



Full wwPDB NMR Structure Validation Report ⓘ

Jun 2, 2020 – 08:09 am BST

PDB ID : 3ZGP
Title : NMR structure of the catalytic domain from *E. faecium* L,D- transpeptidase acylated by ertapenem
Authors : Lecoq, L.; Triboulet, S.; Dubee, V.; Bougault, C.; Hugonnet, J.E.; Arthur, M.; Simorre, J.P.
Deposited on : 2012-12-18

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
Mogul	:	1.8.5 (274361), CSD as541be (2020)
buster-report	:	1.1.7 (2018)
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

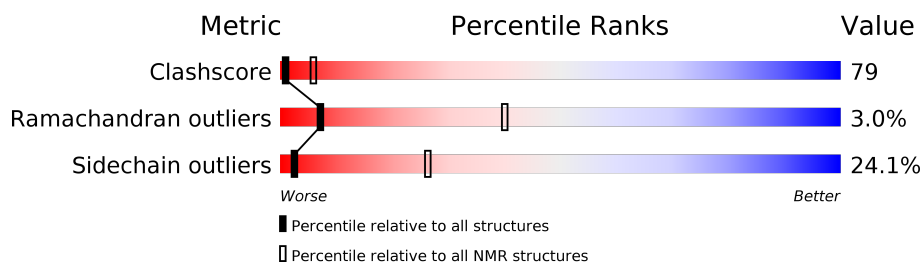
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 92%.

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	129	

2 Ensemble composition and analysis

This entry contains 20 models. Model 10 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:342-A:394, A:404-A:412, A:418-A:424, A:428-A:466 (108)	0.10	10

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 1 clusters and 1 single-model cluster was found.

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

3 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 2040 atoms, of which 980 are hydrogens and 0 are deuteriums.

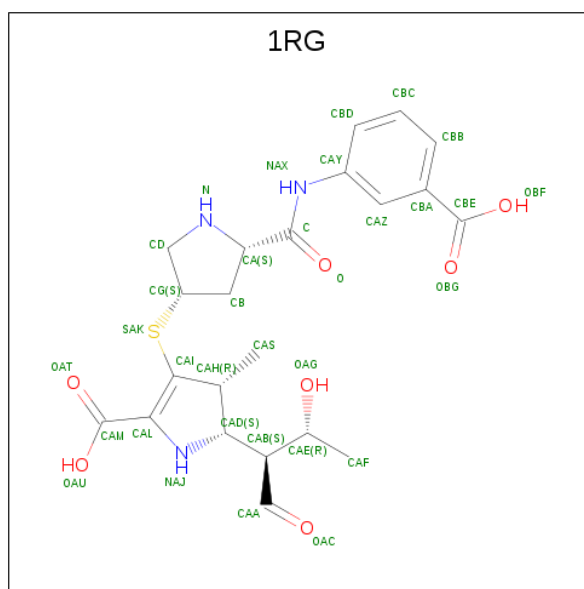
- Molecule 1 is a protein called ERFK/YBIS/YCFS/YNHG.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	129	1982	657	955	161	203	6	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	338	GLY	-	expression tag	UNP Q3Y185
A	339	HIS	-	expression tag	UNP Q3Y185
A	340	MET	-	expression tag	UNP Q3Y185

- Molecule 2 is (4R,5S)-3-({(3S,5S)-5-[(3-carboxyphenyl)carbamoyl]pyrrolidin-3-yl}sulfanyl)-5-[(1S,2R)-1-formyl-2-hydroxypropyl]-4-methyl-4,5-dihydro-1H-pyrrole-2-carboxylic acid (three-letter code: 1RG) (formula: C₂₂H₂₇N₃O₇S).



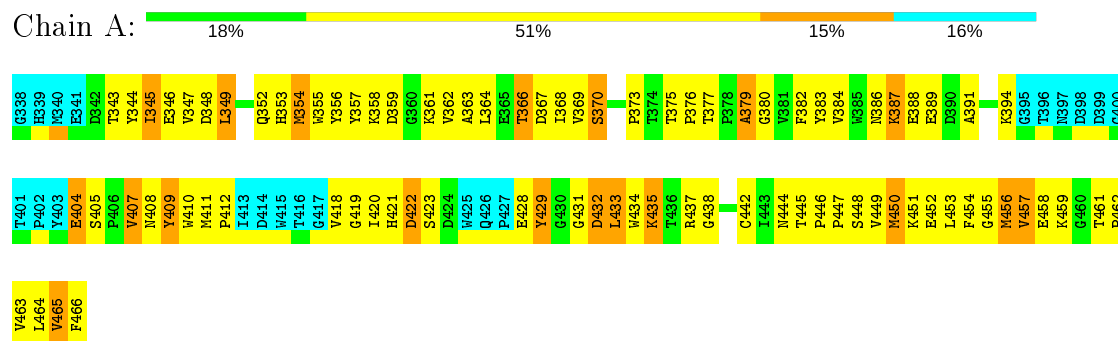
Mol	Chain	Residues	Atoms					
			Total	C	H	N	O	S
2	A	1	58	22	25	3	7	1

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

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

- Molecule 1: ERFK/YBIS/YCFS/YNHG

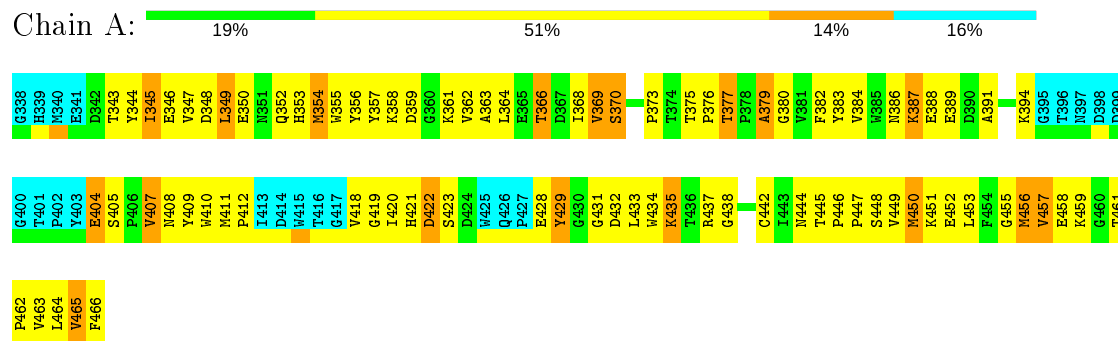


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

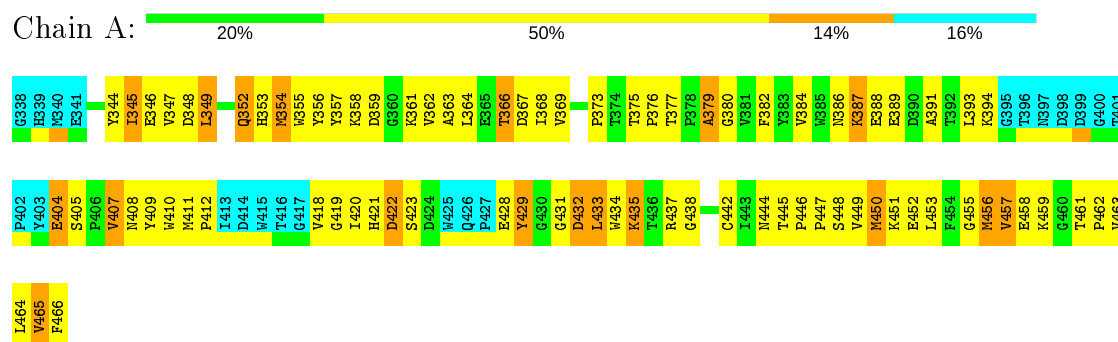
4.2.1 Score per residue for model 1

- Molecule 1: ERFK/YBIS/YCFS/YNHG



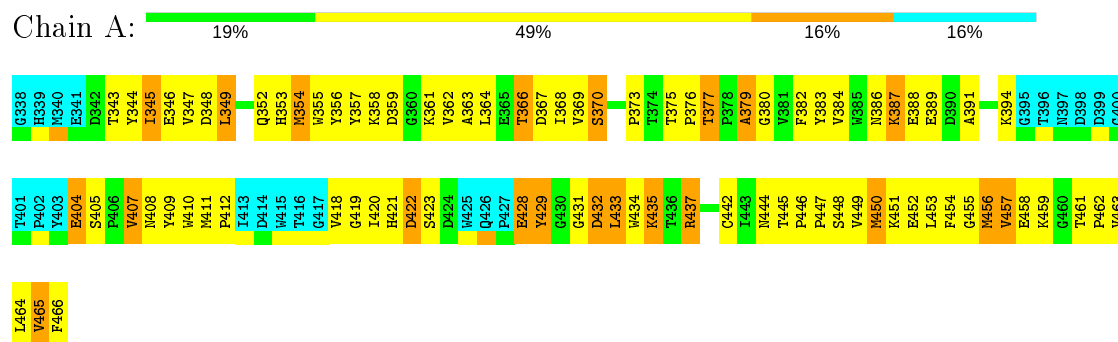
4.2.2 Score per residue for model 2

- Molecule 1: ERFK/YBIS/YCFS/YNHG



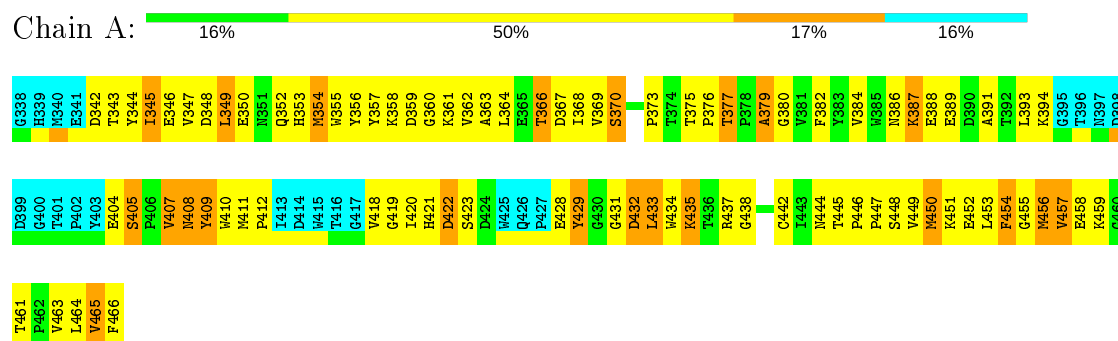
4.2.3 Score per residue for model 3

- Molecule 1: ERFK/YBIS/YCFS/YNHG



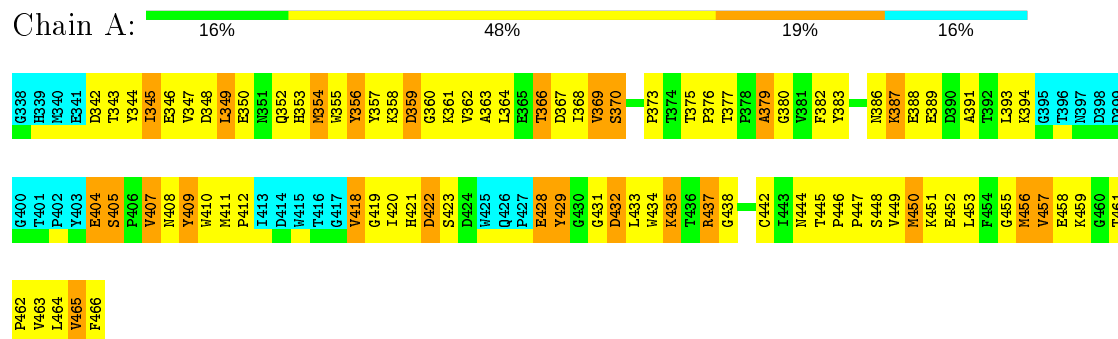
4.2.4 Score per residue for model 4

- Molecule 1: ERFK/YBIS/YCFS/YNHG



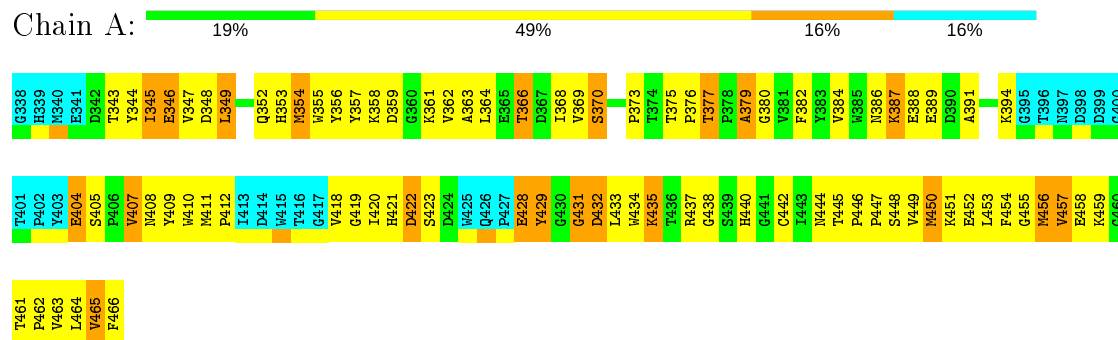
4.2.5 Score per residue for model 5

- Molecule 1: ERFK/YBIS/YCFS/YNHG



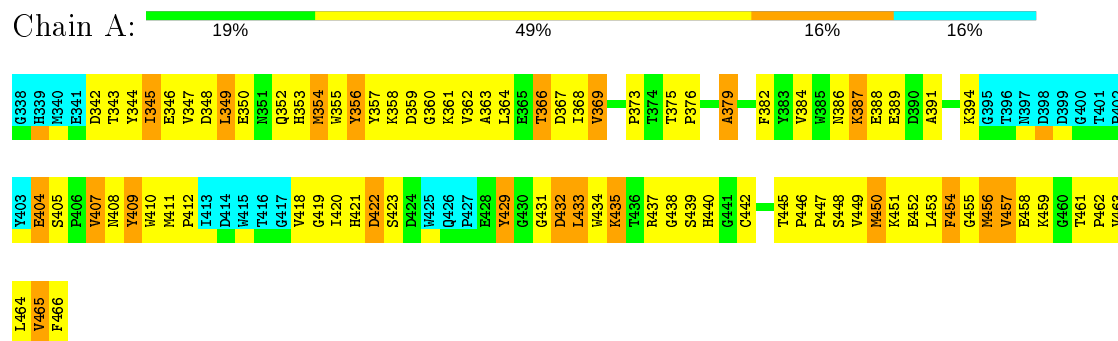
4.2.6 Score per residue for model 6

- Molecule 1: ERFK/YBIS/YCFS/YNHG



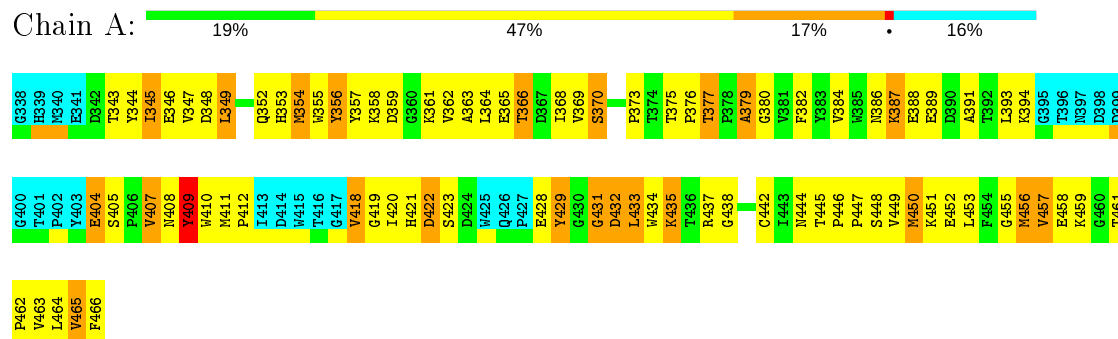
4.2.7 Score per residue for model 7

- Molecule 1: ERFK/YBIS/YCFS/YNHG



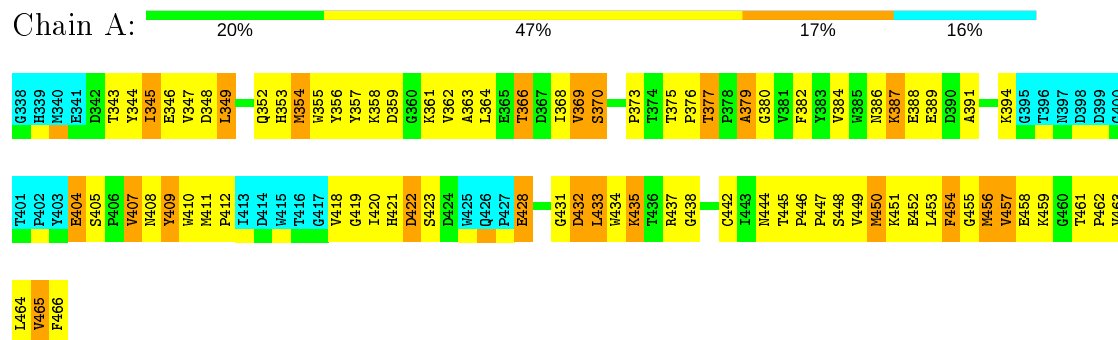
4.2.8 Score per residue for model 8

- Molecule 1: ERFK/YBIS/YCFS/YNHG



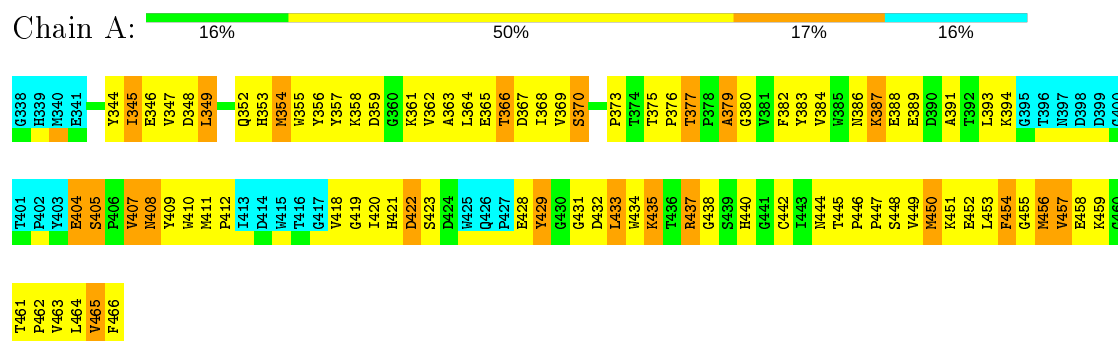
4.2.9 Score per residue for model 9

- Molecule 1: ERFK/YBIS/YCFS/YNHG



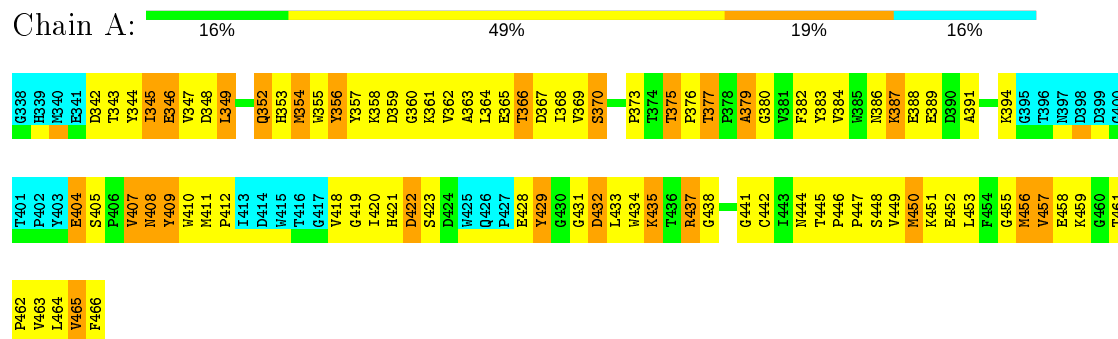
4.2.10 Score per residue for model 10 (medoid)

- Molecule 1: ERFK/YBIS/YCFS/YNHG



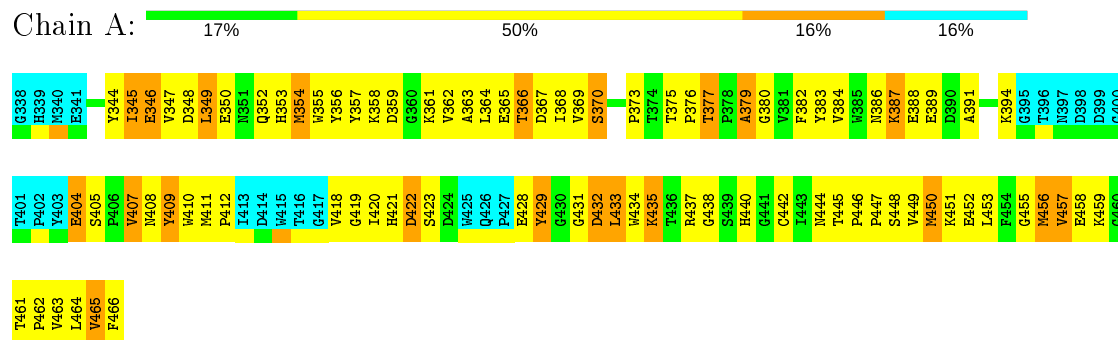
4.2.11 Score per residue for model 11

- Molecule 1: ERFK/YBIS/YCFS/YNHG



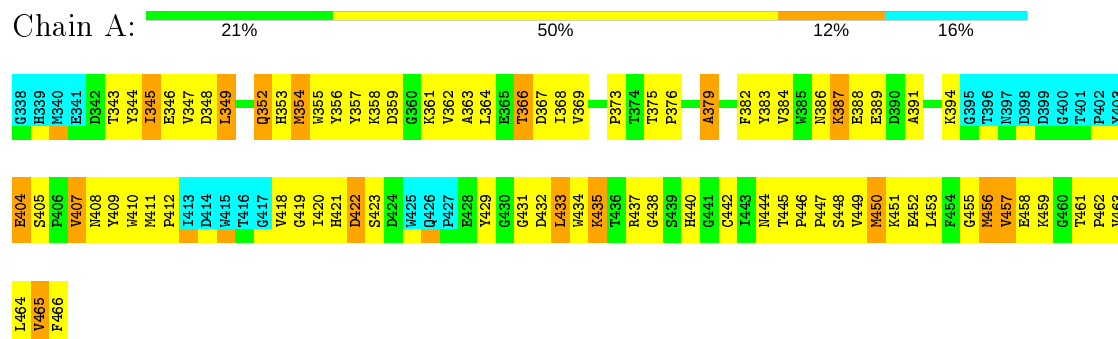
4.2.12 Score per residue for model 12

- Molecule 1: ERFK/YBIS/YCFS/YNHG



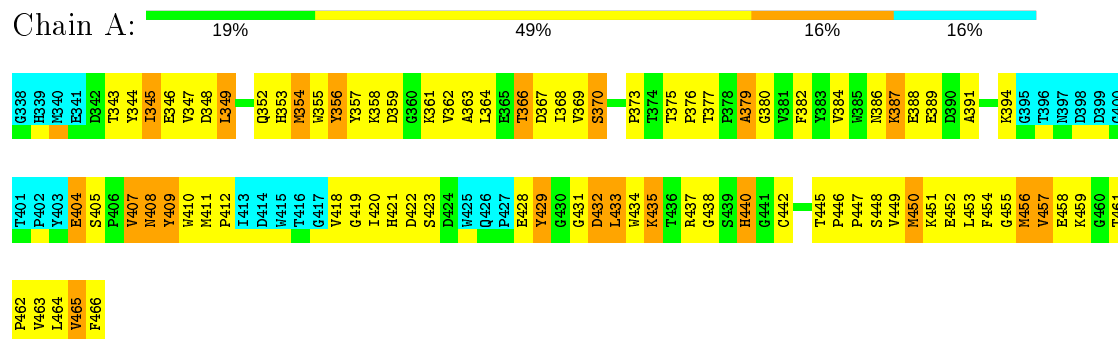
4.2.13 Score per residue for model 13

- Molecule 1: ERFK/YBIS/YCFS/YNHG



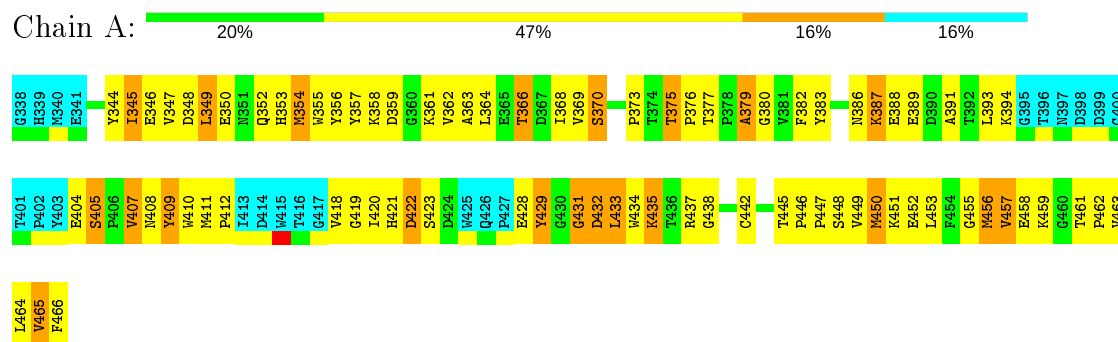
4.2.14 Score per residue for model 14

- Molecule 1: ERFK/YBIS/YCFS/YNHG



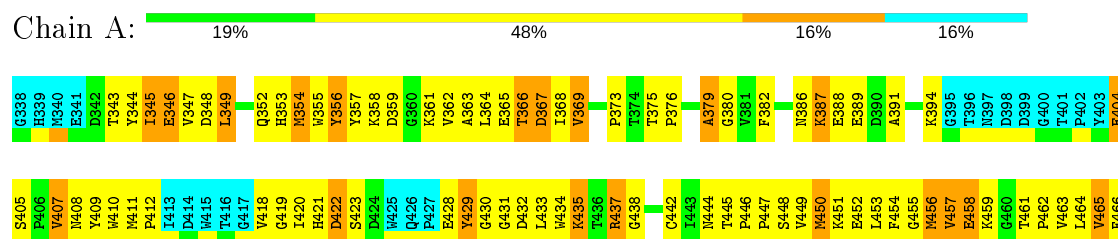
4.2.15 Score per residue for model 15

- Molecule 1: ERFK/YBIS/YCFS/YNHG



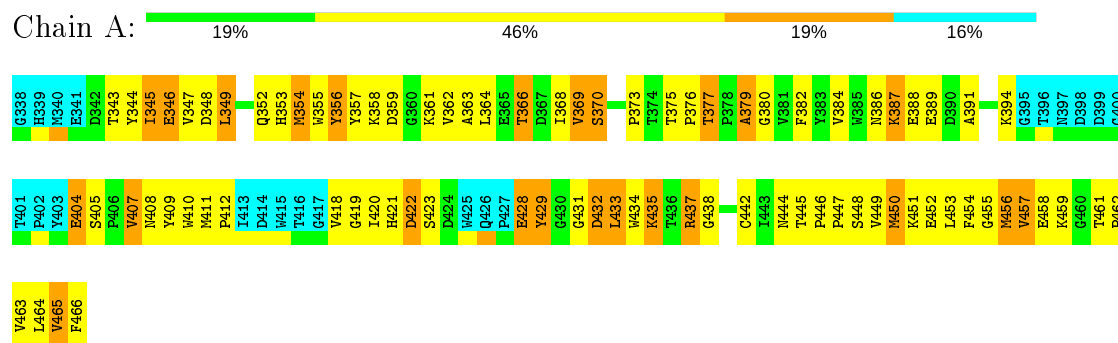
4.2.16 Score per residue for model 16

- Molecule 1: ERFK/YBIS/YCFS/YNHG



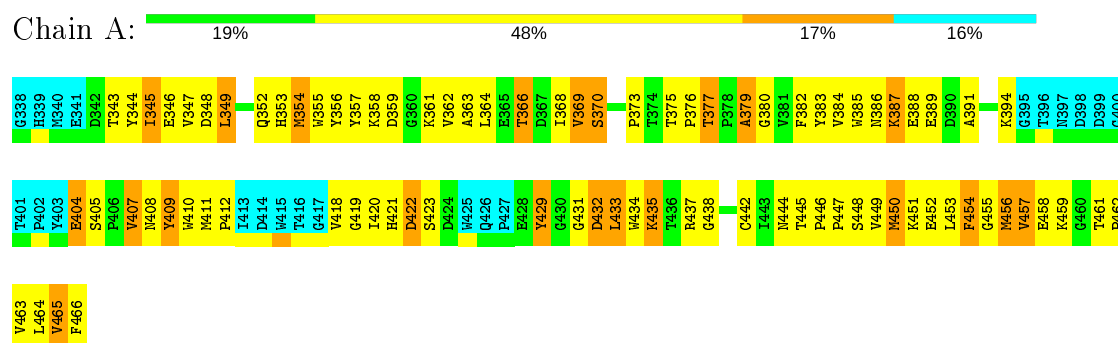
4.2.17 Score per residue for model 17

- Molecule 1: ERFK/YBIS/YCFS/YNHG



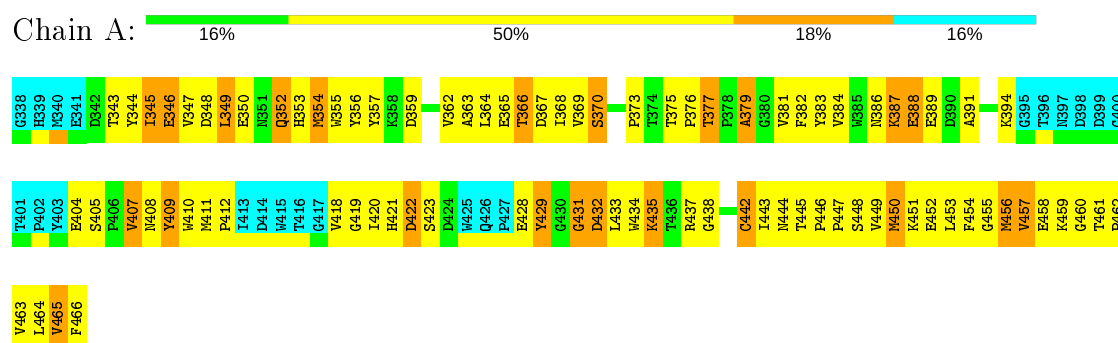
4.2.18 Score per residue for model 18

- Molecule 1: ERFK/YBIS/YCFS/YNHG



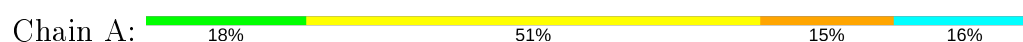
4.2.19 Score per residue for model 19

- Molecule 1: ERFK/YBIS/YCFS/YNHG



4.2.20 Score per residue for model 20

- Molecule 1: ERFK/YBIS/YCFS/YNHG



K338	K339	K340	E341	D342	T343	Y344	I345	E346	Y347	D348	L349	E350	H351	Q352	H353	K354	V355	Y356	Y357	K358	D359	G360	K361	V362	L363	L364	E365	T366	D367	I368	V369			P373	T374	T375	P376	T377			P378	A379	G380	V381	F382	Y383	Y384	H385	N386	K387	E388	E389	D390	A391			K394	G395	T396	N397	D398	D399	G400																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																											
T401	P402	Y403	E404	S405	P406	V407	M408	Y409	W410	M411	P412	L413	D414	W415	T416	G417	V418	G419	I420	H421	D422	S423	D424	W425	Q426	P427	E428	Y429	G430	G431	D432	L433	W434	K435	T436	R437	G438																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																					

5 Refinement protocol and experimental data overview

The models were refined using the following method: *ARIA2.3*.

Of the 1700 calculated structures, 20 were deposited, based on the following criterion: *TOTAL ENERGY*.

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

Software name	Classification	Version
CNS1.2	refinement	
UNIO	structure solution	10
TALOS	structure solution	
CCPNMR ANALYSIS	structure solution	ANALYSIS

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 6 of this report.

Chemical shift file(s)	input_cs.cif
Number of chemical shift lists	1
Total number of shifts	1573
Number of shifts mapped to atoms	1573
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	92%

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

COVALENT-GEOMETRY INFOmissingINFO

5.1 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	860	817	815	131±4
2	A	33	25	24	7±2
All	All	17860	16840	16780	2723

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 79.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:349:LEU:HD21	1:A:465:VAL:HG23	0.96	1.33	5	20
1:A:450:MET:SD	1:A:453:LEU:HD23	0.85	2.11	6	20
2:A:130:1RG:CAM	2:A:130:1RG:HBA	0.84	2.02	7	3
1:A:433:LEU:HD22	1:A:437:ARG:HD2	0.84	1.48	5	6
1:A:343:THR:CG2	1:A:356:TYR:OH	0.82	2.27	5	7
1:A:352:GLN:OE1	1:A:369:VAL:HA	0.76	1.81	18	4
1:A:391:ALA:HB3	1:A:407:VAL:HG12	0.76	1.56	4	20
1:A:379:ALA:HB1	1:A:466:PHE:HA	0.75	1.59	17	19
1:A:368:ILE:HG22	1:A:445:THR:HA	0.73	1.60	19	20
1:A:364:LEU:HD21	1:A:449:VAL:O	0.73	1.83	9	20
1:A:429:TYR:OH	1:A:447:PRO:HD3	0.72	1.85	14	18
1:A:349:LEU:H	1:A:349:LEU:HD22	0.71	1.44	12	12
2:A:130:1RG:OAU	2:A:130:1RG:HBA	0.71	1.86	2	2
1:A:344:TYR:CD2	1:A:464:LEU:HD13	0.70	2.21	19	20
1:A:446:PRO:O	1:A:449:VAL:HG22	0.70	1.86	14	16
1:A:349:LEU:HD22	1:A:349:LEU:H	0.70	1.46	17	8
1:A:389:GLU:HA	1:A:408:ASN:O	0.69	1.88	7	20
1:A:388:GLU:O	1:A:409:TYR:HA	0.68	1.89	15	20
2:A:130:1RG:HBD	2:A:130:1RG:O	0.68	1.88	20	9
2:A:130:1RG:O	2:A:130:1RG:HBD	0.68	1.89	13	11
1:A:375:THR:OG1	2:A:130:1RG:HA	0.68	1.89	12	2
1:A:386:ASN:O	1:A:412:PRO:HD2	0.67	1.89	5	20
1:A:422:ASP:OD1	1:A:450:MET:HB2	0.67	1.90	14	1
1:A:442:CYS:HB3	2:A:130:1RG:HBSB	0.66	1.64	10	18
1:A:382:PHE:HB2	1:A:463:VAL:CG2	0.66	2.21	13	19
1:A:420:ILE:HG22	1:A:450:MET:SD	0.66	2.31	14	20
1:A:433:LEU:HG	1:A:437:ARG:HD2	0.65	1.68	20	13
1:A:346:GLU:CD	1:A:466:PHE:HE1	0.65	1.95	6	2
1:A:434:TRP:CH2	1:A:435:LYS:HE3	0.65	2.26	17	20
1:A:375:THR:HG21	2:A:130:1RG:NAX	0.64	2.07	7	2
1:A:346:GLU:CD	1:A:466:PHE:CE1	0.64	2.71	17	7
1:A:364:LEU:HD22	1:A:456:MET:HE1	0.64	1.69	18	20
1:A:433:LEU:HG	1:A:437:ARG:CD	0.63	2.23	9	14
1:A:347:VAL:HG23	1:A:464:LEU:O	0.63	1.93	18	19
1:A:407:VAL:HG22	1:A:422:ASP:O	0.63	1.93	14	20
2:A:130:1RG:OAU	2:A:130:1RG:HD	0.63	1.93	17	4
1:A:379:ALA:HA	1:A:465:VAL:HG22	0.63	1.69	7	20
1:A:364:LEU:HD22	1:A:456:MET:CE	0.62	2.24	7	20
2:A:130:1RG:HBA	2:A:130:1RG:OAU	0.62	1.94	12	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:A:130:1RG:HD	2:A:130:1RG:OAU	0.62	1.93	11	4
1:A:354:MET:HB3	1:A:366:THR:HG22	0.62	1.71	19	20
1:A:453:LEU:O	1:A:457:VAL:HG13	0.62	1.95	7	20
1:A:445:THR:HG22	1:A:449:VAL:CG2	0.61	2.24	14	20
1:A:356:TYR:HB2	1:A:453:LEU:CD1	0.61	2.25	16	20
1:A:387:LYS:HA	1:A:411:MET:SD	0.61	2.36	6	20
1:A:347:VAL:HG22	1:A:354:MET:HG3	0.61	1.72	19	20
1:A:382:PHE:HB2	1:A:463:VAL:HG12	0.60	1.73	1	1
1:A:367:ASP:OD2	1:A:429:TYR:HB2	0.60	1.96	5	10
2:A:130:1RG:CB	2:A:130:1RG:CAM	0.60	2.79	4	1
1:A:387:LYS:HB3	1:A:411:MET:SD	0.60	2.36	7	13
1:A:349:LEU:O	1:A:352:GLN:HG3	0.60	1.97	3	1
2:A:130:1RG:OAC	2:A:130:1RG:NAJ	0.60	2.35	8	9
1:A:382:PHE:CE2	1:A:418:VAL:HG11	0.60	2.32	19	2
1:A:347:VAL:HB	1:A:465:VAL:HB	0.59	1.74	11	20
2:A:130:1RG:NAJ	2:A:130:1RG:OAC	0.59	2.35	12	11
1:A:355:TRP:CD1	1:A:362:VAL:HG11	0.59	2.32	19	20
1:A:354:MET:SD	1:A:445:THR:HG21	0.59	2.38	19	20
1:A:356:TYR:CD1	1:A:453:LEU:CD1	0.58	2.86	18	20
1:A:422:ASP:CG	1:A:450:MET:HB2	0.58	2.18	14	1
1:A:434:TRP:CZ2	1:A:435:LYS:HE3	0.58	2.33	9	20
1:A:388:GLU:HB2	1:A:410:TRP:HB3	0.58	1.76	8	20
1:A:388:GLU:HB3	1:A:391:ALA:HB2	0.58	1.76	16	19
1:A:352:GLN:HB3	1:A:368:ILE:O	0.58	1.98	13	14
1:A:366:THR:OG1	1:A:446:PRO:HG2	0.57	2.00	1	20
1:A:346:GLU:OE1	1:A:347:VAL:N	0.57	2.37	12	6
1:A:393:LEU:HD11	1:A:407:VAL:HG21	0.57	1.75	10	1
1:A:347:VAL:HG22	1:A:354:MET:CG	0.57	2.30	19	20
1:A:349:LEU:N	1:A:349:LEU:HD13	0.57	2.15	19	12
1:A:349:LEU:HD21	1:A:465:VAL:CG2	0.57	2.24	19	1
1:A:349:LEU:HD13	1:A:349:LEU:N	0.57	2.15	7	8
1:A:352:GLN:OE1	1:A:368:ILE:HD12	0.56	2.00	16	2
1:A:346:GLU:OE1	1:A:466:PHE:CE1	0.56	2.58	17	7
1:A:389:GLU:HG2	1:A:409:TYR:CE2	0.56	2.35	10	8
1:A:345:ILE:HD11	1:A:457:VAL:HG11	0.56	1.75	6	20
1:A:379:ALA:HB1	1:A:466:PHE:CA	0.56	2.30	17	18
1:A:428:GLU:HG3	1:A:437:ARG:CD	0.56	2.31	12	16
1:A:434:TRP:CE2	1:A:435:LYS:HG2	0.56	2.36	15	20
1:A:388:GLU:CB	1:A:410:TRP:HB3	0.55	2.30	19	20
1:A:434:TRP:O	1:A:438:GLY:HA2	0.55	2.00	5	19
1:A:356:TYR:CE1	1:A:457:VAL:HG12	0.55	2.36	1	13

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:356:TYR:HD2	1:A:363:ALA:HB3	0.55	1.60	5	20
1:A:386:ASN:HA	1:A:459:LYS:CG	0.55	2.31	12	9
1:A:433:LEU:HG	1:A:437:ARG:HD3	0.55	1.77	9	1
2:A:130:1RG:HBA	2:A:130:1RG:CAM	0.55	2.31	2	1
1:A:418:VAL:HG12	1:A:419:GLY:N	0.55	2.17	18	18
1:A:422:ASP:HB2	1:A:447:PRO:HA	0.54	1.79	19	19
1:A:345:ILE:HD13	1:A:345:ILE:N	0.54	2.17	1	12
1:A:393:LEU:HG	1:A:405:SER:O	0.54	2.02	10	1
1:A:345:ILE:N	1:A:345:ILE:HD13	0.54	2.17	6	8
1:A:370:SER:OG	1:A:377:THR:HG21	0.54	2.03	14	15
1:A:453:LEU:CD1	1:A:456:MET:HE2	0.54	2.33	18	20
1:A:347:VAL:HB	1:A:465:VAL:HA	0.54	1.80	18	14
1:A:366:THR:HG21	1:A:446:PRO:HD2	0.53	1.81	19	20
1:A:347:VAL:O	1:A:465:VAL:HA	0.53	2.02	19	3
1:A:346:GLU:CD	1:A:464:LEU:HB2	0.53	2.24	6	1
1:A:352:GLN:NE2	1:A:434:TRP:CD1	0.53	2.76	16	2
1:A:409:TYR:CD2	1:A:451:LYS:HA	0.53	2.39	7	11
2:A:130:1RG:CAL	2:A:130:1RG:CB	0.53	2.86	4	1
1:A:373:PRO:HG3	1:A:434:TRP:CZ3	0.53	2.39	1	20
2:A:130:1RG:SAK	2:A:130:1RG:OAU	0.53	2.66	20	7
1:A:373:PRO:HD3	1:A:435:LYS:HA	0.53	1.80	10	20
1:A:346:GLU:HG3	1:A:466:PHE:CE1	0.53	2.39	10	13
2:A:130:1RG:O	2:A:130:1RG:CBD	0.53	2.57	17	10
2:A:130:1RG:OAU	2:A:130:1RG:SAK	0.53	2.66	9	11
1:A:345:ILE:HD12	1:A:453:LEU:HD11	0.53	1.81	9	20
1:A:345:ILE:CG2	1:A:453:LEU:HD21	0.53	2.34	19	20
1:A:353:HIS:NE2	1:A:365:GLU:HG2	0.53	2.18	16	7
2:A:130:1RG:CBD	2:A:130:1RG:O	0.53	2.57	8	9
1:A:441:GLY:HA3	2:A:130:1RG:SAK	0.53	2.43	11	1
2:A:130:1RG:CAL	2:A:130:1RG:HBA	0.52	2.33	7	1
1:A:387:LYS:HD3	1:A:387:LYS:H	0.52	1.64	6	9
1:A:389:GLU:HG2	1:A:409:TYR:CE1	0.52	2.40	6	1
1:A:382:PHE:HB2	1:A:463:VAL:HG22	0.52	1.82	8	19
1:A:383:TYR:HD2	1:A:385:TRP:CD1	0.52	2.22	18	1
1:A:379:ALA:CB	1:A:466:PHE:HA	0.52	2.34	17	12
1:A:375:THR:HB	2:A:130:1RG:CAZ	0.52	2.34	11	1
1:A:356:TYR:CD2	1:A:363:ALA:HB3	0.52	2.39	18	20
1:A:366:THR:OG1	1:A:449:VAL:HG11	0.52	2.05	14	20
1:A:448:SER:O	1:A:451:LYS:HG2	0.52	2.04	2	14
1:A:440:HIS:HB2	2:A:130:1RG:OAC	0.52	2.05	14	2
1:A:433:LEU:CA	1:A:437:ARG:HG3	0.52	2.35	3	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:343:THR:HG21	1:A:356:TYR:OH	0.51	2.03	16	7
1:A:366:THR:HG21	1:A:445:THR:HG23	0.51	1.83	16	20
1:A:375:THR:OG1	2:A:130:1RG:N	0.51	2.43	4	1
1:A:437:ARG:CZ	1:A:437:ARG:HB3	0.51	2.35	7	1
1:A:349:LEU:HD11	1:A:465:VAL:HB	0.51	1.81	19	12
1:A:344:TYR:HA	1:A:461:THR:HG23	0.51	1.83	18	20
1:A:352:GLN:OE1	1:A:432:ASP:HA	0.50	2.06	3	1
1:A:433:LEU:CD2	1:A:437:ARG:HD2	0.50	2.31	11	6
1:A:347:VAL:HG12	1:A:348:ASP:N	0.50	2.21	7	19
1:A:408:ASN:N	1:A:408:ASN:HD22	0.50	2.05	14	3
1:A:346:GLU:CD	1:A:347:VAL:N	0.50	2.64	19	6
1:A:356:TYR:HD2	1:A:363:ALA:CB	0.50	2.20	18	20
1:A:432:ASP:HB2	1:A:435:LYS:CD	0.50	2.37	3	15
1:A:433:LEU:HB3	1:A:437:ARG:HG3	0.49	1.83	5	2
1:A:386:ASN:HA	1:A:459:LYS:HG3	0.49	1.84	7	13
1:A:433:LEU:CG	1:A:437:ARG:HD2	0.49	2.35	2	12
1:A:343:THR:HG23	1:A:357:TYR:O	0.49	2.07	19	12
1:A:410:TRP:CE3	1:A:421:HIS:HB3	0.49	2.42	5	20
1:A:356:TYR:CD1	1:A:453:LEU:HD11	0.49	2.42	18	20
1:A:440:HIS:HB3	2:A:130:1RG:HNAJ	0.49	1.68	12	3
2:A:130:1RG:OAC	2:A:130:1RG:CAL	0.49	2.61	19	1
1:A:410:TRP:HE3	1:A:421:HIS:HB3	0.49	1.68	11	20
1:A:375:THR:N	1:A:376:PRO:HD3	0.49	2.23	1	20
1:A:387:LYS:H	1:A:387:LYS:CD	0.49	2.21	16	5
1:A:345:ILE:HD11	1:A:457:VAL:CG1	0.48	2.38	13	18
1:A:451:LYS:HG3	1:A:452:GLU:N	0.48	2.23	20	20
1:A:449:VAL:HG23	1:A:450:MET:N	0.48	2.23	7	20
1:A:356:TYR:O	1:A:362:VAL:HB	0.48	2.08	18	13
1:A:357:TYR:CD1	1:A:362:VAL:HG12	0.48	2.44	19	20
1:A:386:ASN:ND2	1:A:388:GLU:HG2	0.48	2.24	12	11
2:A:130:1RG:O	2:A:130:1RG:HD	0.48	2.08	11	1
1:A:408:ASN:HD22	1:A:408:ASN:N	0.48	2.07	4	1
1:A:347:VAL:O	1:A:466:PHE:N	0.48	2.45	16	17
1:A:433:LEU:CD1	1:A:437:ARG:HD2	0.48	2.39	3	7
1:A:457:VAL:HB	1:A:461:THR:HG21	0.48	1.86	8	20
1:A:407:VAL:CG1	1:A:410:TRP:HB2	0.48	2.39	11	19
1:A:450:MET:HA	1:A:453:LEU:HB2	0.48	1.85	14	20
1:A:419:GLY:O	1:A:442:CYS:HB2	0.48	2.08	19	4
1:A:387:LYS:HB2	1:A:454:PHE:CD2	0.48	2.43	19	7
1:A:356:TYR:HB2	1:A:453:LEU:HD13	0.48	1.83	17	20
1:A:345:ILE:CD1	1:A:457:VAL:HG11	0.48	2.39	12	20

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:394:LYS:HG2	1:A:404:GLU:CG	0.48	2.39	15	20
1:A:383:TYR:OH	1:A:460:GLY:HA2	0.47	2.09	19	1
1:A:387:LYS:H	1:A:387:LYS:HD3	0.47	1.69	2	7
1:A:349:LEU:N	1:A:349:LEU:HD22	0.47	2.21	12	9
1:A:358:LYS:O	1:A:361:LYS:HG2	0.47	2.09	13	17
1:A:407:VAL:HG11	1:A:410:TRP:HB2	0.47	1.85	8	19
1:A:367:ASP:OD2	1:A:430:GLY:HA2	0.47	2.09	16	1
1:A:346:GLU:OE1	1:A:464:LEU:CB	0.47	2.61	6	1
1:A:349:LEU:HD22	1:A:349:LEU:N	0.47	2.22	7	10
1:A:448:SER:O	1:A:451:LYS:HE3	0.47	2.09	8	11
1:A:346:GLU:O	1:A:355:TRP:N	0.47	2.47	1	17
1:A:384:VAL:HG23	1:A:386:ASN:O	0.47	2.08	20	15
1:A:352:GLN:HE22	1:A:432:ASP:CA	0.47	2.23	3	1
1:A:422:ASP:HA	1:A:445:THR:O	0.47	2.09	2	1
1:A:451:LYS:CG	1:A:452:GLU:N	0.46	2.78	20	20
1:A:387:LYS:CD	1:A:387:LYS:H	0.46	2.24	15	9
1:A:356:TYR:CE2	1:A:456:MET:HB2	0.46	2.46	20	13
1:A:423:SER:N	1:A:445:THR:O	0.46	2.48	19	20
1:A:393:LEU:N	1:A:393:LEU:HD23	0.46	2.26	10	1
1:A:464:LEU:HB3	1:A:466:PHE:CE1	0.46	2.45	5	12
1:A:409:TYR:CD1	1:A:451:LYS:HA	0.46	2.46	18	5
1:A:453:LEU:C	1:A:455:GLY:N	0.46	2.69	6	20
1:A:366:THR:HG21	1:A:445:THR:CG2	0.46	2.40	1	13
1:A:411:MET:HE3	1:A:453:LEU:HG	0.46	1.88	5	1
1:A:369:VAL:HB	1:A:433:LEU:HB2	0.46	1.87	7	6
1:A:388:GLU:HB2	1:A:410:TRP:O	0.46	2.09	14	15
1:A:382:PHE:HB2	1:A:463:VAL:CG1	0.46	2.39	1	1
1:A:432:ASP:HB3	1:A:435:LYS:CD	0.46	2.41	19	1
1:A:386:ASN:HA	1:A:459:LYS:HG2	0.46	1.87	11	6
1:A:433:LEU:HD12	1:A:437:ARG:HD2	0.46	1.88	18	2
1:A:418:VAL:HG22	1:A:419:GLY:N	0.46	2.26	11	1
1:A:345:ILE:CG1	1:A:463:VAL:HG12	0.46	2.41	20	14
1:A:394:LYS:HG2	1:A:404:GLU:HG3	0.46	1.86	15	3
1:A:356:TYR:HD1	1:A:453:LEU:HD11	0.46	1.71	6	20
1:A:380:GLY:N	1:A:465:VAL:O	0.45	2.48	17	17
1:A:354:MET:HB2	1:A:368:ILE:CG2	0.45	2.41	16	12
1:A:346:GLU:O	1:A:354:MET:HG2	0.45	2.10	19	1
1:A:382:PHE:CD2	1:A:418:VAL:HG11	0.45	2.46	19	1
1:A:421:HIS:O	1:A:445:THR:HB	0.45	2.12	6	6
1:A:458:GLU:HG3	1:A:461:THR:OG1	0.45	2.11	16	1
1:A:349:LEU:O	1:A:352:GLN:HG2	0.45	2.11	1	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:418:VAL:CG2	1:A:419:GLY:N	0.45	2.80	11	1
1:A:344:TYR:CB	1:A:462:PRO:HD2	0.45	2.41	18	18
1:A:410:TRP:CH2	1:A:419:GLY:HA3	0.45	2.46	1	4
1:A:366:THR:CG2	1:A:446:PRO:HD2	0.45	2.41	7	20
1:A:347:VAL:HB	1:A:465:VAL:CB	0.45	2.41	6	19
1:A:433:LEU:O	1:A:437:ARG:HG3	0.45	2.12	1	5
1:A:410:TRP:CD1	1:A:412:PRO:HD3	0.45	2.46	5	1
1:A:366:THR:HG21	1:A:449:VAL:HG21	0.45	1.89	20	18
1:A:346:GLU:OE2	1:A:466:PHE:HE1	0.44	1.93	6	1
1:A:449:VAL:O	1:A:452:GLU:HB2	0.44	2.12	4	20
1:A:356:TYR:CD1	1:A:453:LEU:HD12	0.44	2.47	13	13
1:A:353:HIS:CD2	1:A:355:TRP:CE2	0.44	3.06	8	17
1:A:344:TYR:O	1:A:357:TYR:N	0.44	2.51	15	19
1:A:387:LYS:H	1:A:387:LYS:HD2	0.44	1.72	7	1
1:A:450:MET:HE3	1:A:450:MET:O	0.44	2.12	1	3
1:A:389:GLU:HG3	1:A:454:PHE:CE2	0.44	2.47	19	1
1:A:364:LEU:HD21	1:A:449:VAL:C	0.44	2.33	5	11
1:A:352:GLN:NE2	1:A:432:ASP:HA	0.44	2.27	3	1
1:A:346:GLU:OE1	1:A:464:LEU:HB2	0.44	2.13	6	1
1:A:393:LEU:HD21	1:A:421:HIS:CG	0.44	2.47	15	3
1:A:343:THR:HA	1:A:357:TYR:O	0.44	2.13	6	5
1:A:352:GLN:OE1	1:A:431:GLY:HA2	0.44	2.12	15	2
1:A:348:ASP:HA	1:A:466:PHE:OXT	0.44	2.13	15	1
1:A:348:ASP:HB2	1:A:355:TRP:CZ3	0.43	2.48	19	10
1:A:346:GLU:OE1	1:A:466:PHE:HE1	0.43	1.93	6	1
1:A:418:VAL:CG1	1:A:419:GLY:N	0.43	2.82	18	15
1:A:442:CYS:HB3	2:A:130:IRG:CAS	0.43	2.43	11	1
1:A:453:LEU:HD12	1:A:456:MET:HE2	0.43	1.89	6	17
1:A:384:VAL:HG21	1:A:411:MET:SD	0.43	2.54	11	9
1:A:344:TYR:HB3	1:A:462:PRO:HD2	0.43	1.91	18	1
1:A:356:TYR:CD2	1:A:456:MET:HG3	0.43	2.49	19	5
1:A:348:ASP:HA	1:A:466:PHE:C	0.43	2.33	5	6
1:A:353:HIS:HD2	1:A:355:TRP:CE2	0.43	2.31	12	15
1:A:384:VAL:HG12	1:A:463:VAL:HG23	0.43	1.90	1	1
1:A:354:MET:SD	1:A:445:THR:CG2	0.43	3.06	19	13
1:A:350:GLU:HG3	1:A:466:PHE:OXT	0.43	2.13	19	1
1:A:349:LEU:HD22	1:A:466:PHE:OXT	0.43	2.13	15	1
1:A:345:ILE:HD13	1:A:356:TYR:CD1	0.42	2.49	5	2
1:A:428:GLU:HG3	1:A:437:ARG:HD3	0.42	1.91	20	2
1:A:352:GLN:HE22	1:A:432:ASP:HA	0.42	1.74	3	1
1:A:347:VAL:O	1:A:465:VAL:CA	0.42	2.67	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:354:MET:HB2	1:A:368:ILE:HG21	0.42	1.90	18	5
1:A:358:LYS:O	1:A:361:LYS:CG	0.42	2.68	10	10
1:A:453:LEU:HD12	1:A:453:LEU:HA	0.42	1.62	19	9
1:A:373:PRO:O	1:A:376:PRO:HG3	0.42	2.15	13	2
1:A:382:PHE:N	1:A:463:VAL:O	0.42	2.47	1	1
1:A:443:ILE:HD12	1:A:443:ILE:N	0.42	2.30	19	1
1:A:345:ILE:HG21	1:A:453:LEU:HD21	0.42	1.91	19	1
2:A:130:1RG:HAD	2:A:130:1RG:HAFA	0.42	1.81	1	6
1:A:345:ILE:HG22	1:A:355:TRP:O	0.42	2.15	5	5
2:A:130:1RG:HAFA	2:A:130:1RG:HAD	0.42	1.80	5	4
1:A:450:MET:O	1:A:450:MET:HE3	0.42	2.15	5	3
1:A:428:GLU:HG3	1:A:433:LEU:HG	0.42	1.90	9	1
1:A:437:ARG:NH1	1:A:437:ARG:HB3	0.42	2.29	7	1
1:A:358:LYS:N	1:A:361:LYS:O	0.42	2.53	20	2
1:A:431:GLY:O	1:A:433:LEU:HG	0.42	2.14	19	2
1:A:446:PRO:HA	1:A:447:PRO:HD3	0.42	1.79	5	5
1:A:434:TRP:CD2	1:A:435:LYS:HG2	0.42	2.50	20	4
1:A:343:THR:HG23	1:A:356:TYR:OH	0.42	2.14	7	1
1:A:347:VAL:N	1:A:464:LEU:O	0.41	2.53	4	6
1:A:367:ASP:O	1:A:429:TYR:HB3	0.41	2.16	13	1
1:A:346:GLU:HB3	1:A:355:TRP:HB2	0.41	1.91	6	1
1:A:344:TYR:CE2	1:A:346:GLU:HB2	0.41	2.49	1	1
1:A:453:LEU:HA	1:A:453:LEU:HD12	0.41	1.63	6	7
1:A:344:TYR:CD2	1:A:464:LEU:CD1	0.41	3.03	6	1
2:A:130:1RG:CD	2:A:130:1RG:O	0.41	2.68	11	1
1:A:394:LYS:HE2	1:A:404:GLU:HG2	0.41	1.92	17	1
1:A:381:VAL:HG13	1:A:381:VAL:O	0.41	2.16	19	1
1:A:345:ILE:HG12	1:A:463:VAL:HG12	0.41	1.92	8	3
1:A:367:ASP:N	1:A:367:ASP:OD1	0.41	2.53	13	1
1:A:342:ASP:HB3	1:A:360:GLY:CA	0.41	2.45	11	3
1:A:393:LEU:HB2	1:A:405:SER:HB2	0.41	1.92	4	3
1:A:432:ASP:HB2	1:A:435:LYS:HD2	0.41	1.93	6	1
2:A:130:1RG:CAL	2:A:130:1RG:HB	0.41	2.46	4	1
1:A:349:LEU:CD2	1:A:349:LEU:H	0.41	2.26	4	1
1:A:377:THR:CG2	1:A:465:VAL:HG21	0.41	2.46	20	1
1:A:432:ASP:HB3	1:A:435:LYS:HD2	0.41	1.92	1	1
1:A:342:ASP:HB3	1:A:360:GLY:N	0.41	2.31	5	1
1:A:448:SER:O	1:A:451:LYS:HE2	0.41	2.15	11	1
1:A:345:ILE:CD1	1:A:345:ILE:N	0.40	2.82	19	3
1:A:420:ILE:HD13	1:A:463:VAL:CG1	0.40	2.46	1	1
1:A:358:LYS:O	1:A:359:ASP:HB2	0.40	2.16	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:384:VAL:HG13	1:A:461:THR:O	0.40	2.17	18	1
1:A:382:PHE:CE2	1:A:418:VAL:HG21	0.40	2.52	15	1
1:A:345:ILE:N	1:A:345:ILE:CD1	0.40	2.83	13	1
1:A:440:HIS:HB3	2:A:130:1RG:OAC	0.40	2.16	6	1
1:A:433:LEU:CB	1:A:437:ARG:HG3	0.40	2.46	3	1
1:A:384:VAL:HB	1:A:411:MET:HB3	0.40	1.93	19	1
1:A:352:GLN:HE22	1:A:432:ASP:N	0.40	2.15	3	1
1:A:354:MET:HB2	1:A:368:ILE:HG12	0.40	1.93	1	1

5.2 Torsion angles ⓘ

5.2.1 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	107/129 (83%)	87±1 (81±1%)	17±1 (16±1%)	3±1 (3±0%)	7	40
All	All	2140/2580 (83%)	1741 (81%)	335 (16%)	64 (3%)	7	40

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	379	ALA	20
1	A	431	GLY	20
1	A	432	ASP	19
1	A	440	HIS	2
1	A	418	VAL	2
1	A	412	PRO	1

5.2.2 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	95/112 (85%)	72±2 (76±2%)	23±2 (24±2%)	2	26
All	All	1900/2240 (85%)	1443 (76%)	457 (24%)	2	26

All 34 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	359	ASP	20
1	A	465	VAL	20
1	A	369	VAL	20
1	A	366	THR	20
1	A	407	VAL	20
1	A	450	MET	20
1	A	345	ILE	20
1	A	458	GLU	20
1	A	456	MET	20
1	A	387	LYS	20
1	A	349	LEU	20
1	A	457	VAL	20
1	A	405	SER	20
1	A	435	LYS	20
1	A	354	MET	20
1	A	422	ASP	19
1	A	429	TYR	18
1	A	404	GLU	17
1	A	444	ASN	17
1	A	370	SER	15
1	A	433	LEU	14
1	A	377	THR	13
1	A	350	GLU	7
1	A	352	GLN	6
1	A	346	GLU	6
1	A	437	ARG	6
1	A	428	GLU	5
1	A	408	ASN	4
1	A	383	TYR	3
1	A	367	ASP	2
1	A	375	THR	2
1	A	388	GLU	1
1	A	442	CYS	1
1	A	439	SER	1

5.2.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.4 Carbohydrates [i](#)

There are no carbohydrates in this entry.

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5.5 Other polymers [i](#)

There are no such molecules in this entry.

5.6 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 92% for the well-defined parts and 91% for the entire structure.

6.1 Chemical shift list 1

File name: input_cs.cif

Chemical shift list name: *assigned_chem_shift_list*

6.1.1 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	1573
Number of shifts mapped to atoms	1573
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	7

6.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	124	0.04 ± 0.15	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	114	-0.06 ± 0.20	None needed (< 0.5 ppm)
$^{13}\text{C}'$	106	0.41 ± 0.14	None needed (< 0.5 ppm)
^{15}N	112	0.24 ± 0.53	None needed (< 0.5 ppm)

6.1.3 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 92%, i.e. 1195 atoms were assigned a chemical shift out of a possible 1293. 0 out of 17 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	499/524 (95%)	203/208 (98%)	198/216 (92%)	98/100 (98%)
Sidechain	560/623 (90%)	346/365 (95%)	208/242 (86%)	6/16 (38%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	136/146 (93%)	68/75 (91%)	61/62 (98%)	7/9 (78%)
Overall	1195/1293 (92%)	617/648 (95%)	467/520 (90%)	111/125 (89%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 91%, i.e. 1389 atoms were assigned a chemical shift out of a possible 1529. 0 out of 17 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	577/625 (92%)	235/248 (95%)	230/258 (89%)	112/119 (94%)
Sidechain	640/718 (89%)	397/421 (94%)	235/279 (84%)	8/18 (44%)
Aromatic	172/186 (92%)	85/95 (89%)	77/78 (99%)	10/13 (77%)
Overall	1389/1529 (91%)	717/764 (94%)	542/615 (88%)	130/150 (87%)

6.1.4 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	446	PRO	HG2	-0.11	3.48 – 0.38	-6.6
1	A	435	LYS	HG3	-0.33	2.76 – -0.04	-6.0
1	A	435	LYS	HG2	-0.18	2.67 – 0.07	-6.0
1	A	423	SER	HB2	2.35	5.18 – 2.58	-5.9
1	A	353	HIS	HD2	4.41	9.28 – 4.78	-5.8
1	A	423	SER	HB3	2.24	5.25 – 2.45	-5.8
1	A	412	PRO	HD3	1.45	5.52 – 1.72	-5.7

6.1.5 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:

