



Full wwPDB NMR Structure Validation Report ⓘ

Mar 8, 2026 – 05:31 PM UTC

PDB ID : 2JWO / pdb_00002jwo
Title : A PHD finger motif in the C-terminus of RAG2 modulates recombination activity
Authors : Ivanov, D.; Hyberts, S.G.; Sun, Z.; Wagner, G.
Deposited on : 2007-10-17

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

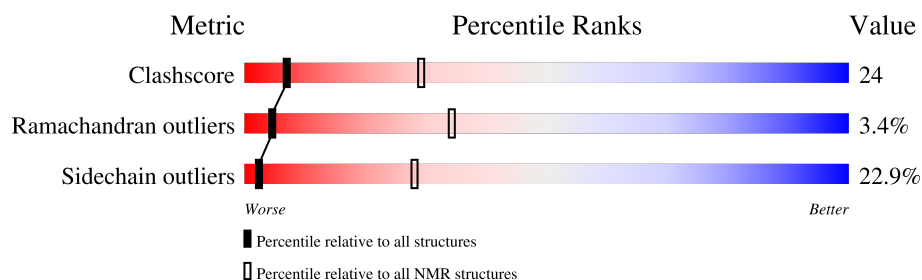
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment was not calculated.

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	82	

2 Ensemble composition and analysis

This entry contains 20 models. Model 8 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:415-A:483 (69)	0.90	8

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 4 clusters and 3 single-model clusters were found.

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

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 1253 atoms, of which 596 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called V(D)J recombination-activating protein 2.

Mol	Chain	Residues	Atoms						Trace
1	A	82	Total	C	H	N	O	S	0
			1251	414	596	109	124	8	

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	406	GLY	-	expression tag	UNP P21784
A	407	PRO	-	expression tag	UNP P21784
A	408	LEU	-	expression tag	UNP P21784
A	409	GLY	-	expression tag	UNP P21784
A	410	SER	-	expression tag	UNP P21784
A	411	PRO	-	expression tag	UNP P21784
A	412	GLU	-	expression tag	UNP P21784
A	413	PHE	-	expression tag	UNP P21784

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

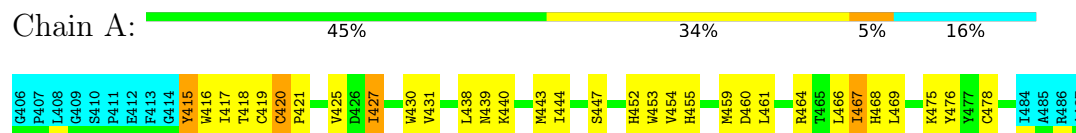
Mol	Chain	Residues	Atoms	
2	A	2	Total	Zn
			2	2

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: V(D)J recombination-activating protein 2

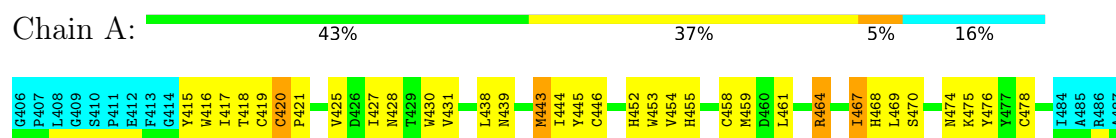


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

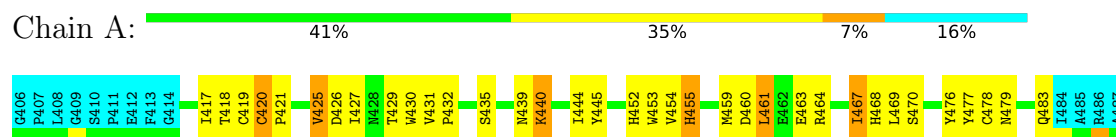
4.2.1 Score per residue for model 1

- Molecule 1: V(D)J recombination-activating protein 2



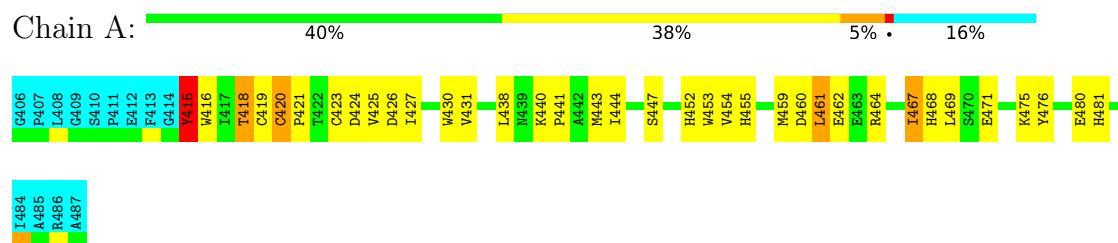
4.2.2 Score per residue for model 2

- Molecule 1: V(D)J recombination-activating protein 2



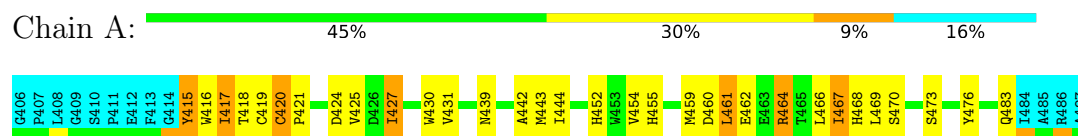
4.2.3 Score per residue for model 3

- Molecule 1: V(D)J recombination-activating protein 2



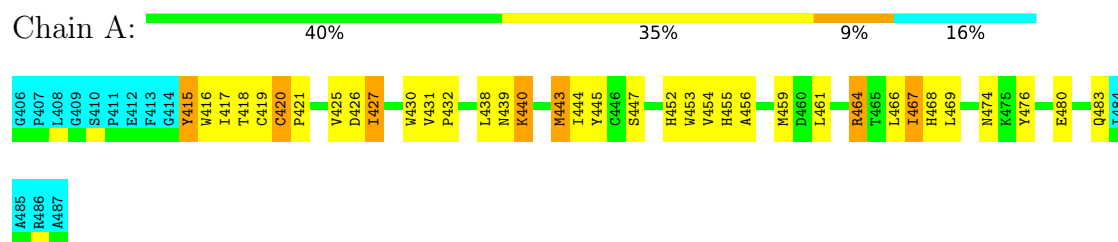
4.2.4 Score per residue for model 4

- Molecule 1: V(D)J recombination-activating protein 2



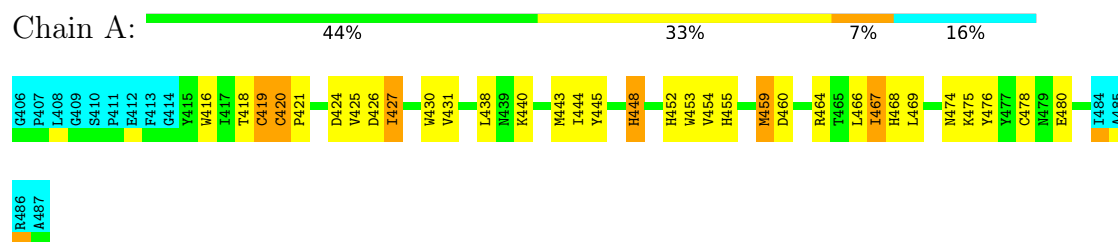
4.2.5 Score per residue for model 5

- Molecule 1: V(D)J recombination-activating protein 2



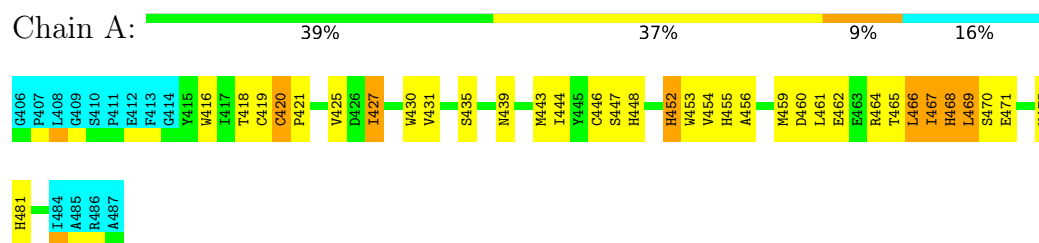
4.2.6 Score per residue for model 6

- Molecule 1: V(D)J recombination-activating protein 2



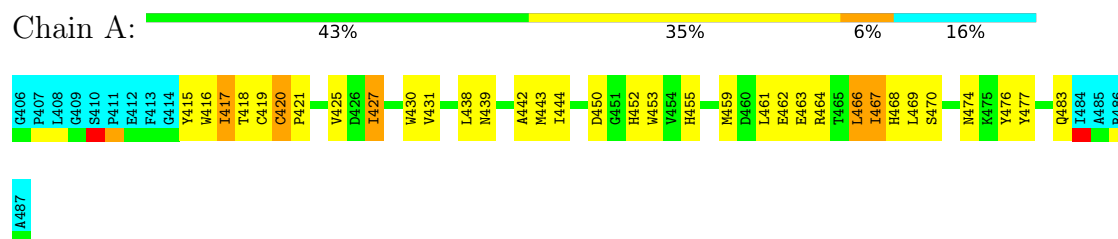
4.2.7 Score per residue for model 7

- Molecule 1: V(D)J recombination-activating protein 2



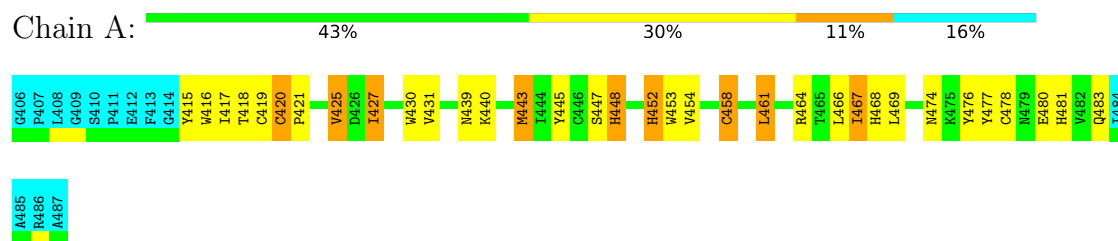
4.2.8 Score per residue for model 8 (medoid)

- Molecule 1: V(D)J recombination-activating protein 2



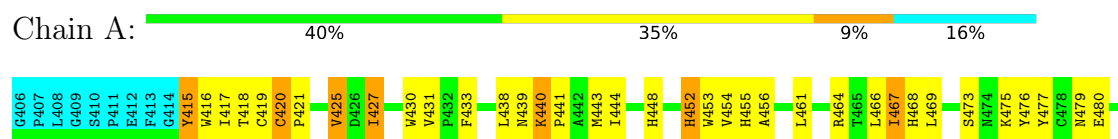
4.2.9 Score per residue for model 9

- Molecule 1: V(D)J recombination-activating protein 2



4.2.10 Score per residue for model 10

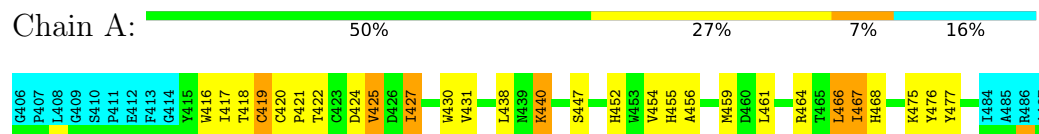
- Molecule 1: V(D)J recombination-activating protein 2





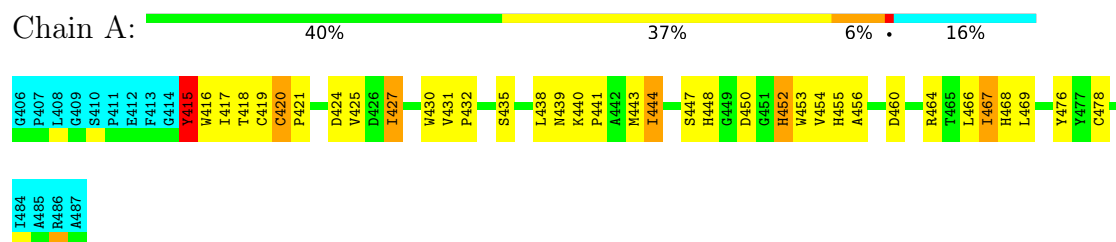
4.2.11 Score per residue for model 11

- Molecule 1: V(D)J recombination-activating protein 2



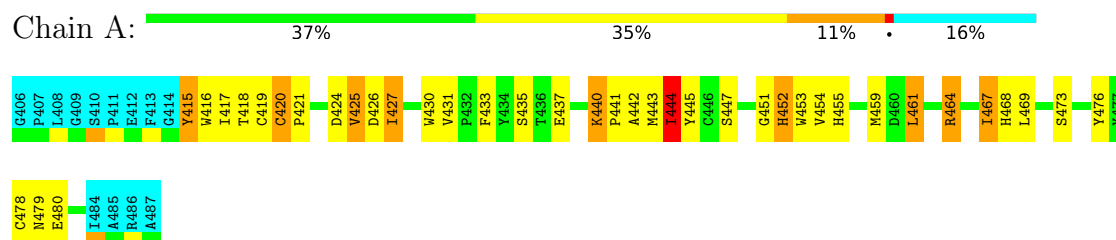
4.2.12 Score per residue for model 12

- Molecule 1: V(D)J recombination-activating protein 2



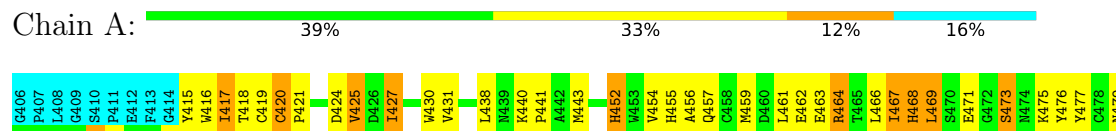
4.2.13 Score per residue for model 13

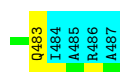
- Molecule 1: V(D)J recombination-activating protein 2



4.2.14 Score per residue for model 14

- Molecule 1: V(D)J recombination-activating protein 2

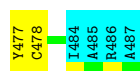
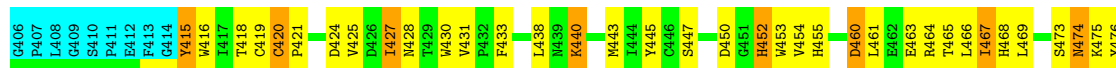




4.2.15 Score per residue for model 15

- Molecule 1: V(D)J recombination-activating protein 2

Chain A: 38% 37% 10% 16%



4.2.16 Score per residue for model 16

- Molecule 1: V(D)J recombination-activating protein 2

Chain A: 34% 41% 9% 16%



4.2.17 Score per residue for model 17

- Molecule 1: V(D)J recombination-activating protein 2

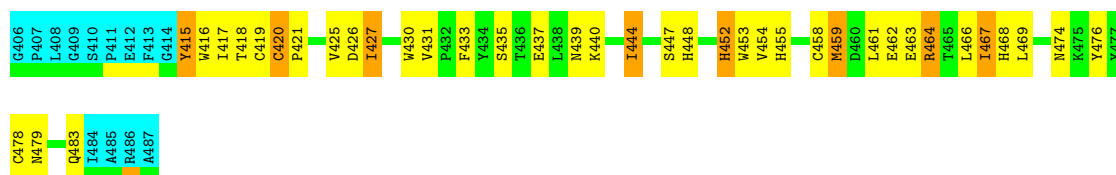
Chain A: 40% 34% 9% 16%



4.2.18 Score per residue for model 18

- Molecule 1: V(D)J recombination-activating protein 2

Chain A: 37% 38% 10% 16%



4.2.19 Score per residue for model 19

- Molecule 1: V(D)J recombination-activating protein 2

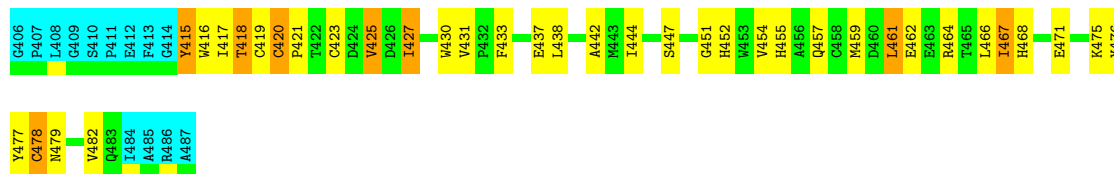
Chain A: 44% 32% 9% 16%



4.2.20 Score per residue for model 20

- Molecule 1: V(D)J recombination-activating protein 2

Chain A: 39% 35% 10% 16%



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
DYANA	structure solution	
X-PLOR NIH	refinement	

No chemical shift data was provided.

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	1.41±0.01	0±0/585 (0.0± 0.0%)	1.55±0.02	1±1/801 (0.2± 0.1%)
All	All	1.41	0/11700 (0.0%)	1.55	25/16020 (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
1	A	0.0±0.0	1.0±0.0
All	All	0	20

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	444	ILE	N-CA-CB	-6.34	105.11	112.34	10	3
1	A	425	VAL	N-CA-CB	-6.27	104.75	111.46	20	13
1	A	420	CYS	N-CA-CB	-6.24	104.87	111.29	17	1
1	A	424	ASP	N-CA-CB	-5.61	105.06	111.79	15	5
1	A	439	ASN	N-CA-CB	-5.59	105.08	111.79	8	2
1	A	419	CYS	N-CA-CB	-5.12	104.09	110.90	11	1

There are no chirality outliers.

All unique planar outliers are listed below.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	464	ARG	Sidechain	20

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	565	506	506	26±3
All	All	11340	10120	10120	518

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 24.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:444:ILE:HD13	1:A:476:TYR:CE1	0.87	2.03	12	6
1:A:417:ILE:HD11	1:A:443:MET:HE1	0.84	1.49	5	5
1:A:469:LEU:HD13	1:A:476:TYR:CE2	0.84	2.08	7	7
1:A:469:LEU:HD22	1:A:476:TYR:CD2	0.80	2.10	12	7
1:A:426:ASP:OD1	1:A:429:THR:HG22	0.80	1.77	2	1
1:A:444:ILE:HG22	1:A:454:VAL:O	0.80	1.77	19	4
1:A:425:VAL:HG21	1:A:455:HIS:ND1	0.79	1.92	11	13
1:A:454:VAL:HG21	1:A:478:CYS:SG	0.79	2.17	20	1
1:A:420:CYS:SG	1:A:459:MET:HE1	0.76	2.20	4	3
1:A:469:LEU:HD11	1:A:476:TYR:CE2	0.74	2.18	4	5
1:A:417:ILE:HD11	1:A:443:MET:CE	0.72	2.14	1	4
1:A:469:LEU:HD11	1:A:476:TYR:CD2	0.71	2.21	5	8
1:A:443:MET:HE2	1:A:454:VAL:HA	0.70	1.61	6	1
1:A:461:LEU:HD11	1:A:476:TYR:OH	0.70	1.86	10	9
1:A:444:ILE:HG21	1:A:476:TYR:OH	0.70	1.86	1	1
1:A:437:GLU:OE2	1:A:442:ALA:HB2	0.69	1.88	13	1
1:A:459:MET:O	1:A:461:LEU:HD12	0.68	1.88	13	1
1:A:469:LEU:HD21	1:A:476:TYR:HB2	0.66	1.68	19	4
1:A:431:VAL:HG23	1:A:432:PRO:HD2	0.66	1.68	12	3
1:A:438:LEU:O	1:A:438:LEU:HD23	0.65	1.91	10	1
1:A:419:CYS:SG	1:A:459:MET:HE1	0.63	2.33	2	1
1:A:443:MET:HE2	1:A:453:TRP:O	0.62	1.94	12	2
1:A:425:VAL:HG23	1:A:458:CYS:SG	0.61	2.35	18	3
1:A:461:LEU:HD11	1:A:476:TYR:CZ	0.60	2.30	14	2
1:A:461:LEU:HD23	1:A:465:THR:CG2	0.60	2.27	7	3
1:A:466:LEU:O	1:A:466:LEU:HD13	0.60	1.95	18	2
1:A:456:ALA:CB	1:A:466:LEU:HD23	0.60	2.26	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:437:GLU:CD	1:A:442:ALA:HB2	0.60	2.22	20	1
1:A:467:ILE:CG2	1:A:468:HIS:N	0.59	2.65	9	20
1:A:479:ASN:O	1:A:482:VAL:HG12	0.59	1.97	20	1
1:A:467:ILE:HG22	1:A:468:HIS:N	0.57	2.15	18	20
1:A:452:HIS:CE1	1:A:454:VAL:CG1	0.57	2.87	20	1
1:A:418:THR:HG23	1:A:418:THR:O	0.57	2.00	16	1
1:A:466:LEU:C	1:A:466:LEU:HD23	0.57	2.23	17	1
1:A:425:VAL:HG21	1:A:455:HIS:CG	0.56	2.35	13	7
1:A:456:ALA:CB	1:A:466:LEU:HD11	0.56	2.29	19	2
1:A:418:THR:HG22	1:A:423:CYS:O	0.56	2.00	3	2
1:A:452:HIS:CE1	1:A:454:VAL:HG11	0.56	2.36	16	3
1:A:442:ALA:CB	1:A:466:LEU:HD11	0.56	2.30	8	2
1:A:425:VAL:HG11	1:A:455:HIS:NE2	0.56	2.16	11	5
1:A:425:VAL:HG21	1:A:455:HIS:CE1	0.56	2.34	13	6
1:A:461:LEU:HD23	1:A:465:THR:HG22	0.56	1.77	16	2
1:A:420:CYS:SG	1:A:459:MET:HE3	0.55	2.41	6	1
1:A:444:ILE:HD13	1:A:476:TYR:CE2	0.55	2.36	7	1
1:A:468:HIS:CD2	1:A:469:LEU:N	0.55	2.75	7	3
1:A:417:ILE:CD1	1:A:443:MET:HE1	0.54	2.30	5	3
1:A:443:MET:HE3	1:A:454:VAL:HA	0.54	1.79	19	1
1:A:417:ILE:HG12	1:A:443:MET:HE1	0.54	1.78	17	3
1:A:444:ILE:HD13	1:A:476:TYR:CZ	0.53	2.39	7	1
1:A:469:LEU:HD21	1:A:476:TYR:CD2	0.53	2.38	4	1
1:A:443:MET:HE3	1:A:453:TRP:CD1	0.53	2.38	16	1
1:A:417:ILE:CG1	1:A:443:MET:HE1	0.53	2.33	4	2
1:A:461:LEU:HD21	1:A:476:TYR:CE2	0.52	2.39	15	2
1:A:456:ALA:CB	1:A:466:LEU:HD12	0.52	2.35	12	1
1:A:468:HIS:CD2	1:A:468:HIS:C	0.51	2.88	4	17
1:A:459:MET:HB2	1:A:461:LEU:HD12	0.51	1.82	3	1
1:A:419:CYS:HB3	1:A:455:HIS:ND1	0.51	2.21	14	6
1:A:442:ALA:HB3	1:A:466:LEU:HD11	0.50	1.83	4	2
1:A:419:CYS:O	1:A:459:MET:HE1	0.50	2.07	6	1
1:A:452:HIS:CD2	1:A:452:HIS:N	0.50	2.80	12	18
1:A:466:LEU:HD13	1:A:466:LEU:C	0.49	2.31	18	2
1:A:425:VAL:HG11	1:A:455:HIS:CE1	0.49	2.43	11	2
1:A:419:CYS:HB2	1:A:454:VAL:HB	0.49	1.84	16	9
1:A:419:CYS:HA	1:A:454:VAL:HG12	0.49	1.83	15	3
1:A:430:TRP:C	1:A:431:VAL:HG13	0.49	2.33	18	17
1:A:421:PRO:C	1:A:422:THR:HG23	0.49	2.30	11	1
1:A:416:TRP:CZ2	1:A:427:ILE:HB	0.49	2.42	14	16
1:A:431:VAL:CG2	1:A:432:PRO:HD2	0.49	2.38	12	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:444:ILE:HD13	1:A:454:VAL:O	0.49	2.08	13	1
1:A:456:ALA:O	1:A:461:LEU:HD12	0.48	2.07	11	4
1:A:416:TRP:CZ3	1:A:427:ILE:N	0.48	2.82	13	10
1:A:453:TRP:C	1:A:454:VAL:HG13	0.47	2.34	7	9
1:A:469:LEU:HD22	1:A:476:TYR:HD2	0.47	1.65	7	2
1:A:444:ILE:HD13	1:A:476:TYR:CD1	0.47	2.41	12	1
1:A:420:CYS:HB2	1:A:421:PRO:HD2	0.47	1.85	11	2
1:A:476:TYR:CD1	1:A:477:TYR:N	0.46	2.83	10	6
1:A:430:TRP:CH2	1:A:440:LYS:N	0.46	2.84	5	1
1:A:420:CYS:CB	1:A:421:PRO:CD	0.46	2.93	16	18
1:A:418:THR:HG22	1:A:420:CYS:O	0.46	2.11	17	1
1:A:421:PRO:O	1:A:422:THR:OG1	0.46	2.31	11	1
1:A:443:MET:HE3	1:A:453:TRP:HD1	0.46	1.70	16	1
1:A:452:HIS:CD2	1:A:452:HIS:H	0.46	2.29	13	18
1:A:461:LEU:HD23	1:A:465:THR:HG21	0.46	1.88	7	1
1:A:477:TYR:N	1:A:477:TYR:CD1	0.46	2.84	19	2
1:A:415:TYR:CE1	1:A:443:MET:CB	0.45	2.99	1	1
1:A:443:MET:HE3	1:A:453:TRP:HB3	0.45	1.89	15	2
1:A:430:TRP:CH2	1:A:440:LYS:C	0.45	2.95	17	11
1:A:469:LEU:HD13	1:A:476:TYR:CD2	0.45	2.45	7	2
1:A:430:TRP:CG	1:A:431:VAL:N	0.45	2.85	5	3
1:A:430:TRP:CD2	1:A:431:VAL:N	0.45	2.85	18	15
1:A:445:TYR:CD1	1:A:445:TYR:O	0.45	2.70	13	2
1:A:444:ILE:CD1	1:A:476:TYR:CE1	0.44	3.00	8	2
1:A:425:VAL:CB	1:A:455:HIS:CE1	0.44	3.01	4	3
1:A:430:TRP:O	1:A:431:VAL:HG13	0.44	2.13	8	6
1:A:443:MET:SD	1:A:455:HIS:CD2	0.44	3.10	1	1
1:A:469:LEU:CD1	1:A:476:TYR:CD2	0.44	2.99	4	3
1:A:415:TYR:CE1	1:A:441:PRO:O	0.44	2.71	12	6
1:A:445:TYR:O	1:A:445:TYR:CG	0.44	2.70	17	2
1:A:444:ILE:CD1	1:A:476:TYR:CE2	0.44	3.01	7	1
1:A:469:LEU:HD21	1:A:476:TYR:HD2	0.43	1.73	4	1
1:A:443:MET:CG	1:A:455:HIS:CD2	0.43	3.01	15	1
1:A:437:GLU:CG	1:A:440:LYS:O	0.43	2.66	18	1
1:A:430:TRP:CZ2	1:A:440:LYS:C	0.43	2.96	12	1
1:A:476:TYR:CD1	1:A:476:TYR:C	0.43	2.96	19	5
1:A:430:TRP:O	1:A:431:VAL:CG1	0.43	2.66	8	9
1:A:445:TYR:O	1:A:445:TYR:CD1	0.43	2.71	17	1
1:A:415:TYR:CD1	1:A:443:MET:SD	0.43	3.11	9	2
1:A:444:ILE:HD13	1:A:476:TYR:HE1	0.43	1.66	18	1
1:A:443:MET:HG2	1:A:455:HIS:CD2	0.43	2.49	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:445:TYR:CD1	1:A:446:CYS:O	0.43	2.72	16	1
1:A:430:TRP:CH2	1:A:440:LYS:O	0.43	2.72	14	1
1:A:445:TYR:CD1	1:A:445:TYR:C	0.42	2.96	9	5
1:A:469:LEU:HD13	1:A:476:TYR:CZ	0.42	2.49	3	1
1:A:476:TYR:CD1	1:A:477:TYR:O	0.42	2.73	11	2
1:A:476:TYR:C	1:A:476:TYR:CD1	0.42	2.98	4	1
1:A:415:TYR:CZ	1:A:441:PRO:O	0.42	2.73	14	1
1:A:454:VAL:CG2	1:A:459:MET:CE	0.42	2.98	18	1
1:A:473:SER:O	1:A:474:ASN:C	0.42	2.60	15	1
1:A:461:LEU:HD21	1:A:476:TYR:HE2	0.42	1.74	9	2
1:A:420:CYS:CB	1:A:421:PRO:HD2	0.42	2.44	16	10
1:A:476:TYR:CE1	1:A:477:TYR:O	0.42	2.73	14	4
1:A:444:ILE:HD13	1:A:444:ILE:N	0.42	2.30	13	1
1:A:444:ILE:CG1	1:A:445:TYR:N	0.42	2.83	5	3
1:A:444:ILE:C	1:A:453:TRP:CE3	0.42	2.98	18	2
1:A:473:SER:O	1:A:474:ASN:CG	0.42	2.63	15	1
1:A:447:SER:O	1:A:477:TYR:CE2	0.42	2.73	20	1
1:A:425:VAL:HB	1:A:455:HIS:CE1	0.41	2.50	15	3
1:A:477:TYR:CD1	1:A:477:TYR:N	0.41	2.87	14	1
1:A:446:CYS:HB3	1:A:452:HIS:CD2	0.41	2.49	7	2
1:A:415:TYR:CE1	1:A:443:MET:SD	0.41	3.13	5	1
1:A:453:TRP:O	1:A:454:VAL:HG13	0.41	2.15	5	1
1:A:415:TYR:HA	1:A:443:MET:HE2	0.41	1.93	10	1
1:A:480:GLU:O	1:A:481:HIS:CD2	0.41	2.73	9	2
1:A:443:MET:HE3	1:A:453:TRP:O	0.41	2.15	1	1
1:A:444:ILE:CG1	1:A:454:VAL:O	0.41	2.69	3	1
1:A:430:TRP:CZ3	1:A:431:VAL:C	0.41	2.99	7	3
1:A:466:LEU:C	1:A:466:LEU:CD1	0.41	2.94	11	2
1:A:438:LEU:CD1	1:A:439:ASN:ND2	0.41	2.84	12	1
1:A:444:ILE:C	1:A:453:TRP:CZ3	0.41	2.99	16	1
1:A:455:HIS:O	1:A:459:MET:HE2	0.41	2.15	18	1
1:A:444:ILE:O	1:A:453:TRP:CE3	0.41	2.74	19	1
1:A:443:MET:SD	1:A:453:TRP:CD1	0.40	3.15	12	1
1:A:443:MET:O	1:A:453:TRP:CZ3	0.40	2.74	15	1
1:A:437:GLU:CG	1:A:442:ALA:HB2	0.40	2.46	20	1
1:A:452:HIS:H	1:A:452:HIS:CD2	0.40	2.35	8	1
1:A:443:MET:HE3	1:A:453:TRP:C	0.40	2.42	1	1
1:A:444:ILE:N	1:A:454:VAL:O	0.40	2.55	4	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	69/82 (84%)	54±3 (79±4%)	12±2 (18±3%)	2±1 (3±2%)	4	34
All	All	1380/1640 (84%)	1089 (79%)	244 (18%)	47 (3%)	4	34

All 14 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	478	CYS	12
1	A	460	ASP	8
1	A	415	TYR	7
1	A	439	ASN	3
1	A	475	LYS	3
1	A	451	GLY	3
1	A	448	HIS	2
1	A	474	ASN	2
1	A	447	SER	2
1	A	455	HIS	1
1	A	450	ASP	1
1	A	440	LYS	1
1	A	473	SER	1
1	A	419	CYS	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	64/72 (89%)	49±3 (77±5%)	15±3 (23±5%)	2	28
All	All	1280/1440 (89%)	987 (77%)	293 (23%)	2	28

All 42 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	467	ILE	20
1	A	418	THR	18
1	A	420	CYS	18
1	A	427	ILE	16
1	A	417	ILE	12
1	A	466	LEU	12
1	A	415	TYR	11
1	A	438	LEU	10
1	A	461	LEU	10
1	A	447	SER	9
1	A	452	HIS	9
1	A	464	ARG	8
1	A	470	SER	8
1	A	440	LYS	8
1	A	462	GLU	8
1	A	475	LYS	8
1	A	459	MET	8
1	A	483	GLN	7
1	A	426	ASP	6
1	A	439	ASN	6
1	A	419	CYS	6
1	A	433	PHE	6
1	A	443	MET	5
1	A	474	ASN	5
1	A	435	SER	5
1	A	463	GLU	5
1	A	479	ASN	5
1	A	471	GLU	5
1	A	480	GLU	5
1	A	460	ASP	4
1	A	473	SER	4
1	A	424	ASP	4
1	A	428	ASN	3
1	A	468	HIS	3
1	A	469	LEU	3
1	A	444	ILE	3
1	A	448	HIS	2
1	A	450	ASP	2
1	A	457	GLN	2
1	A	437	GLU	2
1	A	458	CYS	1

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Mol	Chain	Res	Type	Models (Total)
1	A	478	CYS	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

No chemical shift data were provided