Full wwPDB NMR Structure Validation Report (i)

Feb 22, 2022 – 09:05 AM EST

PDB ID	:	1WI0
Title	:	Solution structure of the PB1 domain of mouse mitogen activated protein kinase kinase 5 (MAP2K5)
Authors	:	Yoneyama, M.; Hayashi, F.; 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:

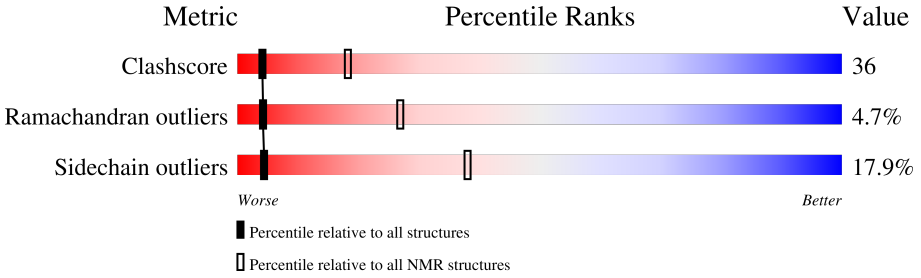
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.26
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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	113	27% 50% • 19%

2 Ensemble composition and analysis (i)

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:17-A:107 (91)	0.20	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 2 clusters and 1 single-model cluster was found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1707 atoms, of which 838 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Mitogen activated protein kinase kinase 5.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	113	1707	544	838	143	177	5	0

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	cloning artifact	UNP Q9WVS7
A	2	SER	-	cloning artifact	UNP Q9WVS7
A	3	SER	-	cloning artifact	UNP Q9WVS7
A	4	GLY	-	cloning artifact	UNP Q9WVS7
A	5	SER	-	cloning artifact	UNP Q9WVS7
A	6	SER	-	cloning artifact	UNP Q9WVS7
A	7	GLY	-	cloning artifact	UNP Q9WVS7
A	108	SER	-	cloning artifact	UNP Q9WVS7
A	109	GLY	-	cloning artifact	UNP Q9WVS7
A	110	PRO	-	cloning artifact	UNP Q9WVS7
A	111	SER	-	cloning artifact	UNP Q9WVS7
A	112	SER	-	cloning artifact	UNP Q9WVS7
A	113	GLY	-	cloning artifact	UNP Q9WVS7

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: Mitogen activated protein kinase kinase 5

Chain A: 27% 50% • 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

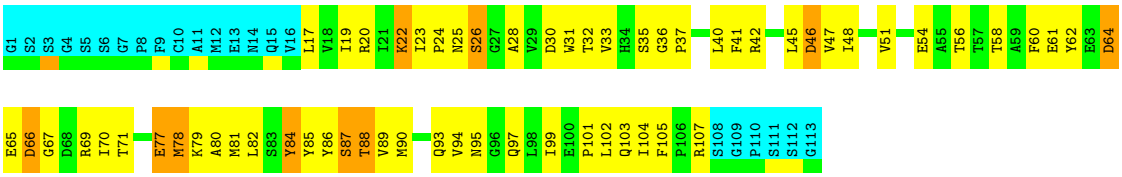
• Molecule 1: Mitogen activated protein kinase kinase 5

Chain A: 27% 48% 5% 19%

4.2.2 Score per residue for model 2 (medoid)

• Molecule 1: Mitogen activated protein kinase kinase 5

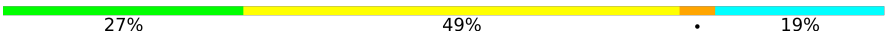
Chain A: 27% 45% 9% 19%

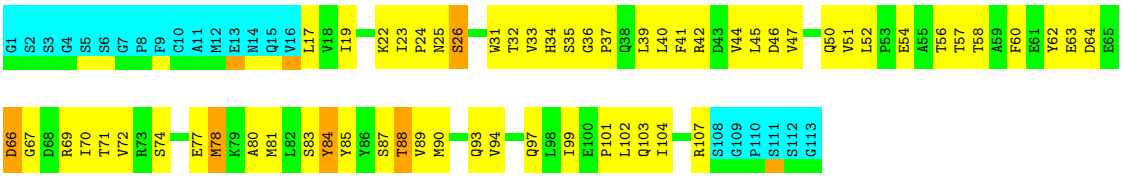


4.2.3 Score per residue for model 3

- Molecule 1: Mitogen activated protein kinase kinase 5

Chain A:

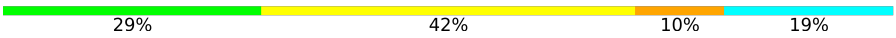


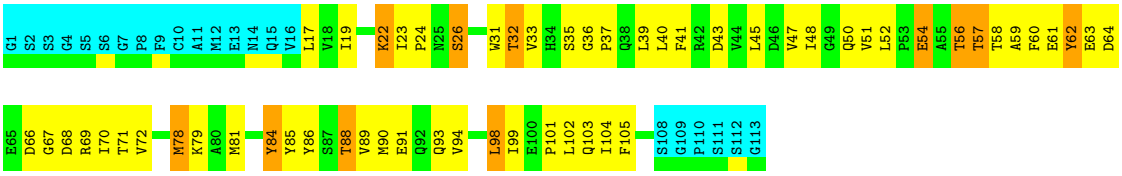


4.2.4 Score per residue for model 4

- Molecule 1: Mitogen activated protein kinase kinase 5

Chain A:

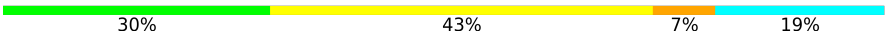


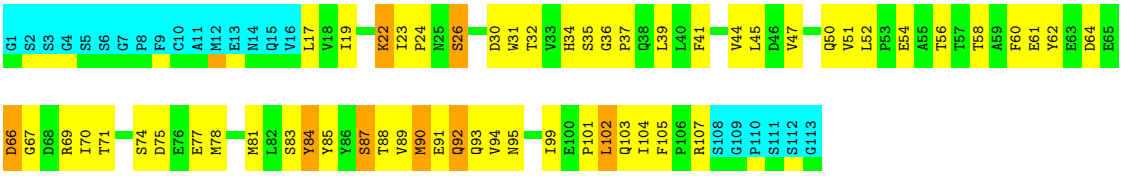


4.2.5 Score per residue for model 5

- Molecule 1: Mitogen activated protein kinase kinase 5

Chain A:





4.2.6 Score per residue for model 6

- Molecule 1: Mitogen activated protein kinase kinase 5

Chain A: 29% 44% 7% 19%

G1 S2 S3 G4 S5 S6 G7 P8 F9 C10 A11 M12 E13 N14 Q15 V16 L17 V18 I19 I23 P24 N25 S26 W31 T32 V33 H34 S35 G36 P37 Q38 L39 L40 F41 R42 D43 V44 L45 D46 V47 I48 V51 L52 P53 E54 A55 T56 T57 T58 A59 F60 E61 Y62 E63 D64 D68

R69 I70 T71 V72 R73 S74 D75 E76 E77 M78 K79 A80 M81 L82 S83 Y84 Y85 Y86 S87 T88 V89 M90 Q93 V94 N95 G96 Q97 L98 I99 E100 P101 L102 Q103 I104 F105 S108 G109 P110 S111 S112 G113

4.2.7 Score per residue for model 7

- Molecule 1: Mitogen activated protein kinase kinase 5

Chain A: 31% 42% 7% 19%

G1 S2 S3 G4 S5 S6 G7 P8 F9 C10 A11 M12 E13 N14 Q15 V16 L17 V18 I19 K22 I23 P24 N25 S26 W31 T32 V33 H34 S35 G36 P37 Q38 L39 L40 F41 R42 D43 V44 L45 D46 V47 I48 V51 E54 A55 T56 T57 T58 A59 F60 E61 Y62 E63 D64 E65 D66

G67 D68 R69 I70 T71 V72 R73 S74 E77 M78 K79 A80 M81 Y84 Y85 T88 V89 M90 E91 Q92 Q93 V94 I99 E100 P101 L102 Q103 I104 R107 S108 G109 P110 S111 S112 G113

4.2.8 Score per residue for model 8

- Molecule 1: Mitogen activated protein kinase kinase 5

Chain A: 35% 38% 7% 19%

G1 S2 S3 G4 S5 S6 G7 P8 F9 C10 A11 M12 E13 N14 Q15 V16 L17 V18 I19 K22 I23 P24 N25 S26 W31 T32 V33 H34 S35 G36 P37 Q38 L39 L40 F41 R42 D43 V44 L45 D46 V47 V51 L52 P53 E54 A55 T56 E61 Y62 E63 D66 G67 D68 R69 I70

T71 V72 E76 E77 M78 K79 A80 M81 L82 Y85 Y86 S87 T88 V89 M90 Q93 V94 N95 I99 E100 P101 L102 Q103 I104 F105 S108 G109 P110 S111 S112 G113

4.2.9 Score per residue for model 9

- Molecule 1: Mitogen activated protein kinase kinase 5

Chain A: 27% 45% 9% 19%

G1 S2 S3 G4 S5 S6 G7 P8 F9 C10 A11 M12 E13 N14 Q15 V16 L17 V18 I19 K22 I23 P24 N25 S26 W31 T32 V33 H34 S35 G36 P37 Q38 L39 L40 F41 R42 D43 V44 L45 D46 V47 I48 V51 L52 P53 E54 A55 T56 T57 T58 A59 F60 E61 Y62 E63 D64 E65

D66 G67 D68 R69 I70 T71 V72 D75 E76 E77 M78 M81 L82 S83 Y84 Y85 Y86 S87 T88 V89 M90 E91 Q92 Q93 V94 L98 I99 E100 P101 L102 Q103 I104 F105 P106 R107 S108 G109 P110 S111 S112 G113

4.2.10 Score per residue for model 10

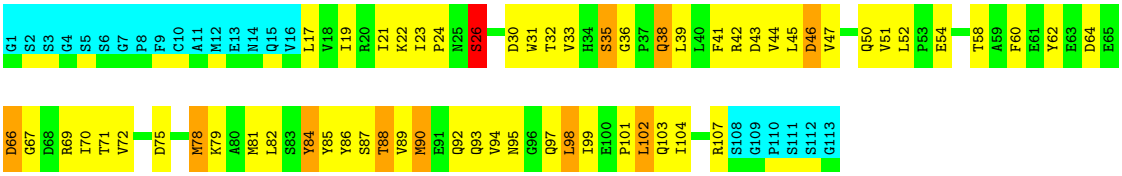
- Molecule 1: Mitogen activated protein kinase kinase 5

Chain A: 30% 44% 6% 19%

4.2.11 Score per residue for model 11

- Molecule 1: Mitogen activated protein kinase kinase 5

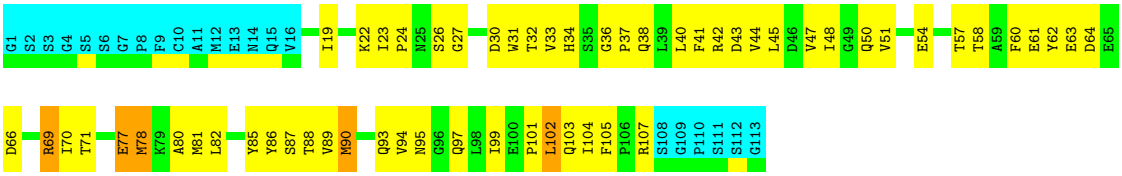
Chain A: 27% 43% 9% • 19%



4.2.12 Score per residue for model 12

- Molecule 1: Mitogen activated protein kinase kinase 5

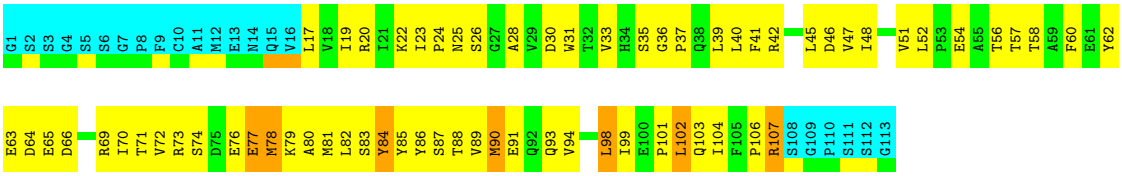
Chain A: 29% 47% • 19%



4.2.13 Score per residue for model 13

- Molecule 1: Mitogen activated protein kinase kinase 5

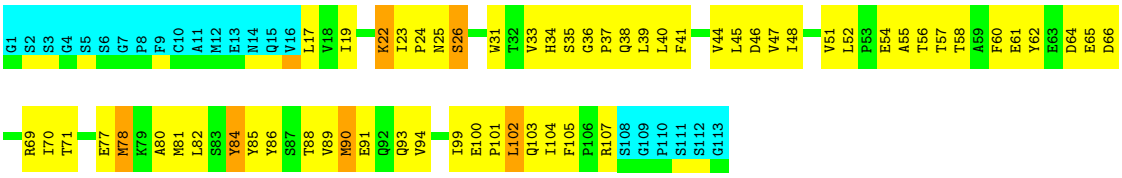
Chain A: 21% 53% 6% 19%



4.2.14 Score per residue for model 14

• Molecule 1: Mitogen activated protein kinase kinase 5

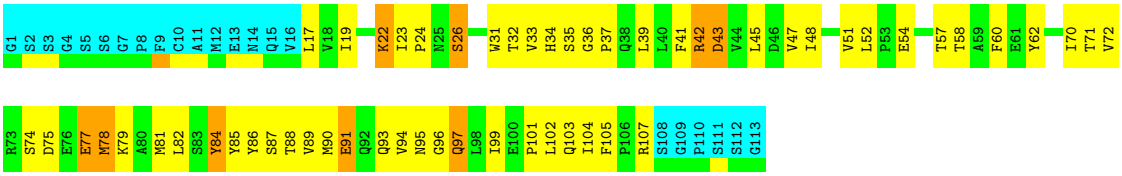
Chain A: 27% 48% 5% 19%



4.2.15 Score per residue for model 15

• Molecule 1: Mitogen activated protein kinase kinase 5

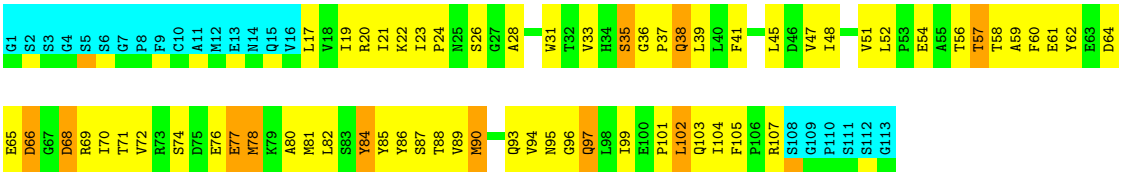
Chain A: 30% 42% 8% 19%



4.2.16 Score per residue for model 16

• Molecule 1: Mitogen activated protein kinase kinase 5

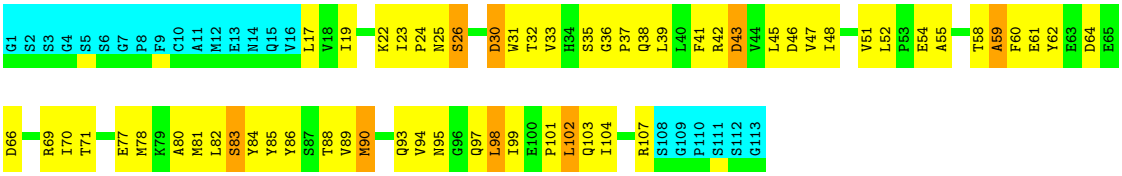
Chain A: 24% 47% 10% 19%



4.2.17 Score per residue for model 17

• Molecule 1: Mitogen activated protein kinase kinase 5

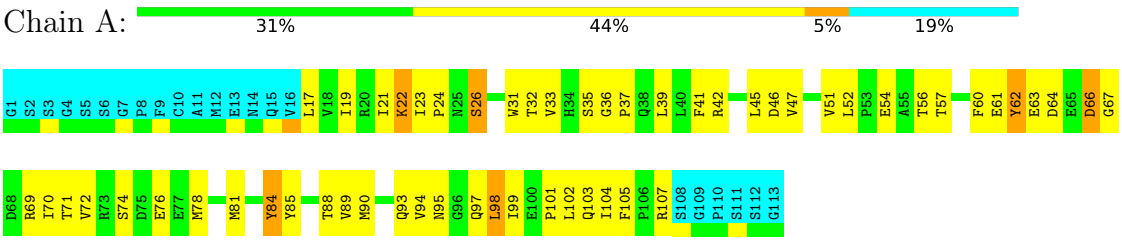
Chain A: 27% 46% 7% 19%



4.2.18 Score per residue for model 18

- Molecule 1: Mitogen activated protein kinase kinase 5

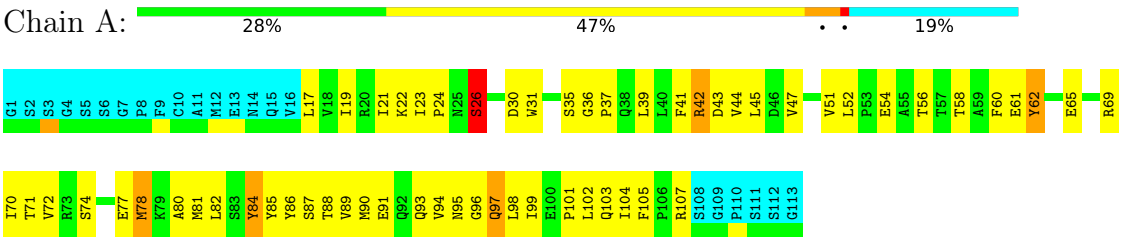
Chain A:



4.2.19 Score per residue for model 19

- Molecule 1: Mitogen activated protein kinase kinase 5

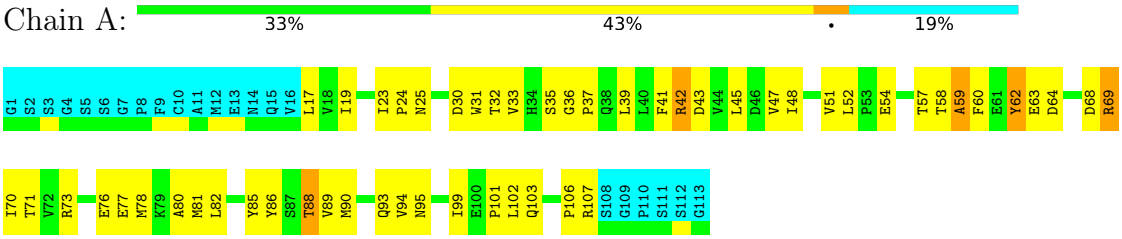
Chain A:



4.2.20 Score per residue for model 20

- Molecule 1: Mitogen activated protein kinase kinase 5

Chain A:



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	1.0.8
CYANA	refinement	1.0.8

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	730	717	717	53±6
All	All	14600	14340	14340	1053

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 36.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:31:TRP:CZ2	1:A:47:VAL:HG21	0.88	2.03	16	20
1:A:81:MET:SD	1:A:102:LEU:HD21	0.81	2.15	17	2
1:A:93:GLN:HG2	1:A:99:ILE:HD11	0.80	1.53	4	20
1:A:90:MET:O	1:A:94:VAL:HG13	0.78	1.78	10	20
1:A:31:TRP:CE2	1:A:47:VAL:HG21	0.78	2.14	5	20
1:A:82:LEU:HD22	1:A:86:TYR:OH	0.76	1.80	8	15
1:A:51:VAL:HG12	1:A:52:LEU:HD12	0.75	1.57	1	16
1:A:31:TRP:CH2	1:A:39:LEU:HD11	0.75	2.16	16	18
1:A:17:LEU:HD12	1:A:85:TYR:CE2	0.74	2.18	4	17
1:A:41:PHE:O	1:A:45:LEU:HD22	0.70	1.86	15	19
1:A:77:GLU:O	1:A:80:ALA:HB3	0.69	1.87	12	12
1:A:93:GLN:CG	1:A:99:ILE:HD11	0.68	2.18	1	20
1:A:31:TRP:O	1:A:33:VAL:HG23	0.67	1.89	20	11
1:A:69:ARG:CZ	1:A:105:PHE:CZ	0.66	2.78	16	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:64:ASP:CG	1:A:70:ILE:HD11	0.65	2.11	11	6
1:A:69:ARG:NE	1:A:105:PHE:CE2	0.65	2.64	8	3
1:A:69:ARG:NE	1:A:105:PHE:CE1	0.65	2.65	12	3
1:A:89:VAL:HG13	1:A:99:ILE:HD12	0.64	1.66	7	14
1:A:52:LEU:HB3	1:A:55:ALA:HB3	0.64	1.68	17	2
1:A:85:TYR:O	1:A:89:VAL:HG23	0.63	1.94	8	20
1:A:41:PHE:CE1	1:A:72:VAL:HG12	0.62	2.29	8	3
1:A:58:THR:O	1:A:59:ALA:HB2	0.62	1.94	20	2
1:A:19:ILE:CG2	1:A:104:ILE:CD1	0.61	2.78	16	18
1:A:19:ILE:HD12	1:A:33:VAL:HG21	0.61	1.70	4	3
1:A:62:TYR:O	1:A:62:TYR:CD1	0.61	2.54	14	19
1:A:51:VAL:HG12	1:A:52:LEU:CD1	0.61	2.26	20	8
1:A:31:TRP:CD2	1:A:47:VAL:HG11	0.60	2.32	12	17
1:A:20:ARG:CZ	1:A:28:ALA:CB	0.60	2.79	13	1
1:A:102:LEU:HG	1:A:104:ILE:HG23	0.59	1.73	16	4
1:A:17:LEU:CD1	1:A:85:TYR:CE2	0.59	2.85	17	12
1:A:64:ASP:OD1	1:A:84:TYR:CD1	0.59	2.55	6	3
1:A:69:ARG:NE	1:A:105:PHE:CZ	0.59	2.70	12	4
1:A:82:LEU:O	1:A:86:TYR:CD2	0.59	2.56	2	11
1:A:17:LEU:HD23	1:A:33:VAL:HG11	0.59	1.74	13	4
1:A:41:PHE:CE1	1:A:60:PHE:CE1	0.59	2.91	6	14
1:A:98:LEU:HD12	1:A:99:ILE:O	0.56	1.99	13	1
1:A:43:ASP:O	1:A:47:VAL:HG23	0.56	2.01	17	3
1:A:84:TYR:CG	1:A:85:TYR:N	0.56	2.73	10	14
1:A:20:ARG:CG	1:A:28:ALA:HB1	0.55	2.31	16	1
1:A:19:ILE:HG23	1:A:104:ILE:HG12	0.55	1.78	16	2
1:A:21:ILE:HG21	1:A:51:VAL:HG11	0.55	1.78	16	1
1:A:31:TRP:HH2	1:A:39:LEU:HD11	0.55	1.59	16	8
1:A:36:GLY:N	1:A:37:PRO:CD	0.55	2.69	12	19
1:A:41:PHE:CZ	1:A:58:THR:O	0.55	2.59	1	15
1:A:69:ARG:CD	1:A:105:PHE:CE1	0.55	2.89	12	1
1:A:70:ILE:HG22	1:A:71:THR:H	0.55	1.60	19	20
1:A:72:VAL:HG11	1:A:78:MET:HG2	0.55	1.78	16	9
1:A:98:LEU:HD12	1:A:99:ILE:N	0.54	2.17	13	1
1:A:84:TYR:C	1:A:84:TYR:CD1	0.54	2.80	10	2
1:A:62:TYR:O	1:A:62:TYR:CG	0.54	2.60	20	20
1:A:31:TRP:CE2	1:A:33:VAL:HG22	0.53	2.38	9	9
1:A:60:PHE:CZ	1:A:72:VAL:HG11	0.52	2.40	13	1
1:A:48:ILE:HD13	1:A:57:THR:HG21	0.52	1.81	6	2
1:A:91:GLU:O	1:A:94:VAL:HG22	0.52	2.04	19	3
1:A:62:TYR:CE2	1:A:81:MET:HB2	0.52	2.40	9	14

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:54:GLU:CG	1:A:54:GLU:O	0.52	2.58	14	5
1:A:62:TYR:CD2	1:A:81:MET:HG3	0.52	2.40	9	5
1:A:85:TYR:O	1:A:89:VAL:CG2	0.51	2.58	8	20
1:A:20:ARG:NE	1:A:28:ALA:HB3	0.51	2.19	2	1
1:A:69:ARG:CD	1:A:105:PHE:CE2	0.51	2.93	16	3
1:A:104:ILE:C	1:A:105:PHE:CD1	0.51	2.84	18	2
1:A:69:ARG:NH2	1:A:105:PHE:CZ	0.51	2.78	9	3
1:A:19:ILE:CG2	1:A:104:ILE:HD11	0.51	2.36	16	6
1:A:62:TYR:CD1	1:A:62:TYR:C	0.51	2.83	14	20
1:A:60:PHE:CD1	1:A:60:PHE:N	0.51	2.79	19	4
1:A:17:LEU:HD23	1:A:33:VAL:CG1	0.51	2.36	13	2
1:A:98:LEU:HD12	1:A:98:LEU:N	0.51	2.21	9	6
1:A:62:TYR:CE2	1:A:70:ILE:HB	0.51	2.41	6	12
1:A:41:PHE:CE1	1:A:60:PHE:CE2	0.50	2.99	13	3
1:A:58:THR:HG22	1:A:58:THR:O	0.50	2.06	19	1
1:A:98:LEU:CD1	1:A:99:ILE:O	0.50	2.59	13	1
1:A:91:GLU:HA	1:A:94:VAL:HG22	0.50	1.83	4	4
1:A:23:ILE:HG23	1:A:24:PRO:HD2	0.50	1.82	11	4
1:A:61:GLU:CB	1:A:70:ILE:O	0.50	2.59	18	12
1:A:31:TRP:CZ3	1:A:44:VAL:HA	0.50	2.41	12	7
1:A:62:TYR:CD2	1:A:81:MET:HB2	0.50	2.42	6	4
1:A:54:GLU:CA	1:A:54:GLU:OE1	0.49	2.59	9	3
1:A:32:THR:O	1:A:32:THR:HG23	0.49	2.07	18	5
1:A:68:ASP:O	1:A:70:ILE:CD1	0.49	2.59	9	2
1:A:57:THR:O	1:A:58:THR:CB	0.49	2.58	13	2
1:A:38:GLN:O	1:A:38:GLN:CG	0.49	2.60	17	1
1:A:19:ILE:HG21	1:A:104:ILE:CD1	0.49	2.38	1	5
1:A:81:MET:CE	1:A:102:LEU:HD21	0.49	2.38	12	3
1:A:62:TYR:CD2	1:A:81:MET:SD	0.49	3.06	9	3
1:A:41:PHE:O	1:A:45:LEU:CD2	0.49	2.60	20	8
1:A:58:THR:O	1:A:59:ALA:CB	0.49	2.61	20	2
1:A:39:LEU:O	1:A:78:MET:CE	0.48	2.61	16	2
1:A:70:ILE:HD13	1:A:70:ILE:N	0.48	2.23	20	2
1:A:69:ARG:CZ	1:A:105:PHE:CE2	0.48	2.96	16	1
1:A:62:TYR:CE1	1:A:84:TYR:CD2	0.48	3.02	14	5
1:A:32:THR:OG1	1:A:34:HIS:NE2	0.48	2.46	12	1
1:A:62:TYR:CE2	1:A:81:MET:HG3	0.48	2.43	9	2
1:A:98:LEU:HD12	1:A:98:LEU:C	0.47	2.30	13	1
1:A:23:ILE:CG2	1:A:24:PRO:HD2	0.47	2.39	18	20
1:A:22:LYS:HG3	1:A:105:PHE:CE2	0.47	2.45	15	6
1:A:31:TRP:CG	1:A:47:VAL:HG11	0.47	2.45	16	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:101:PRO:O	1:A:103:GLN:N	0.47	2.48	13	20
1:A:57:THR:HG23	1:A:59:ALA:O	0.47	2.10	9	2
1:A:42:ARG:O	1:A:45:LEU:N	0.47	2.48	12	6
1:A:54:GLU:O	1:A:54:GLU:CG	0.47	2.63	20	3
1:A:58:THR:O	1:A:58:THR:HG22	0.47	2.09	17	1
1:A:41:PHE:CZ	1:A:45:LEU:HD21	0.47	2.45	6	7
1:A:64:ASP:HA	1:A:84:TYR:CE2	0.46	2.45	10	4
1:A:48:ILE:HG21	1:A:57:THR:HG21	0.46	1.86	7	2
1:A:23:ILE:HG22	1:A:26:SER:HB2	0.46	1.85	11	3
1:A:84:TYR:O	1:A:87:SER:N	0.46	2.49	5	8
1:A:20:ARG:CZ	1:A:28:ALA:HB2	0.46	2.41	13	1
1:A:57:THR:HG22	1:A:59:ALA:O	0.46	2.11	20	1
1:A:48:ILE:O	1:A:51:VAL:N	0.46	2.49	7	13
1:A:70:ILE:HG22	1:A:71:THR:N	0.46	2.26	10	7
1:A:102:LEU:O	1:A:104:ILE:HG23	0.46	2.11	14	2
1:A:62:TYR:CZ	1:A:70:ILE:HG13	0.46	2.46	12	3
1:A:42:ARG:O	1:A:46:ASP:N	0.45	2.47	1	8
1:A:23:ILE:HD11	1:A:51:VAL:CG1	0.45	2.41	19	16
1:A:88:THR:CG2	1:A:89:VAL:N	0.45	2.79	2	6
1:A:40:LEU:C	1:A:78:MET:CE	0.45	2.85	13	6
1:A:17:LEU:N	1:A:33:VAL:O	0.45	2.50	11	5
1:A:42:ARG:O	1:A:43:ASP:C	0.45	2.54	12	5
1:A:62:TYR:CD2	1:A:81:MET:CG	0.45	2.99	9	4
1:A:64:ASP:CG	1:A:65:GLU:N	0.45	2.70	16	1
1:A:40:LEU:C	1:A:78:MET:HE1	0.45	2.32	13	4
1:A:104:ILE:C	1:A:105:PHE:CG	0.45	2.89	18	1
1:A:62:TYR:CE2	1:A:81:MET:CB	0.45	3.00	15	3
1:A:35:SER:HB3	1:A:38:GLN:CB	0.44	2.42	10	3
1:A:98:LEU:HD12	1:A:99:ILE:C	0.44	2.33	13	1
1:A:56:THR:HG22	1:A:57:THR:N	0.44	2.27	1	4
1:A:22:LYS:HB3	1:A:105:PHE:CD2	0.44	2.48	10	2
1:A:57:THR:HG23	1:A:106:PRO:HA	0.44	1.88	20	1
1:A:36:GLY:N	1:A:37:PRO:HD2	0.44	2.28	12	2
1:A:39:LEU:O	1:A:78:MET:HE1	0.44	2.13	8	1
1:A:32:THR:OG1	1:A:34:HIS:CD2	0.44	2.70	12	1
1:A:91:GLU:O	1:A:95:ASN:OD1	0.44	2.36	5	1
1:A:65:GLU:CG	1:A:66:ASP:N	0.44	2.80	16	2
1:A:62:TYR:CG	1:A:81:MET:HG3	0.44	2.48	6	12
1:A:20:ARG:NE	1:A:28:ALA:CB	0.44	2.81	13	2
1:A:33:VAL:O	1:A:34:HIS:HB2	0.44	2.13	12	1
1:A:47:VAL:O	1:A:50:GLN:N	0.43	2.49	12	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:85:TYR:O	1:A:89:VAL:N	0.43	2.47	5	3
1:A:41:PHE:CD1	1:A:72:VAL:HG12	0.43	2.48	8	2
1:A:20:ARG:HG3	1:A:28:ALA:HB1	0.43	1.89	16	1
1:A:51:VAL:C	1:A:52:LEU:HD12	0.43	2.33	4	1
1:A:104:ILE:O	1:A:105:PHE:CG	0.43	2.71	18	1
1:A:17:LEU:HD22	1:A:82:LEU:CD2	0.43	2.43	2	1
1:A:88:THR:O	1:A:91:GLU:N	0.43	2.49	9	2
1:A:54:GLU:O	1:A:54:GLU:CD	0.43	2.57	20	5
1:A:57:THR:O	1:A:59:ALA:N	0.43	2.45	7	1
1:A:64:ASP:OD1	1:A:67:GLY:N	0.43	2.51	7	1
1:A:19:ILE:HD12	1:A:31:TRP:CE3	0.43	2.49	11	1
1:A:45:LEU:HD12	1:A:57:THR:O	0.43	2.14	18	1
1:A:23:ILE:CD1	1:A:51:VAL:CG1	0.43	2.96	5	3
1:A:23:ILE:CG2	1:A:26:SER:HB2	0.43	2.43	18	1
1:A:80:ALA:O	1:A:83:SER:N	0.43	2.52	17	1
1:A:90:MET:C	1:A:90:MET:SD	0.43	2.97	5	5
1:A:105:PHE:CD1	1:A:105:PHE:N	0.43	2.86	5	1
1:A:59:ALA:HB3	1:A:107:ARG:HE	0.43	1.73	16	1
1:A:23:ILE:HD13	1:A:52:LEU:HD11	0.43	1.91	20	1
1:A:85:TYR:O	1:A:89:VAL:CB	0.42	2.67	8	17
1:A:34:HIS:CD2	1:A:34:HIS:N	0.42	2.87	14	3
1:A:41:PHE:CE1	1:A:72:VAL:O	0.42	2.72	3	2
1:A:70:ILE:N	1:A:70:ILE:HD13	0.42	2.29	14	1
1:A:92:GLN:CB	1:A:99:ILE:HD13	0.42	2.44	10	3
1:A:62:TYR:CE2	1:A:81:MET:CG	0.42	3.02	9	1
1:A:62:TYR:CZ	1:A:81:MET:HA	0.42	2.50	17	6
1:A:20:ARG:HE	1:A:28:ALA:HB3	0.42	1.75	2	1
1:A:92:GLN:NE2	1:A:98:LEU:O	0.42	2.52	9	1
1:A:30:ASP:CG	1:A:30:ASP:O	0.42	2.58	19	2
1:A:68:ASP:O	1:A:70:ILE:HD13	0.42	2.14	9	1
1:A:32:THR:O	1:A:32:THR:CG2	0.42	2.68	11	2
1:A:66:ASP:O	1:A:67:GLY:C	0.42	2.59	5	9
1:A:24:PRO:O	1:A:25:ASN:C	0.42	2.58	3	6
1:A:84:TYR:O	1:A:85:TYR:C	0.42	2.57	3	9
1:A:64:ASP:CB	1:A:70:ILE:HD11	0.42	2.45	11	2
1:A:63:GLU:OE2	1:A:69:ARG:NH2	0.41	2.52	20	1
1:A:92:GLN:HB2	1:A:99:ILE:CD1	0.41	2.45	5	1
1:A:77:GLU:N	1:A:77:GLU:CD	0.41	2.74	15	1
1:A:18:VAL:HG13	1:A:30:ASP:HB3	0.41	1.90	10	1
1:A:78:MET:C	1:A:80:ALA:N	0.41	2.73	12	1
1:A:63:GLU:HG3	1:A:69:ARG:CZ	0.41	2.45	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:74:SER:C	1:A:76:GLU:N	0.41	2.74	1	1
1:A:90:MET:SD	1:A:90:MET:C	0.41	2.98	12	3
1:A:64:ASP:HB3	1:A:70:ILE:HD11	0.41	1.92	20	1
1:A:32:THR:HG23	1:A:32:THR:O	0.41	2.15	5	1
1:A:73:ARG:CG	1:A:107:ARG:NH2	0.41	2.84	13	1
1:A:69:ARG:NH2	1:A:105:PHE:CE1	0.41	2.88	16	1
1:A:63:GLU:OE2	1:A:69:ARG:CZ	0.41	2.68	20	1
1:A:77:GLU:O	1:A:80:ALA:CB	0.41	2.64	12	1
1:A:36:GLY:CA	1:A:86:TYR:OH	0.41	2.68	4	1
1:A:106:PRO:O	1:A:107:ARG:C	0.41	2.59	9	1
1:A:85:TYR:CD1	1:A:102:LEU:HD13	0.41	2.50	5	1
1:A:35:SER:O	1:A:36:GLY:C	0.41	2.59	11	1
1:A:96:GLY:O	1:A:97:GLN:C	0.41	2.60	15	3
1:A:19:ILE:HG12	1:A:102:LEU:HD23	0.41	1.91	17	2
1:A:17:LEU:HD21	1:A:19:ILE:HD11	0.41	1.92	20	1
1:A:30:ASP:O	1:A:30:ASP:CG	0.41	2.59	17	2
1:A:64:ASP:OD1	1:A:66:ASP:N	0.41	2.54	16	1
1:A:19:ILE:HG21	1:A:104:ILE:HD13	0.40	1.93	13	1
1:A:64:ASP:OD1	1:A:68:ASP:N	0.40	2.50	4	1
1:A:56:THR:HG23	1:A:57:THR:N	0.40	2.31	6	1
1:A:19:ILE:HD12	1:A:31:TRP:CZ3	0.40	2.51	6	1
1:A:68:ASP:O	1:A:69:ARG:O	0.40	2.39	6	1
1:A:20:ARG:NH2	1:A:28:ALA:HB2	0.40	2.31	13	1
1:A:92:GLN:HB2	1:A:99:ILE:HD13	0.40	1.92	5	1
1:A:63:GLU:OE1	1:A:103:GLN:OE1	0.40	2.40	13	1
1:A:61:GLU:O	1:A:105:PHE:N	0.40	2.55	16	1
1:A:64:ASP:OD1	1:A:64:ASP:C	0.40	2.60	16	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	91/113 (81%)	70±2 (77±3%)	16±3 (18±3%)	4±1 (5±1%)	4	27
All	All	1820/2260 (81%)	1410 (77%)	324 (18%)	86 (5%)	4	27

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	102	LEU	20
1	A	69	ARG	18
1	A	26	SER	17
1	A	97	GLN	12
1	A	56	THR	11
1	A	107	ARG	3
1	A	59	ALA	2
1	A	32	THR	1
1	A	64	ASP	1
1	A	27	GLY	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	82/98 (84%)	67±2 (82±2%)	15±2 (18±2%)	4 38
All	All	1640/1960 (84%)	1346 (82%)	294 (18%)	4 38

All 39 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	78	MET	20
1	A	88	THR	20
1	A	22	LYS	17
1	A	26	SER	17
1	A	35	SER	17
1	A	66	ASP	14
1	A	84	TYR	14
1	A	95	ASN	13
1	A	54	GLU	12
1	A	77	GLU	12
1	A	107	ARG	12
1	A	90	MET	11
1	A	74	SER	9
1	A	98	LEU	9

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Mol	Chain	Res	Type	Models (Total)
1	A	57	THR	7
1	A	63	GLU	7
1	A	30	ASP	6
1	A	46	ASP	6
1	A	79	LYS	6
1	A	87	SER	6
1	A	43	ASP	6
1	A	76	GLU	6
1	A	32	THR	5
1	A	83	SER	5
1	A	75	ASP	5
1	A	38	GLN	5
1	A	62	TYR	4
1	A	42	ARG	4
1	A	65	GLU	3
1	A	21	ILE	3
1	A	64	ASP	2
1	A	73	ARG	2
1	A	91	GLU	2
1	A	68	ASP	2
1	A	56	THR	1
1	A	92	GLN	1
1	A	94	VAL	1
1	A	45	LEU	1
1	A	100	GLU	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