



Full wwPDB NMR Structure Validation Report ⓘ

Sep 28, 2020 – 11:45 AM EDT

PDB ID : 6XRG
Title : Abl 1b isoform inactive2 state
Authors : Xie, T.; Saleh, T.; Rossi, P.; Kalodimos, C.G.
Deposited on : 2020-07-12

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

We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<https://www.wwpdb.org/validation/2017/NMRValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

Cyrange : Kirchner and Güntert (2011)
NmrClust : Kelley et al. (1996)
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : 2.14.6
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.14.6

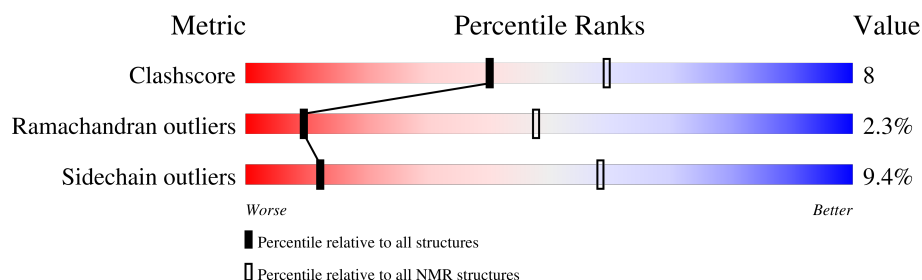
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 9%.

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	287	

2 Ensemble composition and analysis

This entry contains 20 models. Model 6 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:254-A:406, A:422-A:517 (249)	0.54	6

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 2 clusters. No single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 4633 atoms, of which 2293 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Tyrosine-protein kinase ABL1.

Mol	Chain	Residues	Atoms						Trace
1	A	287	Total	C	H	N	O	S	0
			4633	1504	2293	379	441	16	

There are 3 discrepancies between the modelled and reference sequences:

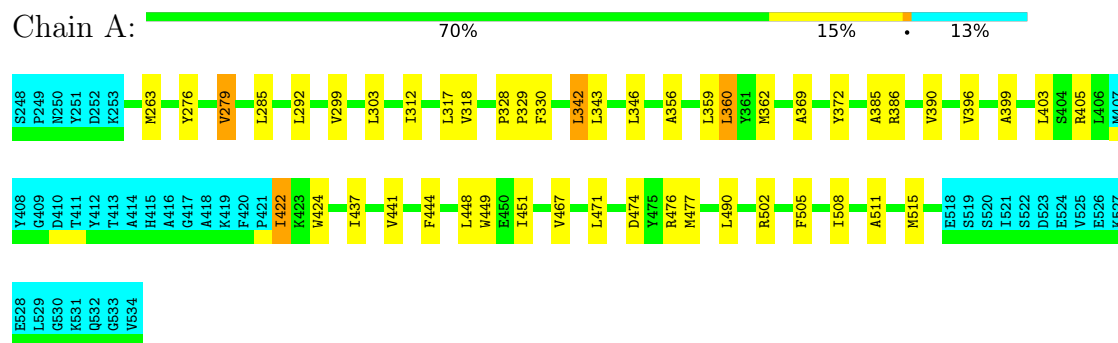
Chain	Residue	Modelled	Actual	Comment	Reference
A	269	GLU	GLY	engineered mutation	UNP P00519
A	309	LEU	MET	engineered mutation	UNP P00519
A	408	TYR	THR	engineered mutation	UNP P00519

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

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

- Molecule 1: Tyrosine-protein kinase ABL1

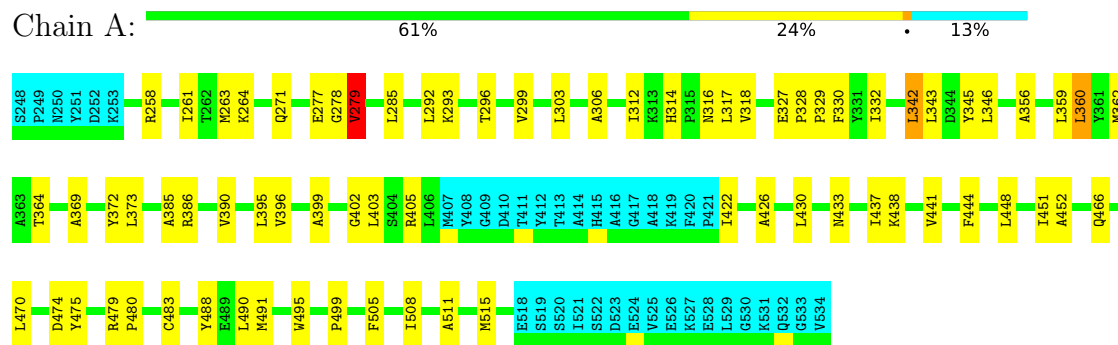


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

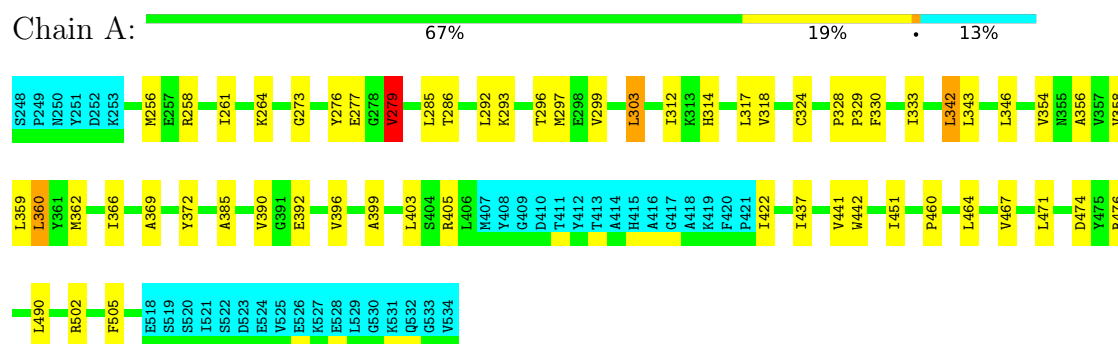
4.2.1 Score per residue for model 1

- Molecule 1: Tyrosine-protein kinase ABL1



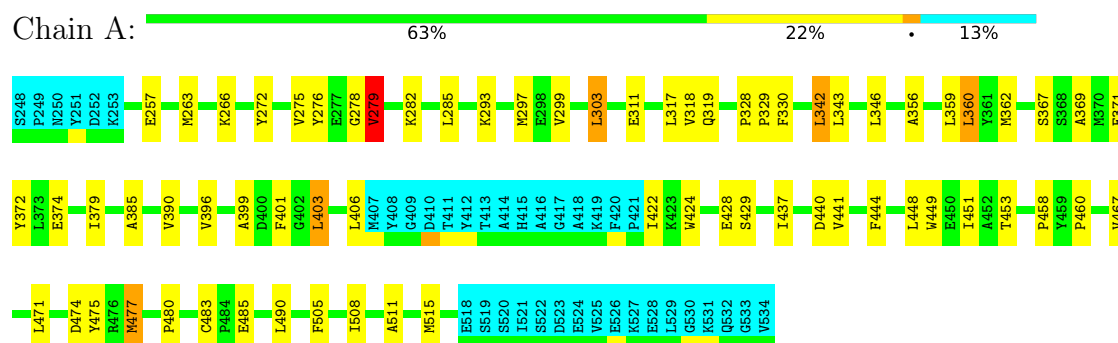
4.2.2 Score per residue for model 2

- Molecule 1: Tyrosine-protein kinase ABL1



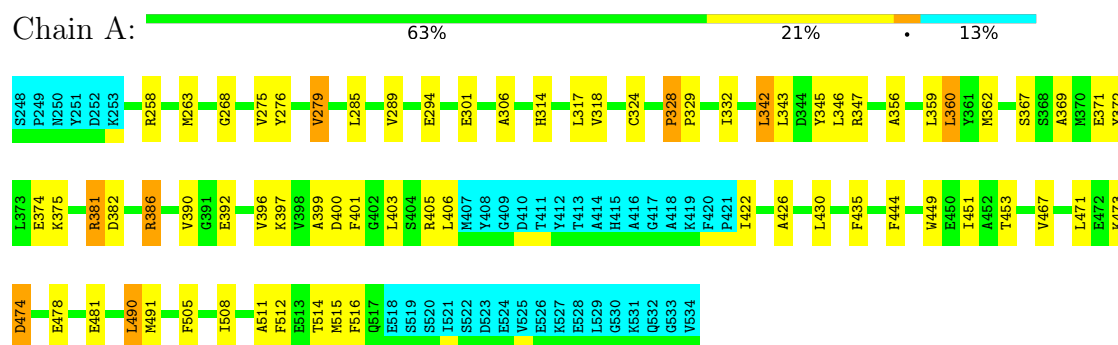
4.2.3 Score per residue for model 3

- Molecule 1: Tyrosine-protein kinase ABL1



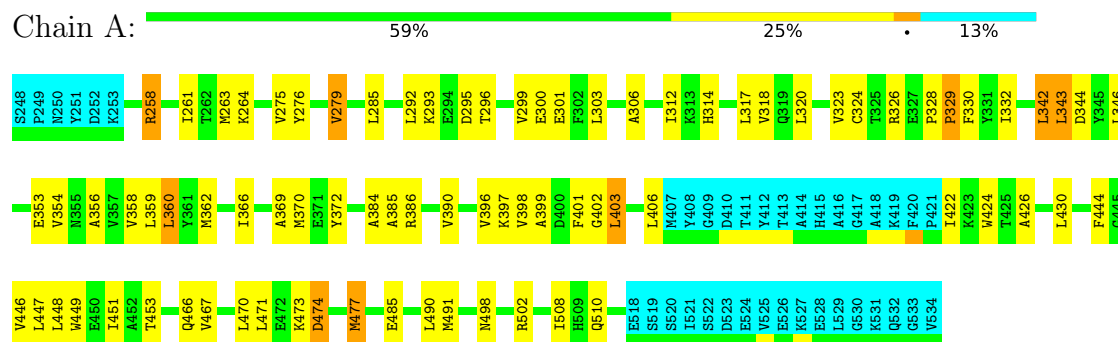
4.2.4 Score per residue for model 4

- Molecule 1: Tyrosine-protein kinase ABL1



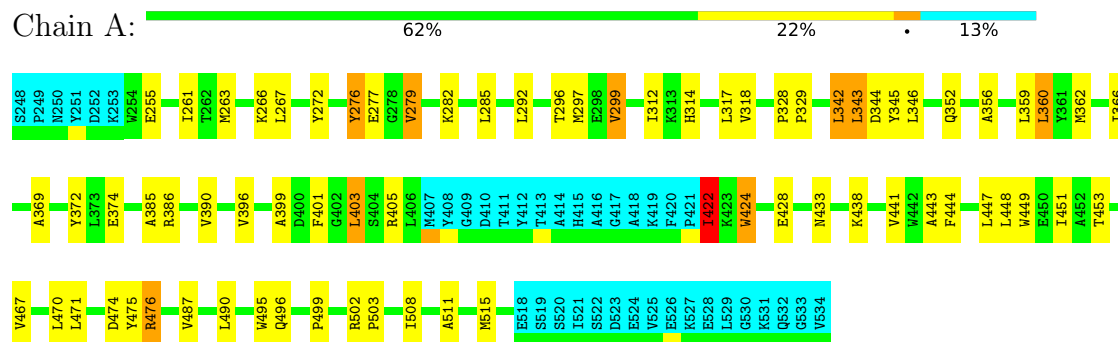
4.2.5 Score per residue for model 5

- Molecule 1: Tyrosine-protein kinase ABL1



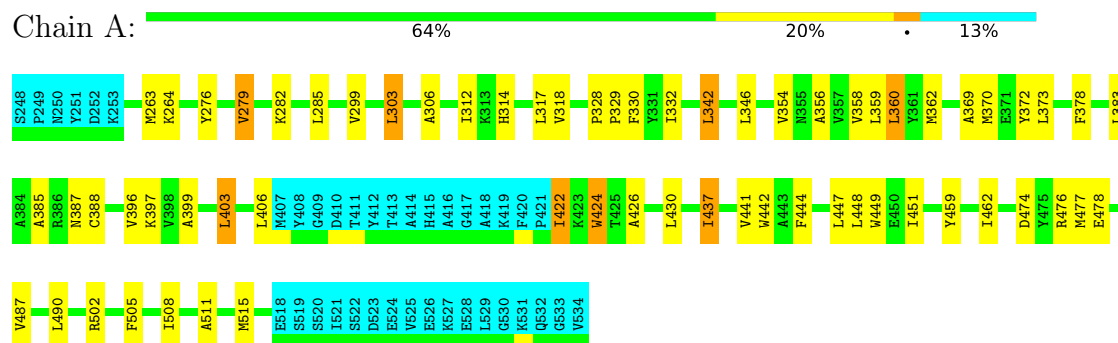
4.2.6 Score per residue for model 6 (medoid)

- Molecule 1: Tyrosine-protein kinase ABL1



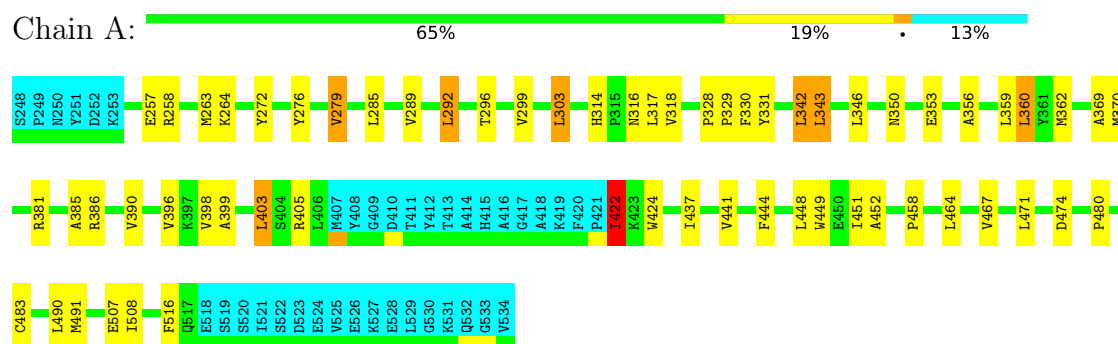
4.2.7 Score per residue for model 7

- Molecule 1: Tyrosine-protein kinase ABL1



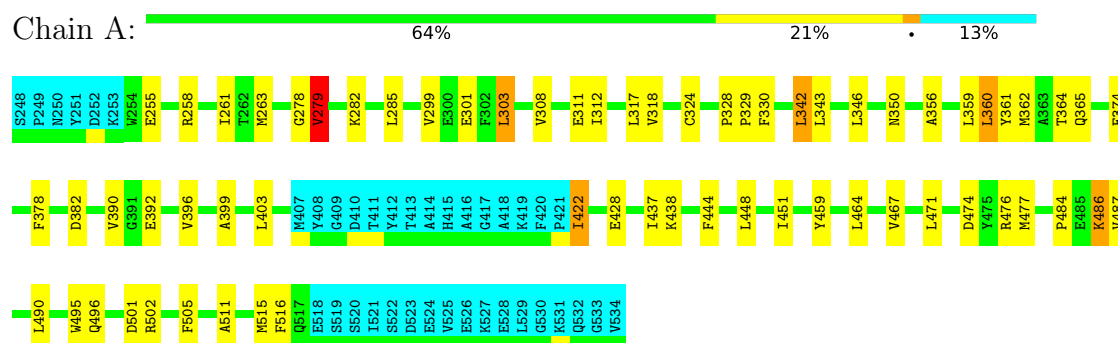
4.2.8 Score per residue for model 8

- Molecule 1: Tyrosine-protein kinase ABL1



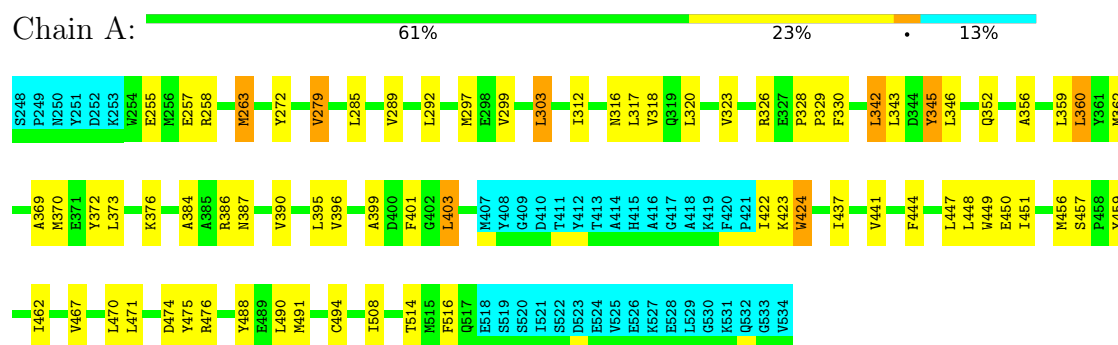
4.2.9 Score per residue for model 9

- Molecule 1: Tyrosine-protein kinase ABL1



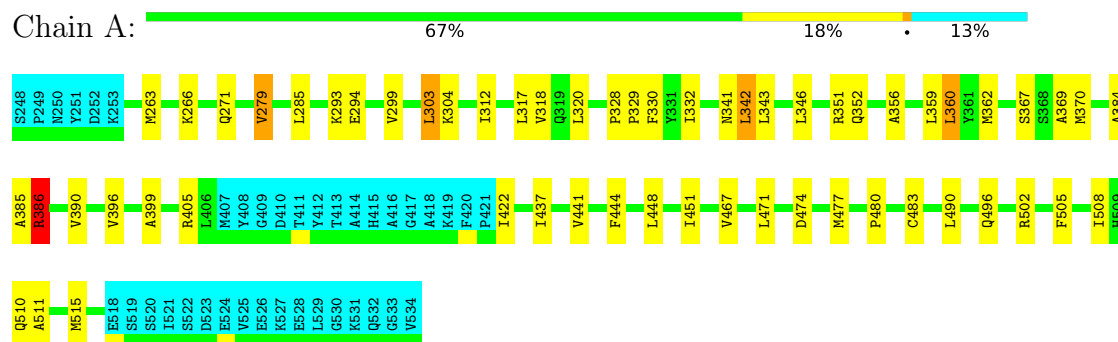
4.2.10 Score per residue for model 10

- Molecule 1: Tyrosine-protein kinase ABL1



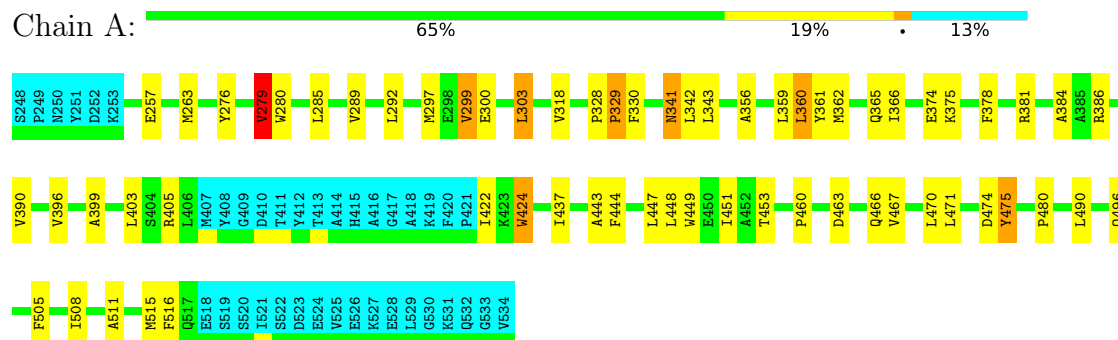
4.2.14 Score per residue for model 14

- Molecule 1: Tyrosine-protein kinase ABL1



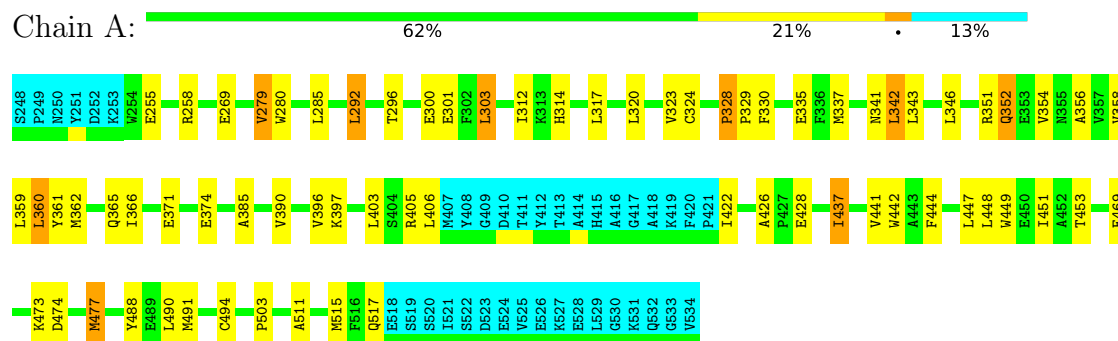
4.2.15 Score per residue for model 15

- Molecule 1: Tyrosine-protein kinase ABL1



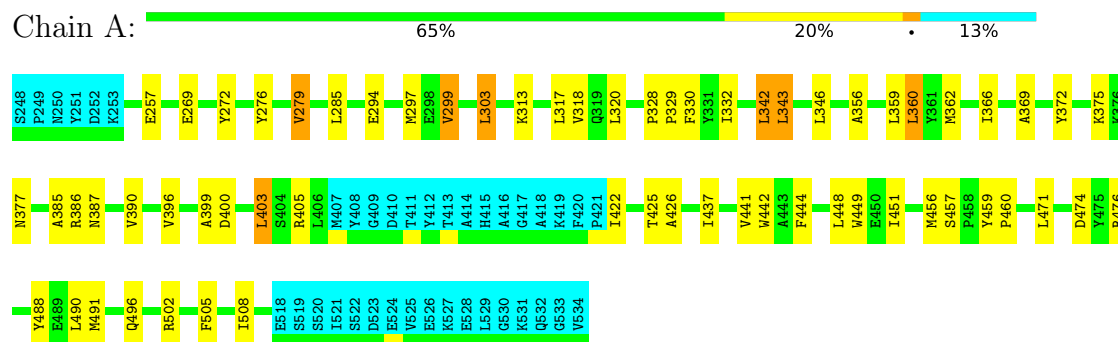
4.2.16 Score per residue for model 16

- Molecule 1: Tyrosine-protein kinase ABL1



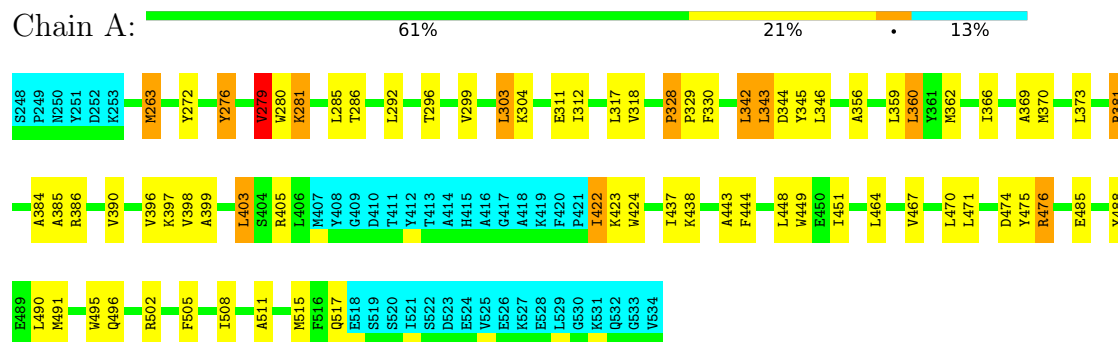
4.2.17 Score per residue for model 17

- Molecule 1: Tyrosine-protein kinase ABL1



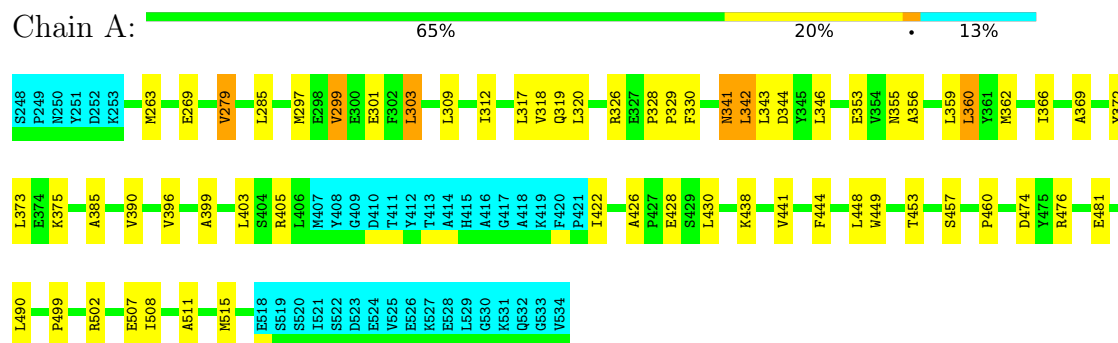
4.2.18 Score per residue for model 18

- Molecule 1: Tyrosine-protein kinase ABL1



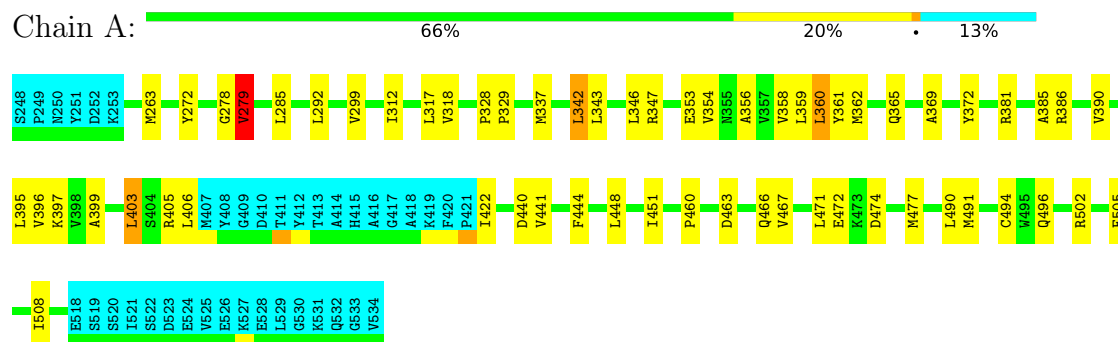
4.2.19 Score per residue for model 19

- Molecule 1: Tyrosine-protein kinase ABL1



4.2.20 Score per residue for model 20

- Molecule 1: Tyrosine-protein kinase ABL1



5 Refinement protocol and experimental data overview

The models were refined using the following method: *molecular dynamics*.

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *target function*.

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

Software name	Classification	Version
CNS	refinement	
CYANA	structure calculation	
TALOS	geometry optimization	
PSVS	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)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	553
Number of shifts mapped to atoms	553
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	9%

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](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the (average) root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.89±0.01	0±0/2101 (0.0± 0.0%)	0.73±0.01	0±0/2846 (0.0± 0.0%)
All	All	0.89	2/42020 (0.0%)	0.73	1/56920 (0.0%)

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	0.2±0.4
All	All	0	4

All unique bond outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	424	TRP	NE1-CE2	-5.77	1.30	1.37	8	2

All unique angle outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	386	ARG	NE-CZ-NH1	5.84	123.22	120.30	14	1

There are no chirality outliers.

All unique planar outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	328	PRO	Peptide	3
1	A	402	GLY	Peptide	1

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	2048	2021	2016	31±5
All	All	40960	40420	40320	619

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 8.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:317:LEU:HD21	1:A:369:ALA:HB1	0.69	1.63	1	16
1:A:297:MET:HB2	1:A:299:VAL:HG12	0.67	1.65	15	2
1:A:312:ILE:HD11	1:A:317:LEU:HD22	0.67	1.66	12	14
1:A:458:PRO:HA	1:A:477:MET:SD	0.65	2.32	12	1
1:A:303:LEU:HD22	1:A:330:PHE:CZ	0.62	2.29	5	15
1:A:292:LEU:HD12	1:A:296:THR:HG21	0.61	1.73	2	9
1:A:403:LEU:H	1:A:403:LEU:HD12	0.61	1.55	10	1
1:A:359:LEU:HD22	1:A:451:ILE:HG23	0.61	1.72	18	14
1:A:362:MET:HB2	1:A:396:VAL:HG23	0.61	1.73	9	2
1:A:359:LEU:HA	1:A:362:MET:SD	0.61	2.36	5	15
1:A:256:MET:SD	1:A:333:ILE:HG21	0.61	2.36	12	2
1:A:390:VAL:HG22	1:A:396:VAL:HG22	0.60	1.71	1	19
1:A:385:ALA:HA	1:A:388:CYS:SG	0.60	2.36	7	1
1:A:370:MET:SD	1:A:398:VAL:HG11	0.60	2.37	18	3
1:A:312:ILE:HD12	1:A:373:LEU:HD21	0.59	1.74	13	3
1:A:386:ARG:HH22	1:A:400:ASP:HA	0.59	1.57	4	1
1:A:318:VAL:HG21	1:A:399:ALA:HB2	0.59	1.73	10	19
1:A:362:MET:HG3	1:A:396:VAL:HG21	0.59	1.73	16	1
1:A:449:TRP:CE3	1:A:491:MET:SD	0.58	2.96	10	4
1:A:386:ARG:NH2	1:A:400:ASP:HA	0.58	2.14	4	1
1:A:386:ARG:HG3	1:A:403:LEU:HD13	0.58	1.75	6	4
1:A:403:LEU:HD22	1:A:406:LEU:HD22	0.57	1.75	7	3
1:A:477:MET:SD	1:A:495:TRP:CZ2	0.57	2.97	9	1
1:A:258:ARG:HB3	1:A:324:CYS:SG	0.57	2.40	5	1
1:A:452:ALA:HB1	1:A:483:CYS:SG	0.57	2.39	8	3
1:A:491:MET:HA	1:A:494:CYS:SG	0.57	2.38	16	3
1:A:438:LYS:HD3	1:A:499:PRO:HB3	0.57	1.76	1	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:297:MET:HG3	1:A:299:VAL:HG12	0.56	1.77	19	1
1:A:384:ALA:HB1	1:A:386:ARG:HH11	0.56	1.61	14	1
1:A:456:MET:SD	1:A:460:PRO:HG3	0.56	2.41	17	1
1:A:423:LYS:HG3	1:A:467:VAL:HG21	0.56	1.76	12	1
1:A:441:VAL:HG13	1:A:508:ILE:HD11	0.56	1.77	17	3
1:A:422:ILE:HG12	1:A:430:LEU:HD22	0.55	1.77	12	2
1:A:341:ASN:ND2	1:A:344:ASP:HB3	0.55	2.16	19	1
1:A:342:LEU:HB3	1:A:385:ALA:HB1	0.55	1.78	6	14
1:A:320:LEU:HD21	1:A:323:VAL:HG23	0.55	1.79	5	5
1:A:258:ARG:HB2	1:A:324:CYS:SG	0.54	2.42	4	4
1:A:441:VAL:HG11	1:A:503:PRO:O	0.54	2.03	6	2
1:A:480:PRO:HB2	1:A:483:CYS:SG	0.54	2.43	14	2
1:A:422:ILE:HG23	1:A:464:LEU:HD21	0.54	1.80	12	1
1:A:356:ALA:O	1:A:360:LEU:HD22	0.53	2.04	18	20
1:A:467:VAL:O	1:A:471:LEU:HG	0.53	2.04	13	15
1:A:261:ILE:HG22	1:A:263:MET:SD	0.53	2.44	6	5
1:A:374:GLU:HB2	1:A:437:ILE:HG13	0.53	1.80	16	1
1:A:441:VAL:HG11	1:A:502:ARG:HE	0.53	1.64	14	1
1:A:370:MET:SD	1:A:373:LEU:HG	0.53	2.44	11	1
1:A:422:ILE:HG12	1:A:425:THR:HB	0.52	1.79	13	1
1:A:384:ALA:HA	1:A:424:TRP:CH2	0.52	2.39	10	3
1:A:488:TYR:HA	1:A:491:MET:SD	0.52	2.44	17	3
1:A:386:ARG:NE	1:A:403:LEU:HD13	0.52	2.20	10	1
1:A:437:ILE:HD11	1:A:505:PHE:HE2	0.52	1.63	9	1
1:A:386:ARG:HG2	1:A:403:LEU:HD22	0.52	1.81	10	1
1:A:437:ILE:HG23	1:A:438:LYS:HD2	0.52	1.82	18	1
1:A:441:VAL:HG22	1:A:505:PHE:CE2	0.51	2.39	14	6
1:A:272:TYR:HB3	1:A:292:LEU:HA	0.51	1.80	6	7
1:A:488:TYR:HA	1:A:491:MET:HG2	0.51	1.83	1	1
1:A:463:ASP:HB2	1:A:466:GLN:HG2	0.51	1.82	15	1
1:A:442:TRP:HB2	1:A:502:ARG:HH22	0.51	1.64	2	1
1:A:312:ILE:HD12	1:A:373:LEU:HD11	0.50	1.82	11	1
1:A:337:MET:SD	1:A:397:LYS:HE2	0.50	2.46	16	1
1:A:316:ASN:HA	1:A:395:LEU:HD21	0.50	1.84	12	4
1:A:424:TRP:CZ3	1:A:443:ALA:HB1	0.50	2.40	6	2
1:A:401:PHE:HD2	1:A:403:LEU:HD21	0.50	1.65	6	1
1:A:486:LYS:HB3	1:A:515:MET:HG2	0.50	1.82	9	1
1:A:343:LEU:HD23	1:A:344:ASP:H	0.50	1.65	11	3
1:A:480:PRO:HG2	1:A:483:CYS:SG	0.50	2.47	12	1
1:A:477:MET:HG3	1:A:491:MET:SD	0.50	2.47	13	1
1:A:422:ILE:HG12	1:A:464:LEU:HD11	0.49	1.84	18	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:496:GLN:HG3	1:A:501:ASP:HB3	0.49	1.82	9	1
1:A:436:SER:HB2	1:A:438:LYS:HG2	0.49	1.84	13	1
1:A:444:PHE:O	1:A:448:LEU:HG	0.49	2.07	8	17
1:A:273:GLY:HA2	1:A:293:LYS:HE3	0.49	1.85	2	1
1:A:425:THR:HA	1:A:442:TRP:CH2	0.49	2.41	17	1
1:A:438:LYS:HD3	1:A:499:PRO:HB2	0.49	1.83	19	1
1:A:359:LEU:HD23	1:A:362:MET:SD	0.49	2.47	12	5
1:A:278:GLY:O	1:A:279:VAL:HG13	0.49	2.08	13	7
1:A:337:MET:SD	1:A:397:LYS:HD2	0.49	2.48	20	2
1:A:320:LEU:HD11	1:A:332:ILE:HB	0.49	1.83	14	2
1:A:342:LEU:O	1:A:346:LEU:HG	0.49	2.08	3	15
1:A:444:PHE:HE2	1:A:508:ILE:HG21	0.49	1.68	11	8
1:A:345:TYR:CD2	1:A:390:VAL:HG21	0.49	2.42	1	7
1:A:449:TRP:O	1:A:453:THR:HG22	0.49	2.08	6	9
1:A:256:MET:SD	1:A:261:ILE:HG21	0.48	2.48	2	1
1:A:466:GLN:HG3	1:A:470:LEU:HD23	0.48	1.83	5	1
1:A:424:TRP:HH2	1:A:447:LEU:HD13	0.48	1.68	10	1
1:A:369:ALA:O	1:A:372:TYR:HB3	0.48	2.08	6	9
1:A:263:MET:HE1	1:A:289:VAL:HG21	0.48	1.85	15	3
1:A:267:LEU:H	1:A:276:TYR:HA	0.48	1.68	6	1
1:A:511:ALA:O	1:A:515:MET:HG3	0.48	2.09	14	13
1:A:314:HIS:HB3	1:A:317:LEU:HD12	0.48	1.83	8	1
1:A:487:VAL:HG22	1:A:515:MET:SD	0.48	2.48	6	1
1:A:341:ASN:HB3	1:A:386:ARG:HA	0.48	1.85	14	1
1:A:463:ASP:HB3	1:A:466:GLN:HE21	0.48	1.68	20	1
1:A:354:VAL:HG13	1:A:358:VAL:HB	0.48	1.86	16	7
1:A:362:MET:HB2	1:A:396:VAL:HG21	0.48	1.85	15	8
1:A:370:MET:HA	1:A:373:LEU:HD13	0.48	1.85	7	3
1:A:444:PHE:CE2	1:A:508:ILE:HG21	0.48	2.44	17	9
1:A:442:TRP:HB2	1:A:502:ARG:NH2	0.48	2.23	2	1
1:A:379:ILE:HD11	1:A:440:ASP:HB2	0.48	1.84	3	1
1:A:306:ALA:HB2	1:A:332:ILE:HG21	0.48	1.86	4	4
1:A:424:TRP:HH2	1:A:447:LEU:HB2	0.48	1.69	6	3
1:A:292:LEU:HD23	1:A:292:LEU:H	0.47	1.69	15	2
1:A:505:PHE:HD1	1:A:508:ILE:HD12	0.47	1.70	7	3
1:A:403:LEU:HD22	1:A:406:LEU:HD13	0.47	1.86	3	1
1:A:275:VAL:HG21	1:A:401:PHE:HB3	0.47	1.85	3	3
1:A:456:MET:SD	1:A:457:SER:O	0.47	2.73	10	3
1:A:401:PHE:HB2	1:A:403:LEU:HG	0.47	1.87	10	2
1:A:426:ALA:O	1:A:430:LEU:HG	0.46	2.10	5	5
1:A:297:MET:SD	1:A:297:MET:N	0.46	2.88	2	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:343:LEU:HA	1:A:346:LEU:HD12	0.46	1.87	17	2
1:A:367:SER:HA	1:A:505:PHE:HD1	0.46	1.70	3	3
1:A:384:ALA:HB1	1:A:386:ARG:NH1	0.46	2.24	14	1
1:A:303:LEU:HD22	1:A:330:PHE:CE2	0.46	2.45	16	5
1:A:459:TYR:HB3	1:A:462:ILE:HD11	0.46	1.86	10	2
1:A:381:ARG:HH22	1:A:443:ALA:HB2	0.46	1.70	18	1
1:A:470:LEU:HD13	1:A:475:TYR:CD1	0.46	2.45	6	5
1:A:312:ILE:HG13	1:A:317:LEU:HD13	0.46	1.88	12	2
1:A:437:ILE:O	1:A:441:VAL:HG23	0.46	2.11	2	9
1:A:361:TYR:O	1:A:365:GLN:HG2	0.45	2.11	13	6
1:A:342:LEU:HD12	1:A:346:LEU:HD11	0.45	1.87	11	7
1:A:386:ARG:HD2	1:A:403:LEU:HD22	0.45	1.87	6	1
1:A:380:HIS:ND1	1:A:381:ARG:N	0.45	2.65	13	1
1:A:359:LEU:HD22	1:A:451:ILE:CG2	0.45	2.42	3	9
1:A:343:LEU:HD22	1:A:344:ASP:N	0.45	2.26	6	1
1:A:341:ASN:N	1:A:341:ASN:HD22	0.45	2.09	15	1
1:A:362:MET:HB2	1:A:396:VAL:CG2	0.45	2.42	12	7
1:A:343:LEU:HD23	1:A:386:ARG:HH21	0.45	1.72	15	1
1:A:459:TYR:CE1	1:A:471:LEU:HD21	0.45	2.47	17	2
1:A:477:MET:SD	1:A:477:MET:N	0.45	2.89	16	2
1:A:314:HIS:HB2	1:A:317:LEU:HB2	0.45	1.88	16	1
1:A:264:LYS:HB2	1:A:277:GLU:HG3	0.45	1.88	2	2
1:A:342:LEU:HB2	1:A:385:ALA:O	0.45	2.12	1	2
1:A:444:PHE:HB2	1:A:505:PHE:HE1	0.45	1.72	17	1
1:A:387:ASN:HB3	1:A:403:LEU:HD11	0.44	1.89	10	1
1:A:375:LYS:HA	1:A:375:LYS:HE2	0.44	1.90	4	1
1:A:304:LYS:HE3	1:A:304:LYS:HA	0.44	1.89	11	1
1:A:449:TRP:CE2	1:A:477:MET:HG2	0.44	2.48	7	1
1:A:257:GLU:HG2	1:A:327:GLU:HG3	0.44	1.87	11	1
1:A:480:PRO:HB2	1:A:483:CYS:HB3	0.44	1.88	8	1
1:A:442:TRP:CD1	1:A:495:TRP:HA	0.44	2.48	12	1
1:A:335:GLU:HG2	1:A:337:MET:SD	0.44	2.53	13	2
1:A:469:GLU:O	1:A:473:LYS:HG2	0.44	2.13	16	1
1:A:426:ALA:HB2	1:A:442:TRP:CD2	0.43	2.47	17	1
1:A:466:GLN:O	1:A:470:LEU:HG	0.43	2.13	1	1
1:A:491:MET:SD	1:A:495:TRP:CH2	0.43	3.11	1	1
1:A:362:MET:O	1:A:366:ILE:HG13	0.43	2.14	6	6
1:A:437:ILE:HD11	1:A:505:PHE:CD2	0.43	2.48	1	1
1:A:263:MET:SD	1:A:276:TYR:CE1	0.43	3.12	18	1
1:A:383:LEU:HA	1:A:387:ASN:HD21	0.43	1.74	7	1
1:A:343:LEU:HB2	1:A:386:ARG:NH2	0.43	2.28	1	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:303:LEU:HD23	1:A:303:LEU:N	0.43	2.28	14	2
1:A:372:TYR:HD2	1:A:373:LEU:HD12	0.43	1.73	12	1
1:A:490:LEU:HD21	1:A:512:PHE:CZ	0.43	2.48	4	1
1:A:424:TRP:CH2	1:A:458:PRO:HG3	0.43	2.49	13	1
1:A:318:VAL:CG2	1:A:399:ALA:HB2	0.43	2.44	15	5
1:A:426:ALA:HB2	1:A:442:TRP:HB3	0.43	1.90	7	1
1:A:422:ILE:HG13	1:A:464:LEU:HD21	0.43	1.91	9	1
1:A:271:GLN:HG3	1:A:402:GLY:HA3	0.42	1.91	1	1
1:A:487:VAL:HA	1:A:515:MET:HE1	0.42	1.91	7	1
1:A:308:VAL:O	1:A:311:GLU:HG2	0.42	2.14	9	1
1:A:438:LYS:HD2	1:A:499:PRO:HB2	0.42	1.91	6	1
1:A:317:LEU:CD2	1:A:369:ALA:HB1	0.42	2.44	12	2
1:A:351:ARG:HD3	1:A:352:GLN:H	0.42	1.73	12	1
1:A:370:MET:HB3	1:A:505:PHE:CD1	0.42	2.50	14	1
1:A:381:ARG:HG2	1:A:435:PHE:CD1	0.42	2.50	4	1
1:A:385:ALA:N	1:A:447:LEU:HD13	0.42	2.30	5	2
1:A:496:GLN:NE2	1:A:502:ARG:HB2	0.42	2.30	14	1
1:A:366:ILE:HD11	1:A:396:VAL:HG11	0.42	1.91	17	3
1:A:476:ARG:HA	1:A:495:TRP:CZ3	0.42	2.49	6	2
1:A:312:ILE:HD13	1:A:317:LEU:HD13	0.42	1.91	16	1
1:A:457:SER:HB2	1:A:460:PRO:HB3	0.42	1.92	19	2
1:A:279:VAL:HG13	1:A:286:THR:HA	0.42	1.92	18	2
1:A:484:PRO:HG2	1:A:487:VAL:HG23	0.42	1.92	9	1
1:A:496:GLN:HG2	1:A:502:ARG:HB2	0.42	1.91	17	1
1:A:422:ILE:HG21	1:A:464:LEU:HD11	0.42	1.92	8	1
1:A:282:LYS:HG2	1:A:283:TYR:H	0.42	1.74	12	1
1:A:343:LEU:HB2	1:A:386:ARG:HH21	0.42	1.75	1	1
1:A:268:GLY:HA3	1:A:406:LEU:HD12	0.42	1.92	4	1
1:A:316:ASN:ND2	1:A:369:ALA:HB2	0.42	2.30	8	1
1:A:272:TYR:O	1:A:293:LYS:HG3	0.41	2.14	3	1
1:A:297:MET:N	1:A:297:MET:SD	0.41	2.93	11	1
1:A:449:TRP:CZ2	1:A:477:MET:HG3	0.41	2.50	3	1
1:A:279:VAL:HB	1:A:280:TRP:H	0.41	1.63	15	1
1:A:426:ALA:HB2	1:A:442:TRP:CE3	0.41	2.50	16	1
1:A:473:LYS:O	1:A:474:ASP:HB2	0.41	2.16	4	2
1:A:437:ILE:HD11	1:A:505:PHE:CE2	0.41	2.50	15	1
1:A:449:TRP:HB2	1:A:491:MET:SD	0.41	2.56	8	2
1:A:289:VAL:HG11	1:A:331:TYR:HD2	0.41	1.75	8	1
1:A:442:TRP:HZ2	1:A:471:LEU:HD22	0.41	1.75	11	1
1:A:351:ARG:HD2	1:A:352:GLN:N	0.41	2.30	14	2
1:A:281:LYS:HD3	1:A:281:LYS:H	0.41	1.75	18	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:428:GLU:HG3	1:A:429:SER:N	0.41	2.31	3	1
1:A:511:ALA:O	1:A:514:THR:HB	0.41	2.16	4	1
1:A:293:LYS:NZ	1:A:295:ASP:HB3	0.41	2.31	5	1
1:A:387:ASN:HB2	1:A:400:ASP:HA	0.41	1.91	17	1
1:A:309:LEU:HB3	1:A:320:LEU:HB2	0.41	1.93	19	1
1:A:496:GLN:O	1:A:502:ARG:HD2	0.41	2.16	20	1
1:A:449:TRP:CH2	1:A:480:PRO:HD3	0.41	2.51	15	1
1:A:384:ALA:HA	1:A:424:TRP:CZ3	0.41	2.51	18	1
1:A:343:LEU:HD23	1:A:386:ARG:HE	0.40	1.75	1	1
1:A:446:VAL:HG13	1:A:477:MET:HE1	0.40	1.94	5	1
1:A:297:MET:HB3	1:A:299:VAL:HG12	0.40	1.93	17	1
1:A:496:GLN:HB3	1:A:502:ARG:HH21	0.40	1.76	18	1
1:A:373:LEU:HB3	1:A:378:PHE:CD1	0.40	2.52	13	1
1:A:375:LYS:NZ	1:A:375:LYS:HB2	0.40	2.30	19	1
1:A:384:ALA:HB2	1:A:424:TRP:CZ2	0.40	2.52	5	1
1:A:422:ILE:HD12	1:A:464:LEU:HD11	0.40	1.92	12	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	249/287 (87%)	231±2 (93±1%)	13±2 (5±1%)	6±1 (2±0%)	9	48
All	All	4980/5740 (87%)	4616 (93%)	250 (5%)	114 (2%)	9	48

All 11 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	329	PRO	20
1	A	279	VAL	20
1	A	328	PRO	20
1	A	474	ASP	20
1	A	299	VAL	17
1	A	301	GLU	6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	460	PRO	5
1	A	422	ILE	3
1	A	499	PRO	1
1	A	300	GLU	1
1	A	517	GLN	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	221/252 (88%)	200±3 (91±1%)	21±3 (9±1%)	12	58
All	All	4420/5040 (88%)	4006 (91%)	414 (9%)	12	58

All 89 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	285	LEU	20
1	A	360	LEU	20
1	A	342	LEU	20
1	A	490	LEU	20
1	A	422	ILE	20
1	A	403	LEU	19
1	A	279	VAL	19
1	A	343	LEU	16
1	A	405	ARG	15
1	A	303	LEU	12
1	A	276	TYR	11
1	A	263	MET	10
1	A	476	ARG	10
1	A	502	ARG	7
1	A	477	MET	7
1	A	378	PHE	6
1	A	257	GLU	6
1	A	516	PHE	6
1	A	374	GLU	6
1	A	314	HIS	6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	381	ARG	5
1	A	437	ILE	5
1	A	258	ARG	5
1	A	353	GLU	5
1	A	428	GLU	4
1	A	485	GLU	4
1	A	282	LYS	4
1	A	294	GLU	4
1	A	397	LYS	4
1	A	372	TYR	4
1	A	326	ARG	4
1	A	269	GLU	4
1	A	352	GLN	3
1	A	424	TRP	3
1	A	293	LYS	3
1	A	300	GLU	3
1	A	386	ARG	3
1	A	392	GLU	3
1	A	496	GLN	3
1	A	341	ASN	3
1	A	304	LYS	3
1	A	264	LYS	3
1	A	347	ARG	3
1	A	478	GLU	3
1	A	371	GLU	3
1	A	329	PRO	3
1	A	510	GLN	3
1	A	266	LYS	3
1	A	475	TYR	2
1	A	319	GLN	2
1	A	292	LEU	2
1	A	377	ASN	2
1	A	498	ASN	2
1	A	438	LYS	2
1	A	364	THR	2
1	A	375	LYS	2
1	A	280	TRP	2
1	A	481	GLU	2
1	A	433	ASN	2
1	A	507	GLU	2
1	A	350	ASN	2
1	A	311	GLU	2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	313	LYS	2
1	A	472	GLU	2
1	A	271	GLN	2
1	A	351	ARG	1
1	A	406	LEU	1
1	A	255	GLU	1
1	A	488	TYR	1
1	A	305	GLU	1
1	A	277	GLU	1
1	A	479	ARG	1
1	A	345	TYR	1
1	A	423	LYS	1
1	A	440	ASP	1
1	A	272	TYR	1
1	A	327	GLU	1
1	A	281	LYS	1
1	A	429	SER	1
1	A	376	LYS	1
1	A	297	MET	1
1	A	486	LYS	1
1	A	355	ASN	1
1	A	514	THR	1
1	A	517	GLN	1
1	A	328	PRO	1
1	A	395	LEU	1
1	A	450	GLU	1
1	A	382	ASP	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 monosaccharides in this entry.

6.6 Ligand geometry

There are no ligands in this entry.

6.7 Other polymers

There are no such molecules in this entry.

6.8 Polymer linkage issues

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 9% for the well-defined parts and 8% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: 07112020_inactive2_BMRB.cs.str

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	553
Number of shifts mapped to atoms	553
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	3

7.1.2 Chemical shift referencing

No chemical shift referencing corrections were calculated (not enough data).

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 9%, i.e. 272 atoms were assigned a chemical shift out of a possible 3192. 0 out of 44 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	0/1225 (0%)	0/488 (0%)	0/498 (0%)	0/239 (0%)
Sidechain	214/1641 (13%)	105/964 (11%)	109/610 (18%)	0/67 (0%)
Aromatic	58/326 (18%)	44/168 (26%)	14/141 (10%)	0/17 (0%)
Overall	272/3192 (9%)	149/1620 (9%)	123/1249 (10%)	0/323 (0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 8%, i.e. 294 atoms were assigned a chemical shift out of a possible 3625. 0 out of 47 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	0/1411 (0%)	0/562 (0%)	0/574 (0%)	0/275 (0%)
Sidechain	236/1847 (13%)	116/1086 (11%)	120/688 (17%)	0/73 (0%)
Aromatic	58/367 (16%)	44/189 (23%)	14/159 (9%)	0/19 (0%)
Overall	294/3625 (8%)	160/1837 (9%)	134/1421 (9%)	0/367 (0%)

7.1.4 Statistically unusual chemical shifts [i](#)

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	453	THR	HG21	-0.20	2.29 – -0.01	-5.8
1	A	453	THR	HG22	-0.20	2.29 – -0.01	-5.8
1	A	453	THR	HG23	-0.20	2.29 – -0.01	-5.8

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

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:

