Full wwPDB NMR Structure Validation Report (i)

Feb 22, 2022 – 09:48 AM EST

PDB ID	:	1WI1
Title	:	Solution structure of the PH domain of human calcium-dependent activator protein for secretion (CAPS)
Authors	:	Yoneyama, M.; Izumi, K.; Yoshida, M.; Tochio, N.; Koshiba, S.; Inoue, M.; Kigawa, T.; Yokoyama, S.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on	:	2004-05-28

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 (i) symbol.

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

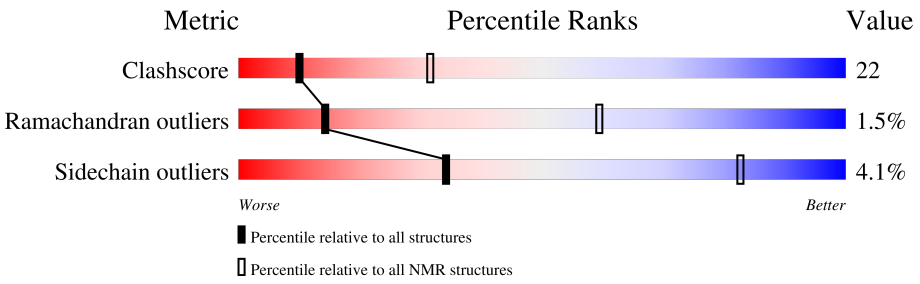
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.26
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.26

1 Overall quality at a glance (i)

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	126	51% 30% 19%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 4 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:9-A:44, A:52-A:117 (102)	0.21	4

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 3 single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1956 atoms, of which 960 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called calcium-dependent activator protein for secretion, CAPS.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	126	1956	633	960	172	187	4	0

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	cloning artifact	UNP Q8NFR0
A	2	SER	-	cloning artifact	UNP Q8NFR0
A	3	SER	-	cloning artifact	UNP Q8NFR0
A	4	GLY	-	cloning artifact	UNP Q8NFR0
A	5	SER	-	cloning artifact	UNP Q8NFR0
A	6	SER	-	cloning artifact	UNP Q8NFR0
A	7	GLY	-	cloning artifact	UNP Q8NFR0
A	121	SER	-	cloning artifact	UNP Q8NFR0
A	122	GLY	-	cloning artifact	UNP Q8NFR0
A	123	PRO	-	cloning artifact	UNP Q8NFR0
A	124	SER	-	cloning artifact	UNP Q8NFR0
A	125	SER	-	cloning artifact	UNP Q8NFR0
A	126	GLY	-	cloning artifact	UNP Q8NFR0

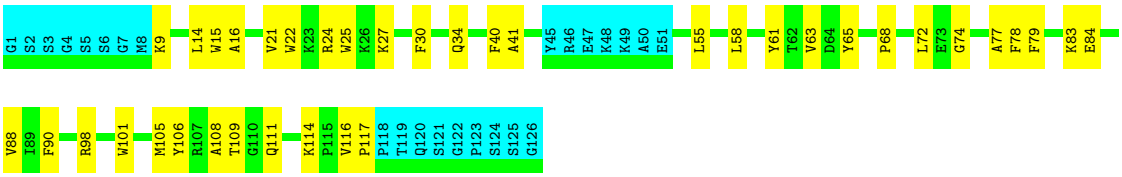
4 Residue-property plots (i)

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: calcium-dependent activator protein for secretion, CAPS

Chain A: 51% 30% 19%



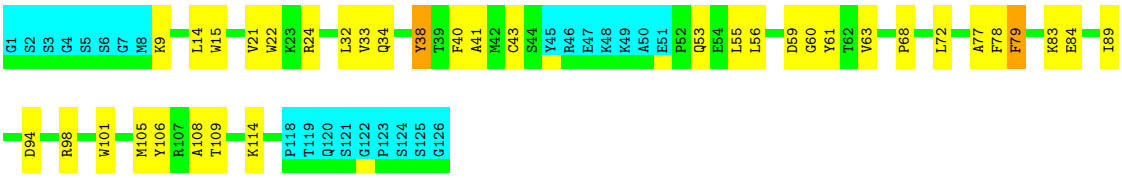
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: calcium-dependent activator protein for secretion, CAPS

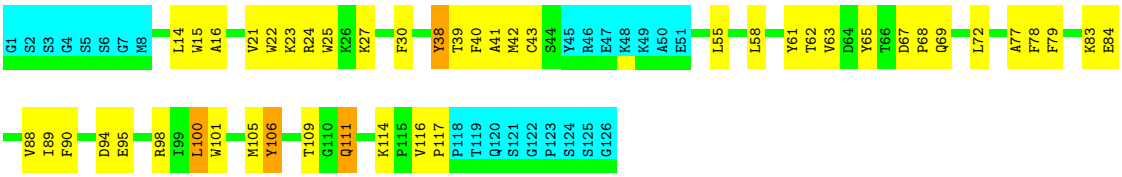
Chain A: 52% 27% • 19%



4.2.2 Score per residue for model 2

• Molecule 1: calcium-dependent activator protein for secretion, CAPS

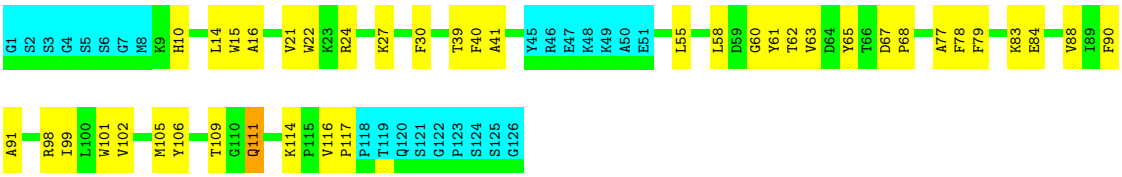
Chain A: 44% 33% • 19%



4.2.3 Score per residue for model 3

- Molecule 1: calcium-dependent activator protein for secretion, CAPS

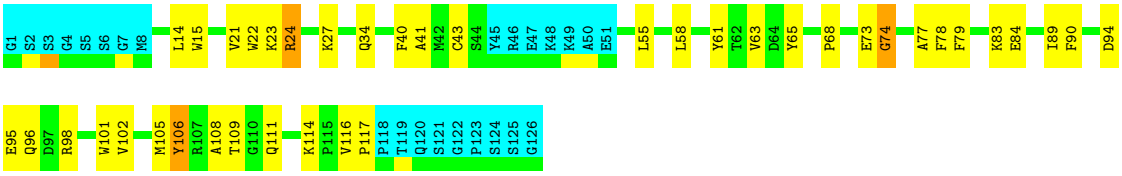
Chain A:



4.2.4 Score per residue for model 4 (medoid)

- Molecule 1: calcium-dependent activator protein for secretion, CAPS

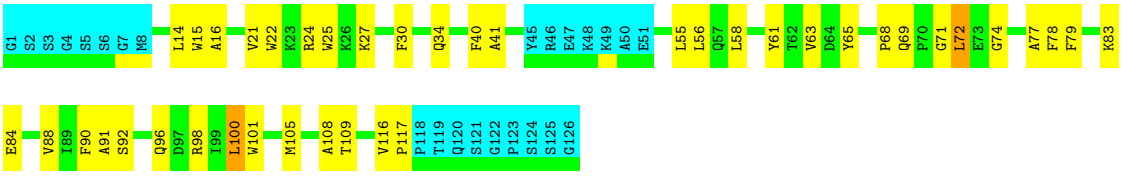
Chain A:



4.2.5 Score per residue for model 5

- Molecule 1: calcium-dependent activator protein for secretion, CAPS

Chain A:



4.2.6 Score per residue for model 6

- Molecule 1: calcium-dependent activator protein for secretion, CAPS

Chain A: 49% 32% 19%

G1 S2 S3 G4 S5 S6 G7 M8 K9 L14 W15 A16 V21 W22 W25 K26 K27 F30 V31 L32 F40 A41 Y45 R46 E47 K48 K49 A50 E51 L55 L56 Q57 L58 Y61 T62 V63 D64 P68 L72 A77 F78 F79 K83 E84 V88 I89 F90

A91 S92 E95 R98 I99 L100 W101 V102 M105 Y106 R107 A108 T109 G110 Q111 V116 P117 P118 T119 Q120 S121 G122 P123 S124 S125 G126

4.2.7 Score per residue for model 7

- Molecule 1: calcium-dependent activator protein for secretion, CAPS

Chain A: 42% 36% • 19%

G1 S2 S3 G4 S5 S6 G7 M8 K9 H10 S11 L14 W15 A16 V21 W22 W25 K26 K27 V31 L32 F40 A41 Y45 R46 E47 K48 K49 A50 E51 P52 Q53 E54 L55 L56 Q57 L58 D59 G60 Y61 T62 V63 D64 Y65 T66 D67 P68 E73 G74 G75 R76 A77 F78

F79 K83 E84 F90 R98 I99 L100 W101 V102 M105 A108 T109 G110 Q111 S112 H113 K114 P115 V116 P117 P118 T119 Q120 S121 G122 P123 S124 S125 G126

4.2.8 Score per residue for model 8

- Molecule 1: calcium-dependent activator protein for secretion, CAPS

Chain A: 48% 30% • 19%

G1 S2 S3 G4 S5 S6 G7 M8 K9 L14 W15 V21 W22 K23 R24 W25 K26 K27 R28 F29 F30 Y31 L32 V33 Q34 F40 A41 Y45 R46 E47 K48 K49 A50 E51 E54 L55 L58 Y61 T62 V63 D64 Y65 T66 D67 P68 L72 F78 F79 K83 E84

V88 I89 F90 D94 D97 W101 M105 Y106 R107 A108 T109 K114 P115 V116 P117 P118 T119 Q120 S121 G122 P123 S124 S125 G126

4.2.9 Score per residue for model 9

- Molecule 1: calcium-dependent activator protein for secretion, CAPS

Chain A: 53% 25% • 19%

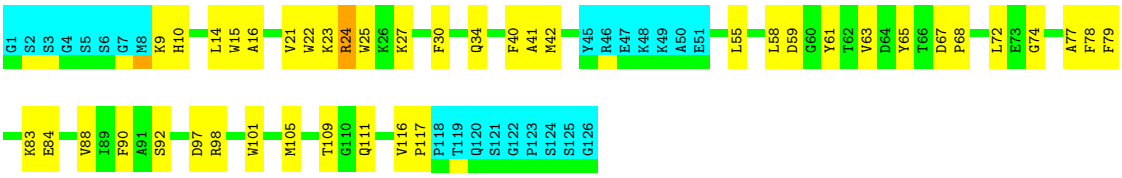
G1 S2 S3 G4 S5 S6 G7 M8 L14 W15 V21 W22 W25 K26 K27 R28 F29 F30 Q34 Y38 T39 F40 A41 Y45 R46 E47 K48 K49 A50 E51 P52 Q53 E54 L55 L56 Y61 T62 V63 D64 P68 L72 E73 G74 A77 F78 F79 K83 E84

R98 I99 L100 W101 V102 Q103 A108 H113 K114 P115 P118 T119 Q120 S121 G122 P123 S124 S125 G126

4.2.10 Score per residue for model 10

• Molecule 1: calcium-dependent activator protein for secretion, CAPS

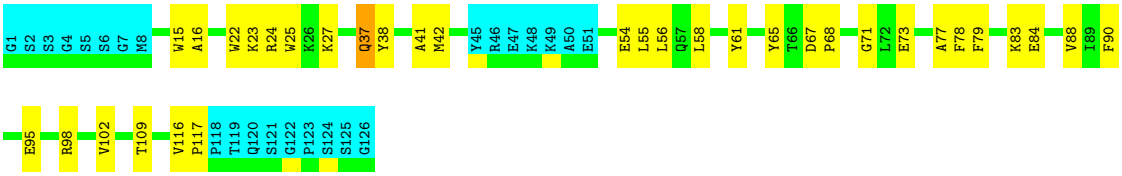
Chain A: 48% 33% • 19%



4.2.11 Score per residue for model 11

• Molecule 1: calcium-dependent activator protein for secretion, CAPS

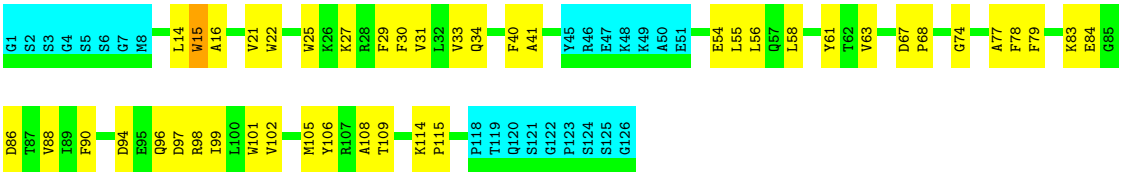
Chain A: 54% 26% • 19%



4.2.12 Score per residue for model 12

• Molecule 1: calcium-dependent activator protein for secretion, CAPS

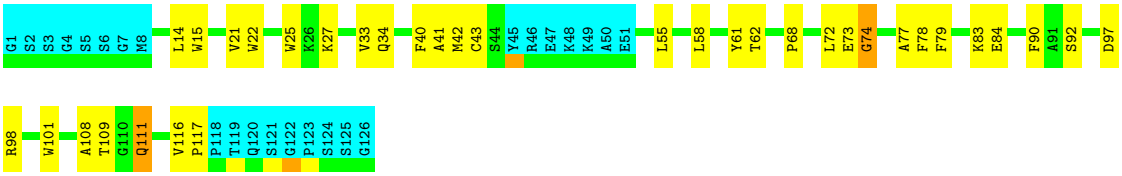
Chain A: 46% 34% • 19%



4.2.13 Score per residue for model 13

• Molecule 1: calcium-dependent activator protein for secretion, CAPS

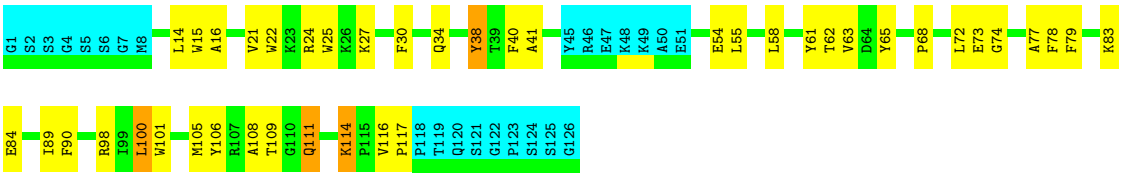
Chain A: 53% 26% • 19%



4.2.14 Score per residue for model 14

• Molecule 1: calcium-dependent activator protein for secretion, CAPS

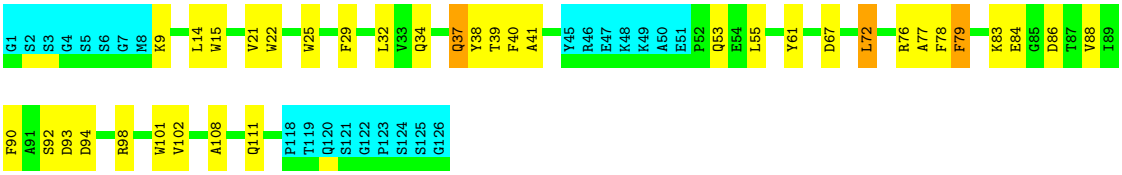
Chain A: 48% 30% • 19%



4.2.15 Score per residue for model 15

• Molecule 1: calcium-dependent activator protein for secretion, CAPS

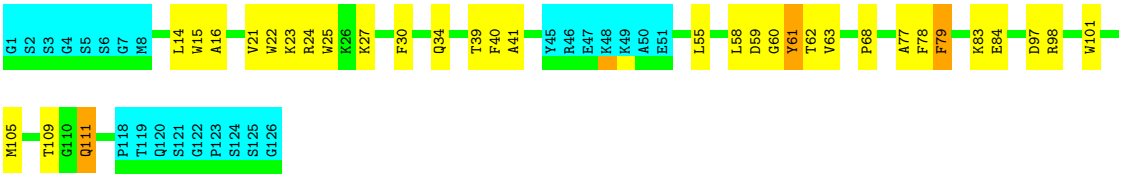
Chain A: 52% 26% • 19%



4.2.16 Score per residue for model 16

• Molecule 1: calcium-dependent activator protein for secretion, CAPS

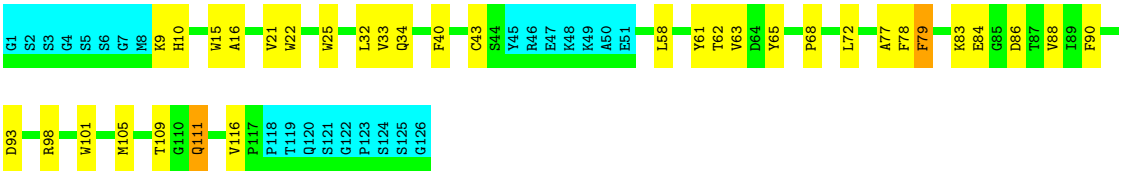
Chain A: 55% 24% • 19%



4.2.17 Score per residue for model 17

• Molecule 1: calcium-dependent activator protein for secretion, CAPS

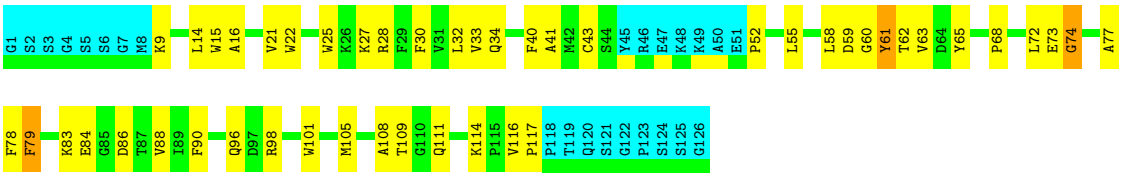
Chain A: 54% 25% • 19%



4.2.18 Score per residue for model 18

• Molecule 1: calcium-dependent activator protein for secretion, CAPS

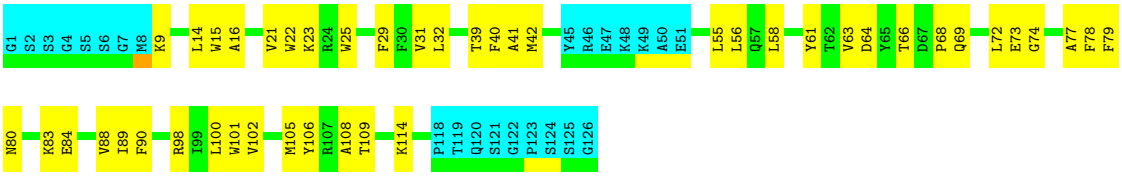
Chain A: 44% 35% • 19%



4.2.19 Score per residue for model 19

• Molecule 1: calcium-dependent activator protein for secretion, CAPS

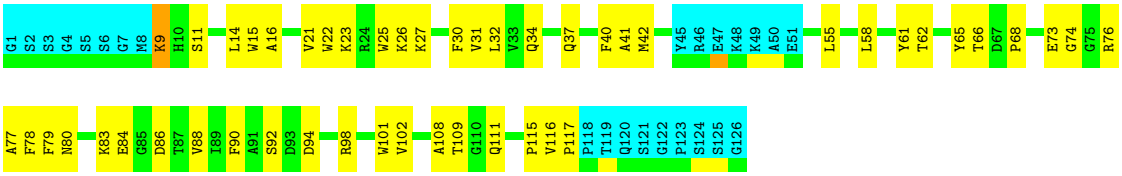
Chain A: 45% 36% 19%



4.2.20 Score per residue for model 20

• Molecule 1: calcium-dependent activator protein for secretion, CAPS

Chain A: 42% 38% • 19%



5 Refinement protocol and experimental data overview (i)

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

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *structures with the least restraint violations, target function*.

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

Software name	Classification	Version
CYANA	structure solution	2.0.17
CYANA	refinement	2.0.17

No chemical shift data was provided.

6 Model quality (i)

6.1 Standard geometry (i)

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 (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
1	A	832	807	805	36±5
All	All	16640	16140	16100	710

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 22.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:41:ALA:HB1	1:A:55:LEU:HD11	0.95	1.38	11	8
1:A:61:TYR:O	1:A:109:THR:HG21	0.84	1.71	12	9
1:A:25:TRP:CD2	1:A:72:LEU:HD22	0.78	2.13	19	9
1:A:98:ARG:O	1:A:102:VAL:HG23	0.77	1.78	19	5
1:A:14:LEU:HD11	1:A:101:TRP:CE2	0.76	2.15	19	17
1:A:58:LEU:O	1:A:109:THR:HG22	0.75	1.81	6	6
1:A:62:THR:HG23	1:A:111:GLN:CD	0.74	2.03	13	7
1:A:77:ALA:HB1	1:A:98:ARG:HD3	0.73	1.58	19	17
1:A:41:ALA:HB1	1:A:55:LEU:HD21	0.72	1.60	12	11
1:A:88:VAL:HG12	1:A:90:PHE:CE1	0.70	2.22	19	13
1:A:55:LEU:HD12	1:A:56:LEU:N	0.69	2.01	1	3
1:A:21:VAL:HG23	1:A:22:TRP:CE3	0.69	2.22	13	18
1:A:58:LEU:HB3	1:A:109:THR:HG22	0.67	1.67	14	14
1:A:40:PHE:HB2	1:A:108:ALA:HB1	0.66	1.65	4	8

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:77:ALA:HB1	1:A:98:ARG:CD	0.65	2.21	19	5
1:A:41:ALA:HB1	1:A:55:LEU:CD2	0.65	2.22	12	9
1:A:25:TRP:CE3	1:A:72:LEU:HD22	0.64	2.28	8	6
1:A:15:TRP:CB	1:A:25:TRP:CZ2	0.63	2.81	9	10
1:A:63:VAL:HG11	1:A:105:MET:HB2	0.63	1.71	3	13
1:A:16:ALA:HB2	1:A:90:PHE:CD2	0.63	2.28	7	8
1:A:63:VAL:HG11	1:A:105:MET:CB	0.63	2.23	12	14
1:A:16:ALA:HB3	1:A:30:PHE:CZ	0.61	2.30	20	9
1:A:105:MET:O	1:A:109:THR:HG23	0.61	1.96	5	7
1:A:33:VAL:HG23	1:A:43:CYS:SG	0.61	2.35	18	1
1:A:9:LYS:HB2	1:A:32:LEU:HD23	0.61	1.73	7	9
1:A:69:GLN:HG2	1:A:89:ILE:HD13	0.61	1.73	19	1
1:A:65:TYR:CD2	1:A:116:VAL:O	0.60	2.55	11	3
1:A:65:TYR:CD1	1:A:116:VAL:O	0.59	2.55	2	8
1:A:25:TRP:CZ3	1:A:72:LEU:HD13	0.59	2.31	14	2
1:A:62:THR:HG23	1:A:111:GLN:OE1	0.59	1.96	18	8
1:A:76:ARG:O	1:A:78:PHE:CE2	0.58	2.57	15	1
1:A:88:VAL:CG1	1:A:90:PHE:CE1	0.58	2.87	19	8
1:A:41:ALA:CB	1:A:55:LEU:HD21	0.58	2.27	12	5
1:A:14:LEU:HD11	1:A:101:TRP:CZ2	0.58	2.34	15	7
1:A:15:TRP:CE3	1:A:27:LYS:N	0.57	2.72	5	2
1:A:56:LEU:HD11	1:A:61:TYR:OH	0.57	1.99	5	1
1:A:76:ARG:O	1:A:78:PHE:CD2	0.57	2.58	15	1
1:A:37:GLN:OE1	1:A:38:TYR:CE1	0.56	2.58	15	1
1:A:9:LYS:CB	1:A:32:LEU:HD23	0.56	2.30	18	1
1:A:41:ALA:CB	1:A:55:LEU:HD11	0.56	2.28	4	6
1:A:15:TRP:HB2	1:A:25:TRP:CZ2	0.55	2.37	15	14
1:A:65:TYR:CE2	1:A:116:VAL:O	0.55	2.60	4	1
1:A:77:ALA:HB3	1:A:92:SER:OG	0.54	2.02	6	5
1:A:14:LEU:HD11	1:A:101:TRP:NE1	0.54	2.18	2	1
1:A:79:PHE:CE2	1:A:90:PHE:CB	0.54	2.91	12	7
1:A:15:TRP:HB3	1:A:25:TRP:CZ2	0.53	2.37	9	2
1:A:79:PHE:CE2	1:A:90:PHE:HB2	0.53	2.38	12	4
1:A:79:PHE:CD1	1:A:79:PHE:N	0.53	2.76	7	11
1:A:63:VAL:HG11	1:A:105:MET:HB3	0.53	1.79	12	4
1:A:55:LEU:HD12	1:A:56:LEU:H	0.52	1.63	1	3
1:A:43:CYS:SG	1:A:55:LEU:HD13	0.52	2.44	4	2
1:A:57:GLN:O	1:A:61:TYR:CD2	0.52	2.63	6	1
1:A:56:LEU:HD11	1:A:61:TYR:CZ	0.52	2.40	7	1
1:A:15:TRP:N	1:A:15:TRP:CD1	0.52	2.78	10	12
1:A:116:VAL:HG13	1:A:117:PRO:HD2	0.51	1.82	8	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:76:ARG:O	1:A:78:PHE:CD1	0.51	2.63	7	1
1:A:77:ALA:HB1	1:A:98:ARG:HD2	0.51	1.82	18	1
1:A:40:PHE:CG	1:A:108:ALA:HB1	0.51	2.40	15	5
1:A:116:VAL:HG23	1:A:117:PRO:HD2	0.51	1.83	4	7
1:A:15:TRP:HB2	1:A:25:TRP:CH2	0.51	2.40	9	3
1:A:10:HIS:HB3	1:A:101:TRP:CH2	0.51	2.41	10	2
1:A:42:MET:HG2	1:A:58:LEU:HD11	0.51	1.83	11	4
1:A:39:THR:C	1:A:40:PHE:CD1	0.51	2.84	15	6
1:A:41:ALA:HB1	1:A:55:LEU:CD1	0.51	2.29	20	4
1:A:14:LEU:HD22	1:A:91:ALA:O	0.51	2.06	3	2
1:A:100:LEU:N	1:A:100:LEU:CD2	0.50	2.74	14	3
1:A:73:GLU:CG	1:A:73:GLU:O	0.50	2.60	7	1
1:A:40:PHE:CD1	1:A:108:ALA:HA	0.50	2.42	13	1
1:A:65:TYR:CE1	1:A:116:VAL:C	0.50	2.85	18	2
1:A:28:ARG:HG2	1:A:30:PHE:CE2	0.49	2.42	18	2
1:A:22:TRP:CD1	1:A:54:GLU:OE1	0.49	2.66	11	1
1:A:68:PRO:HB3	1:A:78:PHE:CD2	0.49	2.43	5	17
1:A:22:TRP:CZ2	1:A:30:PHE:CE2	0.49	3.00	6	3
1:A:99:ILE:HG22	1:A:103:GLN:OE1	0.49	2.07	9	1
1:A:65:TYR:CE2	1:A:116:VAL:C	0.49	2.86	17	1
1:A:79:PHE:CD2	1:A:90:PHE:HB2	0.49	2.42	20	13
1:A:61:TYR:O	1:A:109:THR:CG2	0.48	2.61	4	2
1:A:22:TRP:CD1	1:A:54:GLU:CD	0.48	2.87	12	2
1:A:72:LEU:HD11	1:A:89:ILE:HD13	0.48	1.84	1	1
1:A:67:ASP:N	1:A:67:ASP:OD1	0.48	2.46	15	1
1:A:29:PHE:CZ	1:A:31:VAL:CG2	0.48	2.96	12	1
1:A:33:VAL:CG2	1:A:43:CYS:SG	0.48	3.02	17	2
1:A:66:THR:HG21	1:A:80:ASN:ND2	0.48	2.23	19	2
1:A:100:LEU:H	1:A:100:LEU:HD12	0.48	1.68	19	1
1:A:61:TYR:CE2	1:A:83:LYS:HB2	0.48	2.44	20	1
1:A:62:THR:CG2	1:A:111:GLN:OE1	0.48	2.60	13	4
1:A:37:GLN:OE1	1:A:38:TYR:CE2	0.48	2.67	11	1
1:A:34:GLN:HB2	1:A:40:PHE:CE2	0.48	2.44	17	5
1:A:69:GLN:N	1:A:69:GLN:CD	0.48	2.68	5	1
1:A:21:VAL:O	1:A:23:LYS:N	0.48	2.47	8	1
1:A:61:TYR:CE1	1:A:83:LYS:HB2	0.47	2.44	7	15
1:A:55:LEU:HD23	1:A:55:LEU:C	0.47	2.30	5	2
1:A:94:ASP:N	1:A:94:ASP:OD1	0.47	2.46	1	2
1:A:21:VAL:CG2	1:A:22:TRP:CE3	0.47	2.96	13	8
1:A:15:TRP:CD1	1:A:15:TRP:N	0.47	2.81	18	4
1:A:15:TRP:CZ2	1:A:27:LYS:HB2	0.47	2.45	5	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:10:HIS:HB3	1:A:101:TRP:CZ2	0.47	2.44	17	1
1:A:106:TYR:CE2	1:A:114:LYS:HG3	0.47	2.44	2	4
1:A:42:MET:CE	1:A:101:TRP:CZ3	0.47	2.97	19	2
1:A:94:ASP:OD1	1:A:95:GLU:N	0.47	2.48	4	1
1:A:83:LYS:O	1:A:84:GLU:C	0.47	2.52	7	20
1:A:79:PHE:O	1:A:90:PHE:N	0.47	2.47	3	7
1:A:61:TYR:CD1	1:A:83:LYS:HD3	0.47	2.45	8	1
1:A:40:PHE:CE1	1:A:108:ALA:HA	0.47	2.45	15	1
1:A:61:TYR:CD2	1:A:83:LYS:HD3	0.46	2.46	7	13
1:A:106:TYR:C	1:A:106:TYR:CD1	0.46	2.89	2	1
1:A:68:PRO:HB3	1:A:78:PHE:CE2	0.46	2.45	10	6
1:A:68:PRO:HB3	1:A:78:PHE:CD1	0.46	2.45	2	2
1:A:15:TRP:CB	1:A:25:TRP:CH2	0.46	2.99	9	1
1:A:10:HIS:CE1	1:A:100:LEU:HB3	0.46	2.46	7	1
1:A:113:HIS:O	1:A:114:LYS:C	0.46	2.54	9	1
1:A:15:TRP:CH2	1:A:27:LYS:HB2	0.46	2.46	7	5
1:A:34:GLN:HG3	1:A:40:PHE:CZ	0.46	2.46	9	9
1:A:65:TYR:CZ	1:A:102:VAL:HG11	0.46	2.46	11	2
1:A:34:GLN:HG3	1:A:40:PHE:CE1	0.46	2.46	12	1
1:A:89:ILE:HG22	1:A:90:PHE:N	0.45	2.27	14	2
1:A:40:PHE:CD1	1:A:108:ALA:HB1	0.45	2.47	15	3
1:A:25:TRP:CH2	1:A:72:LEU:HD13	0.45	2.46	19	1
1:A:59:ASP:OD1	1:A:59:ASP:N	0.45	2.50	1	1
1:A:15:TRP:CZ2	1:A:27:LYS:HE3	0.45	2.47	14	2
1:A:11:SER:CB	1:A:31:VAL:HG22	0.45	2.41	7	1
1:A:94:ASP:OD1	1:A:97:ASP:CG	0.45	2.55	8	1
1:A:102:VAL:CG1	1:A:115:PRO:HB2	0.45	2.42	20	2
1:A:15:TRP:CZ2	1:A:27:LYS:HD3	0.45	2.47	4	5
1:A:52:PRO:O	1:A:54:GLU:N	0.45	2.49	7	1
1:A:16:ALA:CB	1:A:90:PHE:CD2	0.45	2.99	19	1
1:A:60:GLY:O	1:A:61:TYR:C	0.45	2.55	3	5
1:A:73:GLU:O	1:A:74:GLY:C	0.45	2.55	14	6
1:A:22:TRP:O	1:A:24:ARG:N	0.45	2.49	16	6
1:A:98:ARG:O	1:A:101:TRP:N	0.45	2.50	6	2
1:A:63:VAL:O	1:A:64:ASP:CG	0.45	2.55	9	1
1:A:65:TYR:CE1	1:A:102:VAL:HG11	0.44	2.47	3	2
1:A:69:GLN:OE1	1:A:89:ILE:HG21	0.44	2.13	2	1
1:A:69:GLN:OE1	1:A:72:LEU:HD12	0.44	2.13	2	1
1:A:15:TRP:CZ2	1:A:27:LYS:HD2	0.44	2.48	5	1
1:A:15:TRP:CD1	1:A:74:GLY:O	0.44	2.70	12	1
1:A:37:GLN:O	1:A:37:GLN:NE2	0.44	2.51	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:61:TYR:CG	1:A:83:LYS:HD3	0.44	2.48	1	3
1:A:79:PHE:CE2	1:A:90:PHE:HB3	0.44	2.47	20	2
1:A:28:ARG:HG3	1:A:30:PHE:CE1	0.44	2.48	8	1
1:A:76:ARG:O	1:A:78:PHE:CE1	0.43	2.71	7	1
1:A:102:VAL:CG1	1:A:115:PRO:CB	0.43	2.96	12	2
1:A:89:ILE:CG2	1:A:90:PHE:N	0.43	2.81	14	1
1:A:79:PHE:CD1	1:A:98:ARG:HG3	0.43	2.48	3	1
1:A:80:ASN:OD1	1:A:80:ASN:C	0.43	2.57	19	1
1:A:37:GLN:OE1	1:A:38:TYR:CD2	0.43	2.71	11	1
1:A:22:TRP:O	1:A:23:LYS:C	0.43	2.56	19	1
1:A:113:HIS:O	1:A:115:PRO:N	0.43	2.52	9	1
1:A:22:TRP:CZ3	1:A:56:LEU:HB2	0.43	2.49	12	1
1:A:33:VAL:HG12	1:A:34:GLN:N	0.43	2.29	13	3
1:A:77:ALA:HB3	1:A:92:SER:HB2	0.43	1.91	10	1
1:A:106:TYR:CZ	1:A:114:LYS:HG3	0.42	2.48	14	6
1:A:38:TYR:CD1	1:A:38:TYR:N	0.42	2.84	2	3
1:A:53:GLN:OE1	1:A:53:GLN:C	0.42	2.57	9	1
1:A:71:GLY:O	1:A:72:LEU:C	0.42	2.57	5	1
1:A:15:TRP:CE2	1:A:27:LYS:HB2	0.42	2.50	2	8
1:A:22:TRP:C	1:A:24:ARG:N	0.42	2.73	16	5
1:A:34:GLN:HA	1:A:40:PHE:CD2	0.42	2.49	13	1
1:A:95:GLU:CD	1:A:95:GLU:C	0.42	2.78	2	1
1:A:15:TRP:CZ3	1:A:27:LYS:HB2	0.41	2.50	4	1
1:A:21:VAL:O	1:A:22:TRP:C	0.41	2.58	8	2
1:A:22:TRP:NE1	1:A:54:GLU:HB2	0.41	2.31	8	1
1:A:14:LEU:CD1	1:A:101:TRP:CE2	0.41	3.02	2	1
1:A:98:ARG:O	1:A:99:ILE:C	0.41	2.58	6	4
1:A:65:TYR:CD2	1:A:116:VAL:C	0.41	2.94	11	1
1:A:10:HIS:CD2	1:A:101:TRP:CZ2	0.41	3.09	3	1
1:A:15:TRP:CD2	1:A:74:GLY:HA3	0.41	2.50	7	1
1:A:15:TRP:CD2	1:A:27:LYS:HB2	0.41	2.51	8	2
1:A:106:TYR:CD1	1:A:115:PRO:CD	0.41	3.04	8	1
1:A:52:PRO:O	1:A:53:GLN:C	0.41	2.58	7	1
1:A:21:VAL:C	1:A:23:LYS:N	0.41	2.73	8	1
1:A:77:ALA:HB1	1:A:98:ARG:HB2	0.41	1.93	14	1
1:A:98:ARG:O	1:A:102:VAL:CG2	0.40	2.65	11	1
1:A:79:PHE:CZ	1:A:90:PHE:HB3	0.40	2.51	12	1
1:A:76:ARG:N	1:A:76:ARG:HD2	0.40	2.31	15	1
1:A:61:TYR:O	1:A:109:THR:CB	0.40	2.69	1	1
1:A:102:VAL:O	1:A:106:TYR:CB	0.40	2.69	6	1
1:A:56:LEU:HD11	1:A:61:TYR:CE2	0.40	2.51	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:106:TYR:CD1	1:A:106:TYR:C	0.40	2.95	4	1
1:A:71:GLY:O	1:A:73:GLU:OE1	0.40	2.40	11	1
1:A:11:SER:HB2	1:A:31:VAL:HG22	0.40	1.92	20	1
1:A:63:VAL:O	1:A:64:ASP:OD1	0.40	2.40	6	1
1:A:52:PRO:C	1:A:54:GLU:N	0.40	2.75	7	1
1:A:111:GLN:OE1	1:A:113:HIS:O	0.40	2.40	7	1
1:A:114:LYS:HE2	1:A:114:LYS:N	0.40	2.32	7	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	102/126 (81%)	87±3 (86±3%)	13±3 (13±3%)	2±1 (2±1%)	14	59
All	All	2040/2520 (81%)	1749 (86%)	260 (13%)	31 (2%)	14	59

All 10 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	111	GLN	10
1	A	74	GLY	7
1	A	23	LYS	5
1	A	72	LEU	2
1	A	61	TYR	2
1	A	53	GLN	1
1	A	22	TRP	1
1	A	99	ILE	1
1	A	59	ASP	1
1	A	29	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	87/105 (83%)	83±2 (96±2%)	4±2 (4±2%)	34 82
All	All	1740/2100 (83%)	1669 (96%)	71 (4%)	34 82

All 25 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	67	ASP	7
1	A	79	PHE	6
1	A	24	ARG	5
1	A	86	ASP	5
1	A	38	TYR	4
1	A	94	ASP	4
1	A	96	GLN	4
1	A	97	ASP	4
1	A	53	GLN	3
1	A	100	LEU	3
1	A	59	ASP	3
1	A	114	LYS	3
1	A	37	GLN	3
1	A	106	TYR	2
1	A	95	GLU	2
1	A	28	ARG	2
1	A	64	ASP	2
1	A	93	ASP	2
1	A	15	TRP	1
1	A	54	GLU	1
1	A	29	PHE	1
1	A	9	LYS	1
1	A	23	LYS	1
1	A	26	LYS	1
1	A	76	ARG	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)

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 (i)

No chemical shift data were provided