



Full wwPDB NMR Structure Validation Report ⓘ

Feb 17, 2022 – 08:15 AM EST

PDB ID : 1NWD
Title : Solution Structure of Ca²⁺/Calmodulin bound to the C-terminal Domain of Petunia Glutamate Decarboxylase
Authors : Yap, K.L.; Yuan, T.; Mal, T.K.; Vogel, H.J.; Ikura, M.
Deposited on : 2003-02-06

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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:

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 : 2.26
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.26

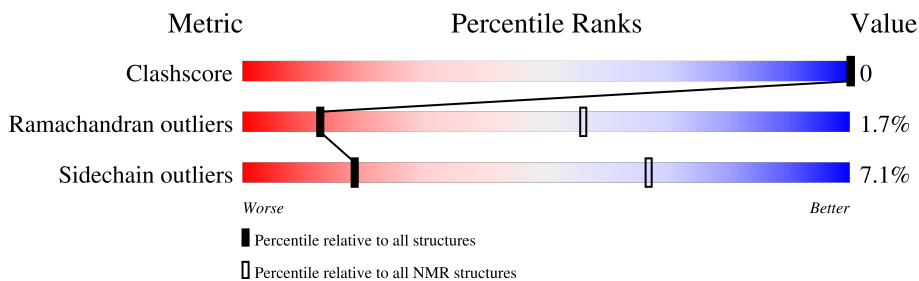
1 Overall quality at a glance

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	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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	148	
2	B	28	
2	C	28	

2 Ensemble composition and analysis i

This entry contains 20 models. Model 12 is the overall representative, medoid model (most similar to other models). The authors have identified model 4 as representative, based on the following criterion: *lowest energy*.

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:7-A:75, A:80-A:148, B:6-B:26, C:6-C:26 (180)	0.56	12

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 3 clusters and 1 single-model cluster was found.

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

3 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3235 atoms, of which 1597 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Calmodulin.

Mol	Chain	Residues	Atoms					Trace	
			Total	C	H	N	O		S
1	A	148	2263	714	1097	188	255	9	0

- Molecule 2 is a protein called Glutamate decarboxylase.

Mol	Chain	Residues	Atoms					Trace	
			Total	C	H	N	O		S
2	B	28	484	149	250	40	44	1	0
2	C	28	484	149	250	40	44	1	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1	GLY	-	cloning artifact	UNP Q07346
B	2	SER	-	cloning artifact	UNP Q07346
C	1	GLY	-	cloning artifact	UNP Q07346
C	2	SER	-	cloning artifact	UNP Q07346

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

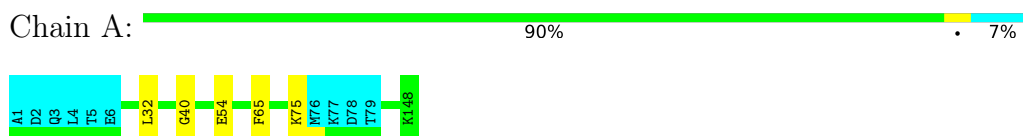
Mol	Chain	Residues	Atoms	
			Total	Ca
3	A	4	4	4

4 Residue-property plots

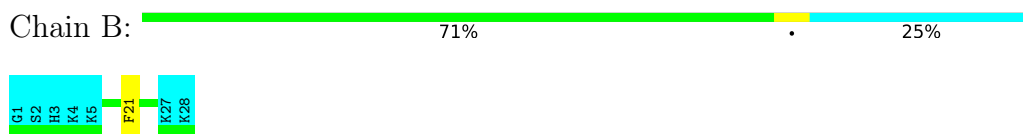
4.1 Average score per residue in the NMR ensemble

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.

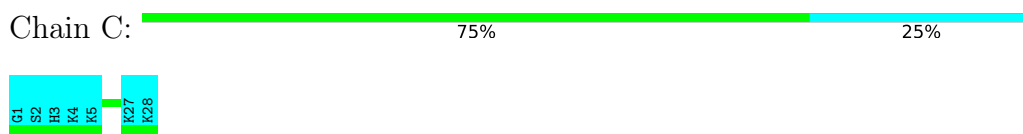
- Molecule 1: Calmodulin



- Molecule 2: Glutamate decarboxylase



- Molecule 2: Glutamate decarboxylase

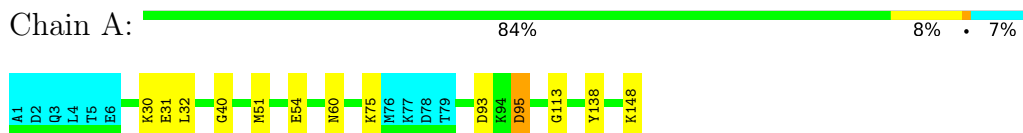


4.2 Scores per residue for each member of the ensemble

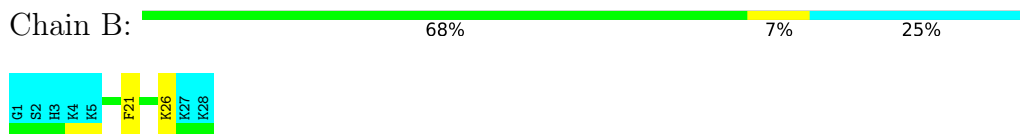
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

- Molecule 1: Calmodulin



- Molecule 2: Glutamate decarboxylase

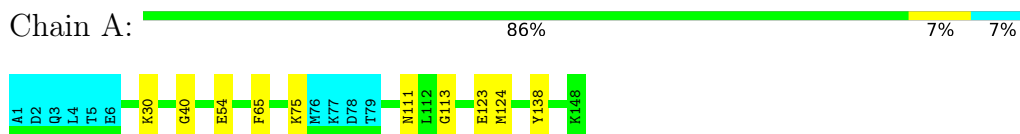


- Molecule 2: Glutamate decarboxylase



4.2.2 Score per residue for model 2

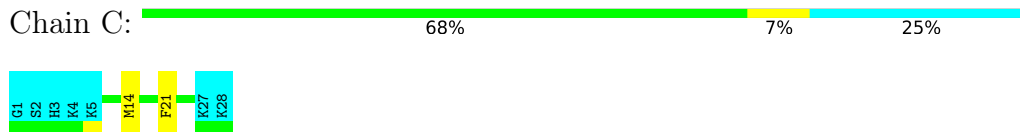
- Molecule 1: Calmodulin



- Molecule 2: Glutamate decarboxylase

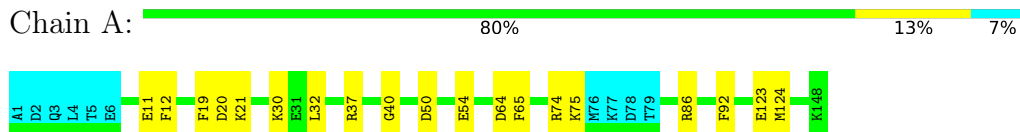


- Molecule 2: Glutamate decarboxylase



4.2.3 Score per residue for model 3

- Molecule 1: Calmodulin



- Molecule 2: Glutamate decarboxylase



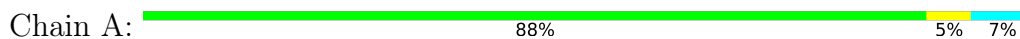


- Molecule 2: Glutamate decarboxylase



4.2.4 Score per residue for model 4

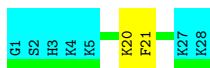
- Molecule 1: Calmodulin



- Molecule 2: Glutamate decarboxylase

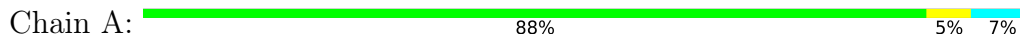


- Molecule 2: Glutamate decarboxylase



4.2.5 Score per residue for model 5

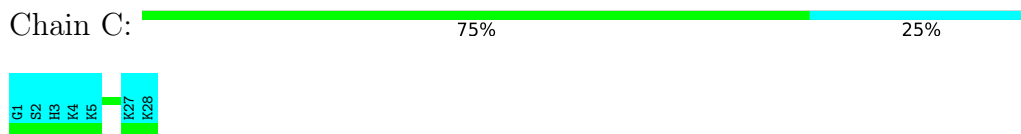
- Molecule 1: Calmodulin



- Molecule 2: Glutamate decarboxylase

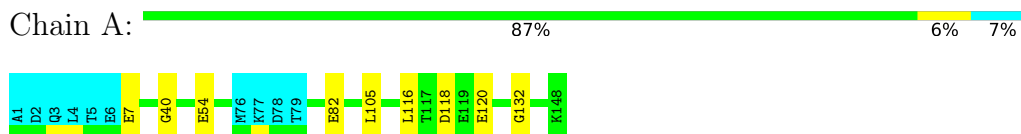


- Molecule 2: Glutamate decarboxylase

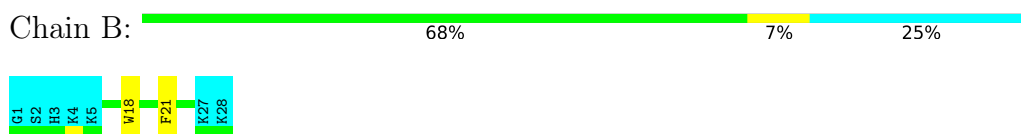


4.2.6 Score per residue for model 6

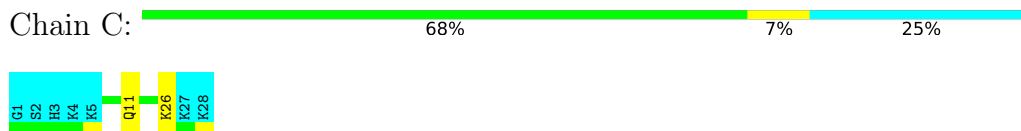
- Molecule 1: Calmodulin



- Molecule 2: Glutamate decarboxylase

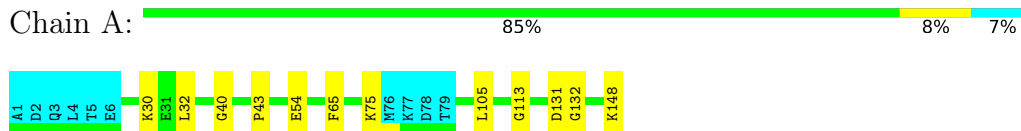


- Molecule 2: Glutamate decarboxylase

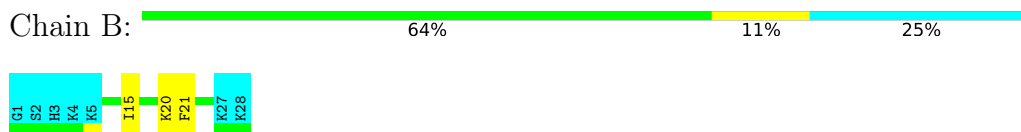


4.2.7 Score per residue for model 7

- Molecule 1: Calmodulin



- Molecule 2: Glutamate decarboxylase



- Molecule 2: Glutamate decarboxylase



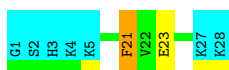


4.2.8 Score per residue for model 8

- Molecule 1: Calmodulin



- Molecule 2: Glutamate decarboxylase

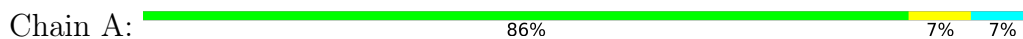


- Molecule 2: Glutamate decarboxylase



4.2.9 Score per residue for model 9

- Molecule 1: Calmodulin



- Molecule 2: Glutamate decarboxylase

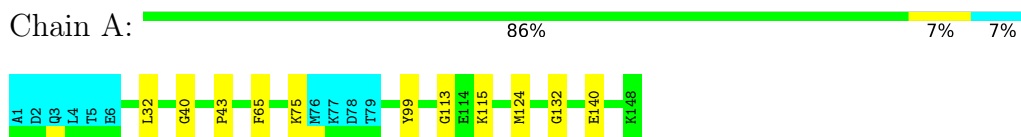


- Molecule 2: Glutamate decarboxylase



4.2.10 Score per residue for model 10

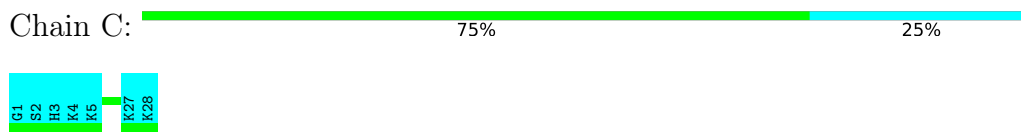
- Molecule 1: Calmodulin



- Molecule 2: Glutamate decarboxylase

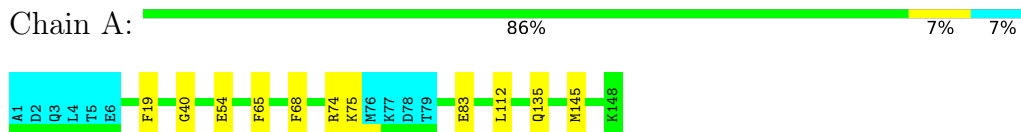


- Molecule 2: Glutamate decarboxylase

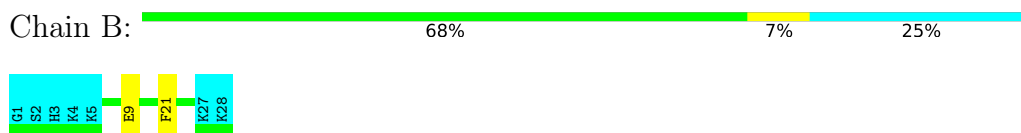


4.2.11 Score per residue for model 11

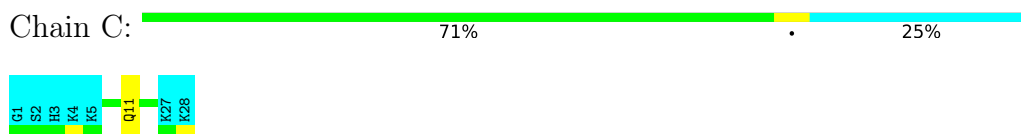
- Molecule 1: Calmodulin



- Molecule 2: Glutamate decarboxylase




- Molecule 2: Glutamate decarboxylase



4.2.12 Score per residue for model 12 (medoid)

- Molecule 1: Calmodulin

Chain A:  84% 9% 7%



- Molecule 2: Glutamate decarboxylase

Chain B:  64% 11% 25%




- Molecule 2: Glutamate decarboxylase

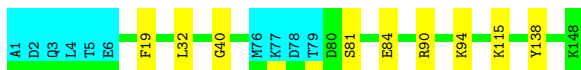
Chain C:  64% 11% 25%



4.2.13 Score per residue for model 13

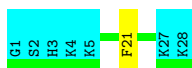
- Molecule 1: Calmodulin

Chain A:  87% 6% 7%



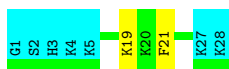
- Molecule 2: Glutamate decarboxylase

Chain B:  71% 0% 25%




- Molecule 2: Glutamate decarboxylase

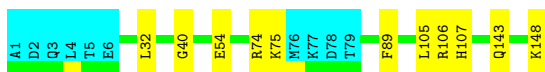
Chain C:  68% 7% 25%



4.2.14 Score per residue for model 14

- Molecule 1: Calmodulin

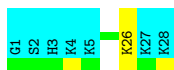
Chain A:  86% 7% 7%



- Molecule 2: Glutamate decarboxylase

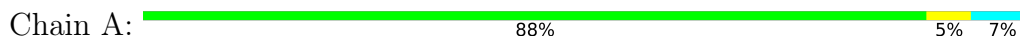


- Molecule 2: Glutamate decarboxylase

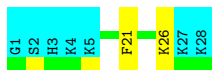


4.2.15 Score per residue for model 15

- Molecule 1: Calmodulin



- Molecule 2: Glutamate decarboxylase

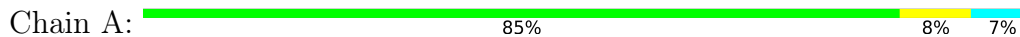


- Molecule 2: Glutamate decarboxylase

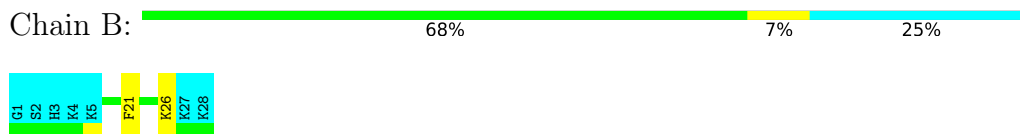


4.2.16 Score per residue for model 16

- Molecule 1: Calmodulin



- Molecule 2: Glutamate decarboxylase

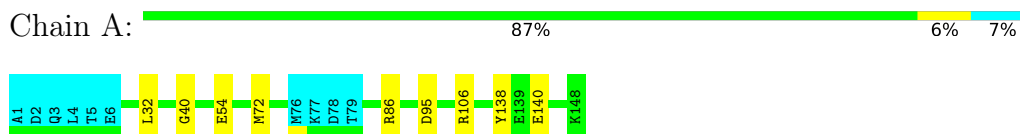


- Molecule 2: Glutamate decarboxylase

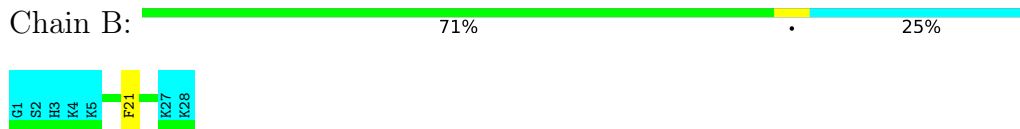


4.2.17 Score per residue for model 17

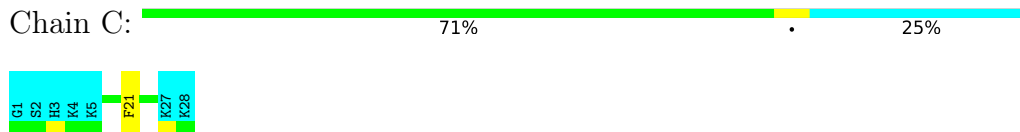
- Molecule 1: Calmodulin



- Molecule 2: Glutamate decarboxylase

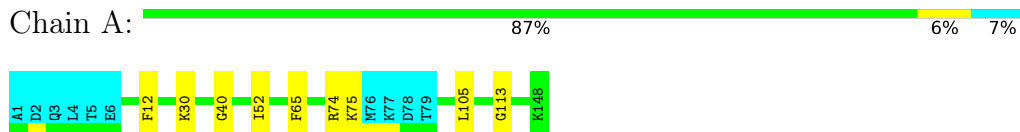


- Molecule 2: Glutamate decarboxylase



4.2.18 Score per residue for model 18

- Molecule 1: Calmodulin

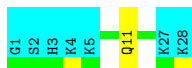


- Molecule 2: Glutamate decarboxylase



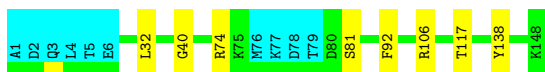
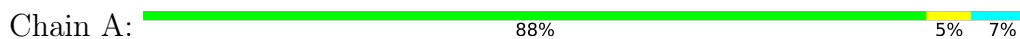


- Molecule 2: Glutamate decarboxylase



4.2.19 Score per residue for model 19

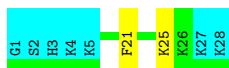
- Molecule 1: Calmodulin



- Molecule 2: Glutamate decarboxylase

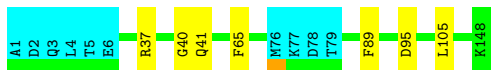
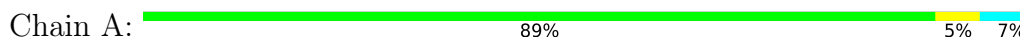


- Molecule 2: Glutamate decarboxylase

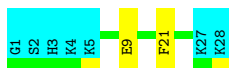


4.2.20 Score per residue for model 20

- Molecule 1: Calmodulin



- Molecule 2: Glutamate decarboxylase



- Molecule 2: Glutamate decarboxylase

Chain C:  68% 7% 25%



5 Refinement protocol and experimental data overview

The models were refined using the following method: *simulated annealing and torsion angle dynamics*.

Of the 200 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
CNS	refinement	1.1
DYANA	structure solution	1.5

No chemical shift data was provided.

6 Model quality [i](#)

6.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section:
CA

There are no covalent bond-length or bond-angle outliers.

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	0.3±0.5
2	B	0.0±0.0	0.1±0.2
All	All	0	8

There are no bond-length outliers.

There are no bond-angle outliers.

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	138	TYR	Sidechain	2
1	A	99	TYR	Sidechain	2
2	B	21	PHE	Sidechain	1
1	A	68	PHE	Sidechain	1
1	A	89	PHE	Sidechain	1
1	A	12	PHE	Sidechain	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
All	All	28920	27620	27600	-

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 -.

There are no clashes.

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	137/148 (93%)	114±3 (83±2%)	20±3 (14±2%)	3±1 (2±1%)	10	49
2	B	21/28 (75%)	20±1 (94±5%)	1±1 (6±5%)	0±0 (0±1%)	32	76
2	C	21/28 (75%)	21±0 (98±2%)	0±0 (2±2%)	0±0 (0±0%)	100	100
All	All	3580/4080 (88%)	3090 (86%)	429 (12%)	61 (2%)	13	56

All 15 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	40	GLY	20
1	A	75	LYS	11
1	A	113	GLY	10
1	A	95	ASP	5
1	A	132	GLY	3
1	A	43	PRO	2
2	B	26	LYS	2
1	A	74	ARG	1
1	A	131	ASP	1
1	A	137	ASN	1
1	A	54	GLU	1
1	A	115	LYS	1
1	A	133	ASP	1
1	A	140	GLU	1
1	A	92	PHE	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	117/126 (93%)	110±3 (94±2%)	7±3 (6±2%)	22 71
2	B	20/26 (77%)	18±1 (89±5%)	2±1 (11±5%)	10 54
2	C	20/26 (77%)	18±1 (91±4%)	2±1 (9±4%)	13 60
All	All	3140/3560 (88%)	2917 (93%)	223 (7%)	18 67

All 77 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)
2	B	21	PHE	20
1	A	32	LEU	12
1	A	54	GLU	11
1	A	65	PHE	11
2	C	21	PHE	9
1	A	37	ARG	7
1	A	105	LEU	7
1	A	148	LYS	6
2	C	26	LYS	6
2	B	15	ILE	6
1	A	30	LYS	5
1	A	74	ARG	5
1	A	138	TYR	4
2	B	20	LYS	4
2	C	14	MET	4
1	A	19	PHE	4
2	C	11	GLN	4
1	A	106	ARG	4
1	A	60	ASN	3
2	B	26	LYS	3
2	C	19	LYS	3
1	A	123	GLU	3
1	A	124	MET	3
1	A	21	LYS	3
1	A	86	ARG	3
2	C	20	LYS	3

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Mol	Chain	Res	Type	Models (Total)
1	A	90	ARG	3
1	A	115	LYS	3
2	B	9	GLU	3
1	A	75	LYS	2
1	A	50	ASP	2
2	C	25	LYS	2
1	A	14	GLU	2
2	B	18	TRP	2
2	C	13	GLU	2
1	A	140	GLU	2
2	B	23	GLU	2
1	A	94	LYS	2
1	A	112	LEU	2
1	A	89	PHE	2
1	A	81	SER	2
1	A	41	GLN	2
1	A	31	GLU	1
1	A	51	MET	1
1	A	93	ASP	1
1	A	95	ASP	1
2	C	12	LEU	1
1	A	111	ASN	1
1	A	11	GLU	1
1	A	12	PHE	1
1	A	20	ASP	1
1	A	64	ASP	1
1	A	92	PHE	1
1	A	87	GLU	1
1	A	7	GLU	1
1	A	82	GLU	1
1	A	116	LEU	1
1	A	118	ASP	1
1	A	120	GLU	1
1	A	137	ASN	1
2	B	11	GLN	1
2	B	12	LEU	1
1	A	83	GLU	1
1	A	135	GLN	1
1	A	145	MET	1
1	A	71	MET	1
2	B	25	LYS	1
2	C	9	GLU	1

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Mol	Chain	Res	Type	Models (Total)
1	A	84	GLU	1
1	A	107	HIS	1
1	A	143	GLN	1
2	B	14	MET	1
1	A	119	GLU	1
1	A	18	LEU	1
1	A	72	MET	1
1	A	52	ILE	1
1	A	117	THR	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](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided