



Full wwPDB NMR Structure Validation Report ⓘ

Mar 25, 2026 – 11:22 AM UTC

PDB ID : 2JZI / pdb_00002jzi
Title : Structure of Calmodulin complexed with the Calmodulin Binding Domain of Calcineurin
Authors : Chyan, C.; Huang, J.; Irene, D.; Lin, T.
Deposited on : 2008-01-09

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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

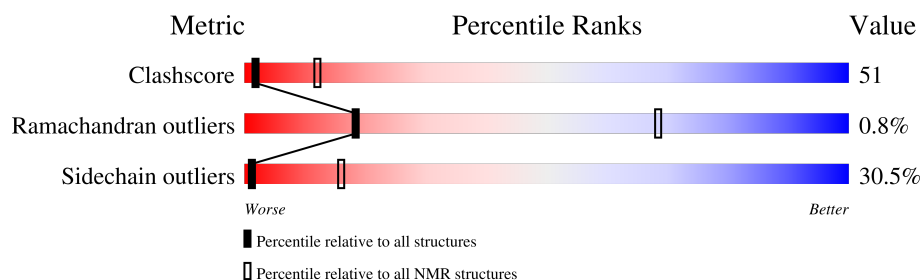
1 Overall quality at a glance

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	148	
2	B	24	

2 Ensemble composition and analysis

This entry contains 20 models. Model 2 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:1-A:72, A:82-A:145, B:1-B:24 (160)	0.32	2

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. No single-model clusters were found.

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

3 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 2694 atoms, of which 1327 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Calmodulin.

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

- Molecule 2 is a protein called Serine/threonine-protein phosphatase 2B catalytic subunit alpha isoform.

Mol	Chain	Residues	Atoms						Trace
2	B	24	Total	C	H	N	O	S	0
			427	124	230	43	29	1	

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

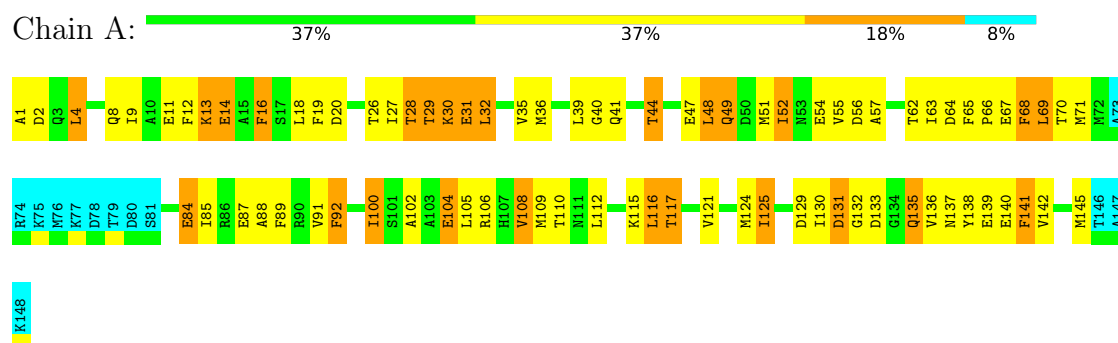
Mol	Chain	Residues	Atoms	
3	A	4	Total	Ca
			4	4

4 Residue-property plots [i](#)

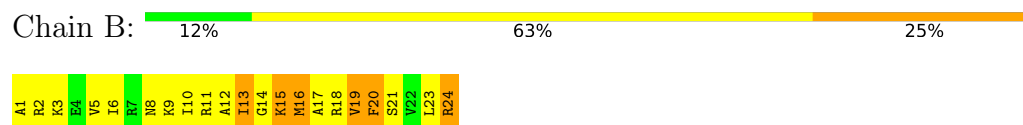
4.1 Average score per residue in the NMR ensemble

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: Calmodulin



- Molecule 2: Serine/threonine-protein phosphatase 2B catalytic subunit alpha isoform

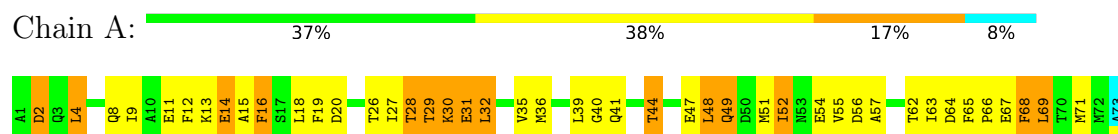


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

- Molecule 1: Calmodulin





- Molecule 2: Serine/threonine-protein phosphatase 2B catalytic subunit alpha isoform

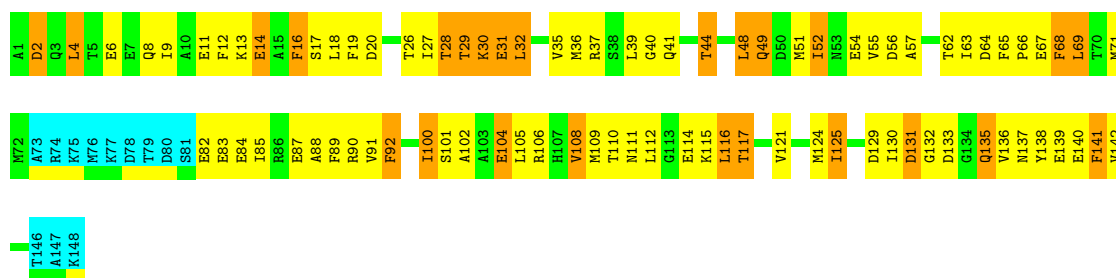
Chain B: 17% 58% 25%



4.2.2 Score per residue for model 2 (medoid)

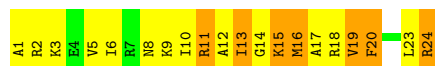
- Molecule 1: Calmodulin

Chain A: 34% 41% 17% 8%



- Molecule 2: Serine/threonine-protein phosphatase 2B catalytic subunit alpha isoform

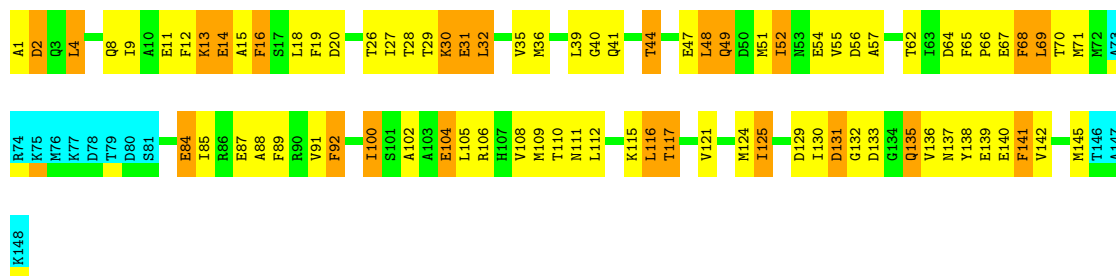
Chain B: 17% 54% 29%



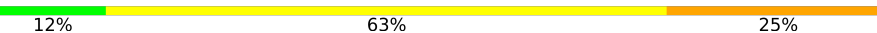
4.2.3 Score per residue for model 3

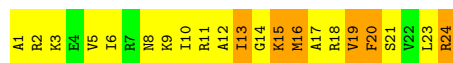
- Molecule 1: Calmodulin

Chain A: 36% 39% 16% 8%



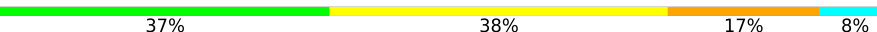
- Molecule 2: Serine/threonine-protein phosphatase 2B catalytic subunit alpha isoform

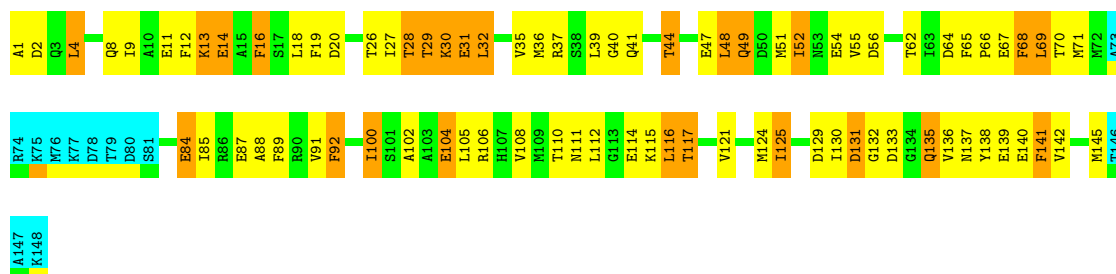
Chain B: 



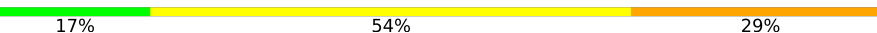
4.2.4 Score per residue for model 4

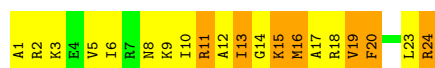
- Molecule 1: Calmodulin

Chain A: 



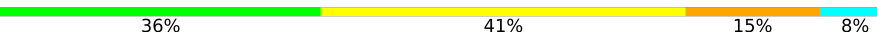
- Molecule 2: Serine/threonine-protein phosphatase 2B catalytic subunit alpha isoform

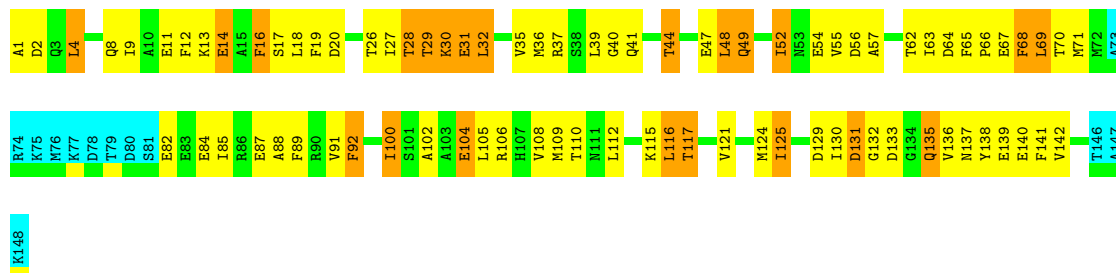
Chain B: 



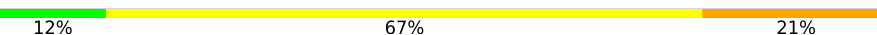
4.2.5 Score per residue for model 5

- Molecule 1: Calmodulin

Chain A: 



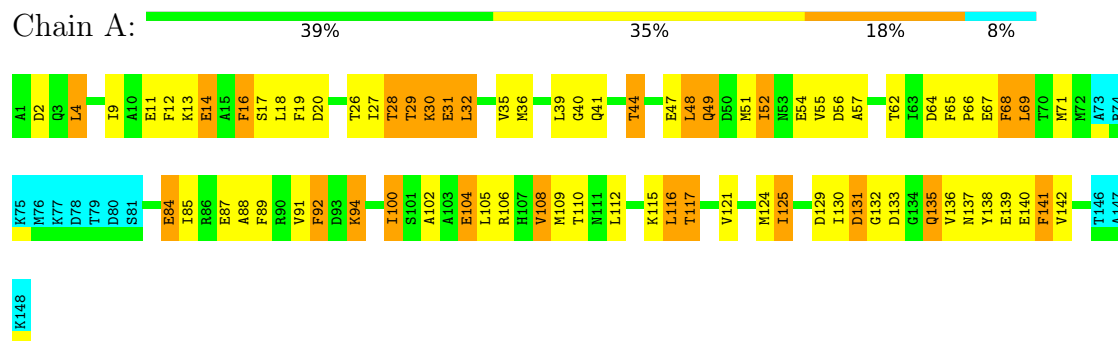
- Molecule 2: Serine/threonine-protein phosphatase 2B catalytic subunit alpha isoform

Chain B: 

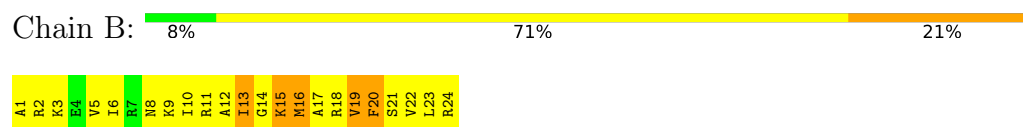


4.2.6 Score per residue for model 6

- Molecule 1: Calmodulin

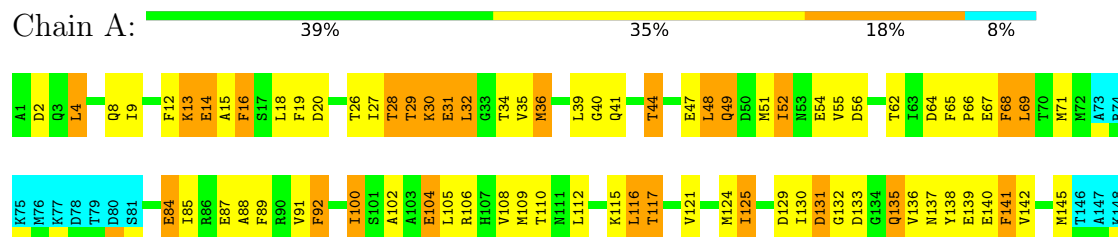


- Molecule 2: Serine/threonine-protein phosphatase 2B catalytic subunit alpha isoform

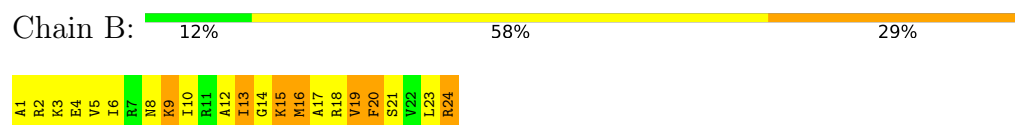


4.2.7 Score per residue for model 7

- Molecule 1: Calmodulin

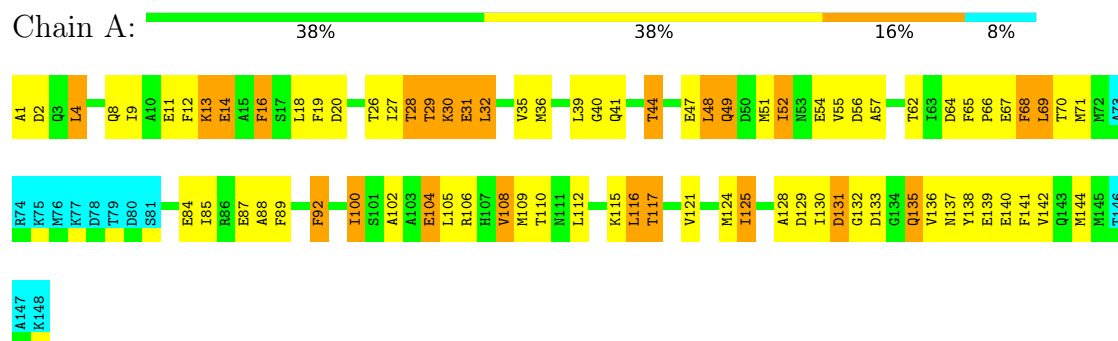


- Molecule 2: Serine/threonine-protein phosphatase 2B catalytic subunit alpha isoform

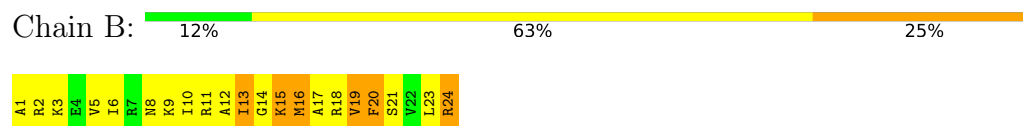


4.2.8 Score per residue for model 8

- Molecule 1: Calmodulin

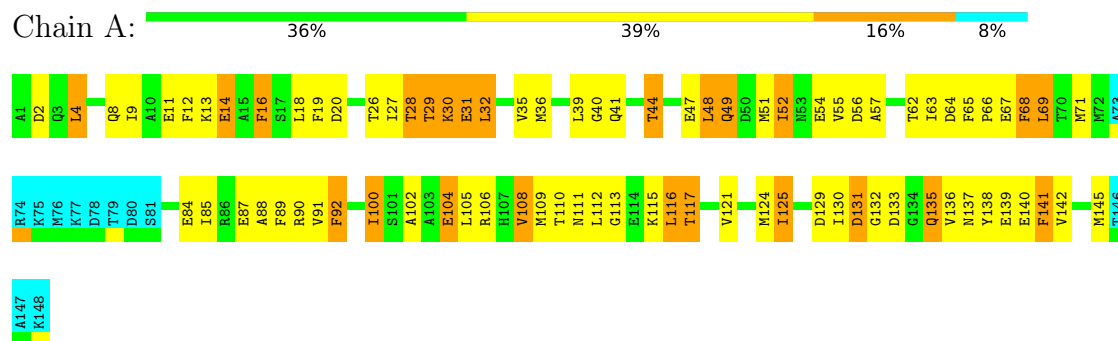


- Molecule 2: Serine/threonine-protein phosphatase 2B catalytic subunit alpha isoform

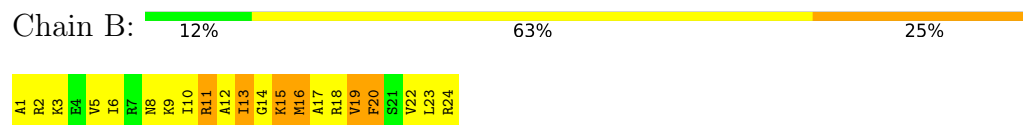


4.2.9 Score per residue for model 9

- Molecule 1: Calmodulin

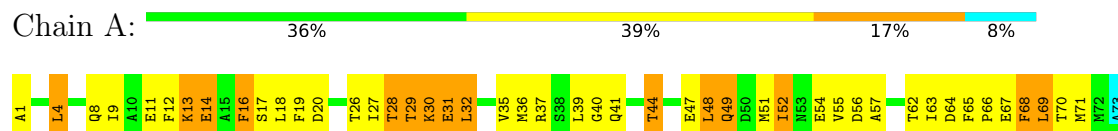


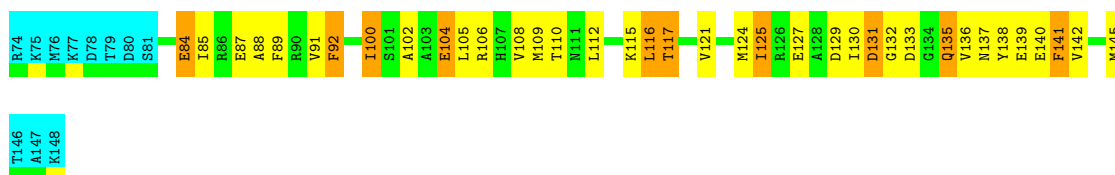
- Molecule 2: Serine/threonine-protein phosphatase 2B catalytic subunit alpha isoform



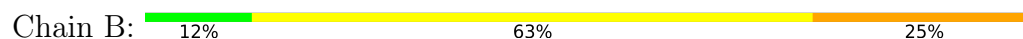
4.2.10 Score per residue for model 10

- Molecule 1: Calmodulin





- Molecule 2: Serine/threonine-protein phosphatase 2B catalytic subunit alpha isoform



4.2.11 Score per residue for model 11

- Molecule 1: Calmodulin

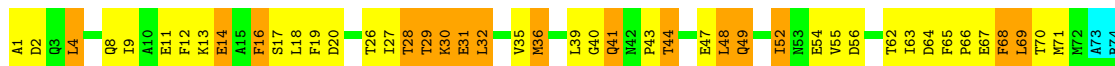
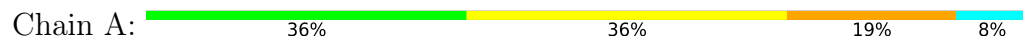


- Molecule 2: Serine/threonine-protein phosphatase 2B catalytic subunit alpha isoform

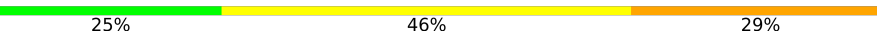


4.2.12 Score per residue for model 12

- Molecule 1: Calmodulin



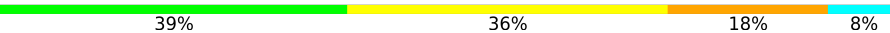
- Molecule 2: Serine/threonine-protein phosphatase 2B catalytic subunit alpha isoform

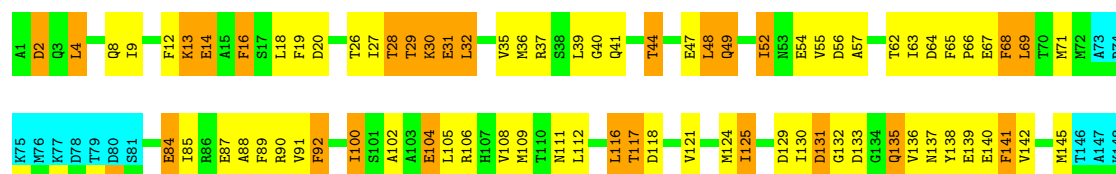
Chain B: 



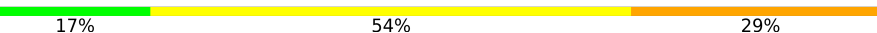
4.2.13 Score per residue for model 13

- Molecule 1: Calmodulin

Chain A: 



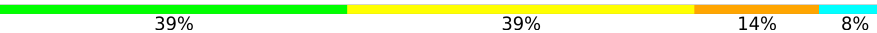
- Molecule 2: Serine/threonine-protein phosphatase 2B catalytic subunit alpha isoform

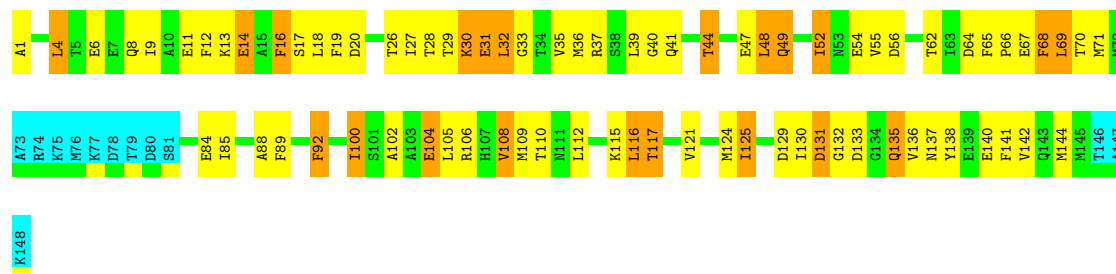
Chain B: 



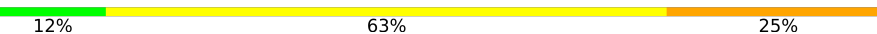
4.2.14 Score per residue for model 14

- Molecule 1: Calmodulin

Chain A: 



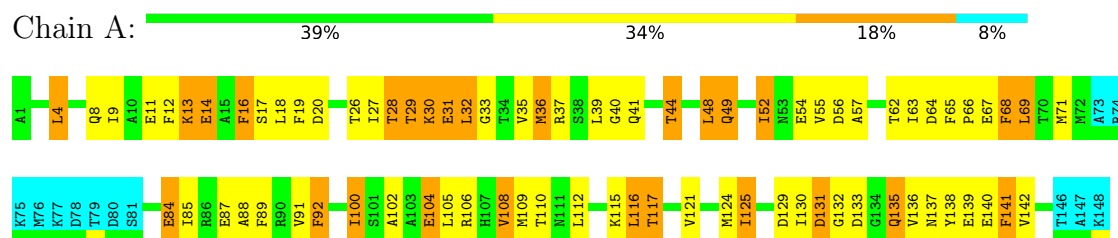
- Molecule 2: Serine/threonine-protein phosphatase 2B catalytic subunit alpha isoform

Chain B: 

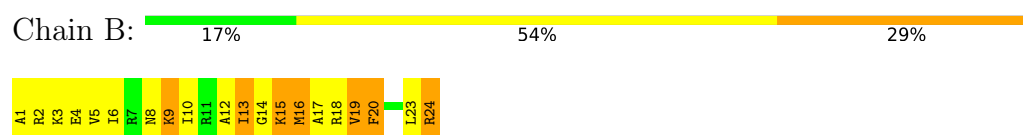


4.2.15 Score per residue for model 15

- Molecule 1: Calmodulin

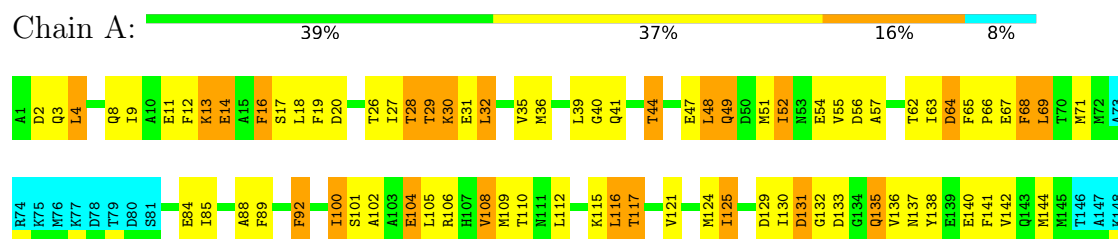


- Molecule 2: Serine/threonine-protein phosphatase 2B catalytic subunit alpha isoform

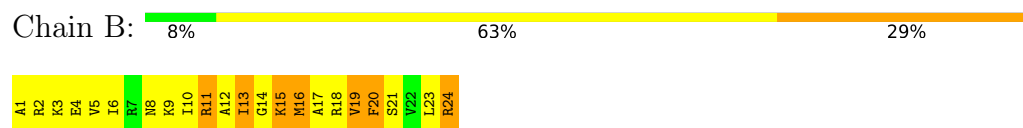


4.2.16 Score per residue for model 16

- Molecule 1: Calmodulin

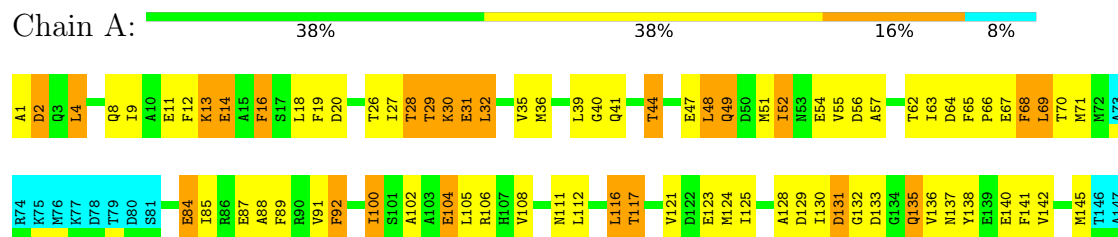


- Molecule 2: Serine/threonine-protein phosphatase 2B catalytic subunit alpha isoform



4.2.17 Score per residue for model 17

- Molecule 1: Calmodulin



K148

- Molecule 2: Serine/threonine-protein phosphatase 2B catalytic subunit alpha isoform

Chain B: 17% 67% 17%

A1 R2 K3 E4 V5 I6 K9 I10 R11 A12 I13 G14 K15 M16 A17 R18 V19 F20 S21 V22 L23 R24

4.2.18 Score per residue for model 18

- Molecule 1: Calmodulin

Chain A: 39% 38% 16% 8%

A1 L4 Q8 I9 A10 E11 F12 K13 A14 A15 F16 S17 L18 F19 D20 T26 L27 T28 T29 K30 E31 L32 V35 M36 L39 Q40 Q41 T44 L48 Q49 D50 M51 I52 N53 E54 V55 D56 A57 T62 I63 D64 F65 P66 E67 F68 L69 T70 M71 M72 A73 R74 K75

M76 K77 D78 T79 S81 E84 I85 R86 E87 A88 F89 R90 F91 I100 S101 A102 A103 E104 R105 H106 V108 M109 L112 L116 T117 V121 D122 E123 M124 I125 A128 D129 I130 D131 G132 D133 G134 Q135 V136 N137 Y138 E139 F140 F141 V142 T146 A147 K148

- Molecule 2: Serine/threonine-protein phosphatase 2B catalytic subunit alpha isoform

Chain B: 17% 58% 25%

A1 R2 K3 E4 V5 I6 K9 I10 R11 A12 I13 G14 K15 M16 A17 R18 V19 F20 S21 V22 L23 R24

4.2.19 Score per residue for model 19

- Molecule 1: Calmodulin

Chain A: 39% 36% 17% 8%

A1 D2 L4 Q8 I9 A10 E11 F12 K13 A14 A15 F16 S17 L18 F19 D20 T26 L27 T28 T29 K30 E31 L32 G33 V35 M36 L39 Q40 Q41 T44 E47 L48 Q49 I52 N53 E54 V55 D56 A57 T62 I63 D64 F65 P66 E67 F68 L69 T70 M71 M72 A73

R74 K75 M76 K77 T79 D80 S81 E84 I85 R86 E87 A88 F89 R90 F91 I100 S101 A102 A103 E104 R105 H106 V108 M109 T110 N111 L112 K115 L116 T117 V121 M124 I125 D129 I130 D131 G132 D133 G134 Q135 V136 N137 Y138 E139 F141 V142 Q143 M144 M145 T146

A147 K148

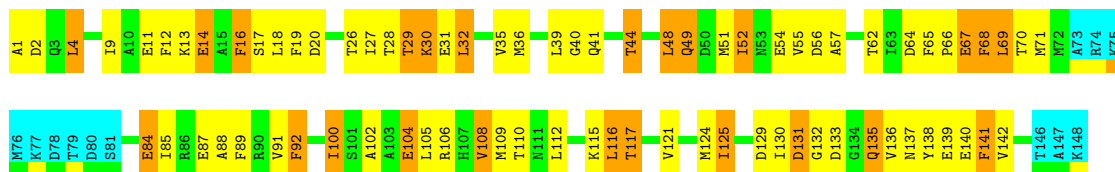
- Molecule 2: Serine/threonine-protein phosphatase 2B catalytic subunit alpha isoform

Chain B: 12% 58% 29%



4.2.20 Score per residue for model 20

• Molecule 1: Calmodulin



• Molecule 2: Serine/threonine-protein phosphatase 2B catalytic subunit alpha isoform



5 Refinement protocol and experimental data overview

The models were refined using the following method: *distance geometry*.

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *back calculated data agree with experimental NOESY spectrum*.

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

Software name	Classification	Version
CNS	refinement	1.2

No chemical shift data was provided.

6 Model quality ⓘ

6.1 Standard geometry ⓘ

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.

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	1073	999	998	101±3
2	B	197	230	230	43±4
All	All	25480	24580	24560	2555

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 51.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:116:LEU:HD12	1:A:121:VAL:HG22	1.06	1.13	3	20
1:A:55:VAL:HG11	2:B:6:ILE:HG21	0.97	1.32	12	20
1:A:100:ILE:HD13	1:A:105:LEU:HD13	0.93	1.37	8	15
1:A:116:LEU:HD12	1:A:121:VAL:CG2	0.86	2.01	17	20
2:B:1:ALA:O	2:B:5:VAL:HG23	0.85	1.72	5	20
2:B:23:LEU:HD12	2:B:24:ARG:N	0.85	1.86	13	18
1:A:117:THR:O	1:A:121:VAL:HG23	0.82	1.75	1	20
1:A:100:ILE:CD1	1:A:105:LEU:HD12	0.81	2.05	17	4
2:B:15:LYS:O	2:B:19:VAL:HG13	0.81	1.75	9	20
1:A:31:GLU:O	1:A:35:VAL:HG23	0.81	1.75	11	20
1:A:100:ILE:HD12	1:A:105:LEU:HD12	0.81	1.52	17	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:71:MET:HG2	2:B:10:ILE:HD13	0.80	1.51	20	20
1:A:18:LEU:HD11	1:A:112:LEU:O	0.80	1.77	15	20
1:A:19:PHE:CE2	1:A:35:VAL:HG21	0.79	2.12	19	20
1:A:55:VAL:HG11	2:B:6:ILE:CG2	0.79	2.06	12	20
1:A:141:PHE:CE1	2:B:23:LEU:HD23	0.78	2.14	10	11
1:A:13:LYS:HA	1:A:16:PHE:CD2	0.76	2.15	2	20
2:B:9:LYS:O	2:B:13:ILE:HD12	0.76	1.79	5	18
1:A:104:GLU:O	1:A:108:VAL:HG23	0.73	1.83	17	20
1:A:108:VAL:O	1:A:112:LEU:HD12	0.73	1.82	11	7
1:A:116:LEU:CD1	1:A:121:VAL:HG22	0.73	2.08	12	20
1:A:100:ILE:CD1	1:A:105:LEU:HD13	0.72	2.13	11	14
1:A:105:LEU:HD11	1:A:124:MET:HG3	0.72	1.59	13	3
1:A:18:LEU:HD21	1:A:112:LEU:HB3	0.71	1.62	10	17
1:A:32:LEU:HD11	1:A:63:ILE:CD1	0.71	2.15	2	5
1:A:57:ALA:HB3	1:A:64:ASP:OD2	0.70	1.86	16	16
2:B:6:ILE:O	2:B:10:ILE:HD12	0.70	1.87	15	19
2:B:5:VAL:HG12	2:B:9:LYS:HD3	0.69	1.63	12	4
1:A:100:ILE:HD12	1:A:105:LEU:HD22	0.69	1.65	8	13
1:A:105:LEU:HD21	1:A:124:MET:HG3	0.69	1.63	12	15
1:A:1:ALA:HB2	1:A:70:THR:OG1	0.69	1.88	20	10
2:B:15:LYS:CE	2:B:15:LYS:N	0.69	2.56	17	20
1:A:106:ARG:HA	1:A:116:LEU:HD11	0.68	1.64	17	20
1:A:29:THR:HG21	1:A:49:GLN:CG	0.68	2.18	20	20
1:A:124:MET:HE1	2:B:23:LEU:O	0.68	1.88	9	7
1:A:32:LEU:HD23	2:B:9:LYS:HD2	0.67	1.67	14	14
1:A:105:LEU:HD21	1:A:124:MET:CG	0.66	2.20	12	3
1:A:71:MET:HB3	2:B:10:ILE:HG21	0.66	1.68	11	18
1:A:19:PHE:HB3	1:A:27:ILE:HD11	0.65	1.69	20	20
1:A:88:ALA:CB	2:B:19:VAL:HG21	0.65	2.22	17	20
2:B:16:MET:O	2:B:19:VAL:HG22	0.65	1.92	13	20
2:B:16:MET:O	2:B:20:PHE:HB2	0.65	1.92	10	17
1:A:29:THR:HB	1:A:48:LEU:HD12	0.64	1.69	1	18
2:B:20:PHE:CD1	2:B:23:LEU:HD21	0.64	2.27	3	20
1:A:18:LEU:HD11	1:A:112:LEU:C	0.64	2.18	17	17
1:A:138:TYR:O	1:A:142:VAL:HG23	0.64	1.91	19	20
1:A:94:LYS:NZ	1:A:108:VAL:HG22	0.63	2.08	6	1
1:A:111:ASN:C	1:A:112:LEU:HD12	0.63	2.19	2	7
1:A:32:LEU:HD11	1:A:63:ILE:HD12	0.63	1.70	10	11
2:B:2:ARG:O	2:B:6:ILE:HG13	0.62	1.94	10	20
1:A:29:THR:HG21	1:A:49:GLN:HG3	0.62	1.72	20	18
1:A:100:ILE:CD1	1:A:105:LEU:HD22	0.62	2.24	19	11

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:6:ILE:HG22	2:B:10:ILE:HD11	0.62	1.71	15	18
2:B:20:PHE:O	2:B:24:ARG:HG2	0.62	1.94	6	9
1:A:44:THR:O	1:A:48:LEU:CD2	0.62	2.48	15	20
2:B:2:ARG:NH1	2:B:5:VAL:HG11	0.62	2.09	19	4
1:A:84:GLU:O	2:B:19:VAL:HG11	0.60	1.96	2	12
1:A:87:GLU:OE2	2:B:12:ALA:HB1	0.60	1.96	8	2
1:A:9:ILE:HG22	1:A:69:LEU:CD2	0.60	2.27	4	20
1:A:87:GLU:O	1:A:91:VAL:HG23	0.60	1.96	3	17
1:A:138:TYR:CE1	1:A:142:VAL:CG2	0.60	2.85	20	20
1:A:27:ILE:HG23	1:A:31:GLU:HB3	0.59	1.74	3	20
1:A:71:MET:CG	2:B:10:ILE:HD13	0.59	2.25	20	20
1:A:88:ALA:HB2	2:B:19:VAL:HG21	0.59	1.74	10	9
1:A:27:ILE:HD12	1:A:68:PHE:CE2	0.59	2.33	17	20
1:A:4:LEU:CD1	1:A:12:PHE:CZ	0.58	2.85	11	20
1:A:84:GLU:HB3	2:B:15:LYS:HB3	0.58	1.73	3	11
1:A:129:ASP:HB2	1:A:136:VAL:HG22	0.58	1.76	7	20
1:A:68:PHE:CE1	2:B:10:ILE:HG23	0.58	2.34	11	19
1:A:9:ILE:HG22	1:A:69:LEU:HD21	0.57	1.76	20	20
2:B:3:LYS:HA	2:B:6:ILE:HD12	0.57	1.76	19	20
1:A:32:LEU:HD23	2:B:9:LYS:CD	0.57	2.30	20	1
1:A:4:LEU:HD12	1:A:69:LEU:CD2	0.56	2.30	11	20
1:A:110:THR:HG23	1:A:115:LYS:HA	0.56	1.76	10	17
1:A:138:TYR:C	1:A:138:TYR:CD1	0.56	2.83	11	20
2:B:13:ILE:O	2:B:17:ALA:HB2	0.56	2.01	12	20
2:B:15:LYS:N	2:B:15:LYS:HE3	0.56	2.16	17	20
2:B:18:ARG:HE	2:B:19:VAL:HG12	0.56	1.61	9	11
1:A:28:THR:HG23	1:A:30:LYS:HG3	0.56	1.78	3	9
1:A:105:LEU:C	1:A:105:LEU:HD23	0.56	2.25	13	4
1:A:48:LEU:O	1:A:52:ILE:CG1	0.56	2.54	1	20
1:A:27:ILE:HD12	1:A:68:PHE:HE2	0.55	1.61	16	20
1:A:30:LYS:CD	1:A:31:GLU:N	0.55	2.70	17	20
1:A:1:ALA:HB2	1:A:70:THR:HA	0.55	1.79	5	1
1:A:18:LEU:C	1:A:18:LEU:HD23	0.54	2.27	10	20
1:A:68:PHE:CD1	2:B:10:ILE:HG23	0.54	2.38	10	17
1:A:108:VAL:HG12	2:B:20:PHE:CE2	0.54	2.38	18	9
1:A:145:MET:O	1:A:145:MET:HE2	0.54	2.01	12	1
1:A:36:MET:HE3	1:A:39:LEU:HD22	0.54	1.80	15	4
2:B:2:ARG:HH12	2:B:5:VAL:HG11	0.54	1.62	19	2
2:B:5:VAL:HG12	2:B:9:LYS:CD	0.54	2.32	19	4
1:A:39:LEU:C	1:A:39:LEU:HD23	0.53	2.28	4	20
1:A:18:LEU:HD21	1:A:112:LEU:CB	0.53	2.32	4	11

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:85:ILE:HG22	1:A:138:TYR:HE1	0.53	1.64	19	20
1:A:36:MET:HB2	2:B:9:LYS:HD2	0.53	1.81	7	4
1:A:89:PHE:CD2	1:A:138:TYR:HB2	0.53	2.39	17	20
1:A:71:MET:CG	2:B:10:ILE:HG21	0.52	2.34	20	2
2:B:15:LYS:O	2:B:18:ARG:HG3	0.52	2.05	7	11
1:A:130:ILE:HG13	1:A:131:ASP:OD1	0.51	2.05	6	20
1:A:14:GLU:O	1:A:18:LEU:CB	0.51	2.59	16	20
1:A:29:THR:CB	1:A:48:LEU:HD12	0.51	2.35	15	6
1:A:20:ASP:CG	1:A:26:THR:O	0.51	2.54	14	20
2:B:18:ARG:HD2	2:B:18:ARG:C	0.51	2.31	7	20
2:B:9:LYS:C	2:B:13:ILE:HD12	0.51	2.31	14	14
1:A:9:ILE:HA	1:A:12:PHE:CD1	0.50	2.42	3	20
1:A:52:ILE:O	1:A:55:VAL:HG22	0.50	2.06	14	20
1:A:16:PHE:CD1	1:A:68:PHE:CD2	0.50	3.00	20	20
2:B:13:ILE:O	2:B:17:ALA:CB	0.50	2.59	1	20
1:A:109:MET:CE	2:B:20:PHE:CD2	0.50	2.95	19	18
2:B:12:ALA:O	2:B:16:MET:HG2	0.50	2.07	3	20
1:A:138:TYR:CE1	1:A:142:VAL:HG21	0.50	2.40	19	6
1:A:131:ASP:O	1:A:132:GLY:C	0.49	2.55	14	20
1:A:12:PHE:CD2	1:A:69:LEU:CD2	0.49	2.95	20	20
1:A:102:ALA:HB1	1:A:121:VAL:CG1	0.49	2.36	19	20
2:B:23:LEU:HD12	2:B:23:LEU:C	0.49	2.32	3	14
1:A:16:PHE:CD1	1:A:16:PHE:N	0.49	2.80	7	20
1:A:131:ASP:OD1	1:A:131:ASP:N	0.49	2.45	8	20
1:A:36:MET:CE	1:A:39:LEU:HD22	0.49	2.38	19	2
1:A:129:ASP:CG	1:A:135:GLN:O	0.49	2.56	10	20
1:A:84:GLU:O	1:A:88:ALA:HB2	0.49	2.07	18	7
1:A:71:MET:CB	2:B:10:ILE:HG21	0.49	2.37	20	6
1:A:28:THR:HA	1:A:62:THR:HG22	0.49	1.85	20	5
1:A:32:LEU:HD23	2:B:9:LYS:HD3	0.49	1.82	20	1
1:A:4:LEU:N	1:A:4:LEU:HD23	0.48	2.23	5	20
1:A:124:MET:HE1	2:B:23:LEU:C	0.48	2.33	9	3
1:A:9:ILE:O	1:A:12:PHE:N	0.48	2.46	14	20
2:B:6:ILE:O	2:B:9:LYS:HG2	0.48	2.09	20	1
1:A:32:LEU:HD13	1:A:52:ILE:CD1	0.48	2.39	7	2
1:A:13:LYS:HA	1:A:16:PHE:CE2	0.47	2.44	13	20
1:A:85:ILE:CG2	1:A:142:VAL:HG22	0.47	2.39	20	5
1:A:92:PHE:CD1	2:B:20:PHE:CE1	0.47	3.03	17	18
1:A:137:ASN:ND2	1:A:138:TYR:H	0.47	2.06	14	20
1:A:112:LEU:HD12	1:A:112:LEU:N	0.47	2.24	2	3
1:A:56:ASP:CG	1:A:62:THR:O	0.47	2.58	19	20

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:55:VAL:CG1	2:B:6:ILE:HG21	0.47	2.25	15	1
1:A:85:ILE:HD13	1:A:145:MET:HE1	0.47	1.87	11	1
2:B:18:ARG:NE	2:B:19:VAL:HG12	0.47	2.25	11	13
1:A:144:MET:CA	1:A:144:MET:HE2	0.47	2.40	19	4
1:A:4:LEU:HB2	1:A:9:ILE:HG23	0.46	1.87	2	20
1:A:12:PHE:O	1:A:16:PHE:CD1	0.46	2.69	13	20
1:A:12:PHE:CE2	1:A:69:LEU:HD23	0.46	2.46	20	10
1:A:55:VAL:HA	1:A:71:MET:HE1	0.46	1.86	6	12
1:A:85:ILE:HG12	1:A:145:MET:HE1	0.46	1.88	13	5
1:A:108:VAL:HG12	2:B:20:PHE:HE2	0.46	1.71	8	11
1:A:65:PHE:N	1:A:66:PRO:HD2	0.46	2.26	20	20
1:A:131:ASP:C	1:A:133:ASP:N	0.46	2.74	6	20
2:B:11:ARG:O	2:B:15:LYS:HG2	0.46	2.11	16	14
1:A:29:THR:HG21	1:A:49:GLN:CB	0.46	2.41	19	5
1:A:27:ILE:HG23	1:A:31:GLU:CB	0.45	2.40	16	19
1:A:84:GLU:CB	2:B:15:LYS:HB3	0.45	2.41	18	11
1:A:19:PHE:CZ	2:B:13:ILE:CG1	0.45	3.00	5	2
2:B:20:PHE:O	2:B:24:ARG:CG	0.45	2.64	6	6
1:A:102:ALA:N	1:A:125:ILE:HD11	0.45	2.27	19	18
1:A:141:PHE:CD1	1:A:141:PHE:C	0.45	2.94	14	13
2:B:19:VAL:O	2:B:22:VAL:HG22	0.45	2.12	10	5
1:A:13:LYS:CB	1:A:65:PHE:CE2	0.45	3.00	11	12
2:B:19:VAL:C	2:B:22:VAL:HG22	0.45	2.37	5	5
1:A:12:PHE:HB3	1:A:16:PHE:CZ	0.45	2.47	9	20
2:B:3:LYS:HA	2:B:6:ILE:CD1	0.45	2.43	1	20
1:A:19:PHE:HE2	1:A:35:VAL:HG21	0.44	1.68	15	5
1:A:13:LYS:HA	1:A:16:PHE:CG	0.44	2.48	11	20
1:A:72:MET:HG2	2:B:10:ILE:HG22	0.44	1.88	11	1
1:A:28:THR:OG1	1:A:29:THR:N	0.44	2.50	15	17
2:B:19:VAL:O	2:B:22:VAL:CG2	0.44	2.65	10	6
1:A:19:PHE:CZ	2:B:13:ILE:HG12	0.44	2.47	20	15
1:A:105:LEU:HD13	1:A:125:ILE:HG12	0.44	1.88	13	1
1:A:104:GLU:CD	1:A:104:GLU:N	0.44	2.76	8	20
1:A:84:GLU:C	2:B:19:VAL:HG11	0.44	2.38	10	1
2:B:6:ILE:C	2:B:10:ILE:HD12	0.44	2.38	15	3
2:B:16:MET:HE3	2:B:16:MET:HB2	0.43	1.71	5	4
1:A:84:GLU:O	1:A:88:ALA:CB	0.43	2.66	18	7
1:A:137:ASN:ND2	1:A:138:TYR:N	0.43	2.66	5	20
1:A:14:GLU:O	1:A:18:LEU:HB3	0.43	2.13	16	15
2:B:20:PHE:O	2:B:23:LEU:HG	0.43	2.13	5	6
2:B:21:SER:HA	2:B:24:ARG:HG2	0.43	1.90	18	10

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:55:VAL:HB	1:A:71:MET:HE3	0.43	1.90	5	4
1:A:51:MET:HE3	2:B:2:ARG:HB2	0.43	1.91	6	1
1:A:28:THR:CG2	1:A:30:LYS:HG3	0.43	2.43	3	5
1:A:85:ILE:CD1	1:A:145:MET:HE1	0.43	2.43	11	1
2:B:5:VAL:O	2:B:9:LYS:HD3	0.43	2.13	19	3
2:B:21:SER:HA	2:B:24:ARG:CG	0.43	2.44	10	2
1:A:19:PHE:HB3	1:A:27:ILE:CD1	0.43	2.43	14	4
1:A:124:MET:HE3	1:A:127:GLU:CG	0.43	2.44	10	1
1:A:67:GLU:OE1	1:A:71:MET:HE2	0.42	2.14	20	1
1:A:64:ASP:O	1:A:68:PHE:HB2	0.42	2.15	20	1
1:A:92:PHE:CE2	1:A:100:ILE:CD1	0.42	3.03	1	3
2:B:14:GLY:C	2:B:15:LYS:HE2	0.42	2.39	18	20
1:A:19:PHE:CD1	1:A:112:LEU:CD2	0.42	3.01	18	4
1:A:12:PHE:CD2	1:A:69:LEU:HD23	0.42	2.50	20	8
1:A:48:LEU:O	1:A:52:ILE:HG13	0.42	2.15	5	4
1:A:4:LEU:HD13	1:A:12:PHE:CZ	0.42	2.50	13	17
1:A:94:LYS:HZ2	1:A:108:VAL:HG22	0.42	1.72	6	1
1:A:105:LEU:HD11	1:A:124:MET:CG	0.42	2.38	13	1
1:A:12:PHE:HB3	1:A:16:PHE:CE1	0.42	2.49	14	20
1:A:44:THR:O	1:A:48:LEU:HD23	0.42	2.15	13	4
2:B:11:ARG:O	2:B:15:LYS:HE3	0.42	2.15	9	2
1:A:105:LEU:HD21	1:A:124:MET:HG2	0.42	1.91	5	1
1:A:124:MET:CE	1:A:128:ALA:HB2	0.42	2.45	18	3
1:A:13:LYS:HB2	1:A:65:PHE:CE2	0.42	2.49	14	4
1:A:44:THR:O	1:A:48:LEU:HG	0.42	2.14	7	1
1:A:11:GLU:O	1:A:14:GLU:CG	0.42	2.68	20	18
1:A:1:ALA:HB2	1:A:70:THR:CB	0.41	2.45	8	3
1:A:30:LYS:O	1:A:34:THR:CB	0.41	2.68	7	2
1:A:102:ALA:HB1	1:A:121:VAL:HG11	0.41	1.93	6	5
2:B:16:MET:HG3	2:B:17:ALA:N	0.41	2.31	6	12
1:A:12:PHE:C	1:A:16:PHE:CE1	0.41	2.99	13	7
1:A:141:PHE:CD1	1:A:141:PHE:O	0.41	2.74	12	3
2:B:15:LYS:CE	2:B:15:LYS:CA	0.41	2.98	17	1
1:A:12:PHE:O	1:A:15:ALA:N	0.41	2.52	7	3
1:A:131:ASP:HB2	1:A:133:ASP:CG	0.40	2.42	6	1
1:A:105:LEU:HD22	1:A:121:VAL:HG13	0.40	1.91	13	1
1:A:84:GLU:OE1	1:A:85:ILE:CG1	0.40	2.70	19	1
2:B:18:ARG:O	2:B:22:VAL:HG13	0.40	2.17	5	1
1:A:33:GLY:O	1:A:37:ARG:CB	0.40	2.69	15	2
1:A:30:LYS:HD3	1:A:30:LYS:C	0.40	2.41	16	1
1:A:89:PHE:HB2	1:A:141:PHE:CE2	0.40	2.52	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:109:MET:O	1:A:113:GLY:N	0.40	2.55	9	1
1:A:41:GLN:HB3	1:A:43:PRO:HD3	0.40	1.93	12	1
1:A:39:LEU:HD23	1:A:40:GLY:N	0.40	2.32	18	1
1:A:19:PHE:CE1	1:A:112:LEU:HD21	0.40	2.52	20	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	135/148 (91%)	127±1 (94±1%)	6±1 (5±1%)	1±1 (1±0%)	16	66
2	B	22/24 (92%)	22±0 (100±1%)	0±0 (0±1%)	0±0 (0±0%)	100	100
All	All	3140/3440 (91%)	2985 (95%)	130 (4%)	25 (1%)	18	68

All 2 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	19
1	A	2	ASP	6

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	116/126 (92%)	82±2 (70±2%)	34±2 (30±2%)	1	17
2	B	20/20 (100%)	13±1 (65±6%)	7±1 (35±6%)	1	9
All	All	2720/2920 (93%)	1890 (69%)	830 (31%)	1	16

All 62 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	4	LEU	20
1	A	14	GLU	20
1	A	16	PHE	20
1	A	30	LYS	20
1	A	32	LEU	20
1	A	41	GLN	20
1	A	44	THR	20
1	A	48	LEU	20
1	A	49	GLN	20
1	A	52	ILE	20
1	A	54	GLU	20
1	A	67	GLU	20
1	A	68	PHE	20
1	A	69	LEU	20
1	A	92	PHE	20
1	A	100	ILE	20
1	A	116	LEU	20
1	A	117	THR	20
1	A	125	ILE	20
1	A	131	ASP	20
1	A	135	GLN	20
1	A	140	GLU	20
2	B	13	ILE	20
2	B	15	LYS	20
2	B	16	MET	20
1	A	104	GLU	19
2	B	19	VAL	19
2	B	20	PHE	19
1	A	8	GLN	18
1	A	29	THR	18
1	A	31	GLU	18
1	A	28	THR	17
1	A	36	MET	17
1	A	47	GLU	16
2	B	24	ARG	15
1	A	139	GLU	14
1	A	141	PHE	14
1	A	51	MET	13
1	A	84	GLU	13
2	B	8	ASN	13
1	A	13	LYS	11

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Mol	Chain	Res	Type	Models (Total)
1	A	17	SER	10
1	A	108	VAL	10
2	B	11	ARG	7
1	A	2	ASP	5
1	A	37	ARG	5
1	A	64	ASP	5
2	B	9	LYS	5
1	A	145	MET	4
1	A	90	ARG	3
1	A	101	SER	3
1	A	94	LYS	3
2	B	4	GLU	3
1	A	6	GLU	2
1	A	82	GLU	2
1	A	114	GLU	2
1	A	123	GLU	2
1	A	83	GLU	1
1	A	112	LEU	1
1	A	118	ASP	1
1	A	3	GLN	1
1	A	107	HIS	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](#)

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