



Full wwPDB NMR Structure Validation Report ⓘ

Oct 10, 2021 – 09:05 PM EDT

PDB ID : 2K7Z
Title : Solution Structure of the Catalytic Domain of Procaspase-8
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Deposited on : 2008-08-28

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:

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 : 2.23.2
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.23.2

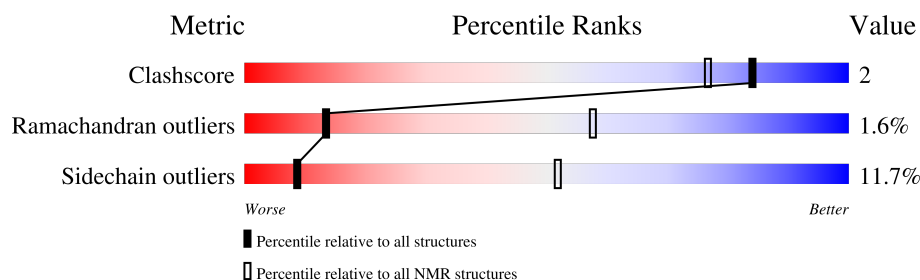
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 80%.

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	266	

2 Ensemble composition and analysis

This entry contains 20 models. Model 1 is the overall representative, medoid model (most similar to other models).

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:225-A:251, A:264-A:361, A:394-A:404, A:421-A:446, A:464-A:479 (178)	1.24	1

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 and 2 single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 3622 atoms, of which 1795 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Caspase-8.

Mol	Chain	Residues	Atoms						Trace
1	A	229	Total	C	H	N	O	S	0
			3622	1160	1795	305	349	13	

There are 4 discrepancies between the modelled and reference sequences:

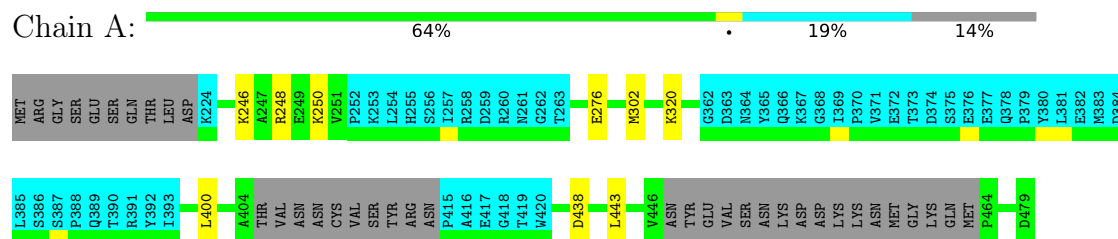
Chain	Residue	Modelled	Actual	Comment	Reference
A	214	MET	-	expression tag	UNP Q14790
A	215	ARG	-	expression tag	UNP Q14790
A	216	GLY	-	expression tag	UNP Q14790
A	360	ALA	CYS	engineered mutation	UNP Q14790

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: Caspase-8

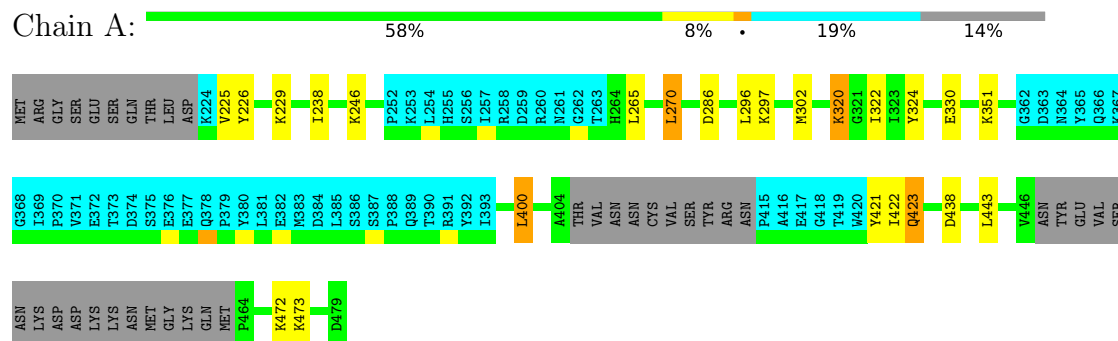


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1 (medoid)

- Molecule 1: Caspase-8



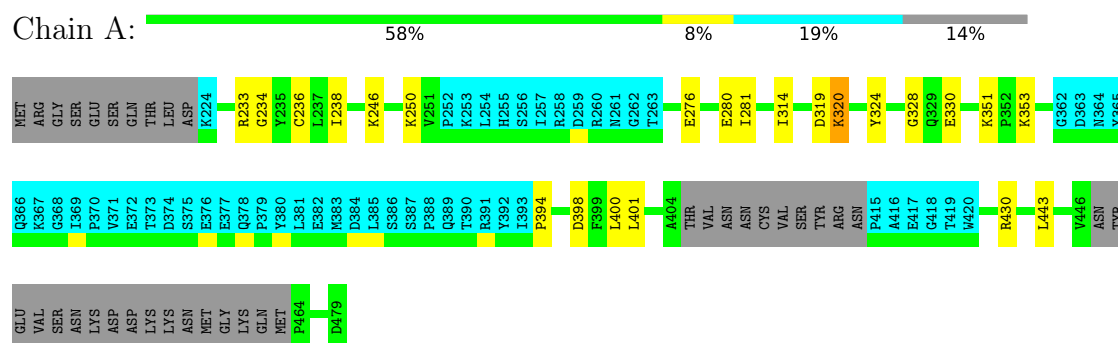
4.2.2 Score per residue for model 2

- Molecule 1: Caspase-8



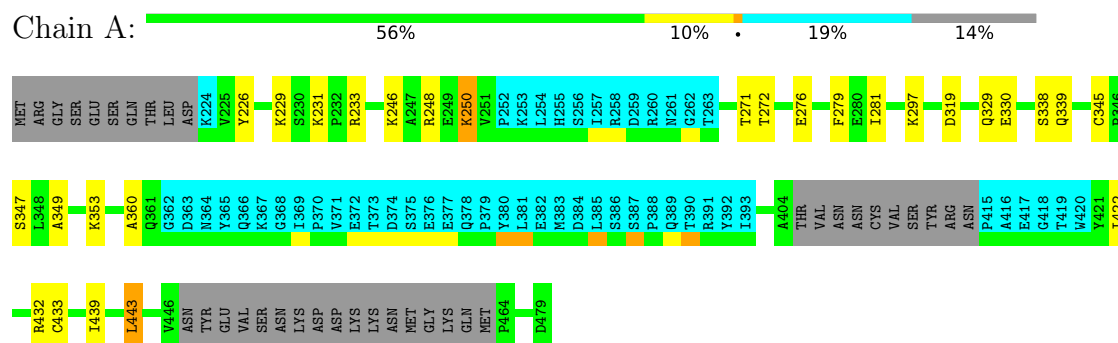
4.2.3 Score per residue for model 3

- Molecule 1: Caspase-8



4.2.4 Score per residue for model 4

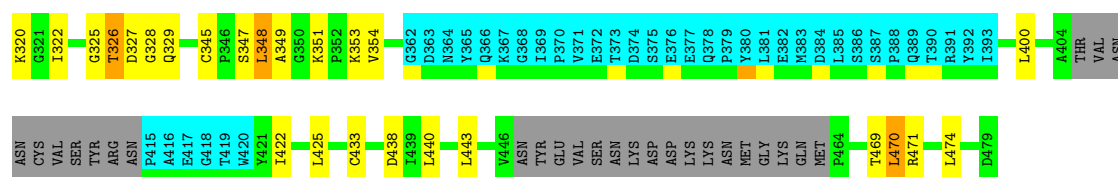
- Molecule 1: Caspase-8



4.2.5 Score per residue for model 5

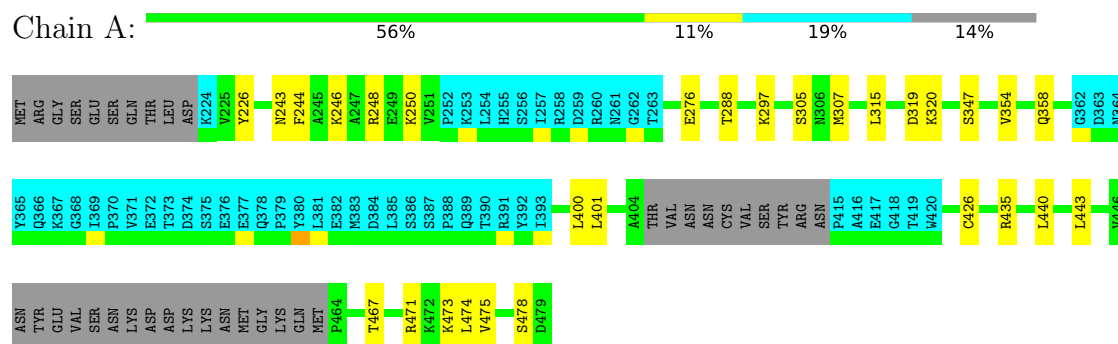
- Molecule 1: Caspase-8





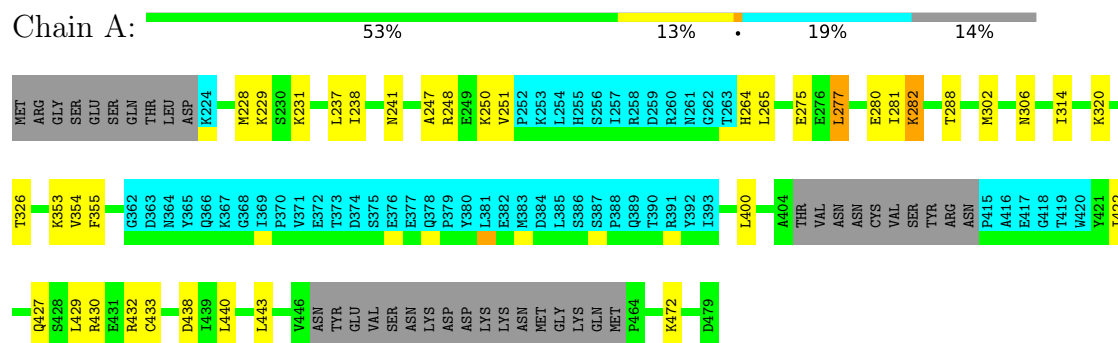
4.2.9 Score per residue for model 9

- Molecule 1: Caspase-8



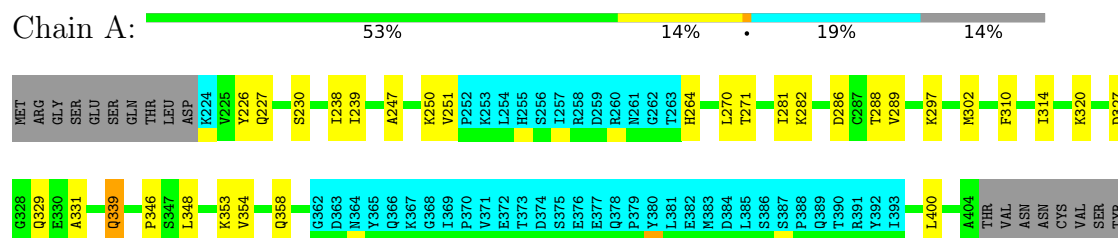
4.2.10 Score per residue for model 10

- Molecule 1: Caspase-8



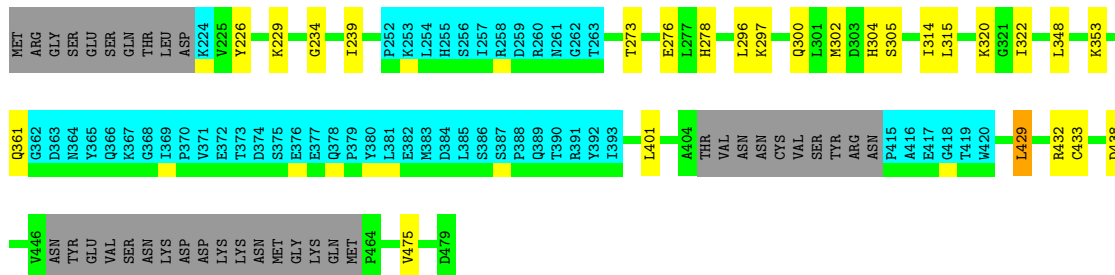
4.2.11 Score per residue for model 11

- Molecule 1: Caspase-8



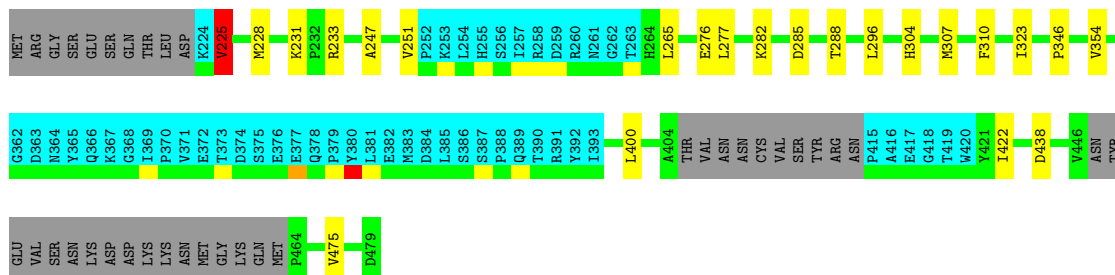
4.2.12 Score per residue for model 12

- Molecule 1: Caspase-8



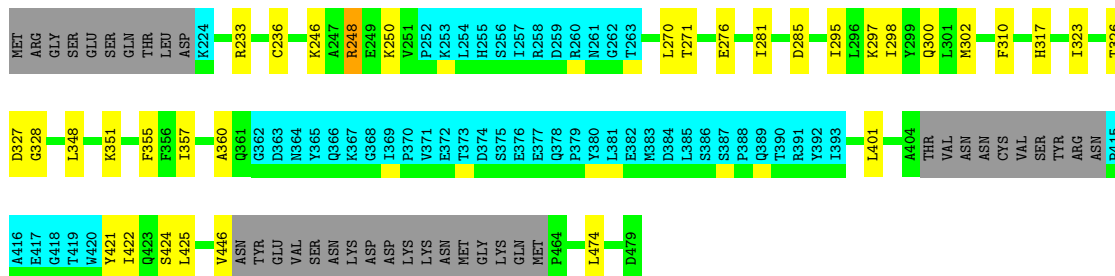
4.2.13 Score per residue for model 13

- Molecule 1: Caspase-8



4.2.14 Score per residue for model 14

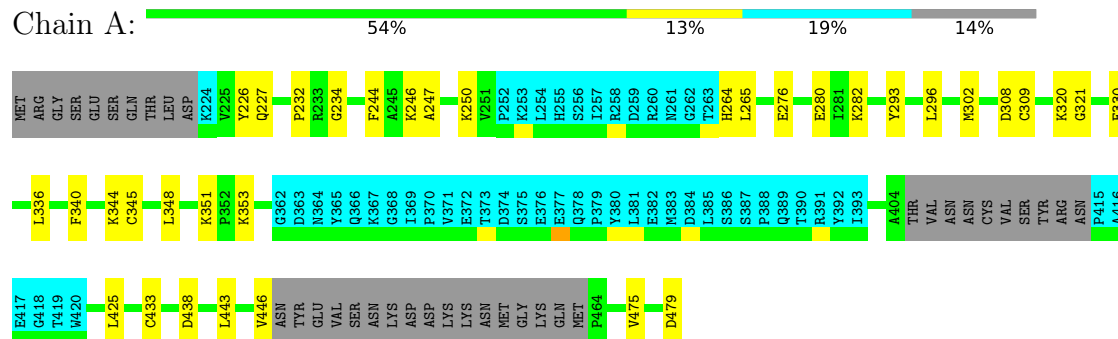
- Molecule 1: Caspase-8



4.2.15 Score per residue for model 15

- Molecule 1: Caspase-8

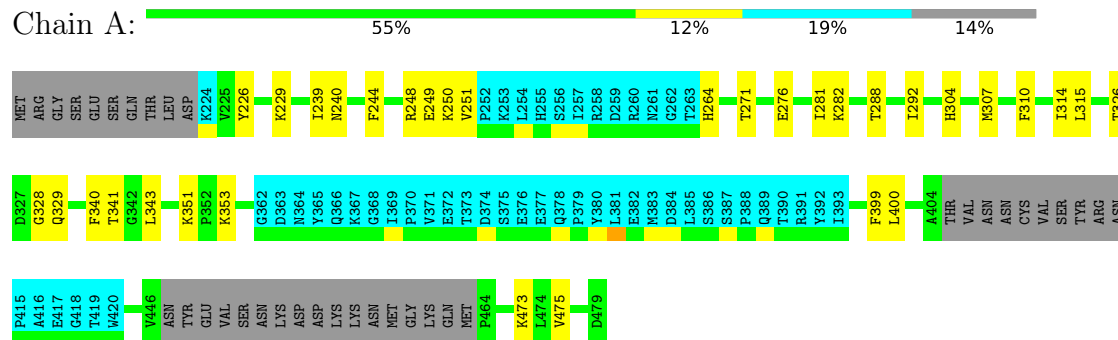
Chain A:



4.2.16 Score per residue for model 16

- Molecule 1: Caspase-8

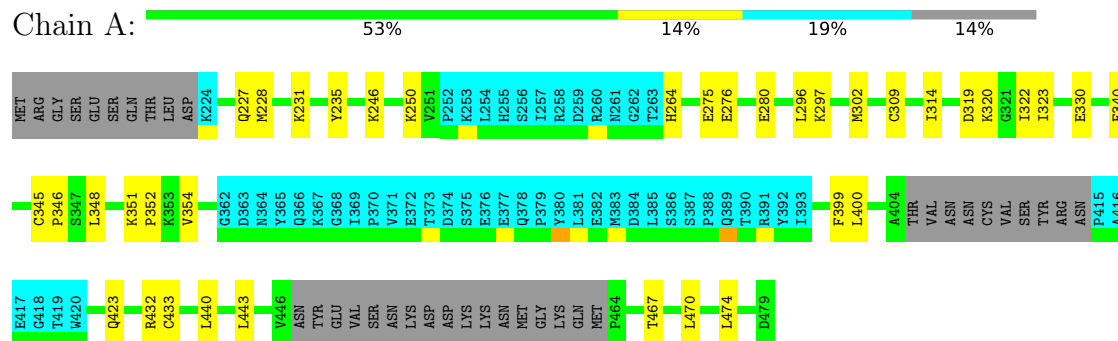
Chain A:



4.2.17 Score per residue for model 17

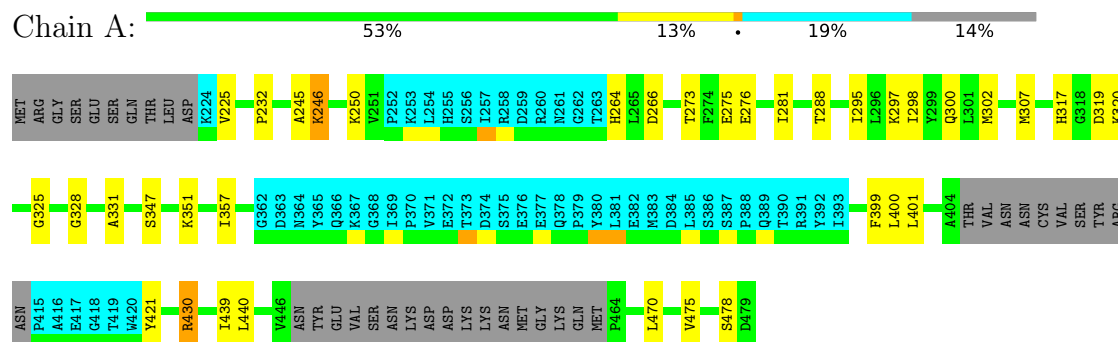
- Molecule 1: Caspase-8

Chain A:



4.2.18 Score per residue for model 18

• Molecule 1: Caspase-8



5 Refinement protocol and experimental data overview

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

Of the 200 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
Amber	geometry optimization	6.0
CYANA	structure solution	2.2
CYANA	refinement	2.2

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	2477
Number of shifts mapped to atoms	2477
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	80%

6 Model quality

6.1 Standard geometry

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	0.66±0.01	0±0/1446 (0.0± 0.0%)	0.87±0.01	0±1/1951 (0.0± 0.0%)
All	All	0.66	0/28920 (0.0%)	0.87	8/39020 (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	0.1±0.2
All	All	0	1

There are no bond-length outliers.

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	432	ARG	NE-CZ-NH1	7.74	124.17	120.30	5	1
1	A	432	ARG	NE-CZ-NH2	-6.61	117.00	120.30	5	1
1	A	430	ARG	NE-CZ-NH1	6.43	123.52	120.30	18	1
1	A	435	ARG	NE-CZ-NH1	5.57	123.08	120.30	9	2
1	A	248	ARG	NE-CZ-NH1	5.55	123.08	120.30	8	1
1	A	327	ASP	CB-CG-OD2	-5.30	113.53	118.30	11	1
1	A	471	ARG	NE-CZ-NH1	5.08	122.84	120.30	8	1

There are no chirality outliers.

All unique planar outliers are listed below.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	421	TYR	Sidechain	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	1416	1407	1407	6±3
All	All	28320	28140	28140	129

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:400:LEU:HD11	1:A:443:LEU:HD11	0.91	1.42	9	4
1:A:354:VAL:HG23	1:A:400:LEU:HD12	0.79	1.55	20	1
1:A:354:VAL:HG13	1:A:400:LEU:HD12	0.77	1.53	9	5
1:A:277:LEU:HD11	1:A:433:CYS:HB3	0.67	1.65	19	1
1:A:271:THR:HG23	1:A:281:ILE:HG21	0.66	1.67	16	6
1:A:400:LEU:HD11	1:A:443:LEU:CD1	0.64	2.23	20	1
1:A:440:LEU:HD11	1:A:470:LEU:HD13	0.62	1.70	5	1
1:A:238:ILE:HD12	1:A:270:LEU:HD13	0.61	1.70	6	1
1:A:225:VAL:HG21	1:A:475:VAL:HG23	0.60	1.71	13	1
1:A:440:LEU:HD13	1:A:470:LEU:HD12	0.59	1.74	18	1
1:A:438:ASP:HA	1:A:475:VAL:HG22	0.58	1.75	5	1
1:A:404:ALA:HB3	1:A:467:THR:HG22	0.56	1.76	7	1
1:A:438:ASP:HB3	1:A:475:VAL:HG22	0.56	1.78	11	4
1:A:444:THR:HG22	1:A:466:PRO:HB2	0.56	1.77	20	1
1:A:331:ALA:HB1	1:A:336:LEU:HD11	0.54	1.80	20	1
1:A:239:ILE:HG21	1:A:292:ILE:HD11	0.54	1.77	16	2
1:A:340:PHE:O	1:A:349:ALA:HB2	0.53	2.03	2	1
1:A:400:LEU:HD23	1:A:440:LEU:HD23	0.53	1.78	8	1
1:A:289:VAL:HG11	1:A:329:GLN:HB2	0.53	1.78	11	1
1:A:440:LEU:HD11	1:A:470:LEU:CD1	0.53	2.34	5	1
1:A:331:ALA:HB3	1:A:336:LEU:HD11	0.53	1.78	19	1
1:A:444:THR:HG22	1:A:466:PRO:CB	0.52	2.35	20	1
1:A:354:VAL:CG2	1:A:474:LEU:HD21	0.52	2.35	17	1
1:A:400:LEU:HD21	1:A:443:LEU:HD11	0.51	1.82	10	1
1:A:239:ILE:HD13	1:A:314:ILE:CD1	0.51	2.36	12	2
1:A:438:ASP:CB	1:A:475:VAL:HG22	0.51	2.35	13	3
1:A:289:VAL:CG2	1:A:331:ALA:HB2	0.51	2.36	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:225:VAL:HG23	1:A:475:VAL:HG21	0.49	1.84	18	1
1:A:352:PRO:HB3	1:A:470:LEU:HD23	0.49	1.84	2	2
1:A:281:ILE:HD12	1:A:281:ILE:H	0.49	1.67	18	1
1:A:440:LEU:HD21	1:A:470:LEU:HD13	0.48	1.84	2	1
1:A:323:ILE:HD12	1:A:323:ILE:H	0.48	1.68	17	1
1:A:355:PHE:HB2	1:A:401:LEU:HD12	0.47	1.86	14	1
1:A:239:ILE:HD13	1:A:314:ILE:HD13	0.47	1.87	12	1
1:A:247:ALA:HB1	1:A:251:VAL:HG23	0.47	1.87	10	1
1:A:279:PHE:CE1	1:A:281:ILE:HD11	0.47	2.44	2	2
1:A:273:THR:HG21	1:A:429:LEU:HD11	0.47	1.87	12	1
1:A:239:ILE:HG22	1:A:315:LEU:HD13	0.46	1.85	5	1
1:A:225:VAL:HG23	1:A:473:LYS:HG2	0.46	1.87	2	1
1:A:354:VAL:HG13	1:A:400:LEU:HD23	0.46	1.88	10	1
1:A:360:ALA:CB	1:A:422:ILE:HG21	0.46	2.40	4	1
1:A:303:ASP:HA	1:A:348:LEU:HD21	0.45	1.86	8	1
1:A:236:CYS:SG	1:A:281:ILE:HG23	0.45	2.51	14	1
1:A:288:THR:HA	1:A:326:THR:HG21	0.45	1.88	8	1
1:A:273:THR:HG21	1:A:430:ARG:HB2	0.45	1.87	20	1
1:A:345:CYS:O	1:A:349:ALA:HB2	0.45	2.12	8	2
1:A:326:THR:HG22	1:A:328:GLY:H	0.45	1.71	14	1
1:A:422:ILE:HG22	1:A:425:LEU:HD13	0.45	1.88	14	1
1:A:400:LEU:HD13	1:A:440:LEU:HD23	0.45	1.89	10	1
1:A:422:ILE:HD12	1:A:422:ILE:H	0.44	1.72	19	2
1:A:400:LEU:CD1	1:A:443:LEU:HD11	0.44	2.41	2	1
1:A:354:VAL:HG13	1:A:400:LEU:HD11	0.44	1.87	6	1
1:A:401:LEU:HD22	1:A:467:THR:HB	0.44	1.89	9	1
1:A:238:ILE:HD13	1:A:270:LEU:HB2	0.44	1.89	1	1
1:A:348:LEU:HD23	1:A:351:LYS:CE	0.44	2.42	14	1
1:A:289:VAL:HG12	1:A:293:TYR:CE1	0.44	2.48	19	1
1:A:247:ALA:HB2	1:A:327:ASP:OD2	0.44	2.13	5	1
1:A:225:VAL:HG22	1:A:226:TYR:CD2	0.44	2.48	1	1
1:A:239:ILE:HG21	1:A:292:ILE:CD1	0.44	2.43	16	1
1:A:237:LEU:HD13	1:A:282:LYS:HB3	0.43	1.91	10	1
1:A:277:LEU:HD21	1:A:433:CYS:HB3	0.43	1.90	10	1
1:A:238:ILE:C	1:A:239:ILE:HD12	0.43	2.34	11	1
1:A:251:VAL:CG2	1:A:322:ILE:HD13	0.43	2.43	2	1
1:A:238:ILE:HD12	1:A:281:ILE:HG21	0.43	1.90	3	2
1:A:348:LEU:HD23	1:A:351:LYS:HE2	0.43	1.91	14	1
1:A:438:ASP:OD1	1:A:473:LYS:HE3	0.43	2.14	7	1
1:A:360:ALA:HB2	1:A:422:ILE:HD11	0.43	1.90	14	1
1:A:352:PRO:CB	1:A:470:LEU:HD23	0.42	2.44	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:394:PRO:HD2	1:A:401:LEU:HD22	0.42	1.91	3	1
1:A:422:ILE:HD12	1:A:425:LEU:HD23	0.42	1.91	8	1
1:A:425:LEU:HD13	1:A:446:VAL:HG11	0.42	1.91	15	1
1:A:225:VAL:HG21	1:A:473:LYS:HG2	0.42	1.89	20	1
1:A:438:ASP:OD2	1:A:473:LYS:HE3	0.42	2.15	1	1
1:A:400:LEU:HD23	1:A:440:LEU:HD22	0.42	1.90	20	1
1:A:295:ILE:HA	1:A:298:ILE:HD12	0.42	1.92	14	3
1:A:247:ALA:HB1	1:A:251:VAL:CG2	0.42	2.45	11	2
1:A:281:ILE:HG22	1:A:283:PRO:HD3	0.42	1.90	20	1
1:A:239:ILE:HD13	1:A:314:ILE:HG23	0.42	1.92	8	1
1:A:473:LYS:HG2	1:A:475:VAL:HG23	0.42	1.91	9	1
1:A:244:PHE:HA	1:A:247:ALA:HB3	0.42	1.91	15	1
1:A:400:LEU:HB2	1:A:470:LEU:HD11	0.42	1.92	18	1
1:A:237:LEU:HD23	1:A:310:PHE:CZ	0.42	2.50	8	1
1:A:440:LEU:HD23	1:A:470:LEU:HD13	0.41	1.91	17	1
1:A:400:LEU:HD21	1:A:443:LEU:CD1	0.41	2.45	5	2
1:A:341:THR:HG22	1:A:343:LEU:H	0.41	1.75	16	1
1:A:225:VAL:HG11	1:A:475:VAL:HB	0.41	1.91	5	1
1:A:293:TYR:CE1	1:A:336:LEU:HD21	0.41	2.50	15	1
1:A:245:ALA:O	1:A:246:LYS:HE2	0.41	2.16	18	1
1:A:424:SER:HB2	1:A:446:VAL:HG13	0.41	1.93	14	1
1:A:473:LYS:HE3	1:A:475:VAL:CG2	0.41	2.44	16	1
1:A:273:THR:HG23	1:A:430:ARG:HB3	0.41	1.92	2	1
1:A:226:TYR:HE1	1:A:475:VAL:HG21	0.41	1.76	15	1
1:A:273:THR:HG23	1:A:430:ARG:CB	0.41	2.46	18	1
1:A:319:ASP:OD1	1:A:320:LYS:HE3	0.41	2.16	3	1
1:A:314:ILE:HD13	1:A:355:PHE:CE1	0.41	2.51	10	1
1:A:354:VAL:HG13	1:A:400:LEU:CD2	0.40	2.46	10	1
1:A:225:VAL:HG22	1:A:228:MET:CE	0.40	2.46	5	1
1:A:440:LEU:HD21	1:A:470:LEU:CD1	0.40	2.46	8	1
1:A:440:LEU:HD21	1:A:474:LEU:HB3	0.40	1.92	9	1
1:A:357:ILE:HG21	1:A:403:MET:CG	0.40	2.46	19	1
1:A:317:HIS:HB2	1:A:357:ILE:HD11	0.40	1.93	14	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	174/266 (65%)	151±4 (87±2%)	21±4 (12±2%)	3±2 (2±1%)	13	57
All	All	3480/5320 (65%)	3012 (87%)	411 (12%)	57 (2%)	13	57

All 35 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	234	GLY	4
1	A	328	GLY	4
1	A	347	SER	4
1	A	286	ASP	3
1	A	232	PRO	3
1	A	346	PRO	3
1	A	229	LYS	2
1	A	423	GLN	2
1	A	248	ARG	2
1	A	443	LEU	2
1	A	285	ASP	2
1	A	325	GLY	2
1	A	422	ILE	2
1	A	320	LYS	1
1	A	226	TYR	1
1	A	465	GLN	1
1	A	324	TYR	1
1	A	241	ASN	1
1	A	336	LEU	1
1	A	442	ILE	1
1	A	444	THR	1
1	A	306	ASN	1
1	A	432	ARG	1
1	A	339	GLN	1
1	A	225	VAL	1
1	A	233	ARG	1
1	A	323	ILE	1
1	A	264	HIS	1
1	A	321	GLY	1
1	A	345	CYS	1
1	A	227	GLN	1
1	A	228	MET	1
1	A	280	GLU	1
1	A	309	CYS	1

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Mol	Chain	Res	Type	Models (Total)
1	A	331	ALA	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	158/239 (66%)	139±4 (88±3%)	19±4 (12±3%)	9	52
All	All	3160/4780 (66%)	2789 (88%)	371 (12%)	9	52

All 102 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	276	GLU	14
1	A	302	MET	13
1	A	250	LYS	12
1	A	246	LYS	11
1	A	320	LYS	11
1	A	353	LYS	10
1	A	296	LEU	9
1	A	297	LYS	9
1	A	231	LYS	9
1	A	248	ARG	9
1	A	351	LYS	8
1	A	288	THR	8
1	A	400	LEU	7
1	A	443	LEU	7
1	A	226	TYR	6
1	A	433	CYS	6
1	A	264	HIS	6
1	A	322	ILE	5
1	A	330	GLU	5
1	A	280	GLU	5
1	A	314	ILE	5
1	A	329	GLN	5
1	A	471	ARG	5
1	A	229	LYS	5

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Mol	Chain	Res	Type	Models (Total)
1	A	319	ASP	5
1	A	265	LEU	5
1	A	315	LEU	5
1	A	399	PHE	5
1	A	307	MET	5
1	A	348	LEU	5
1	A	282	LYS	5
1	A	270	LEU	4
1	A	472	LYS	4
1	A	317	HIS	4
1	A	438	ASP	4
1	A	432	ARG	4
1	A	326	THR	4
1	A	470	LEU	4
1	A	310	PHE	4
1	A	421	TYR	3
1	A	423	GLN	3
1	A	227	GLN	3
1	A	429	LEU	3
1	A	233	ARG	3
1	A	430	ARG	3
1	A	439	ILE	3
1	A	308	ASP	3
1	A	327	ASP	3
1	A	357	ILE	3
1	A	401	LEU	3
1	A	474	LEU	3
1	A	277	LEU	3
1	A	228	MET	3
1	A	305	SER	3
1	A	469	THR	3
1	A	275	GLU	3
1	A	300	GLN	3
1	A	304	HIS	3
1	A	340	PHE	3
1	A	272	THR	2
1	A	279	PHE	2
1	A	339	GLN	2
1	A	437	ASP	2
1	A	235	TYR	2
1	A	241	ASN	2
1	A	251	VAL	2

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Mol	Chain	Res	Type	Models (Total)
1	A	309	CYS	2
1	A	427	GLN	2
1	A	358	GLN	2
1	A	478	SER	2
1	A	324	TYR	1
1	A	422	ILE	1
1	A	395	ASP	1
1	A	425	LEU	1
1	A	236	CYS	1
1	A	398	ASP	1
1	A	338	SER	1
1	A	431	GLU	1
1	A	347	SER	1
1	A	316	SER	1
1	A	243	ASN	1
1	A	244	PHE	1
1	A	426	CYS	1
1	A	230	SER	1
1	A	354	VAL	1
1	A	445	GLU	1
1	A	278	HIS	1
1	A	361	GLN	1
1	A	225	VAL	1
1	A	285	ASP	1
1	A	323	ILE	1
1	A	344	LYS	1
1	A	479	ASP	1
1	A	240	ASN	1
1	A	345	CYS	1
1	A	467	THR	1
1	A	266	ASP	1
1	A	273	THR	1
1	A	444	THR	1
1	A	242	HIS	1
1	A	286	ASP	1
1	A	313	CYS	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 80% for the well-defined parts and 77% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	2477
Number of shifts mapped to atoms	2477
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	6

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	218	-0.13 ± 0.13	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	203	0.31 ± 0.09	None needed (< 0.5 ppm)
$^{13}\text{C}'$	208	0.58 ± 0.18	Should be applied
^{15}N	201	0.86 ± 0.35	Should be applied

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 80%, i.e. 1774 atoms were assigned a chemical shift out of a possible 2211. 21 out of 24 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	854/870 (98%)	337/346 (97%)	351/356 (99%)	166/168 (99%)
Sidechain	869/1153 (75%)	504/679 (74%)	362/430 (84%)	3/44 (7%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	51/188 (27%)	27/102 (26%)	24/80 (30%)	0/6 (0%)
Overall	1774/2211 (80%)	868/1127 (77%)	737/866 (85%)	169/218 (78%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 77%, i.e. 2204 atoms were assigned a chemical shift out of a possible 2845. 25 out of 28 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	1036/1115 (93%)	409/443 (92%)	426/458 (93%)	201/214 (94%)
Sidechain	1095/1499 (73%)	644/885 (73%)	445/553 (80%)	6/61 (10%)
Aromatic	73/231 (32%)	38/124 (31%)	34/99 (34%)	1/8 (12%)
Overall	2204/2845 (77%)	1091/1452 (75%)	905/1110 (82%)	208/283 (73%)

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	246	LYS	CE	58.01	46.00 – 37.80	19.6
1	A	422	ILE	CD1	29.95	21.91 – 5.01	9.8
1	A	248	ARG	NH1	111.52	94.37 – 52.87	9.1
1	A	260	ARG	NH1	111.52	94.37 – 52.87	9.1
1	A	472	LYS	HB2	-0.12	3.03 – 0.53	-7.6
1	A	260	ARG	HD2	1.64	4.27 – 1.97	-6.4

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:

