



Full wwPDB NMR Structure Validation Report ⓘ

Mar 5, 2026 – 06:05 PM UTC

PDB ID : 2GF5 / pdb_00002gf5
Title : Structure of intact FADD (MORT1)
Authors : Carrington, P.E.; Sandu, C.; Wei, Y.; Hill, J.M.; Morisawa, G.; Huang, T.;
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Deposited on : 2006-03-21

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

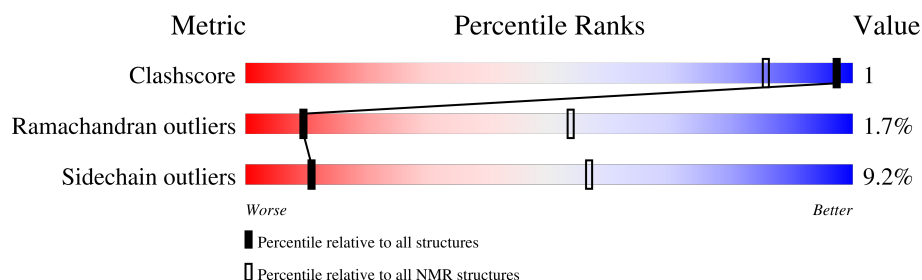
1 Overall quality at a glance

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	191	

2 Ensemble composition and analysis

This entry contains 25 models. Model 22 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative.

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:2-A:190 (189)	1.38	22

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 7 clusters and 1 single-model cluster was found.

Cluster number	Models
1	10, 11, 14, 18, 23
2	5, 7, 8, 20
3	13, 15, 17, 21
4	2, 6, 22
5	1, 19, 24
6	9, 12, 16
7	3, 4
Single-model clusters	25

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 3036 atoms, of which 1527 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called FADD protein.

Mol	Chain	Residues	Atoms						Trace
1	A	191	Total	C	H	N	O	S	0
			3036	929	1527	282	292	6	

There are 2 discrepancies between the modelled and reference sequences:

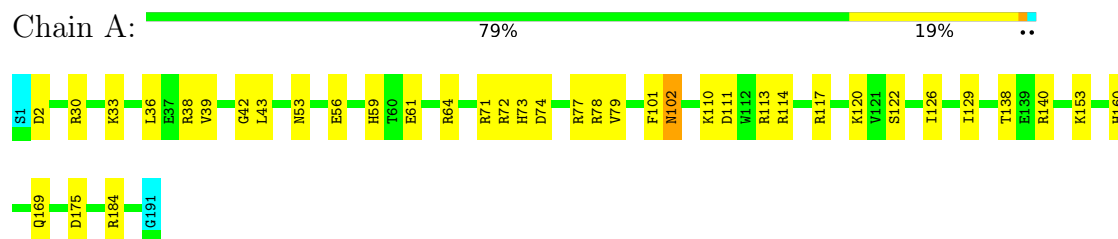
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	SER	-	cloning artifact	UNP Q13158
A	25	TYR	PHE	engineered mutation	UNP Q13158

4 Residue-property plots [i](#)

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: FADD protein

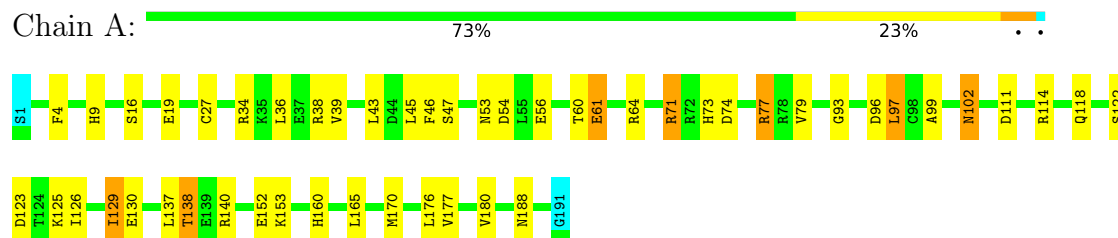


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

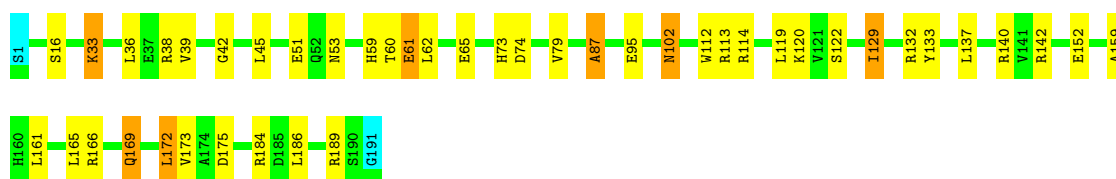
- Molecule 1: FADD protein



4.2.2 Score per residue for model 2

- Molecule 1: FADD protein

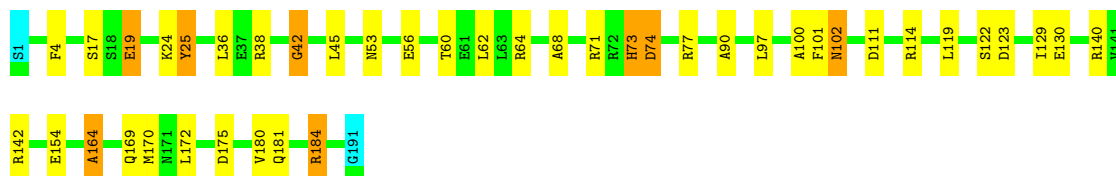




4.2.3 Score per residue for model 3

- Molecule 1: FADD protein

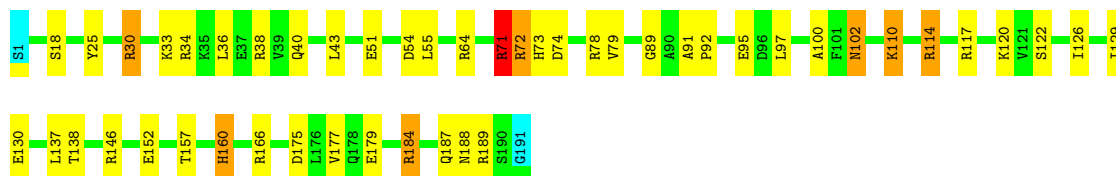
Chain A: 77% 18% ..



4.2.4 Score per residue for model 4

- Molecule 1: FADD protein

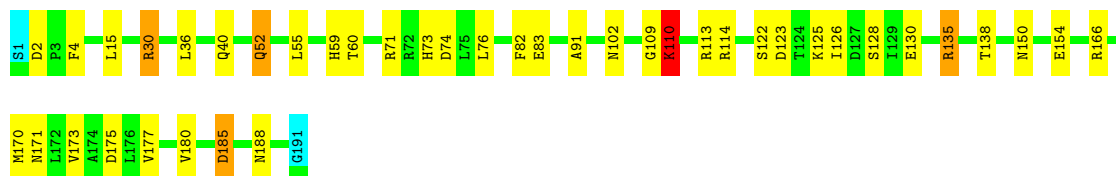
Chain A: 74% 21% ..



4.2.5 Score per residue for model 5

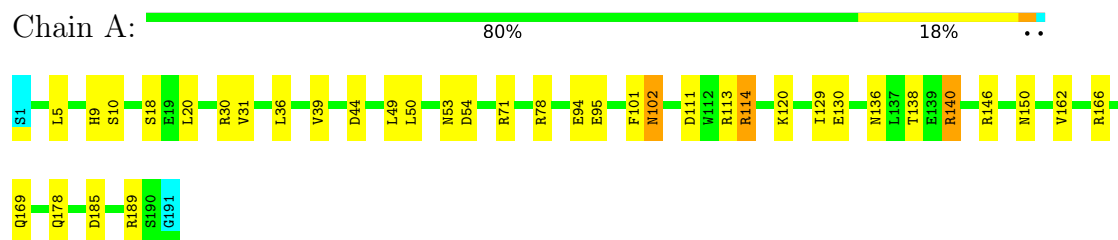
- Molecule 1: FADD protein

Chain A: 77% 19% ...



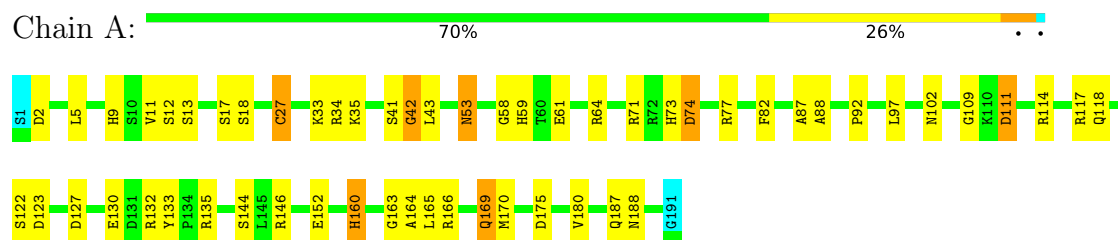
4.2.6 Score per residue for model 6

- Molecule 1: FADD protein



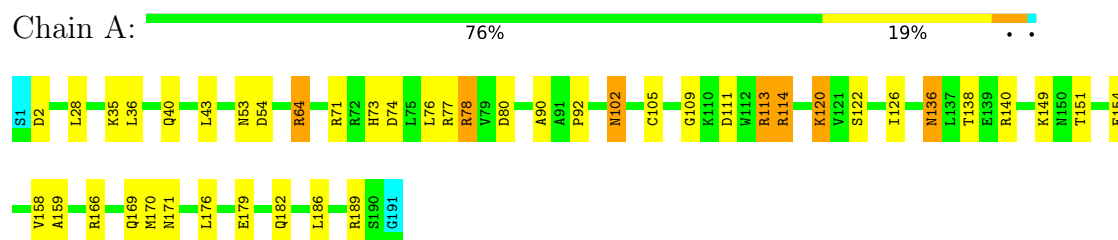
4.2.7 Score per residue for model 7

- Molecule 1: FADD protein



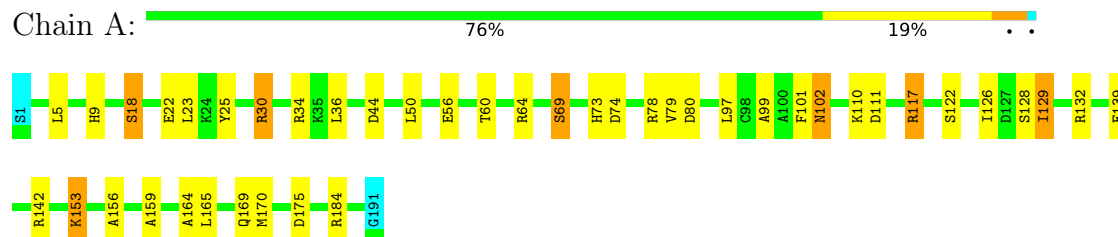
4.2.8 Score per residue for model 8

- Molecule 1: FADD protein



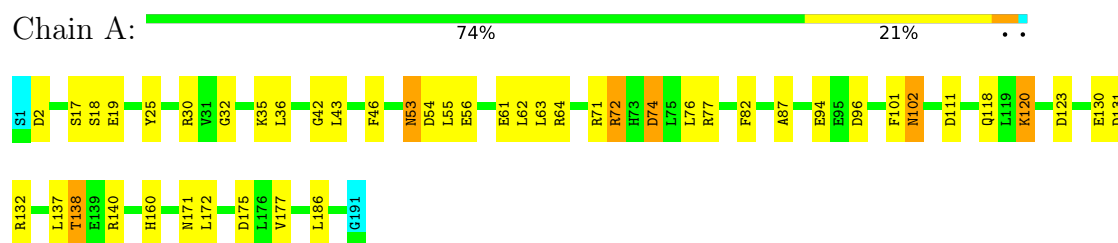
4.2.9 Score per residue for model 9

- Molecule 1: FADD protein



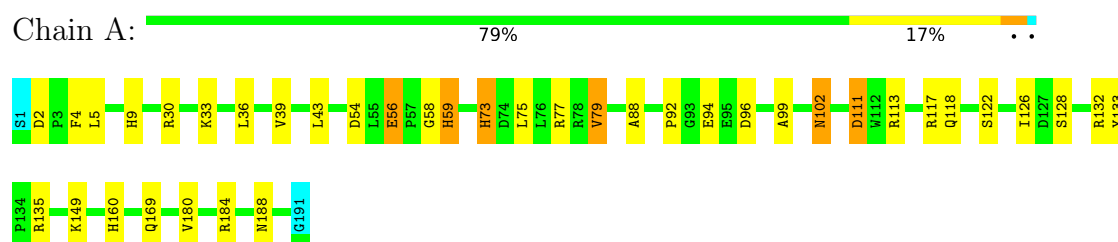
4.2.10 Score per residue for model 10

- Molecule 1: FADD protein



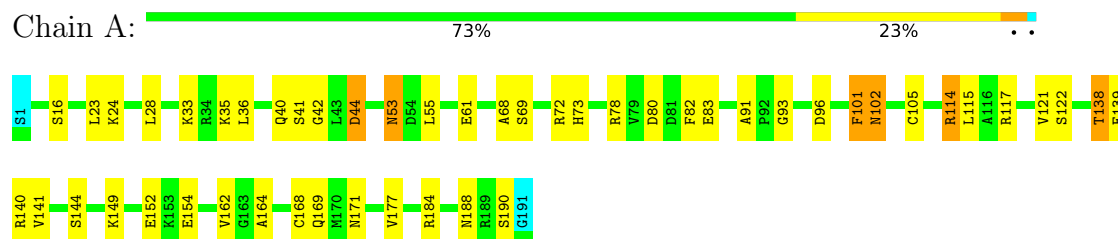
4.2.11 Score per residue for model 11

- Molecule 1: FADD protein



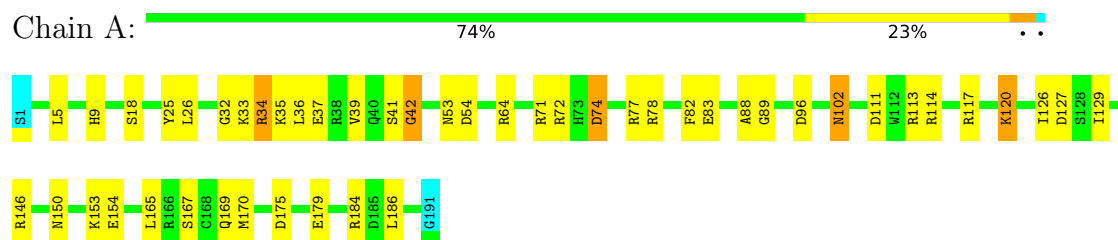
4.2.12 Score per residue for model 12

- Molecule 1: FADD protein



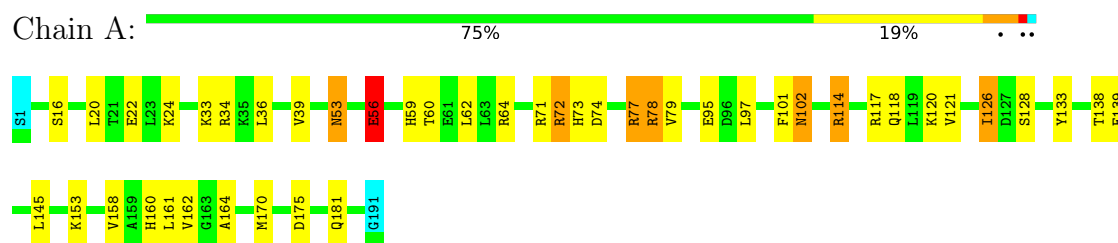
4.2.13 Score per residue for model 13

- Molecule 1: FADD protein



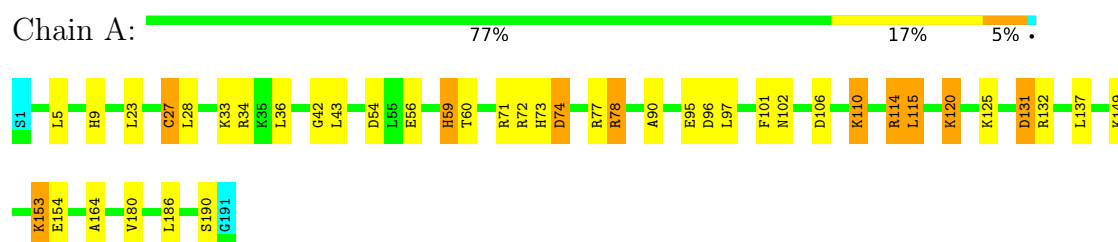
4.2.14 Score per residue for model 14

- Molecule 1: FADD protein



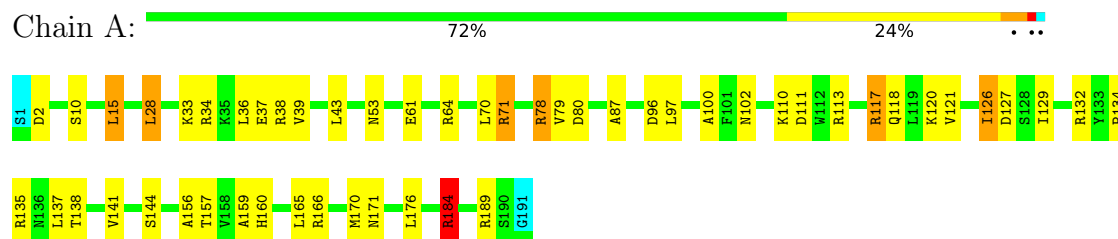
4.2.15 Score per residue for model 15

- Molecule 1: FADD protein



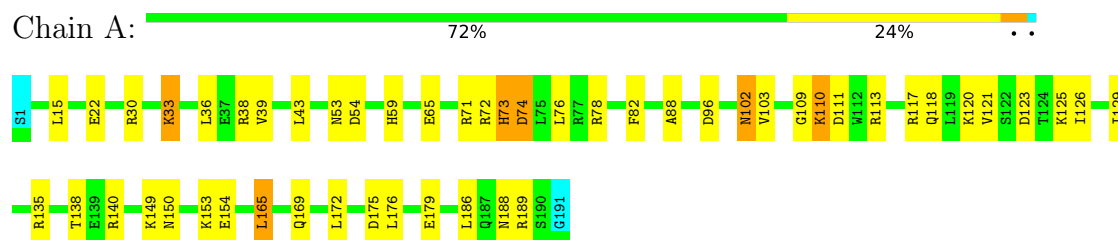
4.2.16 Score per residue for model 16

- Molecule 1: FADD protein



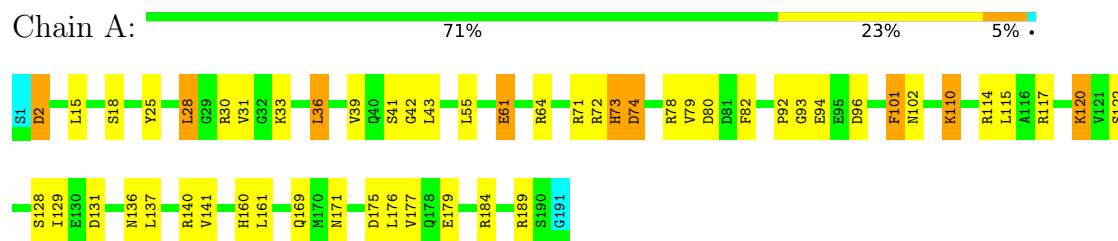
4.2.17 Score per residue for model 17

- Molecule 1: FADD protein



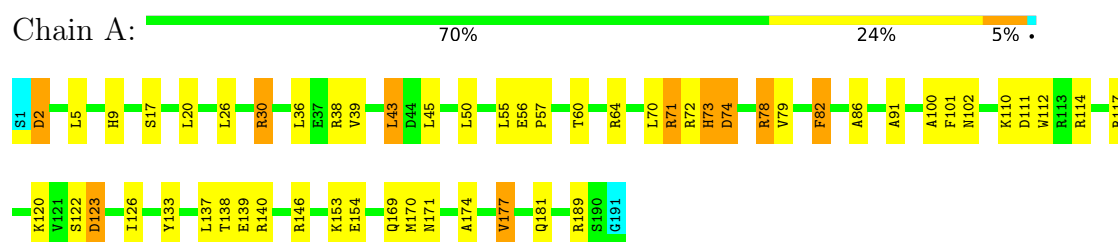
4.2.18 Score per residue for model 18

- Molecule 1: FADD protein



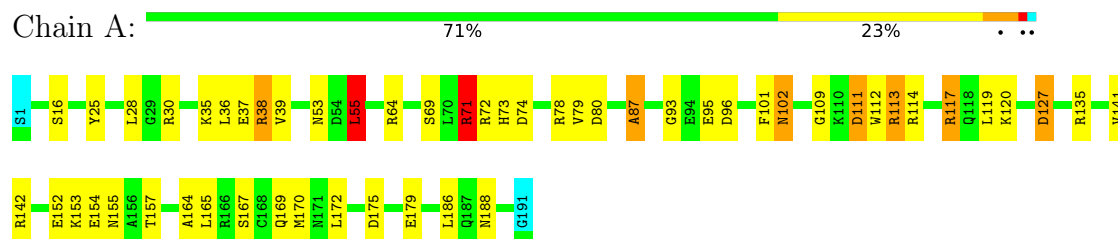
4.2.19 Score per residue for model 19

- Molecule 1: FADD protein



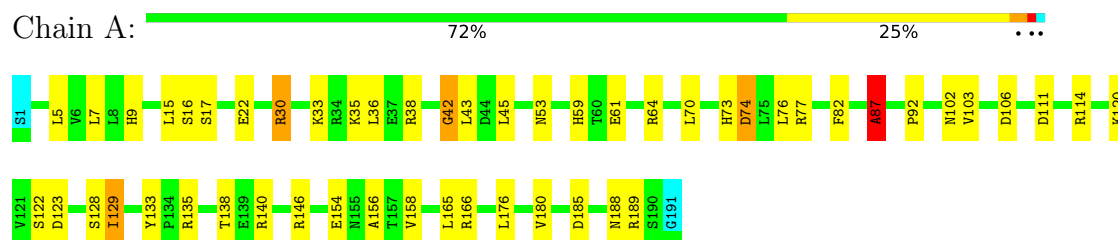
4.2.20 Score per residue for model 20

- Molecule 1: FADD protein



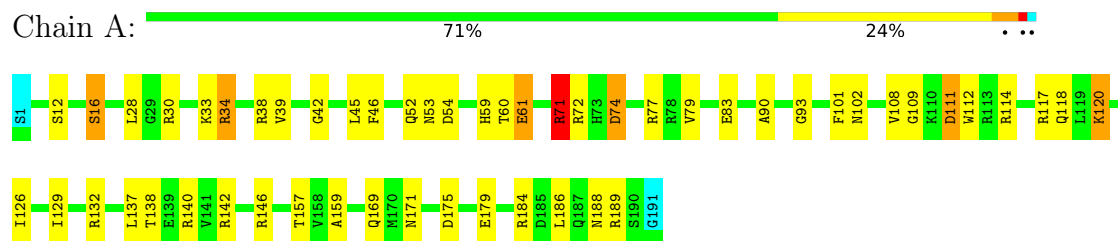
4.2.21 Score per residue for model 21

- Molecule 1: FADD protein



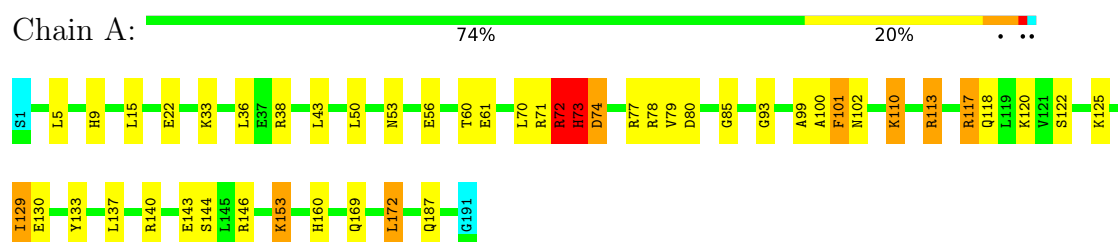
4.2.22 Score per residue for model 22 (medoid)

- Molecule 1: FADD protein



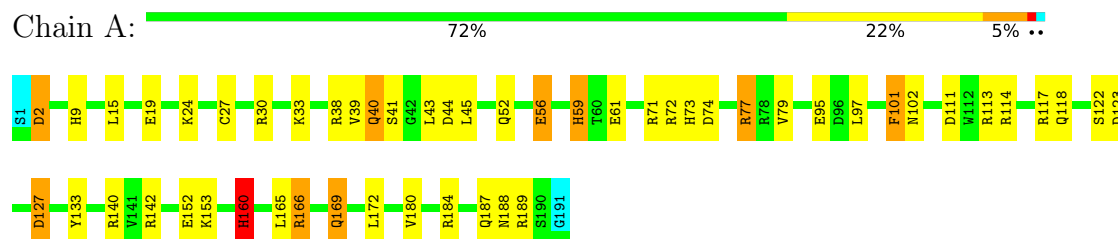
4.2.23 Score per residue for model 23

- Molecule 1: FADD protein



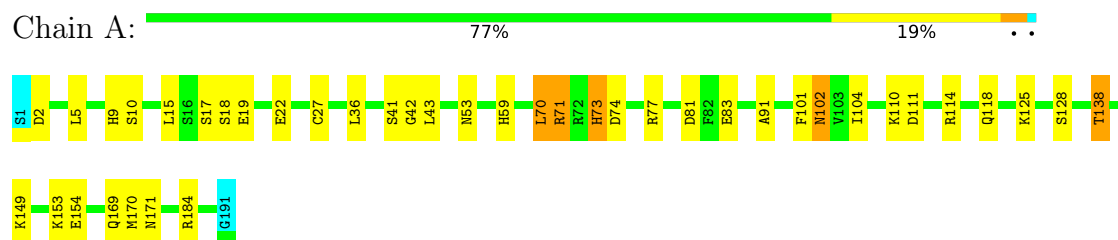
4.2.24 Score per residue for model 24

- Molecule 1: FADD protein



4.2.25 Score per residue for model 25

- Molecule 1: FADD protein



5 Refinement protocol and experimental data overview ⓘ

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

Of the 100 calculated structures, 25 were deposited, based on the following criterion: *25 structures for lowest energy*.

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

Software name	Classification	Version
X-PLOR	refinement	2.12.2
X-PLOR	structure solution	2.12.2

No chemical shift data was provided.

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	1.51±0.01	0±0/1516 (0.0± 0.0%)	1.92±0.04	36±6/2045 (1.8± 0.3%)
All	All	1.51	0/37900 (0.0%)	1.92	908/51125 (1.8%)

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	8.0±3.2
All	All	0	199

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	73	HIS	CA-C-N	10.33	134.48	120.54	7	14
1	A	73	HIS	C-N-CA	10.33	134.48	120.54	7	14
1	A	164	ALA	N-CA-C	9.27	120.99	111.07	12	1
1	A	122	SER	CA-C-N	9.14	132.32	120.44	8	11
1	A	122	SER	C-N-CA	9.14	132.32	120.44	8	11
1	A	53	ASN	CA-CB-CG	8.93	121.53	112.60	10	6
1	A	111	ASP	CA-CB-CG	-8.63	103.97	112.60	13	15
1	A	91	ALA	N-CA-C	8.55	120.08	109.57	5	2
1	A	131	ASP	CA-CB-CG	8.17	120.77	112.60	10	2
1	A	185	ASP	CA-CB-CG	-8.14	104.46	112.60	5	2
1	A	101	PHE	CA-CB-CG	8.00	121.80	113.80	12	9
1	A	122	SER	N-CA-C	7.88	121.61	110.50	2	5
1	A	83	GLU	CA-C-N	7.87	131.14	120.44	12	2
1	A	83	GLU	C-N-CA	7.87	131.14	120.44	12	2
1	A	28	LEU	N-CA-C	7.87	121.82	111.75	20	6

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	74	ASP	CA-CB-CG	-7.79	104.81	112.60	2	4
1	A	114	ARG	N-CA-CB	7.68	121.15	110.01	25	2
1	A	55	LEU	O-C-N	-7.66	114.51	123.25	5	1
1	A	188	ASN	CA-CB-CG	7.61	120.21	112.60	4	6
1	A	114	ARG	CA-C-N	7.56	130.75	120.54	20	10
1	A	114	ARG	C-N-CA	7.56	130.75	120.54	20	10
1	A	39	VAL	N-CA-C	7.51	121.65	109.78	18	8
1	A	2	ASP	N-CA-C	7.49	122.68	109.58	24	3
1	A	127	ASP	CA-CB-CG	7.48	120.08	112.60	24	5
1	A	137	LEU	CA-C-N	7.45	131.14	120.79	23	9
1	A	137	LEU	C-N-CA	7.45	131.14	120.79	23	9
1	A	157	THR	N-CA-CB	7.42	122.77	110.52	16	2
1	A	123	ASP	N-CA-C	7.34	120.15	111.71	1	2
1	A	43	LEU	CA-C-N	7.32	131.80	120.82	16	3
1	A	43	LEU	C-N-CA	7.32	131.80	120.82	16	3
1	A	82	PHE	N-CA-C	7.27	118.85	111.07	12	2
1	A	33	LYS	N-CA-C	7.25	119.18	111.28	22	6
1	A	138	THR	N-CA-C	7.24	119.86	111.02	25	3
1	A	82	PHE	CA-CB-CG	-7.24	106.56	113.80	18	7
1	A	79	VAL	CA-C-N	7.24	130.31	120.54	23	13
1	A	79	VAL	C-N-CA	7.24	130.31	120.54	23	13
1	A	69	SER	N-CA-C	7.15	121.64	112.34	9	2
1	A	28	LEU	CA-C-N	7.14	129.13	120.13	8	1
1	A	28	LEU	C-N-CA	7.14	129.13	120.13	8	1
1	A	95	GLU	CA-C-N	7.05	130.06	120.54	6	4
1	A	95	GLU	C-N-CA	7.05	130.06	120.54	6	4
1	A	72	ARG	CA-C-N	7.05	130.67	120.38	14	6
1	A	72	ARG	C-N-CA	7.05	130.67	120.38	14	6
1	A	123	ASP	CA-CB-CG	-7.05	105.55	112.60	21	4
1	A	94	GLU	N-CA-C	7.04	119.85	111.33	6	4
1	A	53	ASN	N-CA-C	7.03	121.34	111.92	12	1
1	A	102	ASN	CA-CB-CG	7.03	119.63	112.60	12	13
1	A	153	LYS	N-CA-C	7.00	122.85	111.37	17	4
1	A	164	ALA	CA-C-N	6.95	129.47	120.44	14	5
1	A	164	ALA	C-N-CA	6.95	129.47	120.44	14	5
1	A	136	ASN	CA-CB-CG	-6.94	105.66	112.60	8	2
1	A	73	HIS	N-CA-C	6.92	119.41	111.11	20	7
1	A	22	GLU	N-CA-CB	6.92	120.04	110.01	21	2
1	A	37	GLU	N-CA-C	6.91	120.60	111.75	13	2
1	A	96	ASP	CA-CB-CG	-6.91	105.69	112.60	18	6
1	A	32	GLY	CA-C-N	6.90	129.83	120.38	13	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	32	GLY	C-N-CA	6.90	129.83	120.38	13	2
1	A	59	HIS	N-CA-C	6.88	119.89	108.96	11	4
1	A	175	ASP	CA-CB-CG	-6.86	105.74	112.60	9	13
1	A	129	ILE	CA-C-N	6.79	129.71	120.54	6	7
1	A	129	ILE	C-N-CA	6.79	129.71	120.54	6	7
1	A	56	GLU	CB-CA-C	6.79	119.40	109.48	11	2
1	A	39	VAL	N-CA-CB	6.79	118.30	110.49	13	3
1	A	72	ARG	N-CA-C	6.72	120.22	108.52	20	2
1	A	18	SER	N-CA-CB	6.69	120.06	110.16	13	2
1	A	159	ALA	N-CA-C	6.68	120.53	112.38	16	4
1	A	160	HIS	N-CA-CB	6.65	119.89	110.12	4	1
1	A	141	VAL	N-CA-C	6.64	117.40	110.62	16	2
1	A	60	THR	N-CA-C	6.63	121.01	112.26	15	1
1	A	90	ALA	N-CA-C	-6.59	103.91	112.68	3	2
1	A	18	SER	N-CA-C	6.58	119.01	111.11	25	4
1	A	16	SER	N-CA-C	6.58	118.34	110.19	21	2
1	A	54	ASP	N-CA-C	-6.57	105.42	113.50	15	6
1	A	55	LEU	N-CA-C	-6.56	100.81	110.52	10	4
1	A	31	VAL	N-CA-C	-6.55	98.42	107.99	18	1
1	A	111	ASP	N-CA-CB	-6.55	100.78	110.53	22	1
1	A	97	LEU	CA-C-N	6.53	129.03	120.28	14	4
1	A	97	LEU	C-N-CA	6.53	129.03	120.28	14	4
1	A	78	ARG	N-CA-C	6.53	118.40	111.28	16	3
1	A	73	HIS	CA-CB-CG	6.52	120.32	113.80	23	3
1	A	45	LEU	CA-C-N	6.51	129.30	120.38	1	7
1	A	45	LEU	C-N-CA	6.51	129.30	120.38	1	7
1	A	34	ARG	N-CA-C	6.49	118.02	111.07	15	3
1	A	152	GLU	N-CA-CB	6.48	117.81	110.35	12	2
1	A	74	ASP	CA-C-N	6.48	128.96	120.28	18	16
1	A	74	ASP	C-N-CA	6.48	128.96	120.28	18	16
1	A	70	LEU	CA-C-N	6.43	131.42	121.19	25	1
1	A	70	LEU	C-N-CA	6.43	131.42	121.19	25	1
1	A	133	TYR	O-C-N	-6.40	113.96	121.32	11	4
1	A	126	ILE	N-CA-CB	6.40	117.61	110.51	19	2
1	A	177	VAL	N-CA-C	6.39	117.07	110.36	18	2
1	A	117	ARG	N-CA-C	6.39	118.24	111.28	16	6
1	A	149	LYS	N-CA-C	6.38	120.17	112.38	15	3
1	A	168	CYS	N-CA-C	6.32	120.45	112.87	12	1
1	A	153	LYS	CA-C-N	6.29	128.70	120.28	9	1
1	A	153	LYS	C-N-CA	6.29	128.70	120.28	9	1
1	A	68	ALA	N-CA-C	-6.29	105.44	113.23	12	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	54	ASP	CA-C-N	6.28	132.45	122.59	8	1
1	A	54	ASP	C-N-CA	6.28	132.45	122.59	8	1
1	A	170	MET	CG-SD-CE	-6.26	87.13	100.90	1	9
1	A	25	TYR	N-CA-C	6.26	118.10	111.28	20	3
1	A	187	GLN	CA-C-N	6.25	128.57	120.44	4	3
1	A	187	GLN	C-N-CA	6.25	128.57	120.44	4	3
1	A	41	SER	CA-C-N	6.25	133.66	121.41	13	4
1	A	41	SER	C-N-CA	6.25	133.66	121.41	13	4
1	A	104	ILE	N-CA-C	6.24	118.85	111.05	25	1
1	A	128	SER	CA-C-N	6.21	129.28	120.53	18	5
1	A	128	SER	C-N-CA	6.21	129.28	120.53	18	5
1	A	16	SER	CA-C-N	-6.21	111.52	122.26	22	1
1	A	16	SER	C-N-CA	-6.21	111.52	122.26	22	1
1	A	130	GLU	CA-C-N	6.20	128.59	120.28	4	8
1	A	130	GLU	C-N-CA	6.20	128.59	120.28	4	8
1	A	184	ARG	N-CA-C	6.20	118.84	111.33	25	1
1	A	156	ALA	N-CA-C	6.19	118.07	109.15	9	2
1	A	190	SER	N-CA-C	6.17	117.67	111.07	15	1
1	A	25	TYR	N-CA-CB	6.17	118.96	110.01	3	2
1	A	62	LEU	CA-C-N	6.12	128.40	120.44	3	2
1	A	62	LEU	C-N-CA	6.12	128.40	120.44	3	2
1	A	61	GLU	N-CA-C	6.12	118.45	111.11	22	7
1	A	123	ASP	CA-C-N	6.08	128.35	120.44	3	4
1	A	123	ASP	C-N-CA	6.08	128.35	120.44	3	4
1	A	60	THR	CA-C-N	6.08	128.75	120.54	22	7
1	A	60	THR	C-N-CA	6.08	128.75	120.54	22	7
1	A	176	LEU	N-CA-C	6.07	118.68	111.33	17	3
1	A	179	GLU	CA-C-N	6.03	128.66	120.77	4	6
1	A	179	GLU	C-N-CA	6.03	128.66	120.77	4	6
1	A	181	GLN	N-CA-C	6.02	117.64	111.14	3	1
1	A	155	ASN	N-CA-CB	-6.02	102.60	111.51	20	1
1	A	117	ARG	CD-NE-CZ	-6.02	115.98	124.40	9	1
1	A	106	ASP	N-CA-C	6.00	118.31	111.11	21	2
1	A	125	LYS	N-CA-CB	5.99	118.93	110.12	25	2
1	A	35	LYS	N-CA-CB	-5.99	101.34	110.33	13	1
1	A	41	SER	N-CA-C	5.99	116.18	108.34	24	1
1	A	109	GLY	O-C-N	-5.98	118.47	123.73	8	2
1	A	151	THR	CA-C-N	5.97	131.05	122.21	8	1
1	A	151	THR	C-N-CA	5.97	131.05	122.21	8	1
1	A	10	SER	N-CA-C	5.97	118.56	111.33	16	2
1	A	152	GLU	O-C-N	-5.97	114.73	122.37	20	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	9	HIS	CA-C-N	5.96	128.19	120.44	24	2
1	A	9	HIS	C-N-CA	5.96	128.19	120.44	24	2
1	A	165	LEU	N-CA-CB	-5.95	101.14	110.30	21	1
1	A	17	SER	CA-C-N	5.95	128.57	120.54	19	5
1	A	17	SER	C-N-CA	5.95	128.57	120.54	19	5
1	A	88	ALA	CB-CA-C	-5.94	101.32	111.31	13	1
1	A	130	GLU	N-CA-C	5.93	117.74	111.28	10	2
1	A	71	ARG	N-CA-CB	5.92	118.57	110.57	8	4
1	A	60	THR	CA-CB-OG1	5.92	118.48	109.60	1	3
1	A	120	LYS	N-CA-CB	5.91	120.48	110.49	15	4
1	A	157	THR	N-CA-C	-5.91	99.37	109.24	22	2
1	A	100	ALA	CA-C-N	5.90	128.18	120.28	3	5
1	A	100	ALA	C-N-CA	5.90	128.18	120.28	3	5
1	A	91	ALA	CA-C-O	-5.89	115.25	120.19	25	1
1	A	129	ILE	N-CA-CB	5.88	118.10	110.57	21	1
1	A	92	PRO	CA-C-N	5.88	126.62	120.03	21	4
1	A	92	PRO	C-N-CA	5.88	126.62	120.03	21	4
1	A	113	ARG	CA-C-N	5.87	128.42	120.38	6	1
1	A	113	ARG	C-N-CA	5.87	128.42	120.38	6	1
1	A	46	PHE	CA-C-N	5.86	128.06	120.44	1	3
1	A	46	PHE	C-N-CA	5.86	128.06	120.44	1	3
1	A	101	PHE	CA-C-N	5.86	128.06	120.44	22	4
1	A	101	PHE	C-N-CA	5.86	128.06	120.44	22	4
1	A	77	ARG	N-CA-C	5.84	118.43	111.71	14	2
1	A	115	LEU	N-CA-C	5.82	117.30	111.07	15	1
1	A	56	GLU	O-C-N	-5.80	116.39	121.32	1	1
1	A	42	GLY	N-CA-C	5.79	126.91	113.18	21	5
1	A	36	LEU	N-CA-CB	5.79	118.73	110.16	18	1
1	A	93	GLY	CA-C-N	5.79	128.62	120.28	18	6
1	A	93	GLY	C-N-CA	5.79	128.62	120.28	18	6
1	A	122	SER	N-CA-CB	5.79	118.55	110.04	12	3
1	A	121	VAL	N-CA-C	-5.77	101.36	109.21	16	1
1	A	71	ARG	N-CA-C	5.74	120.78	111.37	25	1
1	A	19	GLU	N-CA-CB	5.74	118.55	110.12	1	1
1	A	108	VAL	CA-C-O	5.74	127.10	121.19	22	1
1	A	167	SER	N-CA-C	5.73	119.75	112.87	13	2
1	A	4	PHE	CA-CB-CG	-5.73	108.07	113.80	1	3
1	A	90	ALA	N-CA-CB	5.72	118.63	110.16	22	1
1	A	184	ARG	CA-C-N	5.72	128.27	120.54	22	4
1	A	184	ARG	C-N-CA	5.72	128.27	120.54	22	4
1	A	58	GLY	O-C-N	-5.71	118.65	121.85	7	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	126	ILE	N-CA-C	5.70	117.12	110.62	22	1
1	A	78	ARG	CA-C-N	5.69	128.26	120.46	13	4
1	A	78	ARG	C-N-CA	5.69	128.26	120.46	13	4
1	A	7	LEU	N-CA-C	5.69	117.16	111.07	21	1
1	A	158	VAL	N-CA-CB	5.68	119.11	110.58	21	1
1	A	178	GLN	N-CA-C	5.68	117.47	111.28	6	1
1	A	137	LEU	N-CA-C	5.68	117.33	111.03	15	1
1	A	87	ALA	N-CA-C	5.65	122.84	110.80	21	3
1	A	61	GLU	CA-C-N	5.64	127.78	120.44	1	1
1	A	61	GLU	C-N-CA	5.64	127.78	120.44	1	1
1	A	102	ASN	CB-CA-C	5.64	119.73	110.88	6	3
1	A	176	LEU	CA-C-N	5.63	127.86	120.60	16	2
1	A	176	LEU	C-N-CA	5.63	127.86	120.60	16	2
1	A	22	GLU	CA-C-N	5.63	128.09	120.38	23	2
1	A	22	GLU	C-N-CA	5.63	128.09	120.38	23	2
1	A	113	ARG	N-CA-C	5.61	117.84	111.11	23	1
1	A	144	SER	N-CA-C	5.60	117.83	111.11	23	2
1	A	165	LEU	N-CA-C	5.58	117.81	111.11	17	1
1	A	80	ASP	CA-C-N	5.57	127.74	120.28	8	3
1	A	80	ASP	C-N-CA	5.57	127.74	120.28	8	3
1	A	96	ASP	CA-C-N	5.56	127.67	120.44	13	3
1	A	96	ASP	C-N-CA	5.56	127.67	120.44	13	3
1	A	121	VAL	N-CA-CB	5.55	116.98	110.82	12	1
1	A	125	LYS	N-CA-C	5.55	118.09	111.71	15	1
1	A	111	ASP	N-CA-C	-5.55	105.95	114.16	25	1
1	A	171	ASN	CA-CB-CG	-5.55	107.05	112.60	12	3
1	A	144	SER	N-CA-CB	5.54	118.52	110.26	12	2
1	A	139	GLU	N-CA-C	-5.54	105.39	111.82	12	1
1	A	169	GLN	CA-C-N	-5.54	115.15	122.85	24	1
1	A	169	GLN	C-N-CA	-5.54	115.15	122.85	24	1
1	A	160	HIS	CA-CB-CG	5.53	119.33	113.80	10	3
1	A	61	GLU	N-CA-CB	5.53	118.00	109.98	10	1
1	A	171	ASN	CA-C-N	5.52	127.99	120.54	5	6
1	A	171	ASN	C-N-CA	5.52	127.99	120.54	5	6
1	A	95	GLU	N-CA-C	5.51	116.97	110.97	15	1
1	A	2	ASP	O-C-N	-5.50	116.25	121.20	18	1
1	A	128	SER	N-CA-C	5.50	117.35	111.36	21	1
1	A	154	GLU	N-CA-C	5.48	117.25	111.28	8	4
1	A	39	VAL	CB-CA-C	-5.46	103.05	111.08	14	1
1	A	101	PHE	CB-CA-C	5.45	120.72	110.63	22	3
1	A	78	ARG	N-CA-CB	5.45	117.91	110.01	8	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	128	SER	N-CA-CB	5.44	117.87	109.98	25	1
1	A	88	ALA	N-CA-C	5.42	117.07	108.67	11	1
1	A	114	ARG	CG-CD-NE	-5.41	100.10	112.00	7	1
1	A	83	GLU	N-CA-C	5.41	116.86	111.07	13	1
1	A	20	LEU	N-CA-C	5.40	117.17	111.28	14	2
1	A	171	ASN	N-CA-C	5.39	116.97	111.14	22	1
1	A	39	VAL	O-C-N	-5.39	116.46	122.66	22	1
1	A	43	LEU	N-CA-C	5.38	118.07	111.82	17	1
1	A	174	ALA	N-CA-CB	5.38	117.87	110.07	19	1
1	A	55	LEU	N-CA-CB	-5.38	102.26	110.49	20	2
1	A	4	PHE	N-CA-C	5.38	117.14	111.28	11	1
1	A	112	TRP	N-CA-C	5.37	119.32	112.34	22	1
1	A	31	VAL	CA-C-N	5.37	127.14	121.45	6	1
1	A	31	VAL	C-N-CA	5.37	127.14	121.45	6	1
1	A	20	LEU	CA-C-N	5.37	127.91	120.29	19	1
1	A	20	LEU	C-N-CA	5.37	127.91	120.29	19	1
1	A	161	LEU	CA-C-N	5.36	127.31	120.56	2	3
1	A	161	LEU	C-N-CA	5.36	127.31	120.56	2	3
1	A	18	SER	CA-C-N	5.36	127.41	120.44	9	1
1	A	18	SER	C-N-CA	5.36	127.41	120.44	9	1
1	A	41	SER	CA-C-O	-5.35	115.70	121.38	25	1
1	A	54	ASP	N-CA-CB	-5.35	102.22	110.13	10	1
1	A	69	SER	CA-C-O	5.34	125.52	119.27	20	1
1	A	109	GLY	N-CA-C	-5.32	102.98	110.91	17	2
1	A	76	LEU	CA-C-N	5.32	127.36	120.44	5	1
1	A	76	LEU	C-N-CA	5.32	127.36	120.44	5	1
1	A	15	LEU	N-CA-CB	-5.32	101.95	110.46	16	1
1	A	138	THR	CB-CA-C	-5.31	100.47	110.67	12	1
1	A	81	ASP	N-CA-C	5.30	117.81	111.71	25	1
1	A	105	CYS	CA-C-N	5.29	127.64	120.44	12	2
1	A	105	CYS	C-N-CA	5.29	127.64	120.44	12	2
1	A	102	ASN	N-CA-CB	-5.29	102.35	110.12	25	1
1	A	44	ASP	CA-CB-CG	5.27	117.87	112.60	6	1
1	A	35	LYS	CA-C-N	5.27	127.66	120.54	8	2
1	A	35	LYS	C-N-CA	5.27	127.66	120.54	8	2
1	A	82	PHE	N-CA-CB	5.25	117.57	109.91	18	1
1	A	97	LEU	N-CA-CB	-5.24	102.40	110.20	4	1
1	A	76	LEU	N-CA-CB	5.23	117.55	109.91	10	1
1	A	109	GLY	CA-C-N	5.23	131.53	121.54	5	1
1	A	109	GLY	C-N-CA	5.23	131.53	121.54	5	1
1	A	89	GLY	N-CA-C	-5.23	107.58	115.32	13	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	27	CYS	CA-C-N	5.22	128.01	120.38	24	2
1	A	27	CYS	C-N-CA	5.22	128.01	120.38	24	2
1	A	117	ARG	CA-C-N	5.22	127.23	120.44	7	1
1	A	117	ARG	C-N-CA	5.22	127.23	120.44	7	1
1	A	38	ARG	CG-CD-NE	-5.21	100.54	112.00	16	1
1	A	56	GLU	N-CA-CB	-5.20	101.12	110.37	10	1
1	A	162	VAL	CA-C-N	5.18	125.69	119.94	6	1
1	A	162	VAL	C-N-CA	5.18	125.69	119.94	6	1
1	A	140	ARG	N-CA-CB	5.18	117.47	109.91	6	1
1	A	149	LYS	CA-C-N	5.16	127.92	120.38	17	1
1	A	149	LYS	C-N-CA	5.16	127.92	120.38	17	1
1	A	106	ASP	N-CA-CB	-5.16	102.25	109.94	21	1
1	A	185	ASP	CA-C-N	5.16	127.15	120.44	6	1
1	A	185	ASP	C-N-CA	5.16	127.15	120.44	6	1
1	A	160	HIS	CA-C-N	5.15	127.44	120.44	16	1
1	A	160	HIS	C-N-CA	5.15	127.44	120.44	16	1
1	A	13	SER	N-CA-C	5.15	118.82	112.54	7	1
1	A	51	GLU	CA-C-N	5.14	127.59	120.29	2	1
1	A	51	GLU	C-N-CA	5.14	127.59	120.29	2	1
1	A	170	MET	CB-CA-C	-5.13	103.06	111.68	25	1
1	A	141	VAL	N-CA-CB	5.12	116.55	110.55	12	1
1	A	10	SER	CA-C-N	5.12	127.10	120.70	6	1
1	A	10	SER	C-N-CA	5.12	127.10	120.70	6	1
1	A	44	ASP	N-CA-C	5.12	117.27	111.02	9	2
1	A	72	ARG	N-CA-CB	5.12	119.03	110.53	15	1
1	A	154	GLU	N-CA-CB	-5.11	103.56	110.67	12	1
1	A	79	VAL	N-CA-C	5.11	115.83	110.62	11	1
1	A	99	ALA	CA-C-N	5.11	127.08	120.44	1	4
1	A	99	ALA	C-N-CA	5.11	127.08	120.44	1	4
1	A	37	GLU	CB-CG-CD	5.11	121.28	112.60	16	1
1	A	12	SER	N-CA-CB	5.10	118.19	110.28	7	1
1	A	160	HIS	CB-CG-CD2	-5.10	124.58	131.20	7	1
1	A	125	LYS	CB-CA-C	-5.09	102.90	110.88	17	1
1	A	146	ARG	CA-C-N	5.08	127.69	120.53	21	1
1	A	146	ARG	C-N-CA	5.08	127.69	120.53	21	1
1	A	126	ILE	CA-C-N	5.08	127.85	120.79	11	2
1	A	126	ILE	C-N-CA	5.08	127.85	120.79	11	2
1	A	50	LEU	N-CA-C	5.07	117.70	111.82	23	1
1	A	172	LEU	N-CA-C	5.07	116.49	111.07	23	1
1	A	19	GLU	CA-C-N	5.05	127.05	120.28	3	1
1	A	19	GLU	C-N-CA	5.05	127.05	120.28	3	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	189	ARG	CA-C-N	5.05	127.76	120.38	16	1
1	A	189	ARG	C-N-CA	5.05	127.76	120.38	16	1
1	A	163	GLY	N-CA-C	5.05	119.00	112.83	7	1
1	A	112	TRP	CA-C-N	5.05	127.00	120.44	2	1
1	A	112	TRP	C-N-CA	5.05	127.00	120.44	2	1
1	A	159	ALA	CA-C-N	5.05	127.36	120.54	8	1
1	A	159	ALA	C-N-CA	5.05	127.36	120.54	8	1
1	A	59	HIS	CA-CB-CG	5.04	118.84	113.80	2	1
1	A	12	SER	N-CA-C	5.04	117.50	111.71	22	1
1	A	138	THR	CA-C-N	5.03	127.02	120.28	10	1
1	A	138	THR	C-N-CA	5.03	127.02	120.28	10	1
1	A	110	LYS	N-CA-C	5.03	121.51	110.80	17	1
1	A	15	LEU	CB-CA-C	5.02	118.41	109.38	17	1
1	A	153	LYS	O-C-N	-5.02	116.96	122.38	23	1
1	A	160	HIS	CB-CA-C	-5.01	102.42	110.74	11	1
1	A	145	LEU	CA-C-N	5.01	127.45	120.63	14	1
1	A	145	LEU	C-N-CA	5.01	127.45	120.63	14	1
1	A	76	LEU	N-CA-C	5.01	116.43	111.07	8	1
1	A	47	SER	N-CA-CB	5.01	117.27	110.01	1	1
1	A	28	LEU	CB-CA-C	-5.00	100.75	110.46	12	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	64	ARG	Sidechain	13
1	A	140	ARG	Sidechain	12
1	A	30	ARG	Sidechain	12
1	A	78	ARG	Sidechain	11
1	A	38	ARG	Sidechain	10
1	A	117	ARG	Sidechain	10
1	A	71	ARG	Sidechain	9
1	A	113	ARG	Sidechain	9
1	A	166	ARG	Sidechain	9
1	A	132	ARG	Sidechain	8
1	A	189	ARG	Sidechain	8
1	A	184	ARG	Sidechain	8
1	A	114	ARG	Sidechain	7
1	A	146	ARG	Sidechain	7
1	A	77	ARG	Sidechain	6

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Mol	Chain	Res	Type	Group	Models (Total)
1	A	72	ARG	Sidechain	6
1	A	110	LYS	Peptide	6
1	A	135	ARG	Sidechain	6
1	A	142	ARG	Sidechain	5
1	A	40	GLN	Peptide	4
1	A	34	ARG	Sidechain	4
1	A	133	TYR	Sidechain,Peptide	3
1	A	25	TYR	Sidechain	3
1	A	101	PHE	Sidechain	3
1	A	87	ALA	Peptide	2
1	A	120	LYS	Peptide	2
1	A	2	ASP	Peptide	2
1	A	88	ALA	Peptide	2
1	A	91	ALA	Peptide	2
1	A	160	HIS	Sidechain	2
1	A	89	GLY	Peptide	1
1	A	152	GLU	Peptide	1
1	A	136	ASN	Peptide	1
1	A	111	ASP	Peptide	1
1	A	59	HIS	Sidechain	1
1	A	57	PRO	Peptide	1
1	A	73	HIS	Sidechain	1
1	A	85	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	1498	1517	1513	2±1
All	All	37450	37925	37825	48

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 1.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:5:LEU:O	1:A:9:HIS:CD2	0.52	2.63	11	10
1:A:9:HIS:CD2	1:A:43:LEU:HD11	0.51	2.41	23	3
1:A:165:LEU:HD11	1:A:173:VAL:HG23	0.49	1.84	2	1
1:A:59:HIS:CE1	1:A:83:GLU:OE1	0.49	2.65	22	1
1:A:112:TRP:CD1	1:A:141:VAL:HG12	0.49	2.42	20	1
1:A:59:HIS:CD2	1:A:154:GLU:HG2	0.48	2.44	15	1
1:A:56:GLU:OE2	1:A:59:HIS:CD2	0.47	2.67	24	2
1:A:73:HIS:CE1	1:A:74:ASP:OD2	0.47	2.68	23	2
1:A:97:LEU:HD21	1:A:156:ALA:HB3	0.47	1.84	16	1
1:A:152:GLU:OE2	1:A:160:HIS:CE1	0.46	2.69	24	2
1:A:119:LEU:HD21	1:A:164:ALA:HB2	0.46	1.87	3	1
1:A:55:LEU:H	1:A:55:LEU:CD2	0.45	2.24	20	1
1:A:82:PHE:HA	1:A:86:ALA:HB3	0.45	1.88	19	1
1:A:139:GLU:H	1:A:139:GLU:CD	0.44	2.20	14	1
1:A:59:HIS:CD2	1:A:154:GLU:OE2	0.44	2.71	17	1
1:A:118:GLN:O	1:A:160:HIS:CE1	0.43	2.71	14	1
1:A:109:GLY:C	1:A:111:ASP:H	0.43	2.21	22	2
1:A:115:LEU:HD11	1:A:164:ALA:HA	0.43	1.91	15	1
1:A:111:ASP:HA	1:A:113:ARG:HH11	0.43	1.74	8	1
1:A:75:LEU:O	1:A:79:VAL:HG23	0.43	2.13	11	1
1:A:59:HIS:CE1	1:A:83:GLU:HB3	0.43	2.49	25	1
1:A:125:LYS:HZ2	1:A:143:GLU:CD	0.43	2.21	23	1
1:A:52:GLN:HE21	1:A:52:GLN:HA	0.42	1.73	5	1
1:A:152:GLU:OE1	1:A:160:HIS:CD2	0.42	2.71	7	1
1:A:73:HIS:CE1	1:A:74:ASP:OD1	0.42	2.73	18	1
1:A:133:TYR:CG	1:A:139:GLU:HG3	0.41	2.50	19	1
1:A:118:GLN:C	1:A:120:LYS:H	0.41	2.23	23	1
1:A:24:LYS:HZ3	1:A:44:ASP:CG	0.41	2.22	24	1
1:A:61:GLU:CD	1:A:64:ARG:HH12	0.41	2.23	1	1
1:A:165:LEU:HD23	1:A:165:LEU:C	0.41	2.41	1	1
1:A:157:THR:OG1	1:A:160:HIS:CD2	0.41	2.74	4	1
1:A:59:HIS:HD1	1:A:154:GLU:CD	0.41	2.24	21	1
1:A:19:GLU:H	1:A:19:GLU:CD	0.40	2.24	10	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	189/191 (99%)	165±3 (87±2%)	21±3 (11±2%)	3±1 (2±1%)	9	53
All	All	4725/4775 (99%)	4128 (87%)	518 (11%)	79 (2%)	9	53

All 27 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	169	GLN	12
1	A	42	GLY	10
1	A	53	ASN	8
1	A	120	LYS	6
1	A	87	ALA	5
1	A	110	LYS	5
1	A	27	CYS	3
1	A	71	ARG	3
1	A	16	SER	3
1	A	33	LYS	3
1	A	72	ARG	2
1	A	126	ILE	2
1	A	153	LYS	2
1	A	28	LEU	2
1	A	172	LEU	1
1	A	68	ALA	1
1	A	154	GLU	1
1	A	90	ALA	1
1	A	122	SER	1
1	A	58	GLY	1
1	A	44	ASP	1
1	A	43	LEU	1
1	A	134	PRO	1
1	A	73	HIS	1
1	A	121	VAL	1
1	A	112	TRP	1
1	A	123	ASP	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	165/166 (99%)	150±2 (91±1%)	15±2 (9±1%)	11	56
All	All	4125/4150 (99%)	3745 (91%)	380 (9%)	11	56

All 96 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	102	ASN	24
1	A	36	LEU	22
1	A	138	THR	13
1	A	71	ARG	13
1	A	129	ILE	11
1	A	74	ASP	10
1	A	77	ARG	9
1	A	118	GLN	9
1	A	120	LYS	9
1	A	43	LEU	8
1	A	180	VAL	8
1	A	33	LYS	8
1	A	186	LEU	8
1	A	56	GLU	8
1	A	153	LYS	7
1	A	169	GLN	7
1	A	172	LEU	7
1	A	126	ILE	7
1	A	15	LEU	7
1	A	165	LEU	7
1	A	2	ASP	7
1	A	177	VAL	6
1	A	53	ASN	6
1	A	30	ARG	6
1	A	114	ARG	6
1	A	188	ASN	5
1	A	61	GLU	5
1	A	110	LYS	5
1	A	70	LEU	5
1	A	34	ARG	4
1	A	97	LEU	4
1	A	150	ASN	4
1	A	35	LYS	4
1	A	80	ASP	4
1	A	184	ARG	3
1	A	19	GLU	3

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Mol	Chain	Res	Type	Models (Total)
1	A	24	LYS	3
1	A	52	GLN	3
1	A	50	LEU	3
1	A	23	LEU	3
1	A	73	HIS	3
1	A	55	LEU	3
1	A	16	SER	2
1	A	62	LEU	2
1	A	65	GLU	2
1	A	119	LEU	2
1	A	170	MET	2
1	A	135	ARG	2
1	A	154	GLU	2
1	A	54	ASP	2
1	A	92	PRO	2
1	A	149	LYS	2
1	A	158	VAL	2
1	A	189	ARG	2
1	A	18	SER	2
1	A	140	ARG	2
1	A	40	GLN	2
1	A	101	PHE	2
1	A	115	LEU	2
1	A	162	VAL	2
1	A	26	LEU	2
1	A	113	ARG	2
1	A	95	GLU	2
1	A	181	GLN	2
1	A	27	CYS	2
1	A	131	ASP	2
1	A	22	GLU	2
1	A	76	LEU	2
1	A	103	VAL	2
1	A	38	ARG	2
1	A	127	ASP	2
1	A	51	GLU	1
1	A	125	LYS	1
1	A	173	VAL	1
1	A	185	ASP	1
1	A	49	LEU	1
1	A	11	VAL	1
1	A	187	GLN	1

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Mol	Chain	Res	Type	Models (Total)
1	A	64	ARG	1
1	A	182	GLN	1
1	A	69	SER	1
1	A	139	GLU	1
1	A	63	LEU	1
1	A	59	HIS	1
1	A	96	ASP	1
1	A	190	SER	1
1	A	179	GLU	1
1	A	121	VAL	1
1	A	72	ARG	1
1	A	136	ASN	1
1	A	176	LEU	1
1	A	111	ASP	1
1	A	117	ARG	1
1	A	142	ARG	1
1	A	17	SER	1
1	A	166	ARG	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](#)

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 ⓘ

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided