



Full wwPDB NMR Structure Validation Report ⓘ

Apr 15, 2026 – 10:19 AM UTC

PDB ID : 1AX3 / pdb_00001ax3
Title : SOLUTION NMR STRUCTURE OF B. SUBTILIS IIAGLC, 16 STRUCTURES
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Deposited on : 1997-10-25

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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

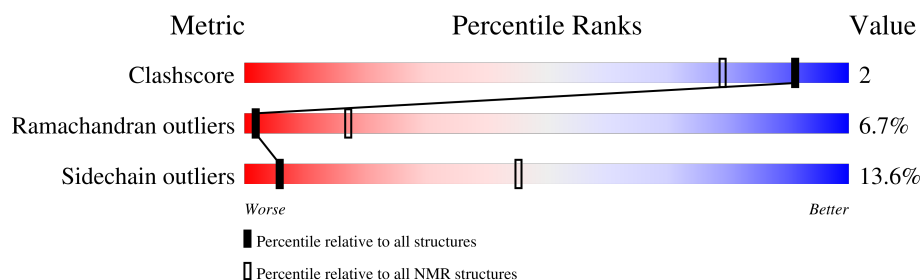
1 Overall quality at a glance

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	162	69% 20% • 10%

2 Ensemble composition and analysis

This entry contains 16 models. Model 5 is the overall representative, medoid model (most similar to other models).

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:15-A:74, A:78-A:162 (145)	0.92	5

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 1 single-model cluster was found.

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

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 2457 atoms, of which 1236 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called GLUCOSE PERMEASE IIA DOMAIN.

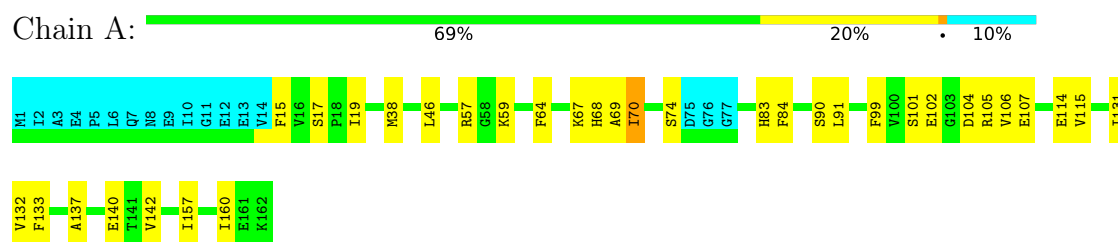
Mol	Chain	Residues	Atoms						Trace
1	A	162	Total	C	H	N	O	S	0
			2457	776	1236	199	242	4	

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: GLUCOSE PERMEASE IIA DOMAIN

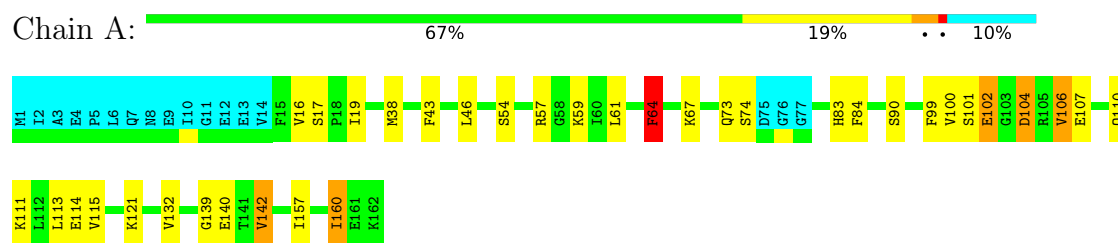


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

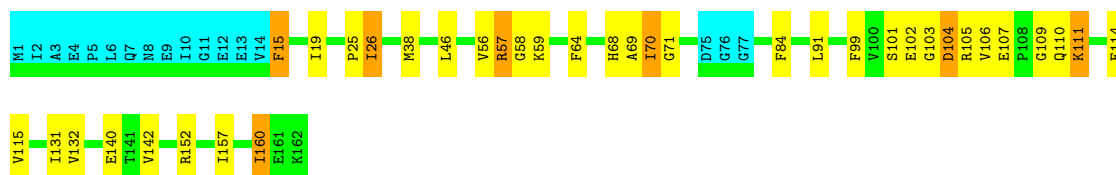
- Molecule 1: GLUCOSE PERMEASE IIA DOMAIN



4.2.2 Score per residue for model 2

- Molecule 1: GLUCOSE PERMEASE IIA DOMAIN

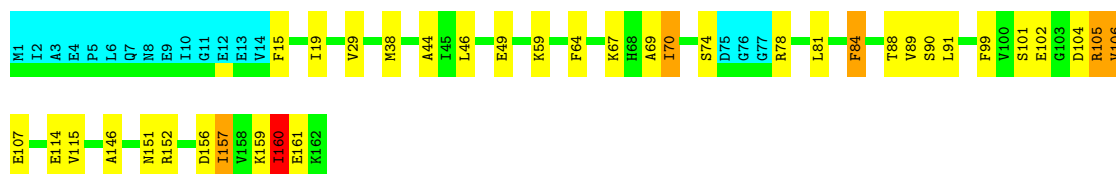




4.2.3 Score per residue for model 3

- Molecule 1: GLUCOSE PERMEASE IIA DOMAIN

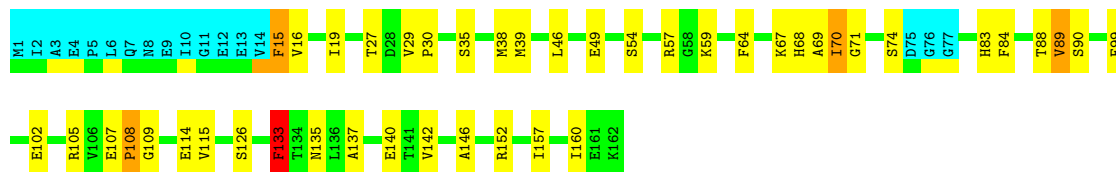
Chain A: 67% 19% 10%



4.2.4 Score per residue for model 4

- Molecule 1: GLUCOSE PERMEASE IIA DOMAIN

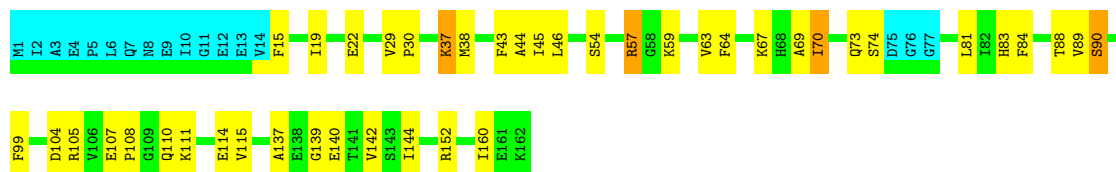
Chain A: 62% 24% 10%



4.2.5 Score per residue for model 5 (medoid)

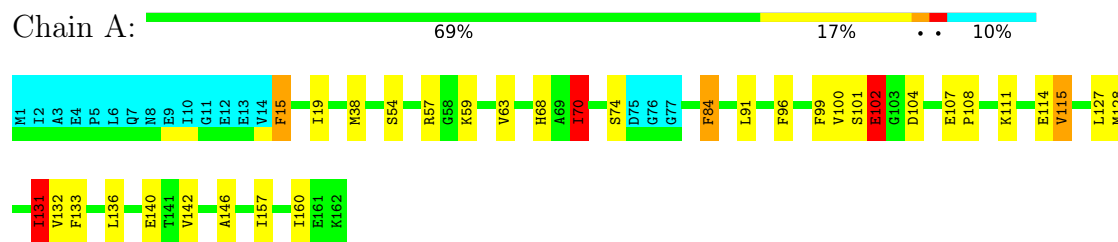
- Molecule 1: GLUCOSE PERMEASE IIA DOMAIN

Chain A: 63% 24% 10%



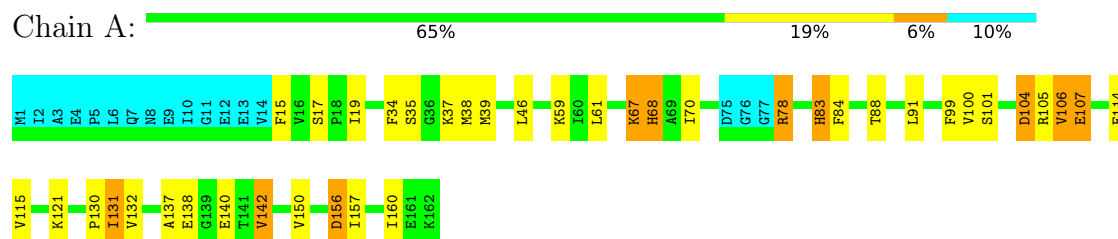
4.2.6 Score per residue for model 6

- Molecule 1: GLUCOSE PERMEASE IIA DOMAIN



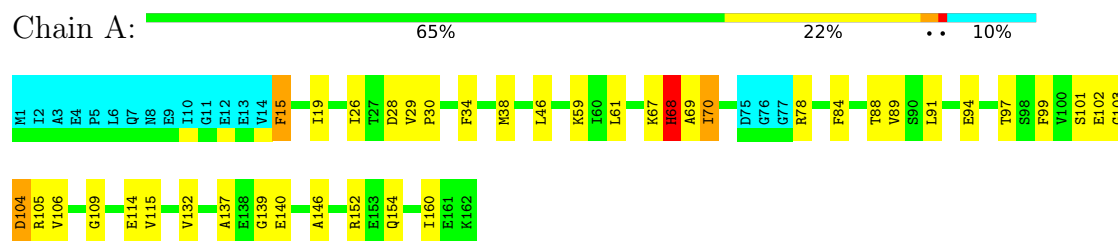
4.2.7 Score per residue for model 7

- Molecule 1: GLUCOSE PERMEASE IIA DOMAIN



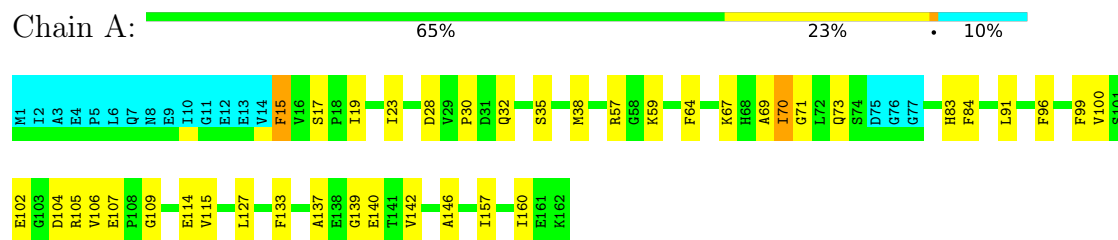
4.2.8 Score per residue for model 8

- Molecule 1: GLUCOSE PERMEASE IIA DOMAIN



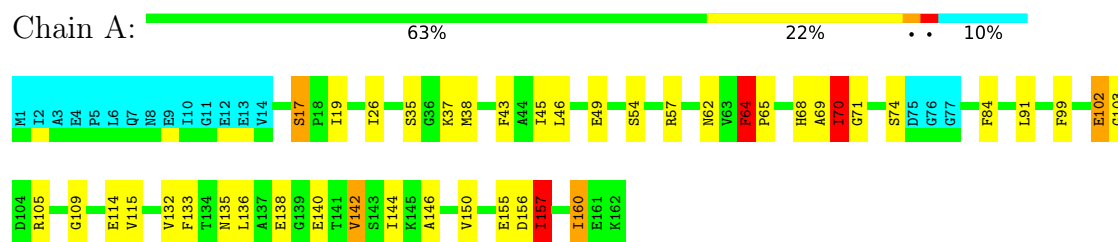
4.2.9 Score per residue for model 9

- Molecule 1: GLUCOSE PERMEASE IIA DOMAIN



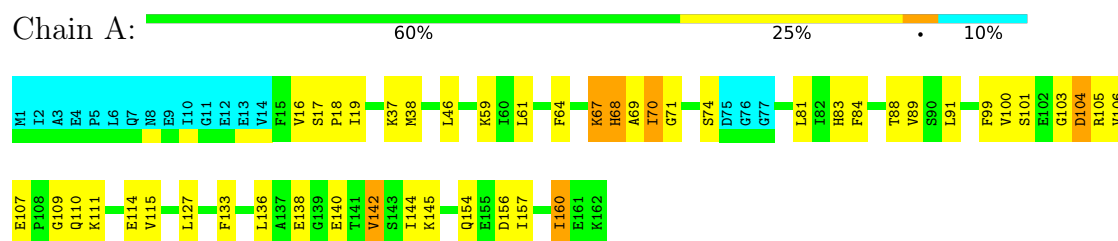
4.2.10 Score per residue for model 10

- Molecule 1: GLUCOSE PERMEASE IIA DOMAIN



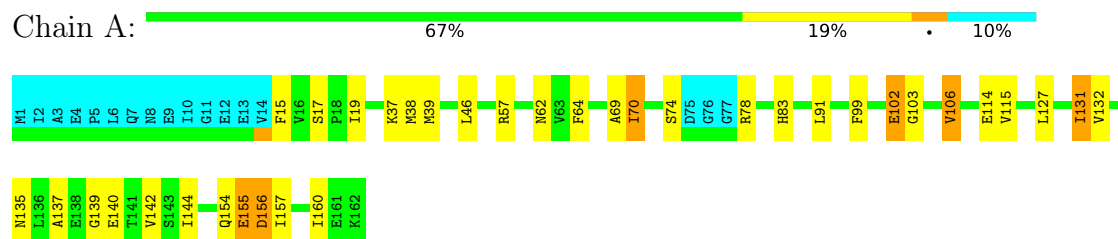
4.2.11 Score per residue for model 11

- Molecule 1: GLUCOSE PERMEASE IIA DOMAIN



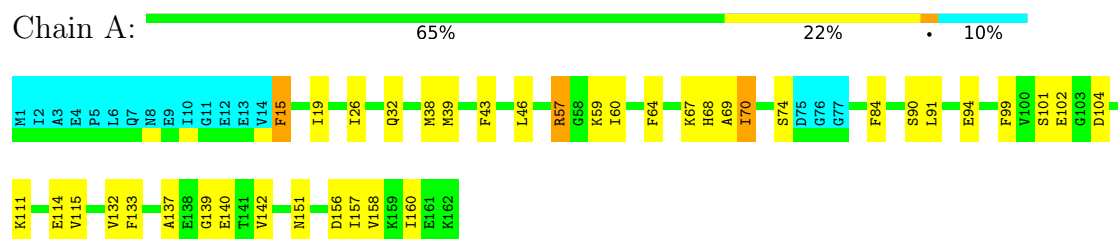
4.2.12 Score per residue for model 12

- Molecule 1: GLUCOSE PERMEASE IIA DOMAIN



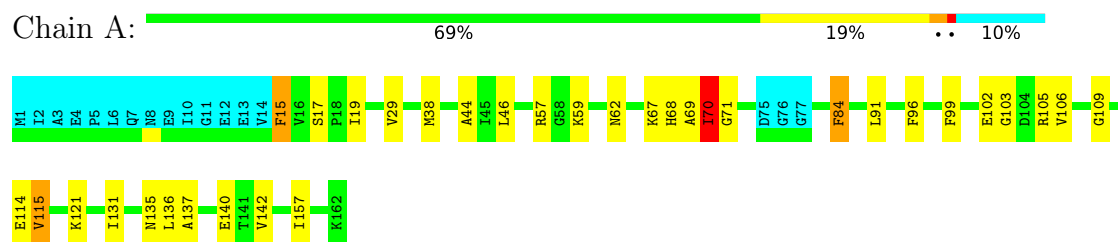
4.2.13 Score per residue for model 13

- Molecule 1: GLUCOSE PERMEASE IIA DOMAIN



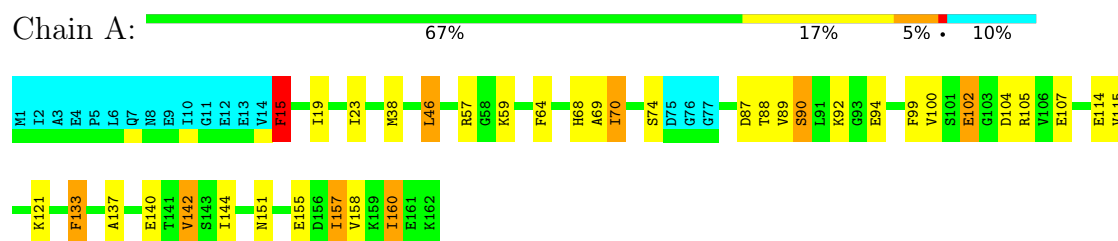
4.2.14 Score per residue for model 14

- Molecule 1: GLUCOSE PERMEASE IIA DOMAIN



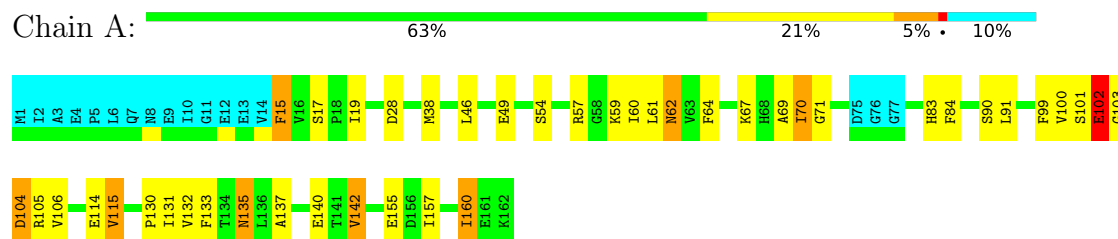
4.2.15 Score per residue for model 15

- Molecule 1: GLUCOSE PERMEASE IIA DOMAIN



4.2.16 Score per residue for model 16

- Molecule 1: GLUCOSE PERMEASE IIA DOMAIN



5 Refinement protocol and experimental data overview

The models were refined using the following method: *DISTANCE GEOMETRY AND MOLECULAR DYNAMICS*.

Of the 100 calculated structures, 16 were deposited, based on the following criterion: *LEAST RESTRAINT VIOLATION AND LOWEST AMBER ENERGY*.

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

Software name	Classification	Version
Amber	refinement	
DISGEO	structure solution	
Amber	structure solution	

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	0.63±0.01	0±0/1117 (0.0± 0.0%)	1.53±0.04	15±4/1514 (1.0± 0.3%)
All	All	0.63	0/17872 (0.0%)	1.53	243/24224 (1.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	Chirality	Planarity
1	A	0.1±0.2	3.4±0.9
All	All	1	55

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	105	ARG	N-CA-C	10.31	125.48	110.42	3	3
1	A	106	VAL	N-CA-C	10.10	130.35	109.34	7	2
1	A	105	ARG	CA-C-N	9.73	139.48	121.97	7	2
1	A	105	ARG	C-N-CA	9.73	139.48	121.97	7	2
1	A	68	HIS	CA-CB-CG	9.41	123.21	113.80	8	3
1	A	69	ALA	CA-C-N	8.32	136.95	121.97	8	13
1	A	69	ALA	C-N-CA	8.32	136.95	121.97	8	13
1	A	70	ILE	N-CA-CB	8.25	124.84	111.23	8	12
1	A	46	LEU	CB-CA-C	7.95	118.04	110.17	13	14
1	A	70	ILE	CB-CA-C	7.94	124.31	111.29	3	13
1	A	103	GLY	CA-C-N	7.67	136.19	121.54	11	3
1	A	103	GLY	C-N-CA	7.67	136.19	121.54	11	3
1	A	57	ARG	N-CA-C	-7.37	97.98	109.25	12	11
1	A	89	VAL	CB-CA-C	7.33	123.31	111.29	15	2
1	A	104	ASP	CA-C-N	7.15	133.16	121.58	2	5

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	104	ASP	C-N-CA	7.15	133.16	121.58	2	5
1	A	114	GLU	N-CA-C	-6.74	97.92	108.90	12	15
1	A	89	VAL	CA-C-N	6.56	134.08	121.54	15	2
1	A	89	VAL	C-N-CA	6.56	134.08	121.54	15	2
1	A	101	SER	N-CA-C	-6.55	102.40	110.65	7	7
1	A	156	ASP	CA-C-N	6.45	130.87	120.30	12	2
1	A	156	ASP	C-N-CA	6.45	130.87	120.30	12	2
1	A	130	PRO	N-CA-CB	6.37	106.49	102.92	16	1
1	A	104	ASP	N-CA-C	6.36	124.34	110.80	11	2
1	A	157	ILE	CB-CA-C	6.26	121.55	111.29	3	2
1	A	107	GLU	CA-C-N	6.21	126.22	119.89	2	4
1	A	107	GLU	C-N-CA	6.21	126.22	119.89	2	4
1	A	70	ILE	CA-C-N	6.20	125.86	121.65	7	1
1	A	70	ILE	C-N-CA	6.20	125.86	121.65	7	1
1	A	71	GLY	N-CA-C	6.09	119.38	110.80	16	6
1	A	46	LEU	N-CA-C	-5.91	98.05	108.69	13	6
1	A	100	VAL	N-CA-CB	5.85	117.50	110.31	9	5
1	A	64	PHE	CA-CB-CG	5.83	119.63	113.80	10	3
1	A	68	HIS	CB-CG-CD2	-5.82	123.64	131.20	13	7
1	A	136	LEU	CA-C-N	5.81	132.63	121.54	14	1
1	A	136	LEU	C-N-CA	5.81	132.63	121.54	14	1
1	A	110	GLN	CA-C-N	5.80	132.62	121.54	5	1
1	A	110	GLN	C-N-CA	5.80	132.62	121.54	5	1
1	A	160	ILE	CA-CB-CG1	5.72	120.13	110.40	3	1
1	A	90	SER	CA-C-N	5.72	128.22	120.38	5	3
1	A	90	SER	C-N-CA	5.72	128.22	120.38	5	3
1	A	37	LYS	CA-C-N	5.62	132.26	121.54	12	5
1	A	37	LYS	C-N-CA	5.62	132.26	121.54	12	5
1	A	109	GLY	CA-C-N	5.61	132.26	121.54	11	2
1	A	109	GLY	C-N-CA	5.61	132.26	121.54	11	2
1	A	142	VAL	CB-CA-C	5.58	119.05	112.68	11	6
1	A	84	PHE	CA-CB-CG	-5.58	108.22	113.80	14	2
1	A	101	SER	CA-C-N	5.57	132.18	121.54	8	2
1	A	101	SER	C-N-CA	5.57	132.18	121.54	8	2
1	A	61	LEU	N-CA-C	-5.57	104.60	111.40	8	2
1	A	18	PRO	N-CA-C	5.54	120.83	113.40	11	1
1	A	155	GLU	CA-C-N	5.51	132.07	121.54	12	1
1	A	155	GLU	C-N-CA	5.51	132.07	121.54	12	1
1	A	114	GLU	CA-C-N	5.41	129.13	121.66	8	1
1	A	114	GLU	C-N-CA	5.41	129.13	121.66	8	1
1	A	135	ASN	CA-CB-CG	5.33	117.93	112.60	16	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	60	ILE	CA-CB-CG1	5.30	119.40	110.40	13	1
1	A	54	SER	CA-C-N	5.25	124.94	119.64	10	2
1	A	54	SER	C-N-CA	5.25	124.94	119.64	10	2
1	A	102	GLU	CB-CA-C	5.25	120.86	110.42	4	2
1	A	29	VAL	CA-C-N	5.23	126.38	119.84	8	2
1	A	29	VAL	C-N-CA	5.23	126.38	119.84	8	2
1	A	106	VAL	CB-CA-C	5.18	119.78	111.29	12	1
1	A	103	GLY	N-CA-C	-5.14	101.00	113.18	16	1
1	A	83	HIS	CB-CG-CD2	-5.14	124.52	131.20	7	1
1	A	56	VAL	N-CA-C	-5.13	101.50	108.06	2	1
1	A	131	ILE	N-CA-C	-5.02	100.52	107.80	6	1
1	A	88	THR	N-CA-C	-5.02	107.29	113.41	8	1
1	A	115	VAL	CB-CA-C	5.00	116.92	110.12	16	1
1	A	87	ASP	CA-C-N	5.00	128.66	121.71	15	1
1	A	87	ASP	C-N-CA	5.00	128.66	121.71	15	1

All unique chiral outliers are listed below.

Mol	Chain	Res	Type	Atoms	Models (Total)
1	A	70	ILE	CA	1

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	99	PHE	Sidechain	16
1	A	84	PHE	Sidechain	14
1	A	15	PHE	Sidechain	9
1	A	133	PHE	Sidechain	7
1	A	64	PHE	Sidechain	3
1	A	34	PHE	Sidechain	2
1	A	43	PHE	Sidechain	1
1	A	57	ARG	Sidechain	1
1	A	78	ARG	Sidechain	1
1	A	96	PHE	Sidechain	1

6.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes

averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	1097	1120	1119	3±1
All	All	17552	17920	17904	55

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

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:140:GLU:HB3	1:A:160:ILE:CG2	0.62	2.24	4	8
1:A:140:GLU:HB3	1:A:160:ILE:HG23	0.56	1.76	10	6
1:A:29:VAL:HG22	1:A:44:ALA:HB2	0.54	1.80	3	2
1:A:133:PHE:HB2	1:A:136:LEU:HD21	0.53	1.79	6	1
1:A:96:PHE:CD1	1:A:115:VAL:HG12	0.51	2.41	14	2
1:A:100:VAL:HB	1:A:102:GLU:CG	0.51	2.36	16	1
1:A:104:ASP:O	1:A:106:VAL:HG22	0.51	2.06	1	1
1:A:146:ALA:HB3	1:A:157:ILE:HG23	0.50	1.83	10	1
1:A:63:VAL:HA	1:A:70:ILE:HG21	0.50	1.83	6	1
1:A:157:ILE:HD12	1:A:157:ILE:H	0.49	1.66	12	1
1:A:133:PHE:CD1	1:A:133:PHE:N	0.48	2.81	4	1
1:A:154:GLN:HB2	1:A:157:ILE:HD13	0.48	1.86	12	1
1:A:140:GLU:CB	1:A:160:ILE:HG23	0.48	2.38	1	6
1:A:43:PHE:CE2	1:A:45:ILE:HD11	0.46	2.46	5	2
1:A:150:VAL:HG23	1:A:157:ILE:HG21	0.45	1.87	10	2
1:A:64:PHE:CE2	1:A:113:LEU:HD21	0.45	2.47	1	1
1:A:29:VAL:CG2	1:A:44:ALA:HB2	0.45	2.42	5	2
1:A:131:ILE:HD12	1:A:131:ILE:N	0.45	2.27	6	1
1:A:68:HIS:ND1	1:A:89:VAL:N	0.45	2.65	8	1
1:A:154:GLN:CB	1:A:157:ILE:HD13	0.44	2.42	11	1
1:A:159:LYS:C	1:A:160:ILE:HD13	0.44	2.37	3	1
1:A:88:THR:O	1:A:90:SER:N	0.43	2.51	5	2
1:A:144:ILE:HG23	1:A:158:VAL:HG22	0.43	1.90	15	1
1:A:133:PHE:CB	1:A:136:LEU:HD11	0.43	2.43	6	1
1:A:160:ILE:HD13	1:A:160:ILE:N	0.42	2.30	3	1
1:A:130:PRO:C	1:A:131:ILE:HD12	0.42	2.40	7	1
1:A:146:ALA:HB2	1:A:157:ILE:HG23	0.41	1.91	6	1
1:A:15:PHE:CZ	1:A:133:PHE:CE1	0.41	3.09	15	1
1:A:43:PHE:CE2	1:A:158:VAL:HG11	0.41	2.51	13	1
1:A:61:LEU:O	1:A:62:ASN:CB	0.40	2.69	16	1
1:A:131:ILE:N	1:A:131:ILE:HD12	0.40	2.31	12	1
1:A:70:ILE:HG22	1:A:71:GLY:N	0.40	2.32	14	1

6.3 Torsion angles

6.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the backbone conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	144/162 (89%)	112±4 (78±3%)	23±4 (16±3%)	10±2 (7±1%)	2	17
All	All	2304/2592 (89%)	1788 (78%)	362 (16%)	154 (7%)	2	17

All 35 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	38	MET	16
1	A	70	ILE	14
1	A	74	SER	10
1	A	104	ASP	10
1	A	137	ALA	10
1	A	102	GLU	9
1	A	17	SER	8
1	A	139	GLY	6
1	A	156	ASP	6
1	A	111	LYS	5
1	A	106	VAL	5
1	A	109	GLY	5
1	A	146	ALA	4
1	A	157	ILE	4
1	A	30	PRO	4
1	A	67	LYS	3
1	A	110	GLN	3
1	A	78	ARG	3
1	A	108	PRO	3
1	A	138	GLU	3
1	A	28	ASP	3
1	A	103	GLY	3
1	A	89	VAL	2
1	A	90	SER	2
1	A	62	ASN	2
1	A	94	GLU	2
1	A	25	PRO	1

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Mol	Chain	Res	Type	Models (Total)
1	A	26	ILE	1
1	A	58	GLY	1
1	A	84	PHE	1
1	A	128	MET	1
1	A	32	GLN	1
1	A	64	PHE	1
1	A	65	PRO	1
1	A	92	LYS	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	126/139 (91%)	109±2 (86±2%)	17±2 (14±2%)	6	45
All	All	2016/2224 (91%)	1741 (86%)	275 (14%)	6	45

All 63 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	19	ILE	16
1	A	115	VAL	16
1	A	59	LYS	14
1	A	142	VAL	14
1	A	15	PHE	13
1	A	91	LEU	12
1	A	105	ARG	10
1	A	67	LYS	10
1	A	102	GLU	9
1	A	132	VAL	9
1	A	64	PHE	8
1	A	83	HIS	8
1	A	157	ILE	7
1	A	160	ILE	7
1	A	107	GLU	7
1	A	131	ILE	6
1	A	106	VAL	5

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Mol	Chain	Res	Type	Models (Total)
1	A	152	ARG	5
1	A	135	ASN	5
1	A	54	SER	4
1	A	121	LYS	4
1	A	26	ILE	4
1	A	49	GLU	4
1	A	35	SER	4
1	A	39	MET	4
1	A	88	THR	4
1	A	144	ILE	4
1	A	127	LEU	4
1	A	155	GLU	4
1	A	16	VAL	3
1	A	73	GLN	3
1	A	57	ARG	3
1	A	81	LEU	3
1	A	151	ASN	3
1	A	68	HIS	3
1	A	61	LEU	2
1	A	90	SER	2
1	A	111	LYS	2
1	A	89	VAL	2
1	A	70	ILE	2
1	A	23	ILE	2
1	A	136	LEU	2
1	A	62	ASN	2
1	A	161	GLU	1
1	A	27	THR	1
1	A	108	PRO	1
1	A	126	SER	1
1	A	133	PHE	1
1	A	22	GLU	1
1	A	37	LYS	1
1	A	63	VAL	1
1	A	78	ARG	1
1	A	94	GLU	1
1	A	97	THR	1
1	A	154	GLN	1
1	A	17	SER	1
1	A	145	LYS	1
1	A	32	GLN	1
1	A	140	GLU	1

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Mol	Chain	Res	Type	Models (Total)
1	A	46	LEU	1
1	A	100	VAL	1
1	A	104	ASP	1
1	A	60	ILE	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 [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided