



Full wwPDB NMR Structure Validation Report ⓘ

Feb 20, 2018 – 05:01 pm GMT

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

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

Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Percentile statistics	:	20171227.v01 (using entries in the PDB archive December 27th 2017)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	trunk30686
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk30686

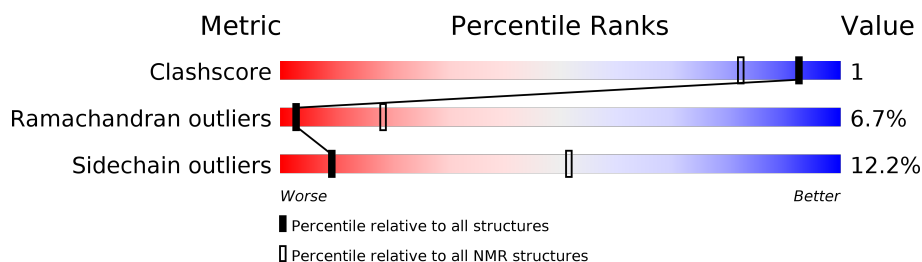
1 Overall quality at a glance

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	136279	12091
Ramachandran outliers	132675	10835
Sidechain outliers	132484	10811

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	

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)	0.53	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

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.

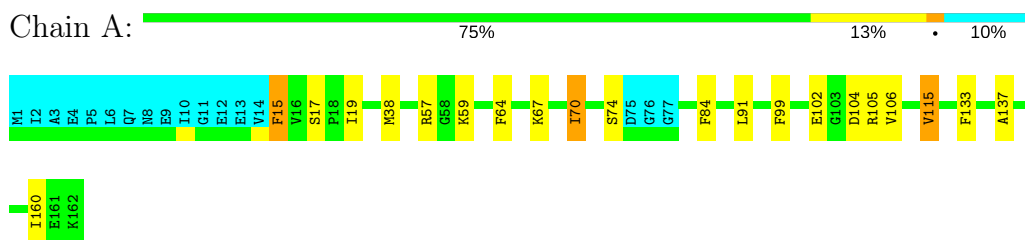
Mol	Chain	Residues	Atoms						Trace
1	A	162	Total	C	H	N	O	S	0
			2457	776	1236	199	242	4	

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA and DNA 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

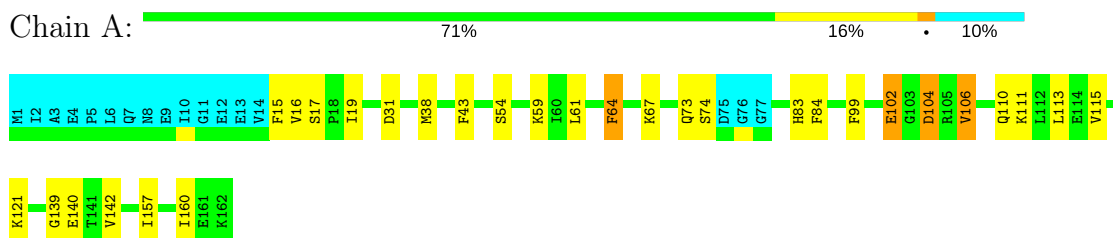


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

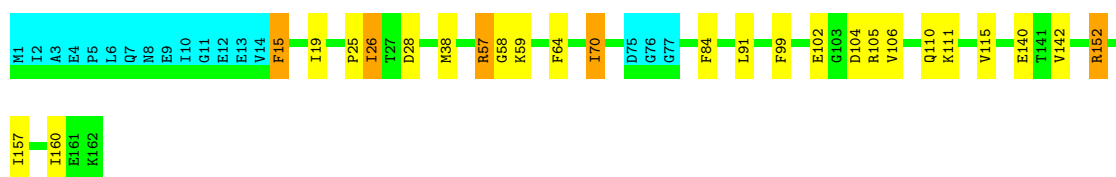
- Molecule 1: GLUCOSE PERMEASE IIA DOMAIN



4.2.2 Score per residue for model 2

- Molecule 1: GLUCOSE PERMEASE IIA DOMAIN

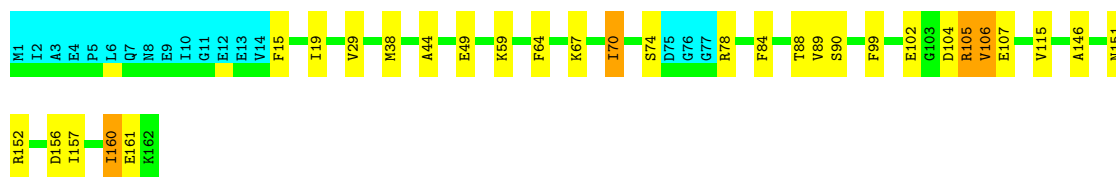




4.2.3 Score per residue for model 3

- Molecule 1: GLUCOSE PERMEASE IIA DOMAIN

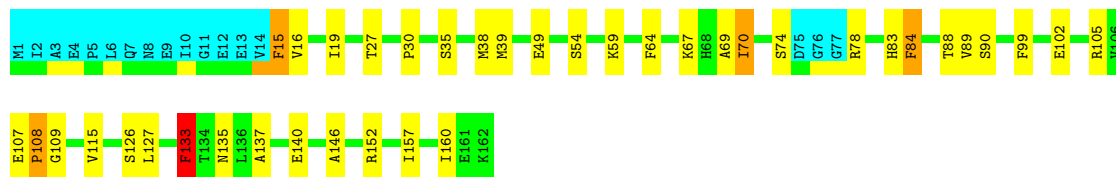
Chain A: 71% 16% 10%



4.2.4 Score per residue for model 4

- Molecule 1: GLUCOSE PERMEASE IIA DOMAIN

Chain A: 65% 21% 10%



4.2.5 Score per residue for model 5 (medoid)

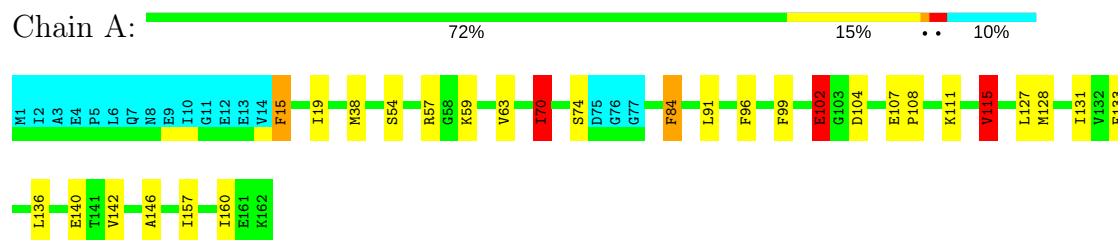
- Molecule 1: GLUCOSE PERMEASE IIA DOMAIN

Chain A: 69% 20% 10%



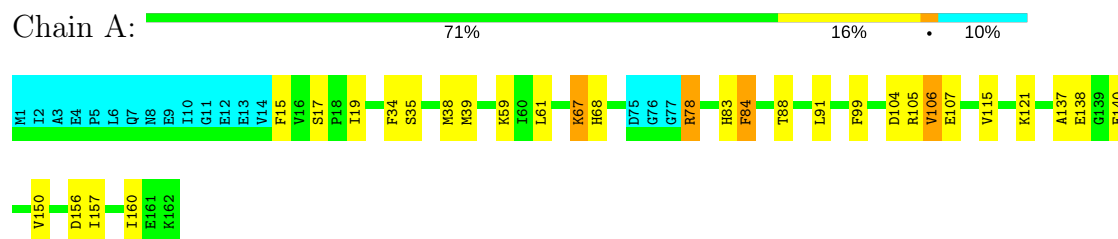
4.2.6 Score per residue for model 6

- Molecule 1: GLUCOSE PERMEASE IIA DOMAIN



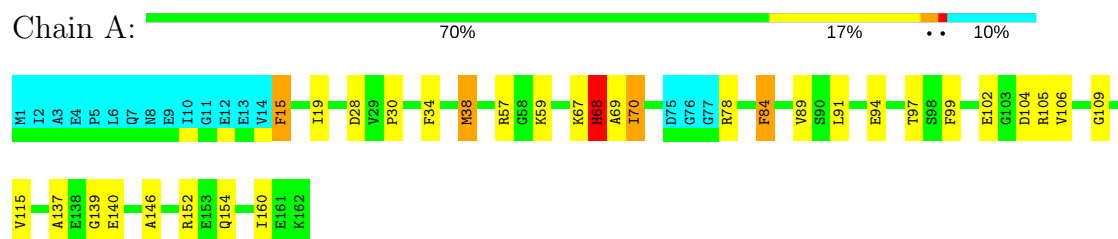
4.2.7 Score per residue for model 7

- Molecule 1: GLUCOSE PERMEASE IIA DOMAIN



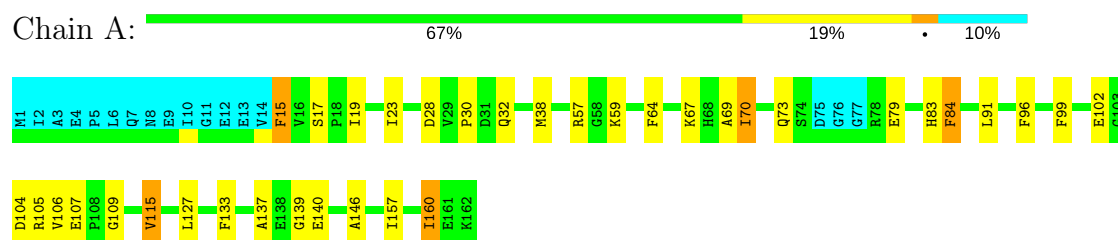
4.2.8 Score per residue for model 8

- Molecule 1: GLUCOSE PERMEASE IIA DOMAIN



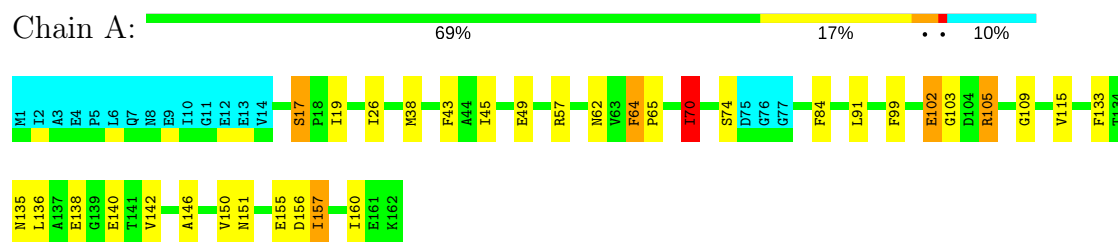
4.2.9 Score per residue for model 9

- Molecule 1: GLUCOSE PERMEASE IIA DOMAIN



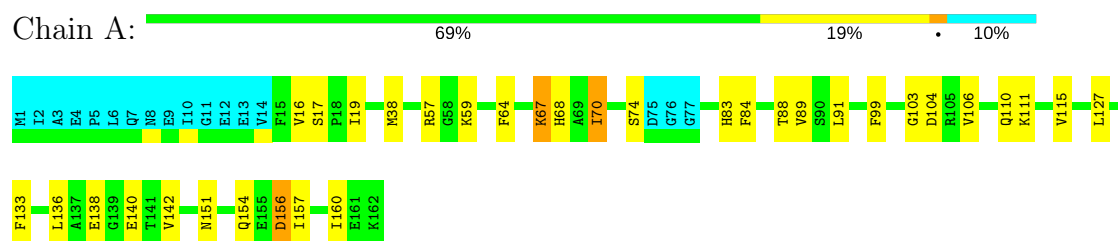
4.2.10 Score per residue for model 10

- Molecule 1: GLUCOSE PERMEASE IIA DOMAIN



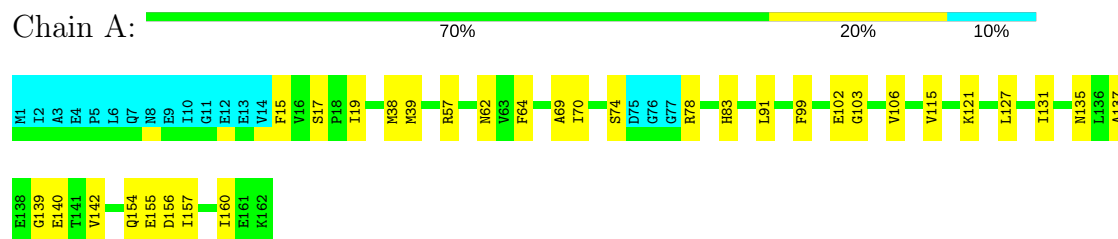
4.2.11 Score per residue for model 11

- Molecule 1: GLUCOSE PERMEASE IIA DOMAIN



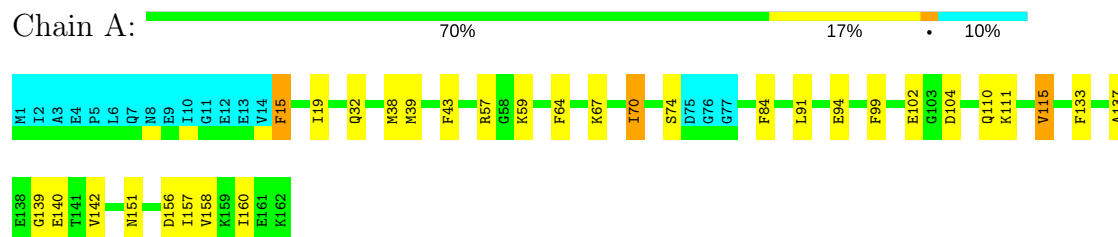
4.2.12 Score per residue for model 12

- Molecule 1: GLUCOSE PERMEASE IIA DOMAIN



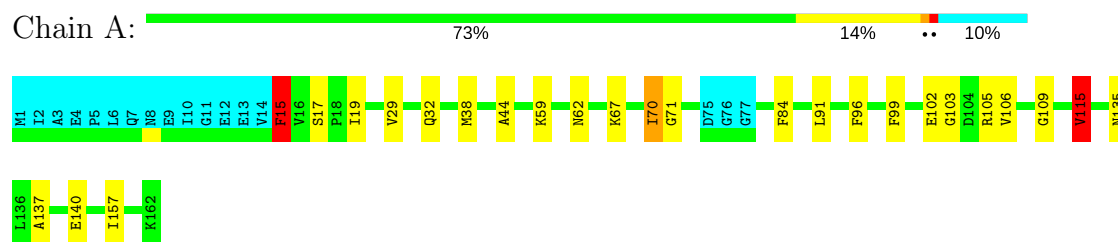
4.2.13 Score per residue for model 13

- Molecule 1: GLUCOSE PERMEASE IIA DOMAIN



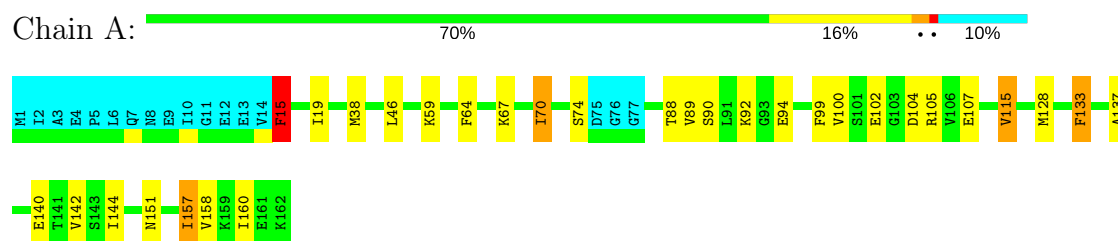
4.2.14 Score per residue for model 14

- Molecule 1: GLUCOSE PERMEASE IIA DOMAIN



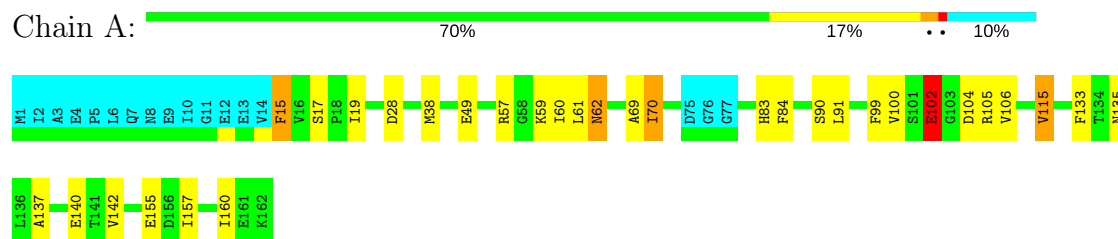
4.2.15 Score per residue for model 15

- 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. No validations of the models with respect to experimental NMR restraints is performed at this time.

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	0.53±0.00	0±0/1117 (0.0±0.0%)	1.12±0.02	3±1/1514 (0.2±0.1%)
All	All	0.53	0/17872 (0.0%)	1.12	44/24224 (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	0.1±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	106	VAL	N-CA-C	7.17	130.35	111.00	7	2
1	A	105	ARG	C-N-CA	7.11	139.48	121.70	7	2
1	A	70	ILE	CB-CA-C	6.35	124.31	111.60	3	11
1	A	89	VAL	CB-CA-C	6.27	123.31	111.40	15	2
1	A	70	ILE	N-CA-CB	6.11	124.84	110.80	8	1
1	A	69	ALA	C-N-CA	6.10	136.95	121.70	8	5
1	A	115	VAL	CG1-CB-CG2	-6.07	101.19	110.90	6	6
1	A	103	GLY	C-N-CA	5.79	136.19	121.70	11	1
1	A	57	ARG	NE-CZ-NH2	-5.74	117.43	120.30	9	4
1	A	68	HIS	CA-CB-CG	5.65	123.21	113.60	8	1
1	A	105	ARG	NE-CZ-NH2	-5.51	117.55	120.30	10	1
1	A	105	ARG	N-CA-C	5.36	125.48	111.00	3	1
1	A	102	GLU	CB-CA-C	5.23	120.86	110.40	4	2
1	A	84	PHE	CB-CG-CD2	-5.18	117.17	120.80	7	2
1	A	15	PHE	CB-CG-CD1	-5.09	117.23	120.80	14	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	152	ARG	NE-CZ-NH2	-5.08	117.76	120.30	2	1
1	A	160	ILE	CG1-CB-CG2	-5.00	100.39	111.40	9	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	96	PHE	Sidechain	1
1	A	78	ARG	Sidechain	1
1	A	57	ARG	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	53

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: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:H	1:A:157:ILE:HD12	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	2
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: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:N	1:A:160:ILE:HD13	0.42	2.30	3	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: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%)	3	18

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	2304/2592 (89%)	1788 (78%)	362 (16%)	154 (7%)	3 18

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	137	ALA	10
1	A	74	SER	10
1	A	104	ASP	10
1	A	102	GLU	9
1	A	17	SER	8
1	A	156	ASP	6
1	A	139	GLY	6
1	A	109	GLY	5
1	A	111	LYS	5
1	A	106	VAL	5
1	A	30	PRO	4
1	A	157	ILE	4
1	A	146	ALA	4
1	A	110	GLN	3
1	A	78	ARG	3
1	A	28	ASP	3
1	A	108	PRO	3
1	A	103	GLY	3
1	A	138	GLU	3
1	A	67	LYS	3
1	A	62	ASN	2
1	A	89	VAL	2
1	A	90	SER	2
1	A	94	GLU	2
1	A	64	PHE	1
1	A	25	PRO	1
1	A	84	PHE	1
1	A	32	GLN	1
1	A	92	LYS	1
1	A	128	MET	1
1	A	26	ILE	1
1	A	58	GLY	1
1	A	65	PRO	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	126/139 (91%)	111±3 (88±2%)	15±3 (12±2%)	9	51
All	All	2016/2224 (91%)	1770 (88%)	246 (12%)	9	51

All 64 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	115	VAL	16
1	A	19	ILE	16
1	A	59	LYS	14
1	A	15	PHE	14
1	A	91	LEU	11
1	A	105	ARG	10
1	A	142	VAL	10
1	A	67	LYS	10
1	A	64	PHE	8
1	A	157	ILE	7
1	A	83	HIS	7
1	A	102	GLU	7
1	A	107	GLU	7
1	A	57	ARG	6
1	A	135	ASN	5
1	A	152	ARG	5
1	A	151	ASN	5
1	A	106	VAL	5
1	A	127	LEU	5
1	A	54	SER	4
1	A	49	GLU	4
1	A	88	THR	4
1	A	39	MET	4
1	A	68	HIS	3
1	A	155	GLU	3
1	A	84	PHE	3
1	A	121	LYS	3
1	A	16	VAL	3
1	A	73	GLN	3

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Mol	Chain	Res	Type	Models (Total)
1	A	32	GLN	3
1	A	35	SER	2
1	A	62	ASN	2
1	A	61	LEU	2
1	A	136	LEU	2
1	A	26	ILE	2
1	A	78	ARG	2
1	A	70	ILE	2
1	A	110	GLN	1
1	A	28	ASP	1
1	A	154	GLN	1
1	A	126	SER	1
1	A	23	ILE	1
1	A	108	PRO	1
1	A	100	VAL	1
1	A	27	THR	1
1	A	133	PHE	1
1	A	60	ILE	1
1	A	90	SER	1
1	A	160	ILE	1
1	A	97	THR	1
1	A	46	LEU	1
1	A	17	SER	1
1	A	161	GLU	1
1	A	38	MET	1
1	A	156	ASP	1
1	A	94	GLU	1
1	A	128	MET	1
1	A	111	LYS	1
1	A	89	VAL	1
1	A	63	VAL	1
1	A	79	GLU	1
1	A	104	ASP	1
1	A	140	GLU	1
1	A	31	ASP	1

6.3.3 RNA ⓘ

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 carbohydrates 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