4
1	A	434	GLU	2
1	A	454	ILE	2
1	A	459	GLU	2
1	A	466	CYS	2
1	A	450	ASN	1
1	A	430	ASN	1
1	A	428	VAL	1
1	A	439	THR	1
1	A	442	GLU	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.6 Ligand geometry ⓘ

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](#)

The completeness of assignment taking into account all chemical shift lists is 49% for the well-defined parts and 49% for the entire structure.

7.1 Chemical shift list 1

File name: BMRB entry 6286

Chemical shift list name: *assigned_chem_shift_list_1*

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	476
Number of shifts mapped to atoms	476
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	4

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	—	—
$^{13}\text{C}_\beta$	0	—	—
$^{13}\text{C}'$	0	—	—
^{15}N	65	0.61 ± 0.41	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 49%, i.e. 343 atoms were assigned a chemical shift out of a possible 707. 0 out of 7 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	148/253 (58%)	99/101 (98%)	0/102 (0%)	49/50 (98%)
Sidechain	169/366 (46%)	164/218 (75%)	0/128 (0%)	5/20 (25%)

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	Total	¹H	¹³C	¹⁵N
Aromatic	26/88 (30%)	26/46 (57%)	0/39 (0%)	0/3 (0%)
Overall	343/707 (49%)	289/365 (79%)	0/269 (0%)	54/73 (74%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 49%, i.e. 453 atoms were assigned a chemical shift out of a possible 921. 0 out of 9 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	197/336 (59%)	132/134 (99%)	0/136 (0%)	65/66 (98%)
Sidechain	228/489 (47%)	220/291 (76%)	0/172 (0%)	8/26 (31%)
Aromatic	28/96 (29%)	28/50 (56%)	0/43 (0%)	0/3 (0%)
Overall	453/921 (49%)	380/475 (80%)	0/351 (0%)	73/95 (77%)

7.1.4 Statistically unusual chemical shifts ⓘ

The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

Mol	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	461	LYS	HE3	0.57	3.86 – 1.96	-12.3
1	A	461	LYS	HE2	0.69	3.87 – 1.97	-11.7
1	A	461	LYS	HD2	-0.11	2.76 – 0.46	-7.5
1	A	469	TYR	HE2	5.03	7.86 – 5.56	-7.3

7.1.5 Random Coil Index (RCI) plots ⓘ

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:

