



Full wwPDB NMR Structure Validation Report ⓘ

Apr 26, 2016 – 11:24 PM BST

PDB ID : 2KMD
Title : Ras signaling requires dynamic properties of Ets1 for phosphorylation-enhanced binding to co-activator CBP
Authors : Nelson, M.L.; Kang, H.; Lee, G.M.; Blaszczyk, A.G.; Lau, D.K.W.; McIntosh, L.P.; Graves, B.J.
Deposited on : 2009-07-27

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
<http://wwpdb.org/validation/2016/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
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : rb-20027457
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027457

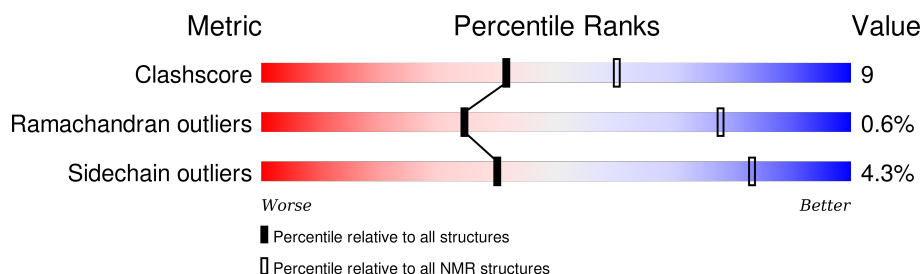
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 92%.

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	114402	11133
Ramachandran outliers	111179	9975
Sidechain outliers	111093	9958

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	113	

2 Ensemble composition and analysis

This entry contains 20 models. Model 8 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 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:55-A:133 (79)	0.22	8

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 6 clusters and 2 single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1771 atoms, of which 874 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Protein C-ets-1.

Mol	Chain	Residues	Atoms								Trace
1	A	111	Total	C	H	N	O	P	S		0
			1771	570	874	146	170	2	9		

There are 3 discrepancies between the modelled and reference sequences:

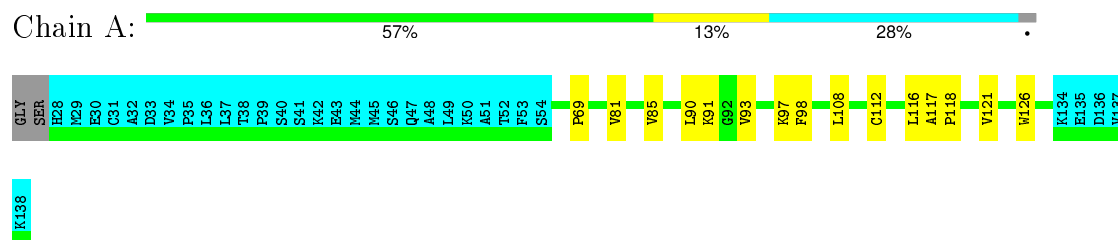
Chain	Residue	Modelled	Actual	Comment	Reference
A	26	GLY	-	EXPRESSION TAG	UNP P27577
A	27	SER	-	EXPRESSION TAG	UNP P27577
A	28	HIS	-	EXPRESSION TAG	UNP P27577

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: Protein C-ets-1

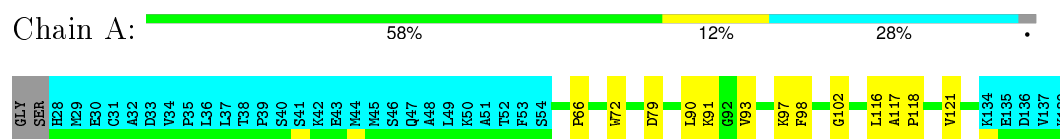


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

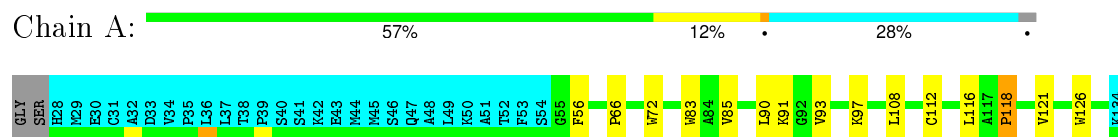
4.2.1 Score per residue for model 1

- Molecule 1: Protein C-ets-1



4.2.2 Score per residue for model 2

- Molecule 1: Protein C-ets-1



E135
D136
V137
K138

4.2.3 Score per residue for model 3

- Molecule 1: Protein C-ets-1

Chain A: 

GLY SER H28 M29 E20 C31 A32 D33 V34 P35 L36 L37 T38 P39 S40 S41 K42 E43 M44 M45 S46 Q47 A48 L49 K50 A51 T52 F53 S54 E74 W80 V81 M82 W83 E87 L90 K91 L108 C112 F113 P118 V121 I124 L125 L129 K134 E135 D136 V137

K138

4.2.4 Score per residue for model 4

- Molecule 1: Protein C-ets-1

Chain A: 

GLY SER H28 M29 E20 C31 A32 D33 V34 P35 L36 L37 T38 P39 S40 S41 K42 E43 M44 M45 S46 Q47 A48 L49 K50 A51 T52 F53 S54 T57 K58 E59 Q60 K67 P68 P69 W80 V81 V85 L90 K91 G92 V93 K97 F98 G106 A107 L108 G109 K110 E111 C112

L116 A117 P118 V121 W126 L129 E130 I131 L132 Q133 K134 E135 D136 V137 K138

4.2.5 Score per residue for model 5

- Molecule 1: Protein C-ets-1

Chain A: 

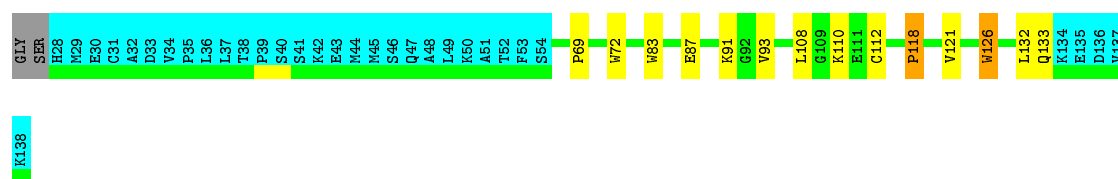
GLY SER H28 M29 E20 C31 A32 D33 V34 P35 L36 L37 T38 P39 S40 S41 K42 E43 M44 M45 S46 Q47 A48 L49 K50 A51 T52 F53 S54 G55 F56 Q60 P69 W83 A84 V85 K91 G92 V93 K97 F98 G102 L116 A117 P118 V121 W126 I131 K134

E135
D136
V137
K138

4.2.6 Score per residue for model 6

- Molecule 1: Protein C-ets-1

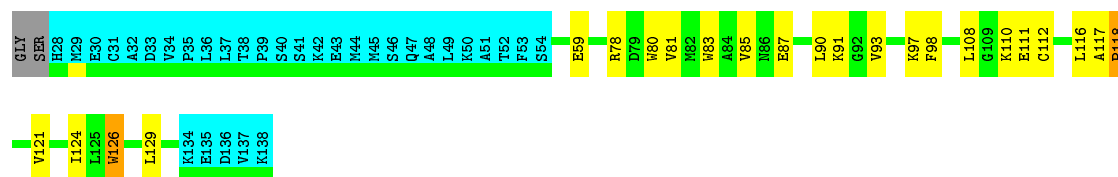
Chain A: 



4.2.7 Score per residue for model 7

- Molecule 1: Protein C-ets-1

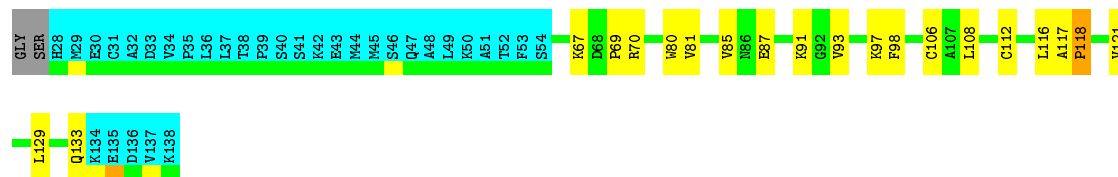
Chain A: 50% 19% 28%



4.2.8 Score per residue for model 8 (medoid)

- Molecule 1: Protein C-ets-1

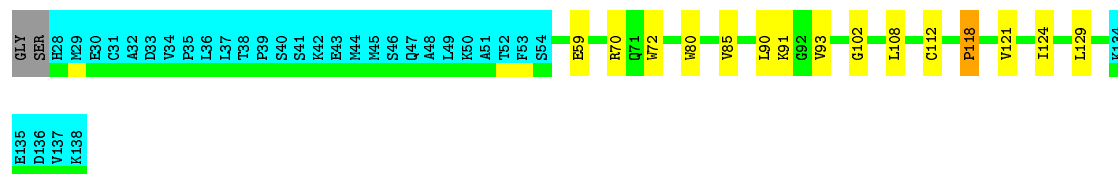
Chain A: 52% 17% 28%



4.2.9 Score per residue for model 9

- Molecule 1: Protein C-ets-1

Chain A: 57% 12% 28%



4.2.10 Score per residue for model 10

- Molecule 1: Protein C-ets-1

Chain A: 



4.2.11 Score per residue for model 11

- Molecule 1: Protein C-ets-1

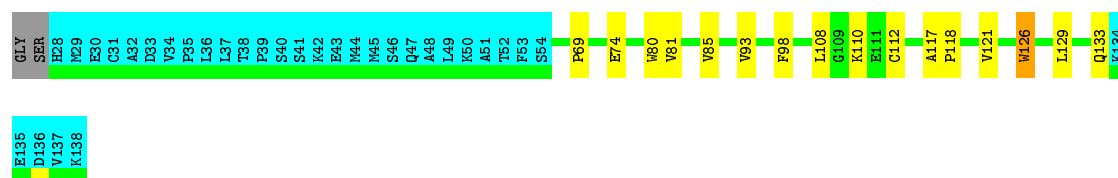
Chain A: 



4.2.12 Score per residue for model 12

- Molecule 1: Protein C-ets-1

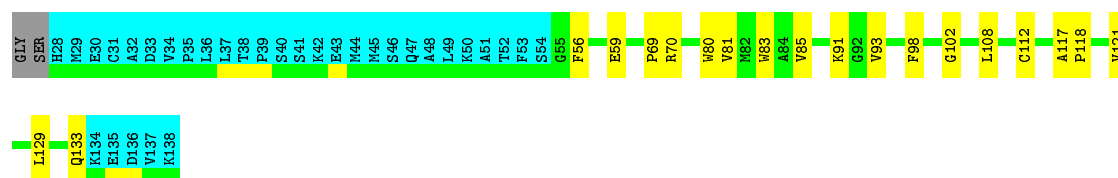
Chain A: 



4.2.13 Score per residue for model 13

- Molecule 1: Protein C-ets-1

Chain A: 



4.2.14 Score per residue for model 14

- Molecule 1: Protein C-ets-1

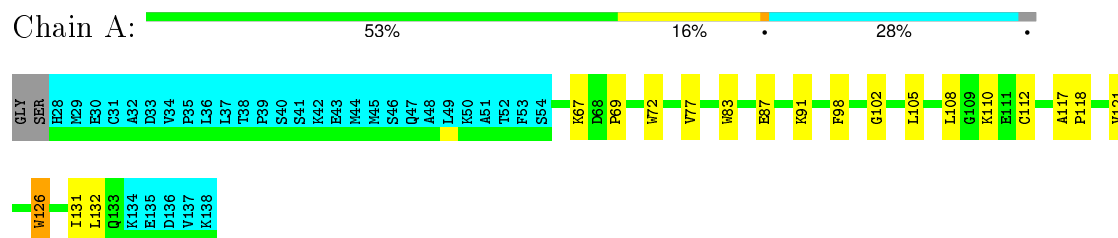
Chain A: 





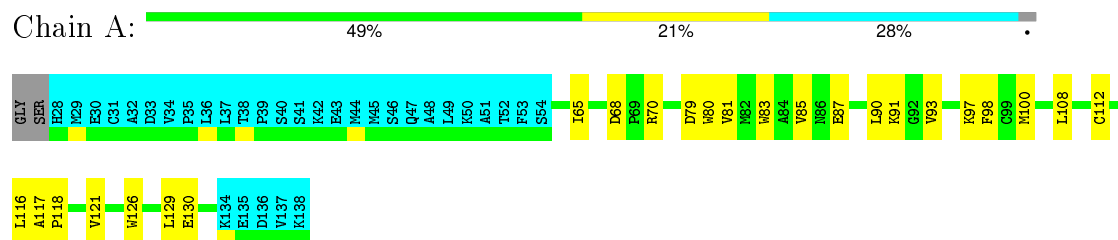
4.2.15 Score per residue for model 15

- Molecule 1: Protein C-ets-1



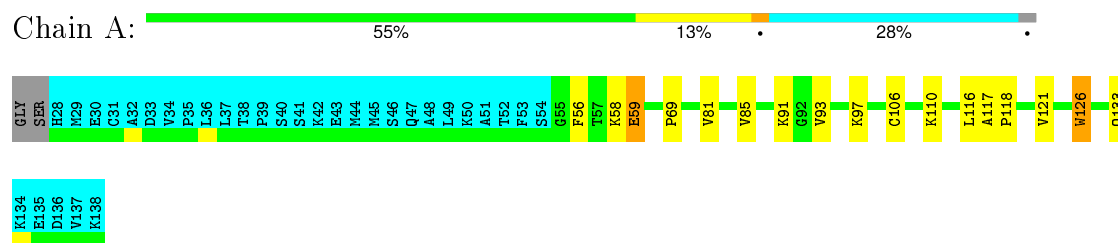
4.2.16 Score per residue for model 16

- Molecule 1: Protein C-ets-1



4.2.17 Score per residue for model 17

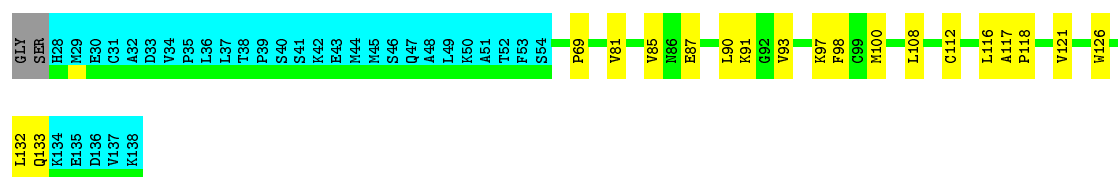
- Molecule 1: Protein C-ets-1



4.2.18 Score per residue for model 18

- Molecule 1: Protein C-ets-1

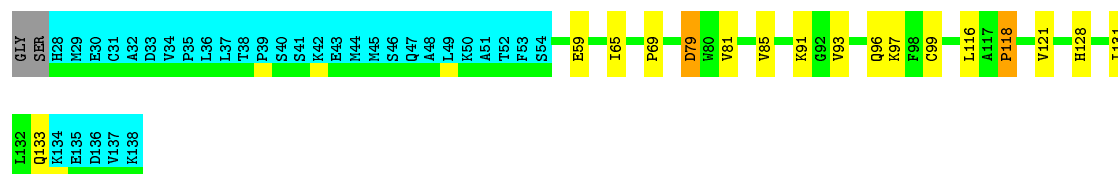




4.2.19 Score per residue for model 19

- Molecule 1: Protein C-ets-1

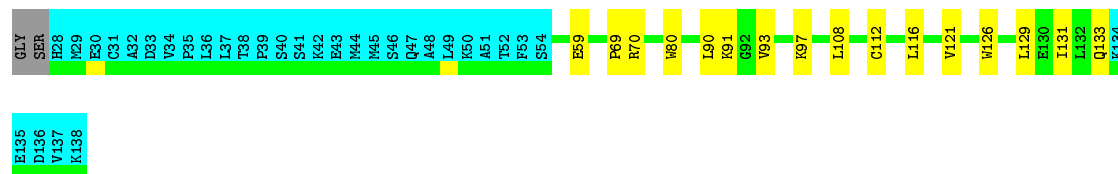
Chain A: 55% 13% 28%



4.2.20 Score per residue for model 20

- Molecule 1: Protein C-ets-1

Chain A: 56% 14% 28%



5 Refinement protocol and experimental data overview

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

Of the 500 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
CYANA	structure solution	
SCULPTOR	refinement	

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	BMRB entry 16426
Number of chemical shift lists	1
Total number of shifts	1419
Number of shifts mapped to atoms	1419
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	92%

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

6 Model quality ⓘ

6.1 Standard geometry ⓘ

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

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	644	627	625	11±4
All	All	12880	12540	12500	226

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 9.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:85:VAL:CG2	1:A:93:VAL:HG11	0.69	2.17	18	13
1:A:118:PRO:HG2	1:A:121:VAL:HG22	0.69	1.65	17	7
1:A:90:LEU:HD13	1:A:121:VAL:HG13	0.64	1.67	11	2
1:A:117:ALA:HB1	1:A:121:VAL:CG2	0.59	2.28	18	7
1:A:118:PRO:HD2	1:A:121:VAL:CG2	0.59	2.27	12	18
1:A:85:VAL:HG21	1:A:93:VAL:HG11	0.59	1.74	18	5
1:A:57:THR:HA	1:A:60:GLN:HG2	0.56	1.75	4	1
1:A:98:PHE:CZ	1:A:117:ALA:HB2	0.54	2.38	18	10
1:A:90:LEU:HB3	1:A:121:VAL:HG12	0.53	1.81	18	2
1:A:98:PHE:HZ	1:A:117:ALA:HB2	0.53	1.62	18	3
1:A:81:VAL:O	1:A:85:VAL:HG23	0.52	2.05	4	10
1:A:69:PRO:HG2	1:A:133:GLN:HG2	0.51	1.83	18	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:118:PRO:CG	1:A:121:VAL:HG22	0.51	2.36	13	7
1:A:90:LEU:HB3	1:A:121:VAL:HG22	0.50	1.84	11	2
1:A:93:VAL:HB	1:A:121:VAL:HG21	0.50	1.83	1	7
1:A:83:TRP:CE2	1:A:87:GLU:HG3	0.49	2.41	15	7
1:A:69:PRO:HD2	1:A:133:GLN:HA	0.49	1.83	13	1
1:A:117:ALA:HB1	1:A:121:VAL:HG23	0.48	1.85	10	5
1:A:108:LEU:HD22	1:A:112:CYS:SG	0.48	2.47	14	1
1:A:80:TRP:CH2	1:A:129:LEU:HB2	0.48	2.44	8	10
1:A:57:THR:HA	1:A:60:GLN:CG	0.48	2.38	4	1
1:A:93:VAL:HB	1:A:121:VAL:HG11	0.48	1.84	20	1
1:A:65:ILE:HD11	1:A:79:ASP:HB3	0.48	1.85	16	2
1:A:69:PRO:HG2	1:A:133:GLN:CG	0.48	2.39	14	2
1:A:108:LEU:HB3	1:A:112:CYS:HB2	0.48	1.86	18	15
1:A:69:PRO:HD3	1:A:132:LEU:CB	0.47	2.39	15	3
1:A:69:PRO:HB2	1:A:106:CYS:SG	0.47	2.49	8	3
1:A:110:LYS:HD3	1:A:126:TRP:CZ2	0.47	2.44	6	6
1:A:72:TRP:HB2	1:A:102:GLY:HA3	0.47	1.86	14	4
1:A:56:PHE:O	1:A:59:GLU:HG3	0.47	2.09	17	1
1:A:85:VAL:HG22	1:A:93:VAL:HG11	0.47	1.86	18	3
1:A:69:PRO:HD3	1:A:132:LEU:HB3	0.47	1.87	6	2
1:A:90:LEU:HB3	1:A:121:VAL:CG1	0.46	2.41	4	3
1:A:90:LEU:HD21	1:A:124:ILE:CD1	0.46	2.40	3	1
1:A:97:LYS:HB3	1:A:116:LEU:HB3	0.46	1.87	1	13
1:A:118:PRO:HG2	1:A:121:VAL:CG2	0.46	2.39	4	2
1:A:113:PHE:CZ	1:A:125:LEU:HB3	0.45	2.47	3	1
1:A:100:MET:SD	1:A:108:LEU:HD11	0.45	2.52	16	3
1:A:69:PRO:HG2	1:A:133:GLN:HG3	0.45	1.89	14	4
1:A:117:ALA:CB	1:A:122:GLY:HA2	0.44	2.42	11	1
1:A:90:LEU:HD13	1:A:121:VAL:HB	0.44	1.90	14	5
1:A:90:LEU:HD21	1:A:124:ILE:HD12	0.44	1.90	7	3
1:A:118:PRO:CD	1:A:121:VAL:HG22	0.43	2.43	13	4
1:A:118:PRO:HD2	1:A:121:VAL:HB	0.43	1.90	11	1
1:A:56:PHE:HB2	1:A:83:TRP:CH2	0.43	2.47	2	3
1:A:69:PRO:O	1:A:102:GLY:HA3	0.43	2.14	5	2
1:A:77:VAL:HG13	1:A:105:LEU:HD22	0.42	1.91	15	1
1:A:91:LYS:HD3	1:A:91:LYS:N	0.42	2.30	5	1
1:A:96:GLN:HA	1:A:99:CYS:SG	0.42	2.55	19	1
1:A:66:PRO:HG2	1:A:72:TRP:CD1	0.42	2.50	1	2
1:A:78:ARG:C	1:A:78:ARG:HD2	0.41	2.36	7	2
1:A:81:VAL:HG13	1:A:125:LEU:HD21	0.41	1.92	3	1
1:A:108:LEU:HB3	1:A:112:CYS:HB3	0.41	1.91	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:90:LEU:HB3	1:A:121:VAL:CG2	0.41	2.45	11	1
1:A:56:PHE:O	1:A:60:GLN:HG2	0.41	2.16	5	1
1:A:70:ARG:CZ	1:A:133:GLN:HB3	0.41	2.46	8	1
1:A:69:PRO:O	1:A:72:TRP:HB2	0.41	2.15	6	1
1:A:90:LEU:CD1	1:A:121:VAL:HG13	0.41	2.44	20	1
1:A:69:PRO:CG	1:A:133:GLN:HG2	0.40	2.47	17	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	79/113 (70%)	74±1 (93±1%)	5±1 (6±1%)	0±0 (1±1%)	34	78
All	All	1580/2260 (70%)	1474 (93%)	97 (6%)	9 (1%)	34	78

All 1 unique Ramachandran outliers are listed below.

Mol	Chain	Res	Type	Models (Total)
1	A	118	PRO	9

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	68/96 (71%)	65±1 (96±1%)	3±1 (4±1%)	40	83
All	All	1360/1920 (71%)	1302 (96%)	58 (4%)	40	83

All 12 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	91	LYS	18
1	A	126	TRP	13
1	A	59	GLU	8
1	A	70	ARG	5
1	A	74	GLU	2
1	A	58	LYS	2
1	A	67	LYS	2
1	A	111	GLU	2
1	A	79	ASP	2
1	A	87	GLU	2
1	A	68	ASP	1
1	A	72	TRP	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains ⓘ

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds for which Mogul statistics could be retrieved, the number of bonds that are observed in the model and the number of bonds that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length is the number of standard deviations the observed value is removed from the expected value. A bond length with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
1	TPO	A	38	1	7,10,11	0.55±0.01	0±0 (0±0%)
1	SEP	A	41	1	7,9,10	0.68±0.01	0±0 (0±0%)

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of angles that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond angle is the number of standard deviations the observed value is removed from the expected value. A bond angle with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
1	TPO	A	38	1	10,14,16	1.31±0.01	0±0 (0±0%)
1	SEP	A	41	1	8,12,14	1.19±0.03	0±0 (0±0%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	TPO	A	38	1	-	0±0,8,11,13	0±0,0,0,0
1	SEP	A	41	1	-	0±0,5,8,10	0±0,0,0,0

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

All unique torsion outliers are listed below.

Mol	Chain	Res	Type	Atoms	Models (Total)
1	A	38	TPO	OG1-CB-CA-N	11

There are no ring outliers.

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

The completeness of assignment taking into account all chemical shift lists is 92% for the well-defined parts and 92% for the entire structure.

7.1 Chemical shift list 1

File name: BMRB entry 16426

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	1419
Number of shifts mapped to atoms	1419
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	6

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	111	-0.23 ± 0.13	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	105	0.14 ± 0.12	None needed (< 0.5 ppm)
$^{13}\text{C}'$	105	-0.29 ± 0.07	None needed (< 0.5 ppm)
^{15}N	105	0.52 ± 0.34	None needed (imprecise)

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 92%, i.e. 930 atoms were assigned a chemical shift out of a possible 1006. 0 out of 14 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	386/389 (99%)	155/155 (100%)	155/158 (98%)	76/76 (100%)
Sidechain	440/499 (88%)	273/293 (93%)	158/186 (85%)	9/20 (45%)

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	Total	¹H	¹³C	¹⁵N
Aromatic	104/118 (88%)	55/62 (89%)	45/48 (94%)	4/8 (50%)
Overall	930/1006 (92%)	483/510 (95%)	358/392 (91%)	89/104 (86%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 92%, i.e. 1258 atoms were assigned a chemical shift out of a possible 1369. 0 out of 19 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	527/535 (99%)	211/213 (99%)	213/218 (98%)	103/104 (99%)
Sidechain	616/699 (88%)	383/412 (93%)	223/262 (85%)	10/25 (40%)
Aromatic	115/135 (85%)	61/71 (86%)	50/54 (93%)	4/10 (40%)
Overall	1258/1369 (92%)	655/696 (94%)	486/534 (91%)	117/139 (84%)

7.1.4 Statistically unusual chemical shifts ⓘ

The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

Mol	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	69	PRO	HA	1.19	6.05 – 2.75	-9.7
1	A	87	GLU	HB3	0.16	3.10 – 0.90	-8.3
1	A	87	GLU	HB2	0.52	3.08 – 0.98	-7.2
1	A	69	PRO	HB3	-0.30	3.81 – 0.21	-6.4
1	A	87	GLU	HG3	0.95	3.31 – 1.21	-6.2
1	A	110	LYS	HG3	-0.36	2.76 – -0.04	-6.1

7.1.5 Random Coil Index (RCI) plots ⓘ

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition.

Random coil index (RCI) for chain A:

