



Full wwPDB NMR Structure Validation Report ⓘ

Mar 9, 2026 – 06:00 AM UTC

PDB ID : 7CWH / pdb_00007cwh
BMRB ID : 36376
Title : Structural basis of RACK7 PHD to read a pediatric glioblastoma-associated histone mutation H3.3G34R
Authors : Lan, W.X.; Li, Z.; Jiao, F.F.; Wang, C.X.; Guo, R.; Cao, C.Y.
Deposited on : 2020-08-28

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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
wwPDB-ShiftChecker : v1.2
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

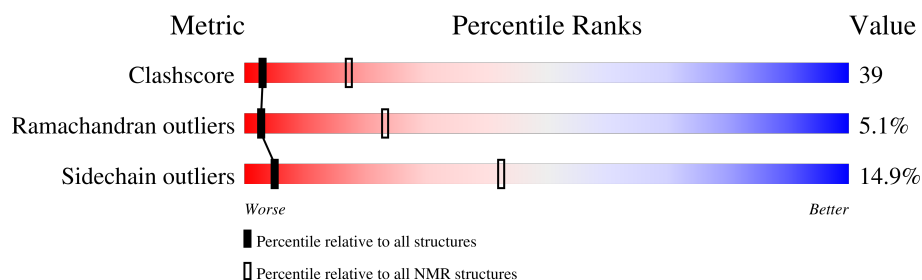
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 86%.

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	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

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	11	
2	B	61	

2 Ensemble composition and analysis

This entry contains 20 models. Model 18 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:34-A:37, B:107-B:154 (52)	0.64	18

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 5 clusters and 2 single-model clusters were found.

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

3 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 1144 atoms, of which 554 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Peptide from Histone H3.3.

Mol	Chain	Residues	Atoms					Trace
1	A	11	Total	C	H	N	O	0
			196	58	102	21	15	

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	34	ARG	GLY	engineered mutation	UNP P84243

- Molecule 2 is a protein called Protein kinase C-binding protein 1.

Mol	Chain	Residues	Atoms						Trace
2	B	61	Total	C	H	N	O	S	0
			946	305	452	85	95	9	

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	
3	B	2	Total	Zn
			2	2

4 Residue-property plots

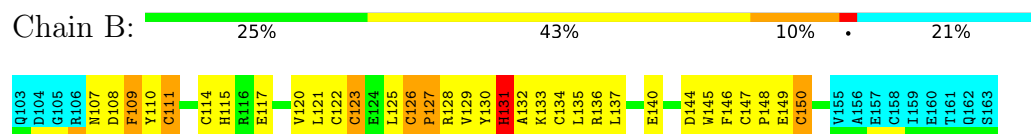
4.1 Average score per residue in the NMR ensemble

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: Peptide from Histone H3.3



- Molecule 2: Protein kinase C-binding protein 1

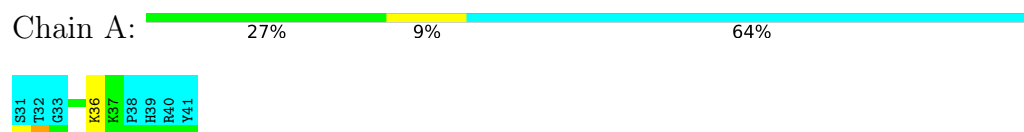


4.2 Scores per residue for each member of the ensemble

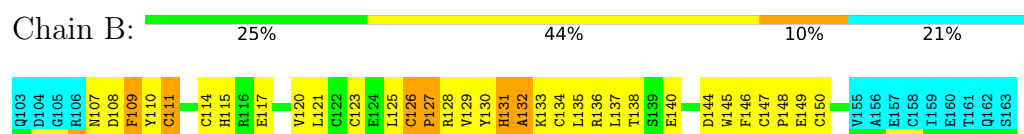
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

- Molecule 1: Peptide from Histone H3.3

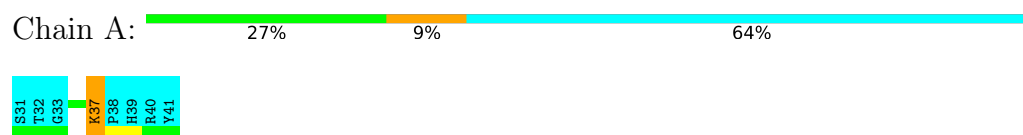


- Molecule 2: Protein kinase C-binding protein 1

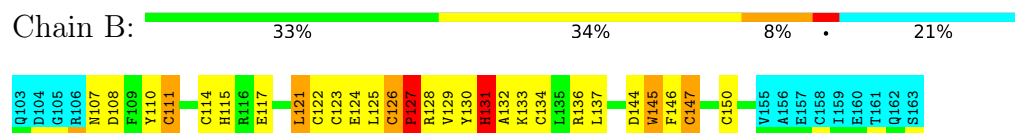


4.2.2 Score per residue for model 2

- Molecule 1: Peptide from Histone H3.3



- Molecule 2: Protein kinase C-binding protein 1

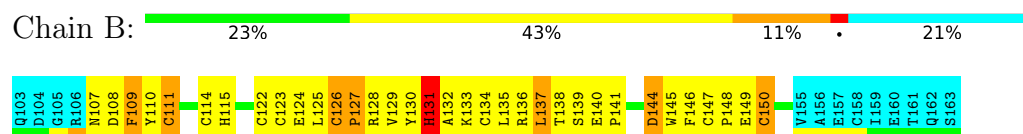


4.2.3 Score per residue for model 3

- Molecule 1: Peptide from Histone H3.3

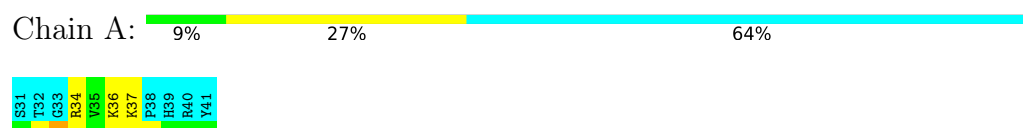


- Molecule 2: Protein kinase C-binding protein 1

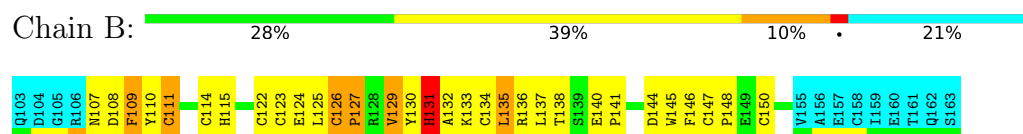


4.2.4 Score per residue for model 4

- Molecule 1: Peptide from Histone H3.3

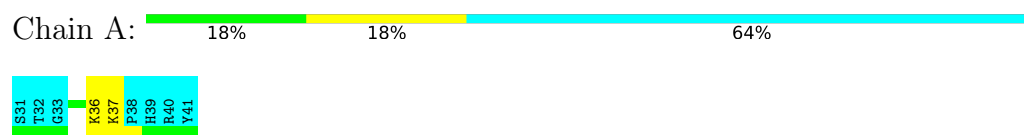


- Molecule 2: Protein kinase C-binding protein 1

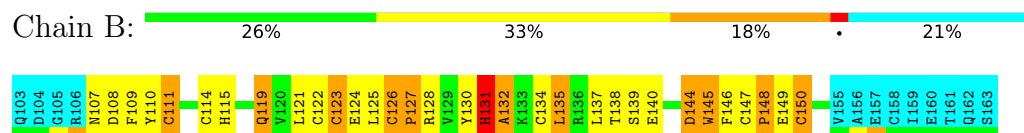


4.2.5 Score per residue for model 5

- Molecule 1: Peptide from Histone H3.3

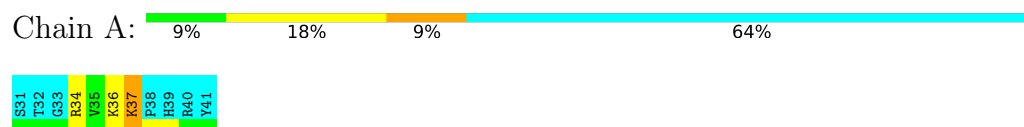


- Molecule 2: Protein kinase C-binding protein 1

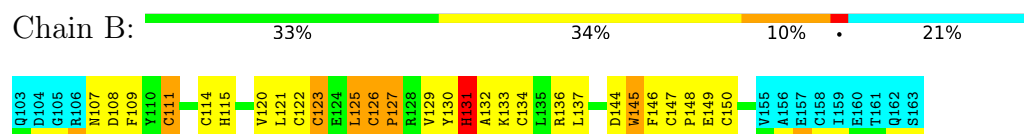


4.2.6 Score per residue for model 6

- Molecule 1: Peptide from Histone H3.3



- Molecule 2: Protein kinase C-binding protein 1

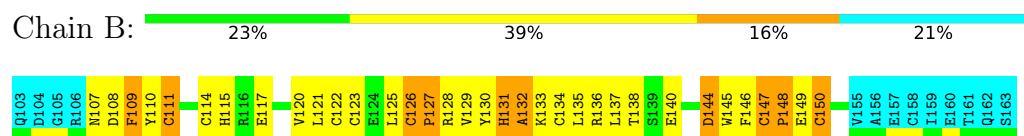


4.2.7 Score per residue for model 7

- Molecule 1: Peptide from Histone H3.3

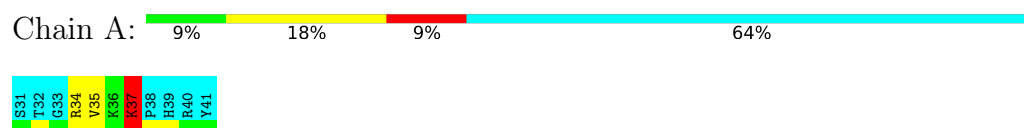


- Molecule 2: Protein kinase C-binding protein 1

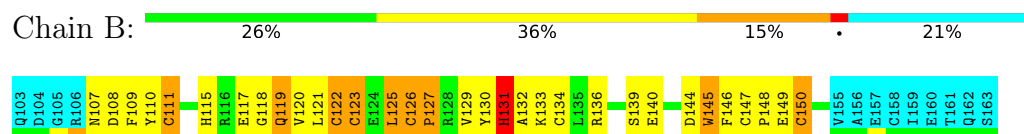


4.2.8 Score per residue for model 8

- Molecule 1: Peptide from Histone H3.3

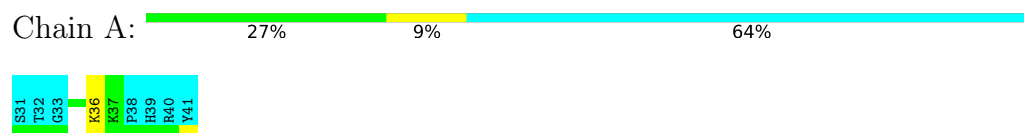


- Molecule 2: Protein kinase C-binding protein 1

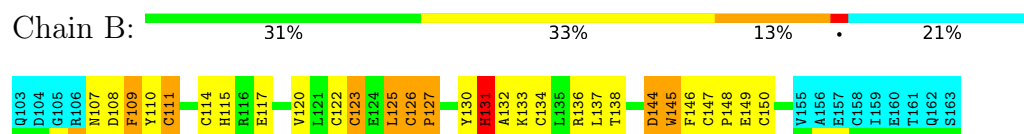


4.2.9 Score per residue for model 9

- Molecule 1: Peptide from Histone H3.3



- Molecule 2: Protein kinase C-binding protein 1

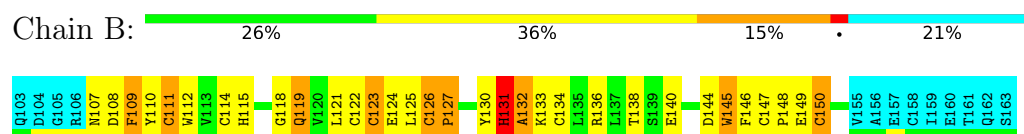


4.2.10 Score per residue for model 10

- Molecule 1: Peptide from Histone H3.3



- Molecule 2: Protein kinase C-binding protein 1

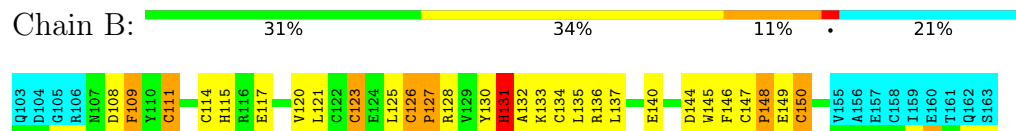


4.2.11 Score per residue for model 11

- Molecule 1: Peptide from Histone H3.3



- Molecule 2: Protein kinase C-binding protein 1

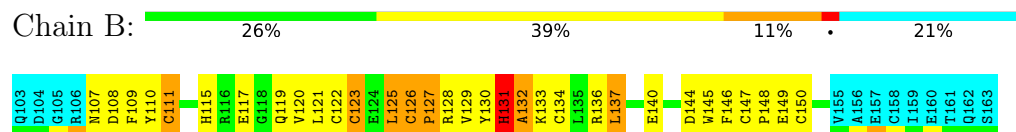


4.2.12 Score per residue for model 12

- Molecule 1: Peptide from Histone H3.3



- Molecule 2: Protein kinase C-binding protein 1

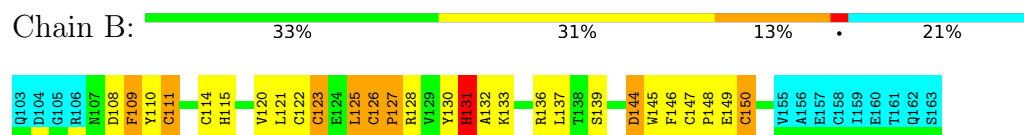


4.2.13 Score per residue for model 13

- Molecule 1: Peptide from Histone H3.3



- Molecule 2: Protein kinase C-binding protein 1

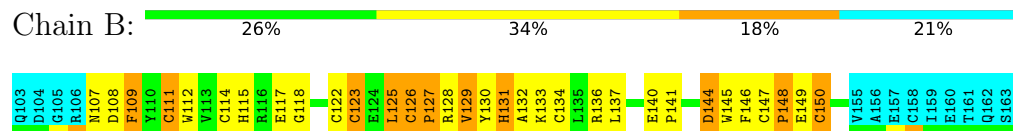


4.2.14 Score per residue for model 14

- Molecule 1: Peptide from Histone H3.3



- Molecule 2: Protein kinase C-binding protein 1

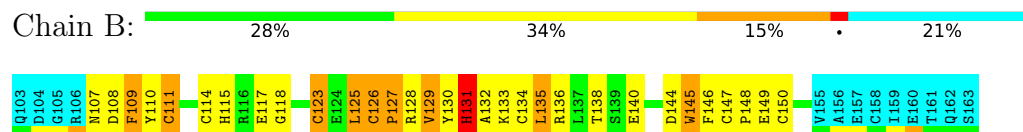


4.2.15 Score per residue for model 15

- Molecule 1: Peptide from Histone H3.3



- Molecule 2: Protein kinase C-binding protein 1

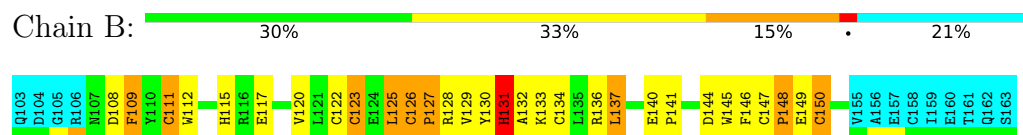


4.2.16 Score per residue for model 16

- Molecule 1: Peptide from Histone H3.3

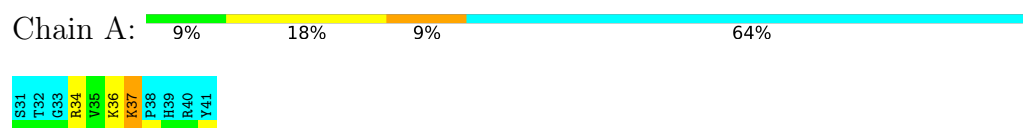


- Molecule 2: Protein kinase C-binding protein 1

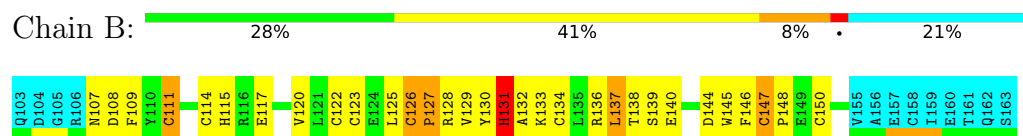


4.2.17 Score per residue for model 17

- Molecule 1: Peptide from Histone H3.3



- Molecule 2: Protein kinase C-binding protein 1

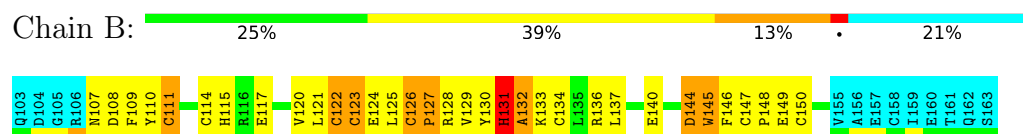


4.2.18 Score per residue for model 18 (medoid)

- Molecule 1: Peptide from Histone H3.3



- Molecule 2: Protein kinase C-binding protein 1

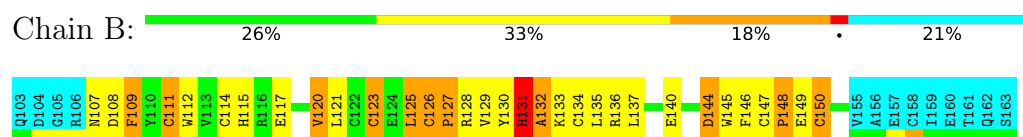


4.2.19 Score per residue for model 19

- Molecule 1: Peptide from Histone H3.3



- Molecule 2: Protein kinase C-binding protein 1



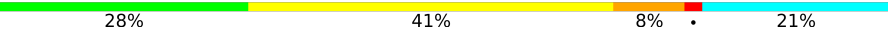
4.2.20 Score per residue for model 20

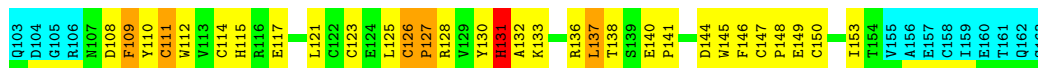
- Molecule 1: Peptide from Histone H3.3

Chain A:  18% 18% 64%



- Molecule 2: Protein kinase C-binding protein 1

Chain B:  28% 41% 8% 21%



5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
CNS	refinement	
X-PLOR NIH	structure calculation	

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	809
Number of shifts mapped to atoms	809
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	86%

6 Model quality [i](#)

6.1 Standard geometry [i](#)

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

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	1.42±0.03	0±0/36 (0.0± 0.0%)	1.32±0.07	0±0/47 (0.0± 0.0%)
2	B	1.43±0.01	0±0/408 (0.0± 0.0%)	1.35±0.01	1±0/555 (0.2± 0.0%)
All	All	1.43	0/8880 (0.0%)	1.35	21/12040 (0.2%)

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
2	B	0.0±0.0	0.8±0.4
All	All	0	17

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
2	B	132	ALA	N-CA-C	-6.05	106.43	113.88	2	20
2	B	127	PRO	CA-N-CD	-5.20	104.72	112.00	2	1

There are no chirality outliers.

All unique planar outliers are listed below.

Mol	Chain	Res	Type	Group	Models (Total)
2	B	131	HIS	Sidechain	17

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	36	48	48	3±2
2	B	395	360	359	33±4
All	All	8660	8160	8140	657

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 39.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:130:TYR:HH	2:B:145:TRP:CD1	0.90	1.83	11	11
2:B:125:LEU:C	2:B:126:CYS:SG	0.77	2.67	5	18
2:B:147:CYS:N	2:B:150:CYS:SG	0.76	2.59	17	20
2:B:130:TYR:HH	2:B:145:TRP:CG	0.76	1.99	8	4
2:B:121:LEU:HD13	2:B:132:ALA:HB2	0.73	1.58	7	4
2:B:130:TYR:OH	2:B:145:TRP:CE3	0.70	2.44	13	3
2:B:111:CYS:CB	2:B:131:HIS:ND1	0.64	2.61	10	20
2:B:126:CYS:O	2:B:127:PRO:C	0.62	2.43	2	20
2:B:107:ASN:ND2	2:B:122:CYS:SG	0.61	2.73	18	8
2:B:109:PHE:CE1	2:B:128:ARG:NH1	0.60	2.68	19	1
2:B:111:CYS:HB2	2:B:131:HIS:ND1	0.60	2.12	2	20
2:B:137:LEU:HD22	2:B:139:SER:O	0.60	1.97	3	2
2:B:125:LEU:HD23	2:B:125:LEU:O	0.59	1.96	4	8
2:B:123:CYS:SG	2:B:130:TYR:CE1	0.59	2.96	13	2
1:A:36:LYS:HZ2	2:B:138:THR:C	0.59	2.06	9	5
2:B:147:CYS:O	2:B:150:CYS:SG	0.58	2.61	7	20
1:A:36:LYS:N	2:B:119:GLN:HE22	0.58	1.95	12	1
2:B:123:CYS:SG	2:B:145:TRP:O	0.58	2.61	2	15
1:A:35:VAL:HG12	2:B:120:VAL:O	0.57	1.98	12	3
2:B:135:LEU:HD12	2:B:135:LEU:N	0.57	2.14	11	1
2:B:130:TYR:OH	2:B:145:TRP:CD1	0.56	2.58	3	3
2:B:130:TYR:OH	2:B:145:TRP:CG	0.56	2.57	8	3
2:B:130:TYR:OH	2:B:145:TRP:CD2	0.56	2.59	6	7
2:B:144:ASP:N	2:B:144:ASP:OD1	0.56	2.37	11	12
2:B:112:TRP:CD1	2:B:112:TRP:H	0.55	2.17	10	2
2:B:146:PHE:C	2:B:150:CYS:SG	0.55	2.90	9	20

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:135:LEU:N	2:B:135:LEU:CD1	0.55	2.69	11	1
2:B:121:LEU:HD23	2:B:122:CYS:H	0.55	1.60	2	1
2:B:112:TRP:CH2	2:B:149:GLU:OE1	0.55	2.60	20	1
1:A:36:LYS:NZ	2:B:137:LEU:O	0.55	2.40	1	15
2:B:121:LEU:HD23	2:B:122:CYS:N	0.54	2.17	2	1
2:B:108:ASP:O	2:B:109:PHE:CD2	0.54	2.61	19	3
1:A:34:ARG:NE	2:B:108:ASP:OD1	0.54	2.40	4	5
2:B:135:LEU:N	2:B:135:LEU:CD2	0.54	2.71	1	1
1:A:34:ARG:NH1	2:B:108:ASP:OD1	0.54	2.41	13	1
1:A:36:LYS:NZ	2:B:138:THR:C	0.53	2.67	9	5
2:B:138:THR:HG22	2:B:138:THR:O	0.53	2.03	7	1
2:B:108:ASP:O	2:B:109:PHE:CG	0.53	2.62	16	4
2:B:111:CYS:O	2:B:115:HIS:N	0.53	2.38	2	19
2:B:133:LYS:O	2:B:136:ARG:N	0.53	2.41	14	19
2:B:137:LEU:N	2:B:137:LEU:HD23	0.53	2.18	2	1
1:A:36:LYS:NZ	2:B:138:THR:O	0.53	2.42	15	1
2:B:121:LEU:O	2:B:130:TYR:CD1	0.53	2.62	20	1
2:B:109:PHE:O	2:B:110:TYR:CD1	0.53	2.62	20	4
2:B:107:ASN:O	2:B:129:VAL:HG21	0.53	2.04	14	1
2:B:110:TYR:CZ	2:B:117:GLU:OE2	0.52	2.61	2	2
2:B:137:LEU:HD21	2:B:139:SER:O	0.52	2.04	13	2
2:B:130:TYR:CD2	2:B:131:HIS:O	0.52	2.62	1	5
2:B:121:LEU:N	2:B:130:TYR:O	0.52	2.41	11	4
2:B:122:CYS:O	2:B:122:CYS:SG	0.52	2.68	10	5
2:B:109:PHE:O	2:B:110:TYR:CD2	0.52	2.62	10	7
2:B:130:TYR:CD1	2:B:131:HIS:O	0.52	2.63	7	5
2:B:135:LEU:N	2:B:135:LEU:HD22	0.51	2.20	1	1
2:B:110:TYR:CE2	2:B:117:GLU:OE2	0.51	2.64	12	1
2:B:125:LEU:O	2:B:125:LEU:CD2	0.51	2.58	5	6
2:B:120:VAL:C	2:B:121:LEU:HD12	0.51	2.31	18	5
2:B:114:CYS:C	2:B:115:HIS:CG	0.51	2.88	15	5
2:B:135:LEU:O	2:B:135:LEU:HD23	0.51	2.06	15	2
2:B:117:GLU:CD	2:B:118:GLY:N	0.51	2.68	15	2
2:B:109:PHE:N	2:B:117:GLU:OE2	0.51	2.44	1	2
2:B:107:ASN:CG	2:B:122:CYS:SG	0.51	2.94	17	2
2:B:137:LEU:CD2	2:B:139:SER:O	0.50	2.59	13	1
1:A:36:LYS:H	2:B:119:GLN:HE22	0.50	1.49	12	1
2:B:112:TRP:HE1	2:B:127:PRO:CB	0.50	2.20	19	2
2:B:147:CYS:O	2:B:149:GLU:N	0.50	2.45	16	17
2:B:121:LEU:HD12	2:B:121:LEU:N	0.50	2.21	7	4
1:A:34:ARG:HE	2:B:108:ASP:CG	0.50	2.14	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:109:PHE:CD2	2:B:110:TYR:N	0.50	2.80	12	5
2:B:137:LEU:CD2	2:B:139:SER:H	0.50	2.20	17	2
2:B:137:LEU:HD23	2:B:138:THR:N	0.49	2.22	17	2
2:B:112:TRP:O	2:B:115:HIS:CD2	0.49	2.65	16	1
2:B:130:TYR:CD1	2:B:130:TYR:C	0.49	2.90	6	4
2:B:127:PRO:O	2:B:128:ARG:C	0.49	2.55	16	15
2:B:131:HIS:HD2	2:B:134:CYS:SG	0.49	2.30	1	18
1:A:36:LYS:H	2:B:119:GLN:NE2	0.49	2.04	12	1
2:B:121:LEU:CD1	2:B:132:ALA:HB2	0.49	2.38	12	3
2:B:130:TYR:CE2	2:B:131:HIS:O	0.49	2.65	1	3
2:B:135:LEU:O	2:B:135:LEU:HD13	0.49	2.08	4	1
2:B:145:TRP:CD1	2:B:146:PHE:N	0.48	2.82	13	1
2:B:114:CYS:O	2:B:115:HIS:CB	0.48	2.61	6	15
2:B:120:VAL:C	2:B:121:LEU:HD22	0.48	2.33	11	3
1:A:35:VAL:CG1	2:B:120:VAL:O	0.48	2.61	16	2
2:B:107:ASN:O	2:B:129:VAL:HG22	0.48	2.09	8	2
2:B:108:ASP:O	2:B:108:ASP:OD1	0.48	2.32	19	8
2:B:107:ASN:HD21	2:B:121:LEU:C	0.47	2.17	1	1
2:B:147:CYS:O	2:B:148:PRO:C	0.47	2.58	5	19
2:B:107:ASN:CG	2:B:107:ASN:O	0.47	2.57	9	1
2:B:146:PHE:CA	2:B:150:CYS:SG	0.47	3.03	5	16
1:A:35:VAL:HG21	2:B:121:LEU:CD2	0.47	2.40	8	1
2:B:126:CYS:O	2:B:127:PRO:O	0.47	2.33	18	3
2:B:137:LEU:H	2:B:137:LEU:CD2	0.47	2.23	2	1
2:B:130:TYR:CE1	2:B:131:HIS:O	0.46	2.69	4	3
2:B:135:LEU:HD21	2:B:148:PRO:CD	0.46	2.40	7	1
2:B:126:CYS:CB	2:B:127:PRO:HD2	0.46	2.39	2	8
2:B:137:LEU:N	2:B:137:LEU:CD2	0.46	2.79	2	1
2:B:135:LEU:HD21	2:B:148:PRO:CG	0.46	2.40	4	1
2:B:125:LEU:O	2:B:126:CYS:SG	0.46	2.74	5	2
2:B:140:GLU:OE1	2:B:141:PRO:O	0.45	2.34	20	5
1:A:36:LYS:O	2:B:140:GLU:OE2	0.45	2.35	1	4
2:B:140:GLU:O	2:B:140:GLU:CD	0.45	2.59	16	1
2:B:121:LEU:HD12	2:B:132:ALA:HB2	0.45	1.88	10	1
2:B:140:GLU:CD	2:B:140:GLU:C	0.45	2.85	20	7
2:B:108:ASP:OD1	2:B:108:ASP:C	0.45	2.60	10	4
2:B:109:PHE:O	2:B:117:GLU:CG	0.45	2.64	8	1
2:B:121:LEU:N	2:B:121:LEU:CD1	0.45	2.80	7	2
2:B:124:GLU:OE2	2:B:144:ASP:CG	0.44	2.61	3	4
1:A:34:ARG:CZ	2:B:108:ASP:OD1	0.44	2.64	13	1
2:B:123:CYS:SG	2:B:124:GLU:N	0.44	2.89	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:34:ARG:CD	2:B:108:ASP:OD1	0.44	2.65	14	1
2:B:147:CYS:C	2:B:149:GLU:N	0.44	2.76	7	10
1:A:36:LYS:O	2:B:140:GLU:CD	0.44	2.61	15	3
2:B:140:GLU:CD	2:B:140:GLU:O	0.44	2.61	5	1
2:B:108:ASP:OD1	2:B:117:GLU:OE1	0.44	2.35	7	2
2:B:109:PHE:N	2:B:117:GLU:OE1	0.44	2.50	9	1
2:B:108:ASP:OD1	2:B:109:PHE:N	0.43	2.51	7	1
1:A:36:LYS:O	2:B:140:GLU:OE1	0.43	2.36	15	1
2:B:108:ASP:OD1	2:B:117:GLU:OE2	0.43	2.36	17	1
2:B:109:PHE:CZ	2:B:128:ARG:NH1	0.43	2.86	19	1
2:B:107:ASN:O	2:B:129:VAL:CG2	0.43	2.66	14	3
2:B:140:GLU:OE2	2:B:141:PRO:O	0.43	2.36	3	2
2:B:108:ASP:OD1	2:B:108:ASP:O	0.43	2.37	10	1
2:B:117:GLU:C	2:B:117:GLU:OE2	0.43	2.61	14	1
2:B:108:ASP:C	2:B:117:GLU:OE2	0.43	2.62	11	2
2:B:124:GLU:OE2	2:B:144:ASP:OD1	0.43	2.36	2	4
2:B:118:GLY:O	2:B:119:GLN:O	0.43	2.37	8	2
2:B:124:GLU:OE1	2:B:144:ASP:CG	0.43	2.61	4	1
2:B:125:LEU:O	2:B:125:LEU:CG	0.43	2.66	4	2
2:B:117:GLU:OE1	2:B:117:GLU:C	0.43	2.61	15	1
2:B:108:ASP:CG	2:B:117:GLU:OE2	0.43	2.62	16	3
2:B:108:ASP:C	2:B:109:PHE:CD2	0.43	2.97	18	1
1:A:35:VAL:CG2	1:A:36:LYS:N	0.43	2.82	3	1
2:B:108:ASP:CG	2:B:117:GLU:OE1	0.43	2.62	7	3
2:B:139:SER:C	2:B:140:GLU:OE1	0.42	2.62	8	1
2:B:140:GLU:CD	2:B:141:PRO:O	0.42	2.62	4	2
2:B:108:ASP:C	2:B:117:GLU:OE1	0.42	2.62	9	1
2:B:109:PHE:O	2:B:110:TYR:CG	0.42	2.72	8	2
2:B:107:ASN:OD1	2:B:120:VAL:O	0.42	2.36	9	1
2:B:108:ASP:OD1	2:B:117:GLU:CD	0.42	2.63	7	1
2:B:127:PRO:O	2:B:129:VAL:N	0.42	2.53	17	1
2:B:135:LEU:O	2:B:136:ARG:CB	0.42	2.68	3	1
2:B:146:PHE:CD1	2:B:146:PHE:N	0.42	2.88	11	2
2:B:137:LEU:HD23	2:B:137:LEU:H	0.41	1.74	2	1
2:B:109:PHE:C	2:B:110:TYR:CD1	0.41	2.98	20	1
2:B:130:TYR:OH	2:B:145:TRP:NE1	0.41	2.53	3	1
2:B:138:THR:O	2:B:138:THR:HG22	0.41	2.14	4	2
2:B:109:PHE:CG	2:B:110:TYR:N	0.41	2.85	12	2
2:B:118:GLY:O	2:B:119:GLN:C	0.41	2.62	10	1
2:B:112:TRP:CZ2	2:B:149:GLU:OE1	0.41	2.74	20	1
2:B:119:GLN:CD	2:B:119:GLN:N	0.41	2.79	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:147:CYS:O	2:B:150:CYS:N	0.41	2.54	7	1
2:B:121:LEU:N	2:B:121:LEU:CD2	0.41	2.84	11	1
1:A:36:LYS:N	2:B:119:GLN:NE2	0.41	2.66	12	1
2:B:117:GLU:CD	2:B:117:GLU:C	0.41	2.89	14	1
2:B:140:GLU:O	2:B:140:GLU:OE2	0.41	2.37	14	1
1:A:34:ARG:NH2	1:A:34:ARG:CB	0.40	2.84	6	1
2:B:146:PHE:O	2:B:147:CYS:C	0.40	2.64	2	1
2:B:135:LEU:HD11	2:B:148:PRO:HG2	0.40	1.92	19	1
2:B:146:PHE:HA	2:B:150:CYS:SG	0.40	2.57	5	1
2:B:135:LEU:O	2:B:135:LEU:CD1	0.40	2.69	4	1
2:B:107:ASN:ND2	2:B:122:CYS:CB	0.40	2.85	8	1

6.3 Torsion angles [i](#)

6.3.1 Protein backbone [i](#)

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	4/11 (36%)	3±1 (78±22%)	1±1 (14±17%)	0±0 (9±12%)	1	12
2	B	48/61 (79%)	41±2 (85±3%)	5±2 (10±3%)	2±1 (5±2%)	3	25
All	All	1040/1440 (72%)	877 (84%)	110 (11%)	53 (5%)	3	23

All 7 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
2	B	127	PRO	20
2	B	109	PHE	15
2	B	148	PRO	6
1	A	37	LYS	5
2	B	119	GLN	3
1	A	34	ARG	2
2	B	107	ASN	2

6.3.2 Protein sidechains [i](#)

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	4/10 (40%)	4±0 (98±8%)	0±0 (2±8%)	42 88
2	B	45/56 (80%)	38±1 (84±2%)	7±1 (16±2%)	4 40
All	All	980/1320 (74%)	834 (85%)	146 (15%)	5 42

All 17 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)
2	B	111	CYS	20
2	B	126	CYS	20
2	B	131	HIS	20
2	B	123	CYS	17
2	B	129	VAL	11
2	B	125	LEU	11
2	B	144	ASP	10
2	B	150	CYS	10
2	B	145	TRP	8
2	B	137	LEU	5
2	B	147	CYS	3
2	B	135	LEU	3
2	B	122	CYS	3
2	B	120	VAL	2
2	B	121	LEU	1
1	A	35	VAL	1
1	A	37	LYS	1

6.3.3 RNA [i](#)

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 oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

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 86% for the well-defined parts and 83% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *RACK_20200827_shifts_convert_revised-4.txt*

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	809
Number of shifts mapped to atoms	809
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	72	0.06 ± 0.45	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	68	-0.03 ± 0.12	None needed (< 0.5 ppm)
$^{13}\text{C}'$	60	0.23 ± 0.17	None needed (< 0.5 ppm)
^{15}N	66	-0.39 ± 0.39	None needed (< 0.5 ppm)

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 86%, i.e. 623 atoms were assigned a chemical shift out of a possible 723. 0 out of 8 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	244/256 (95%)	101/103 (98%)	95/104 (91%)	48/49 (98%)
Sidechain	315/390 (81%)	217/250 (87%)	97/122 (80%)	1/18 (6%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	64/77 (83%)	32/38 (84%)	30/34 (88%)	2/5 (40%)
Overall	623/723 (86%)	350/391 (90%)	222/260 (85%)	51/72 (71%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 83%, i.e. 807 atoms were assigned a chemical shift out of a possible 977. 0 out of 9 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	337/356 (95%)	139/144 (97%)	132/144 (92%)	66/68 (97%)
Sidechain	406/527 (77%)	282/337 (84%)	123/164 (75%)	1/26 (4%)
Aromatic	64/94 (68%)	32/46 (70%)	30/41 (73%)	2/7 (29%)
Overall	807/977 (83%)	453/527 (86%)	285/349 (82%)	69/101 (68%)

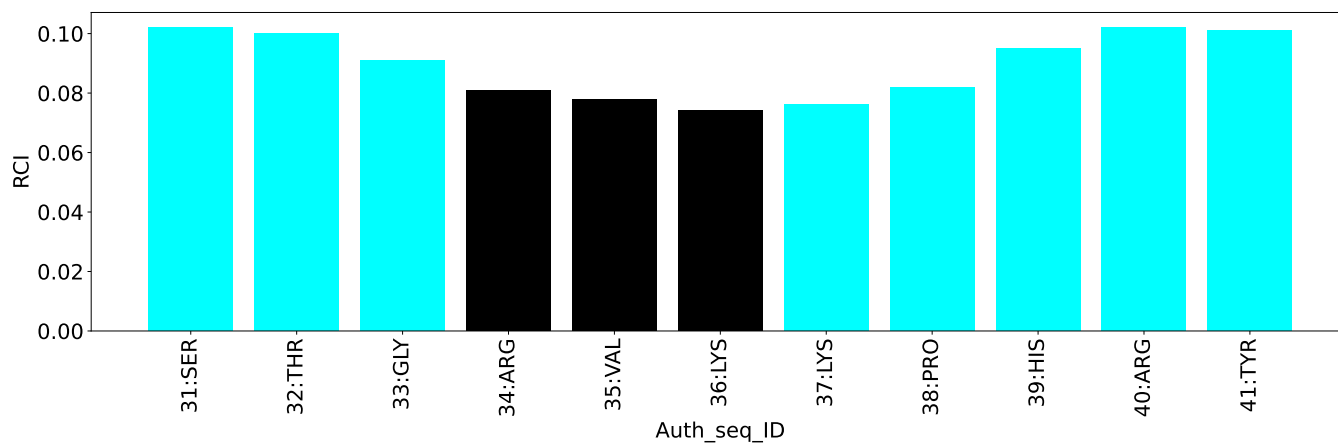
7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

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

The 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. If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A:



Random coil index (RCI) for chain B:

