Full wwPDB NMR Structure Validation Report (i)

Oct 11, 2021 – 06:40 PM EDT

PDB ID	:	2GF5
Title	:	Structure of intact FADD (MORT1)
Authors	:	Carrington, P.E.; Sandu, C.; Wei, Y.; Hill, J.M.; Morisawa, G.; Huang, T.; Gavathiotis, E.; Wei, Y.; Werner, M.H.
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 (i) symbol.

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

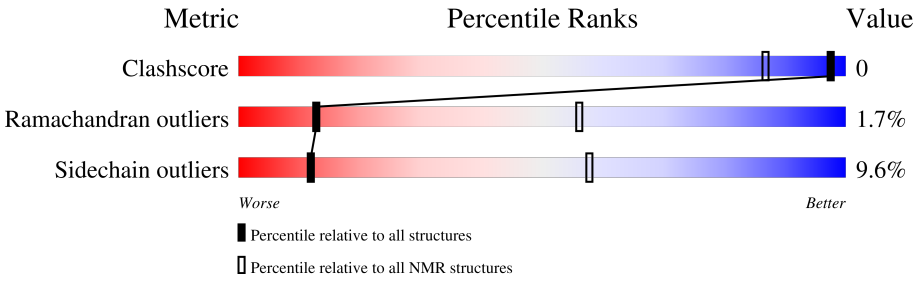
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.23.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

1 Overall quality at a glance (i)

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	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 <=5%

Mol	Chain	Length	Quality of chain
1	A	191	83% 16% ••

2 Ensemble composition and analysis (i)

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)	0.80	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 (i)

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
			Total	C	H	N	O	S	
1	A	191	3036	929	1527	282	292	6	0

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

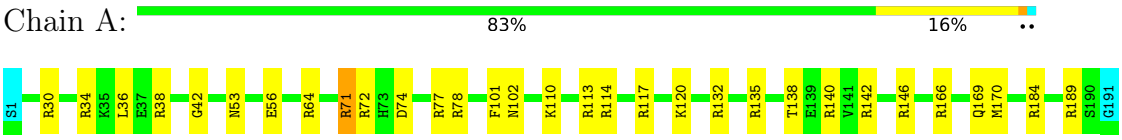
4 Residue-property plots (i)

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

Chain A:



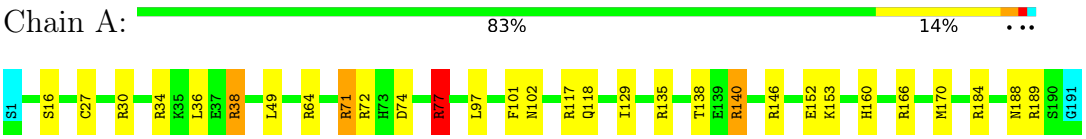
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: FADD protein

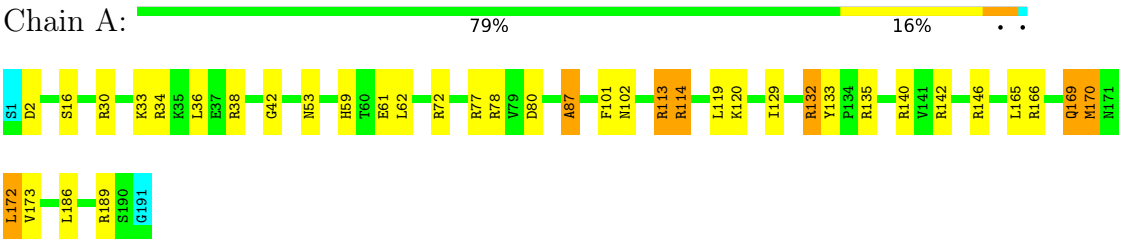
Chain A:



4.2.2 Score per residue for model 2

• Molecule 1: FADD protein

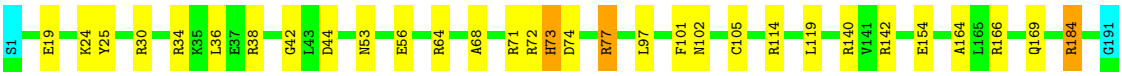
Chain A:



4.2.3 Score per residue for model 3

- Molecule 1: FADD protein

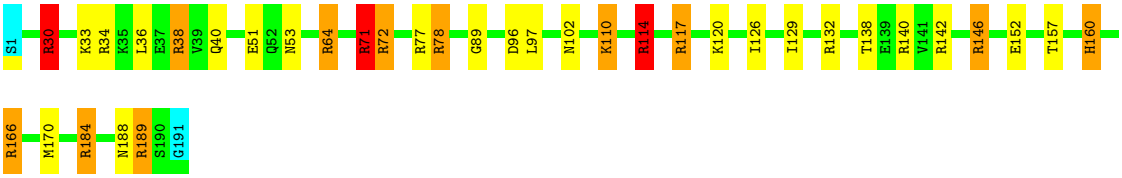
Chain A:



4.2.4 Score per residue for model 4

- Molecule 1: FADD protein

Chain A:



4.2.5 Score per residue for model 5

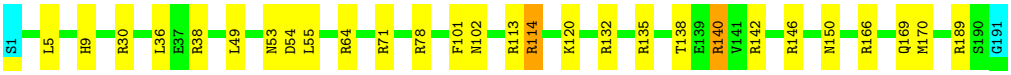
- Molecule 1: FADD protein

Chain A:

4.2.6 Score per residue for model 6

- Molecule 1: FADD protein

Chain A:



4.2.7 Score per residue for model 7

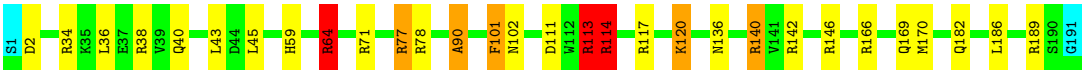
- Molecule 1: FADD protein

Chain A:

4.2.8 Score per residue for model 8

- Molecule 1: FADD protein

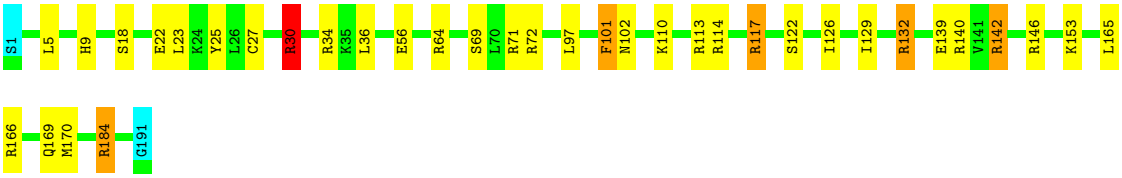
Chain A: 83% 12%



4.2.9 Score per residue for model 9

- Molecule 1: FADD protein

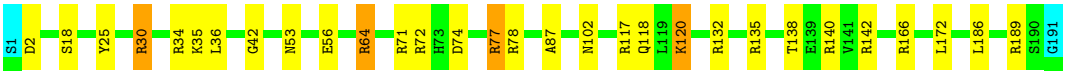
Chain A: 80% 16%



4.2.10 Score per residue for model 10

- Molecule 1: FADD protein

Chain A: 83% 14%



4.2.11 Score per residue for model 11

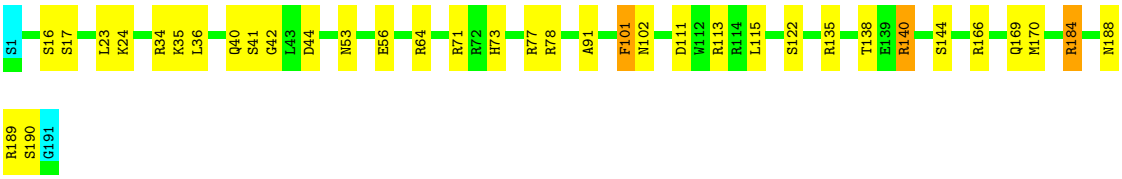
- Molecule 1: FADD protein

Chain A: 82% 15%

4.2.12 Score per residue for model 12

• Molecule 1: FADD protein

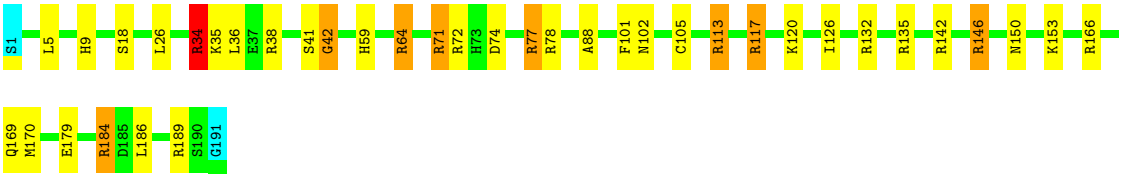
Chain A:



4.2.13 Score per residue for model 13

• Molecule 1: FADD protein

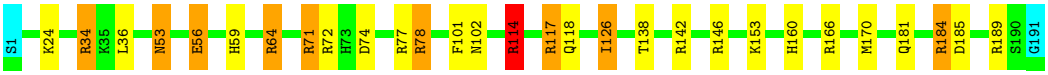
Chain A:



4.2.14 Score per residue for model 14

• Molecule 1: FADD protein

Chain A:



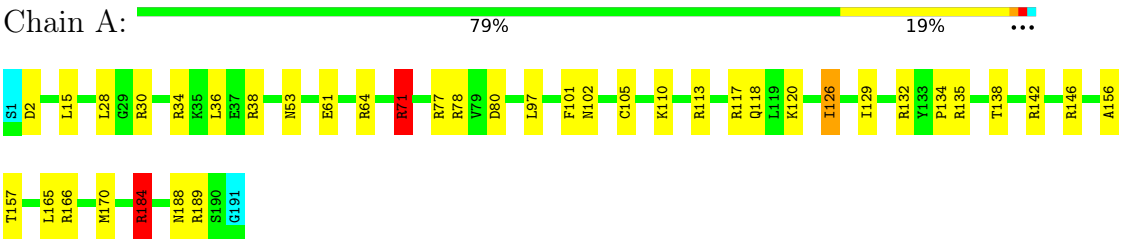
4.2.15 Score per residue for model 15

• Molecule 1: FADD protein

Chain A:

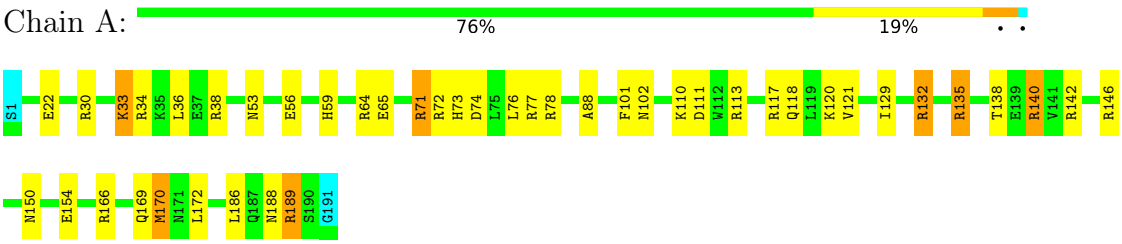
4.2.16 Score per residue for model 16

• Molecule 1: FADD protein



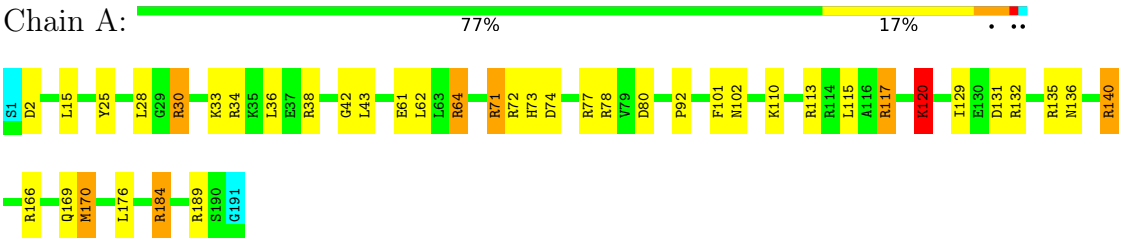
4.2.17 Score per residue for model 17

• Molecule 1: FADD protein



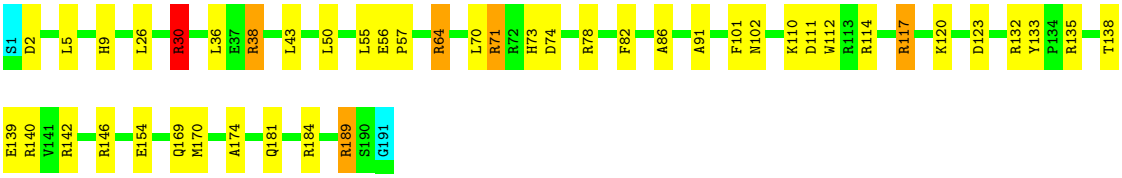
4.2.18 Score per residue for model 18

• Molecule 1: FADD protein



4.2.19 Score per residue for model 19

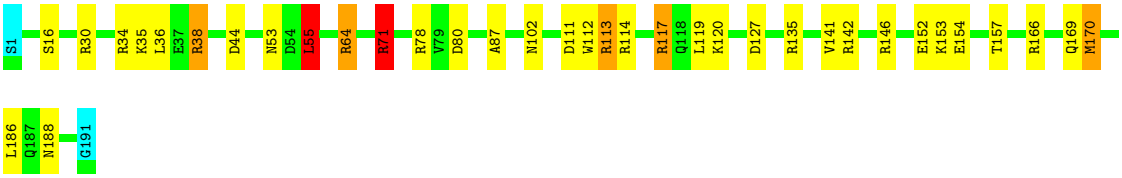
• Molecule 1: FADD protein



4.2.20 Score per residue for model 20

- Molecule 1: FADD protein

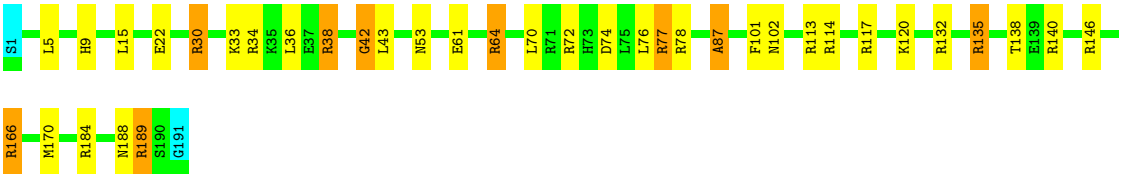
Chain A:



4.2.21 Score per residue for model 21

- Molecule 1: FADD protein

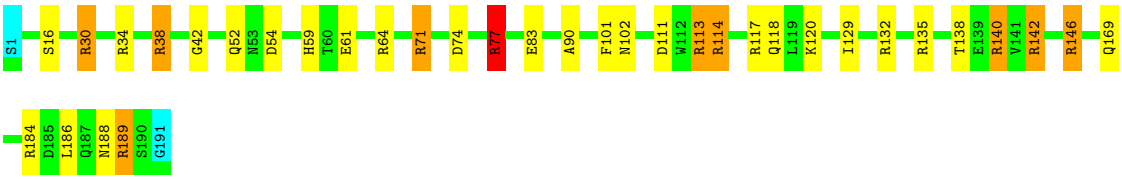
Chain A:



4.2.22 Score per residue for model 22 (medoid)

- Molecule 1: FADD protein

Chain A:



4.2.23 Score per residue for model 23

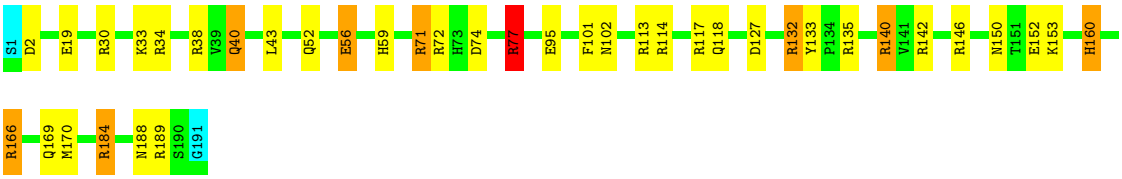
- Molecule 1: FADD protein

Chain A: 79% 15%

4.2.24 Score per residue for model 24

- Molecule 1: FADD protein

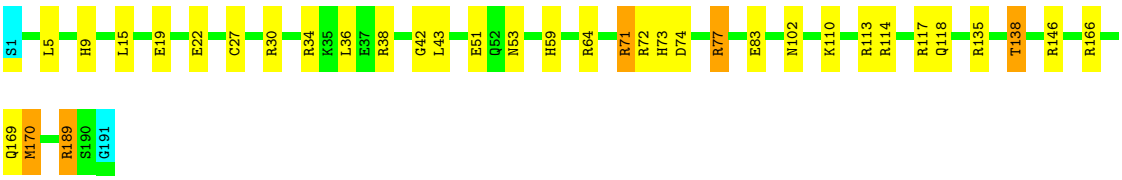
Chain A: 79% 16%



4.2.25 Score per residue for model 25

- Molecule 1: FADD protein

Chain A: 81% 16%



5 Refinement protocol and experimental data overview (i)

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 (i)

6.1 Standard geometry (i)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	1.07±0.00	0±0/1516 (0.0± 0.0%)	1.40±0.04	16±4/2045 (0.8± 0.2%)
All	All	1.07	0/37900 (0.0%)	1.40	390/51125 (0.8%)

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(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	77	ARG	NE-CZ-NH1	11.19	125.89	120.30	8	15
1	A	166	ARG	NE-CZ-NH1	11.01	125.81	120.30	18	17
1	A	64	ARG	NE-CZ-NH1	10.61	125.61	120.30	22	16
1	A	142	ARG	NE-CZ-NH1	10.02	125.31	120.30	11	11
1	A	189	ARG	NE-CZ-NH1	9.01	124.80	120.30	22	17
1	A	184	ARG	NE-CZ-NH1	8.93	124.77	120.30	1	14
1	A	117	ARG	NE-CZ-NH1	8.90	124.75	120.30	20	13
1	A	184	ARG	NE-CZ-NH2	-8.85	115.88	120.30	19	6
1	A	146	ARG	NE-CZ-NH1	8.58	124.59	120.30	16	15
1	A	77	ARG	NE-CZ-NH2	-8.54	116.03	120.30	8	6
1	A	30	ARG	NE-CZ-NH1	8.44	124.52	120.30	16	14
1	A	114	ARG	NE-CZ-NH1	8.36	124.48	120.30	9	10
1	A	71	ARG	NE-CZ-NH1	8.27	124.44	120.30	15	13
1	A	170	MET	CG-SD-CE	-8.17	87.13	100.20	1	19
1	A	72	ARG	NE-CZ-NH1	8.00	124.30	120.30	2	11

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	64	ARG	NE-CZ-NH2	-8.00	116.30	120.30	15	4
1	A	113	ARG	NE-CZ-NH1	7.98	124.29	120.30	13	12
1	A	34	ARG	NE-CZ-NH1	7.97	124.28	120.30	14	13
1	A	132	ARG	NE-CZ-NH1	7.86	124.23	120.30	13	12
1	A	38	ARG	NE-CZ-NH1	7.86	124.23	120.30	4	13
1	A	140	ARG	NE-CZ-NH1	7.82	124.21	120.30	24	11
1	A	101	PHE	CB-CG-CD2	-7.70	115.41	120.80	17	9
1	A	78	ARG	NE-CZ-NH1	7.61	124.11	120.30	2	8
1	A	72	ARG	NE-CZ-NH2	-7.50	116.55	120.30	25	3
1	A	135	ARG	NE-CZ-NH2	-7.28	116.66	120.30	23	6
1	A	166	ARG	NE-CZ-NH2	-7.24	116.68	120.30	18	6
1	A	146	ARG	NE-CZ-NH2	-6.90	116.85	120.30	2	4
1	A	132	ARG	NE-CZ-NH2	-6.81	116.90	120.30	9	5
1	A	25	TYR	CB-CG-CD1	-6.77	116.94	121.00	11	1
1	A	38	ARG	NE-CZ-NH2	-6.71	116.95	120.30	7	2
1	A	157	THR	N-CA-CB	6.56	122.77	110.30	16	3
1	A	117	ARG	NE-CZ-NH2	-6.50	117.05	120.30	11	3
1	A	140	ARG	NE-CZ-NH2	-6.46	117.07	120.30	24	2
1	A	101	PHE	CB-CG-CD1	6.40	125.28	120.80	12	4
1	A	113	ARG	NE-CZ-NH2	-6.38	117.11	120.30	25	2
1	A	18	SER	N-CA-CB	6.37	120.06	110.50	13	1
1	A	135	ARG	NE-CZ-NH1	6.32	123.46	120.30	6	12
1	A	90	ALA	N-CA-CB	6.09	118.63	110.10	22	2
1	A	34	ARG	NE-CZ-NH2	-6.09	117.25	120.30	2	4
1	A	142	ARG	NE-CZ-NH2	-5.88	117.36	120.30	17	4
1	A	114	ARG	N-CA-CB	5.86	121.15	110.60	25	1
1	A	88	ALA	CB-CA-C	-5.85	101.32	110.10	13	1
1	A	30	ARG	NE-CZ-NH2	-5.80	117.40	120.30	11	1
1	A	71	ARG	N-CA-CB	-5.68	100.37	110.60	4	3
1	A	114	ARG	CG-CD-NE	-5.57	100.10	111.80	7	1
1	A	174	ALA	N-CA-CB	5.55	117.87	110.10	19	1
1	A	42	GLY	N-CA-C	5.53	126.91	113.10	21	3
1	A	55	LEU	CB-CG-CD2	5.51	120.37	111.00	20	1
1	A	111	ASP	CB-CG-OD2	5.51	123.26	118.30	17	2
1	A	120	LYS	N-CA-CB	5.49	120.48	110.60	15	4
1	A	114	ARG	NE-CZ-NH2	-5.47	117.56	120.30	9	1
1	A	189	ARG	NE-CZ-NH2	-5.47	117.56	120.30	10	2
1	A	111	ASP	N-CA-CB	-5.46	100.78	110.60	22	1
1	A	117	ARG	CD-NE-CZ	-5.45	115.98	123.60	9	1
1	A	41	SER	C-N-CA	5.41	133.66	122.30	13	2
1	A	122	SER	N-CA-CB	5.37	118.55	110.50	12	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	38	ARG	CG-CD-NE	-5.36	100.54	111.80	16	1
1	A	144	SER	N-CA-CB	5.35	118.52	110.50	12	1
1	A	138	THR	CA-CB-CG2	-5.34	104.93	112.40	25	1
1	A	25	TYR	CB-CG-CD2	-5.33	117.81	121.00	18	1
1	A	80	ASP	CB-CG-OD1	5.31	123.08	118.30	11	2
1	A	78	ARG	NE-CZ-NH2	-5.30	117.65	120.30	14	1
1	A	56	GLU	N-CA-CB	-5.27	101.12	110.60	10	1
1	A	22	GLU	N-CA-CB	5.24	120.04	110.60	21	2
1	A	77	ARG	CD-NE-CZ	5.22	130.91	123.60	8	1
1	A	160	HIS	N-CA-CB	5.16	119.89	110.60	4	1
1	A	101	PHE	CB-CA-C	5.16	120.72	110.40	22	1
1	A	35	LYS	N-CA-CB	-5.14	101.34	110.60	13	1
1	A	12	SER	N-CA-CB	5.13	118.19	110.50	7	1
1	A	55	LEU	O-C-N	-5.12	114.51	122.70	5	1
1	A	73	HIS	C-N-CA	5.11	134.48	121.70	7	1
1	A	44	ASP	CB-CG-OD2	5.08	122.88	118.30	3	1
1	A	55	LEU	N-CA-CB	5.05	120.51	110.40	5	1
1	A	17	SER	N-CA-CB	5.03	118.05	110.50	12	1
1	A	152	GLU	CA-C-N	5.01	128.21	117.20	20	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
1	A	72	ARG	Sidechain	6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group	Models (Total)
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 (i)

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	38

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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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: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: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: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:157:THR:OG1	1:A:160:HIS:CD2	0.41	2.74	4	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	189/191 (99%)	165±3 (87±2%)	21±3 (11±2%)	3±1 (2±1%)	13	56
All	All	4725/4775 (99%)	4128 (87%)	518 (11%)	79 (2%)	13	56

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 (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	165/166 (99%)	149±3 (90±2%)	16±3 (10±2%)	12 58
All	All	4125/4150 (99%)	3730 (90%)	395 (10%)	12 58

All 92 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	23
1	A	36	LEU	22
1	A	71	ARG	15
1	A	74	ASP	12
1	A	138	THR	12
1	A	77	ARG	10
1	A	101	PHE	10
1	A	188	ASN	10
1	A	56	GLU	10
1	A	118	GLN	9
1	A	129	ILE	9
1	A	170	MET	9
1	A	33	LYS	8
1	A	186	LEU	8
1	A	53	ASN	8
1	A	120	LYS	8
1	A	2	ASP	7
1	A	169	GLN	7
1	A	114	ARG	7
1	A	30	ARG	7
1	A	97	LEU	6
1	A	153	LYS	6
1	A	15	LEU	6
1	A	150	ASN	6
1	A	61	GLU	5
1	A	73	HIS	5
1	A	105	CYS	5
1	A	126	ILE	5
1	A	184	ARG	5
1	A	43	LEU	5
1	A	113	ARG	5
1	A	34	ARG	4
1	A	154	GLU	4
1	A	35	LYS	4
1	A	80	ASP	4
1	A	59	HIS	3
1	A	62	LEU	3
1	A	172	LEU	3
1	A	19	GLU	3
1	A	24	LYS	3
1	A	51	GLU	3
1	A	110	LYS	3
1	A	52	GLN	3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	55	LEU	3
1	A	165	LEU	3
1	A	117	ARG	3
1	A	189	ARG	3
1	A	23	LEU	3
1	A	27	CYS	3
1	A	140	ARG	3
1	A	16	SER	2
1	A	49	LEU	2
1	A	119	LEU	2
1	A	96	ASP	2
1	A	45	LEU	2
1	A	135	ARG	2
1	A	185	ASP	2
1	A	54	ASP	2
1	A	92	PRO	2
1	A	18	SER	2
1	A	40	GLN	2
1	A	111	ASP	2
1	A	115	LEU	2
1	A	26	LEU	2
1	A	181	GLN	2
1	A	131	ASP	2
1	A	22	GLU	2
1	A	76	LEU	2
1	A	132	ARG	2
1	A	38	ARG	2
1	A	70	LEU	2
1	A	127	ASP	2
1	A	123	ASP	1
1	A	125	LYS	1
1	A	173	VAL	1
1	A	11	VAL	1
1	A	81	ASP	1
1	A	187	GLN	1
1	A	64	ARG	1
1	A	182	GLN	1
1	A	69	SER	1
1	A	139	GLU	1
1	A	190	SER	1
1	A	179	GLU	1
1	A	65	GLU	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	136	ASN	1
1	A	176	LEU	1
1	A	50	LEU	1
1	A	44	ASP	1
1	A	142	ARG	1
1	A	95	GLU	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 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 (i)

No chemical shift data were provided