



Full wwPDB NMR Structure Validation Report ⓘ

May 28, 2020 – 10:37 pm BST

PDB ID : 2KGL
Title : NMR solution structure of MESD
Authors : Chen, J.; Wang, J.
Deposited on : 2009-03-12

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 ⓘ symbol.

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

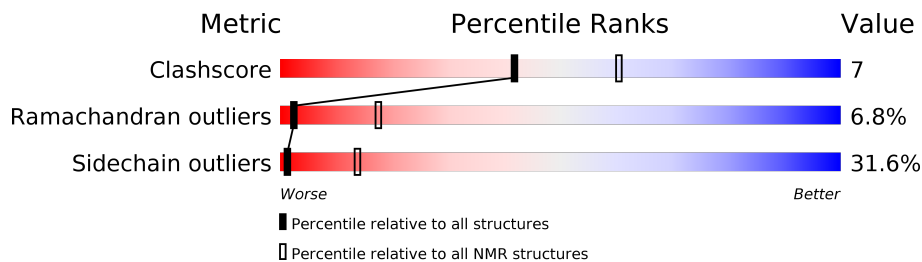
Cyrange : Kirchner and Güntert (2011)
NmrClust : Kelley et al. (1996)
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : 2.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	195	

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:11-A:59, A:64-A:195 (181)	0.73	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 6 single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 3073 atoms, of which 1527 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Mesoderm development candidate 2.

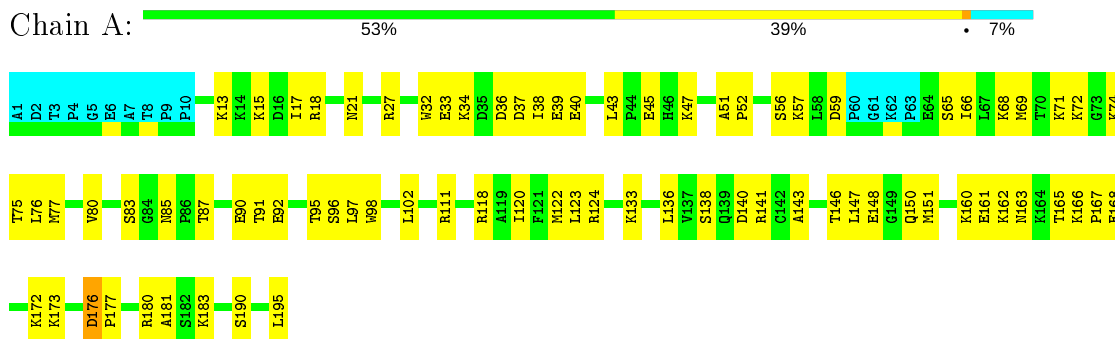
Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	195	3073	960	1527	271	308	7	0

4 Residue-property plots [i](#)

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: Mesoderm development candidate 2

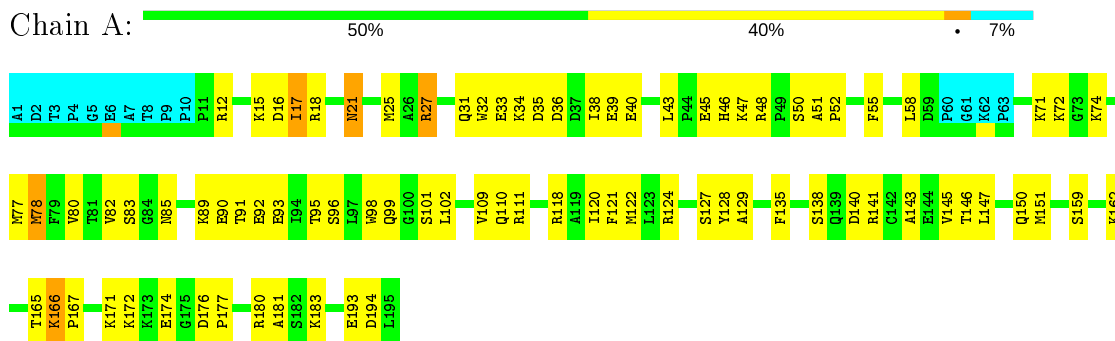


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

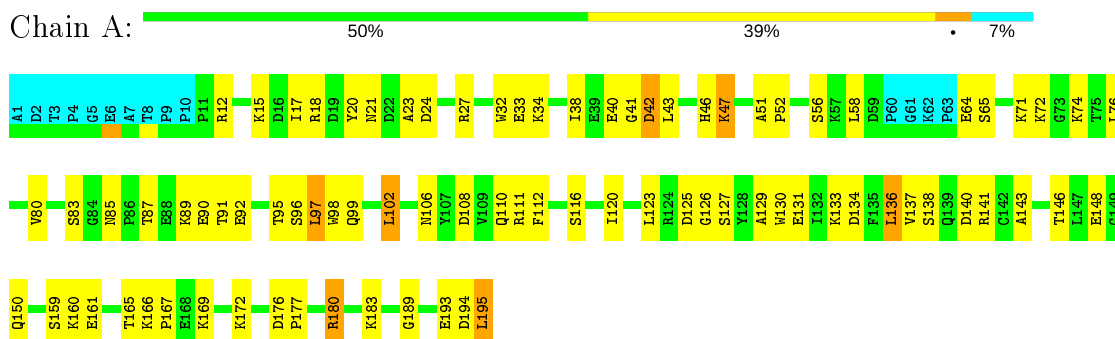
4.2.1 Score per residue for model 1

- Molecule 1: Mesoderm development candidate 2



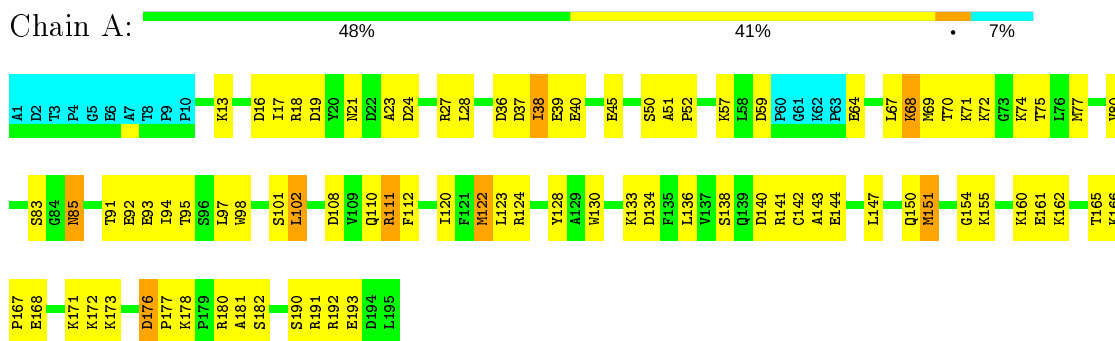
4.2.2 Score per residue for model 2

- Molecule 1: Mesoderm development candidate 2



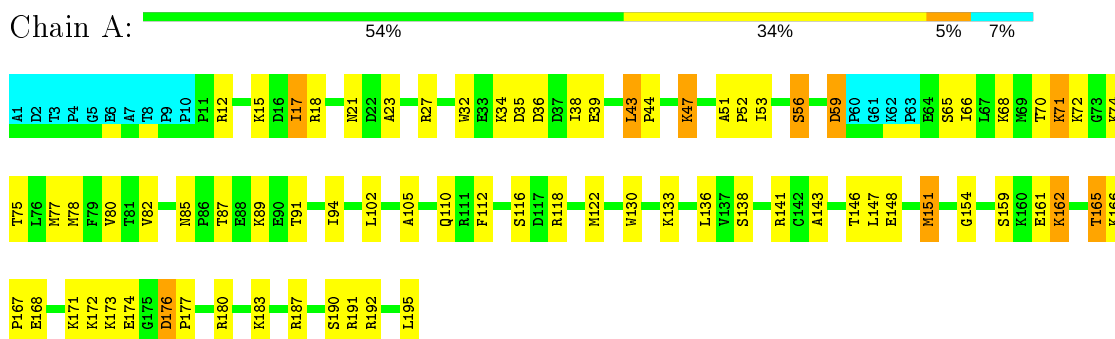
4.2.3 Score per residue for model 3

- Molecule 1: Mesoderm development candidate 2



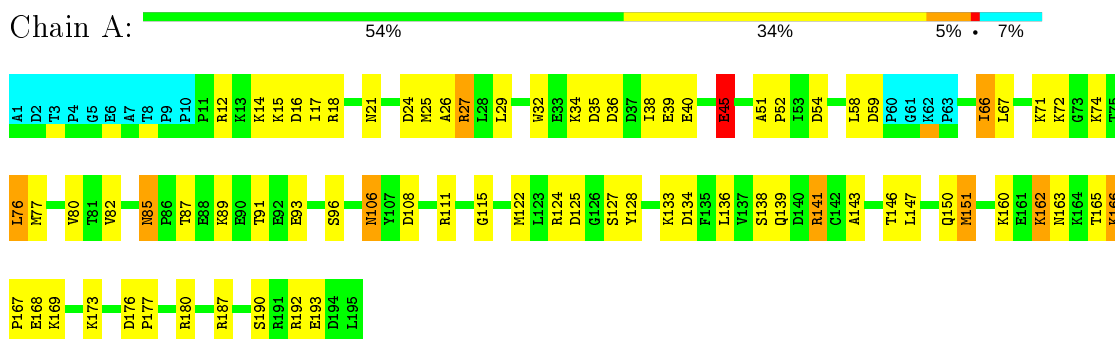
4.2.4 Score per residue for model 4 (medoid)

- Molecule 1: Mesoderm development candidate 2



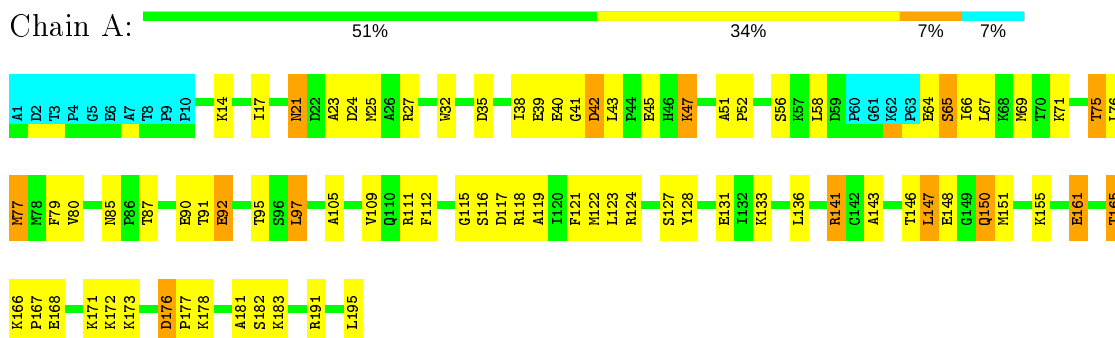
4.2.8 Score per residue for model 8

- Molecule 1: Mesoderm development candidate 2



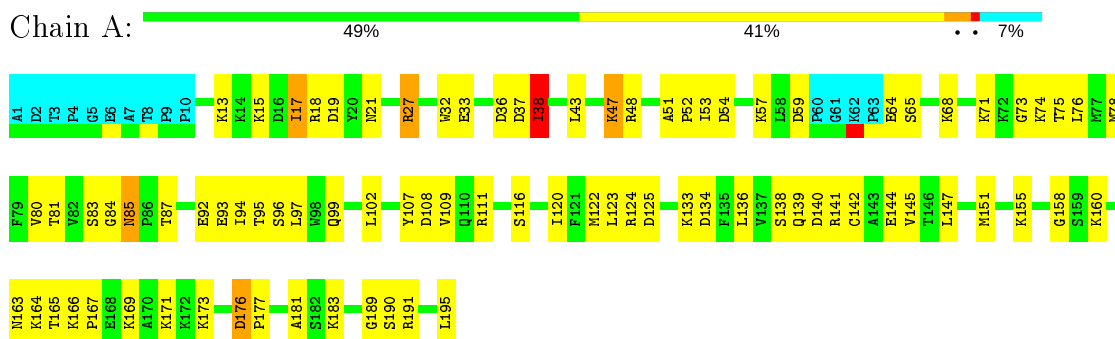
4.2.9 Score per residue for model 9

- Molecule 1: Mesoderm development candidate 2



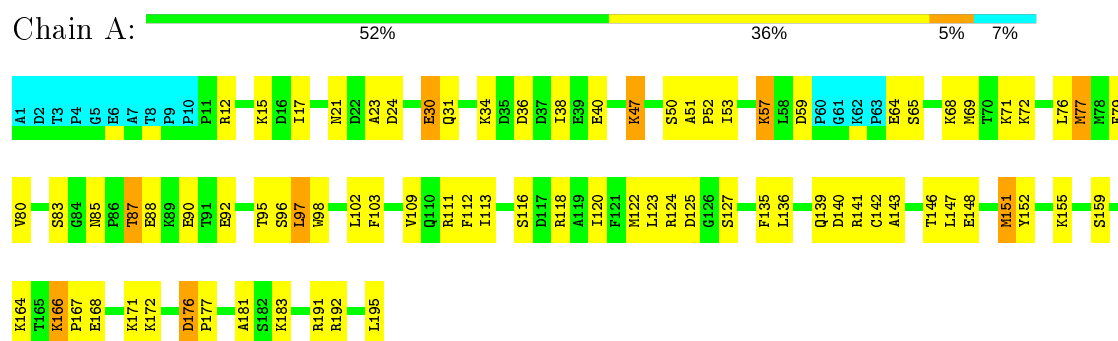
4.2.10 Score per residue for model 10

- Molecule 1: Mesoderm development candidate 2



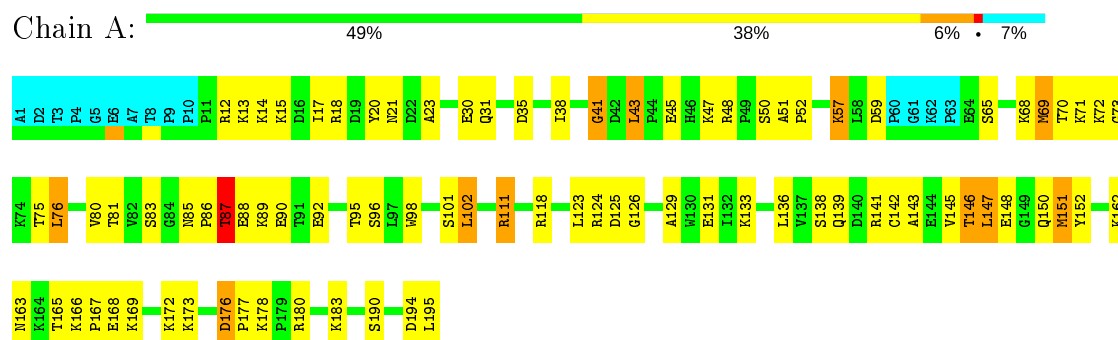
4.2.11 Score per residue for model 11

- Molecule 1: Mesoderm development candidate 2



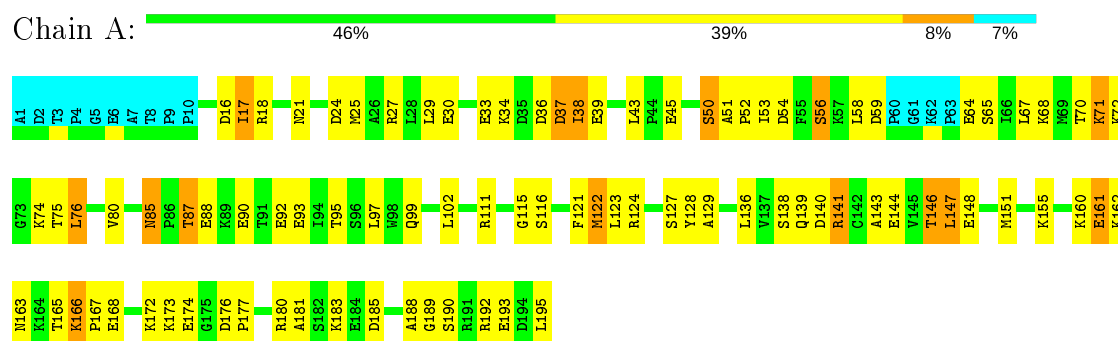
4.2.12 Score per residue for model 12

- Molecule 1: Mesoderm development candidate 2



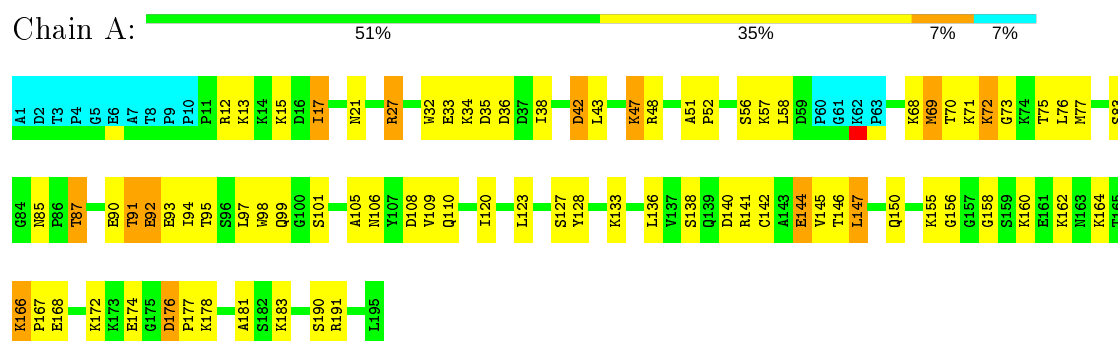
4.2.13 Score per residue for model 13

- Molecule 1: Mesoderm development candidate 2



4.2.14 Score per residue for model 14

- Molecule 1: Mesoderm development candidate 2



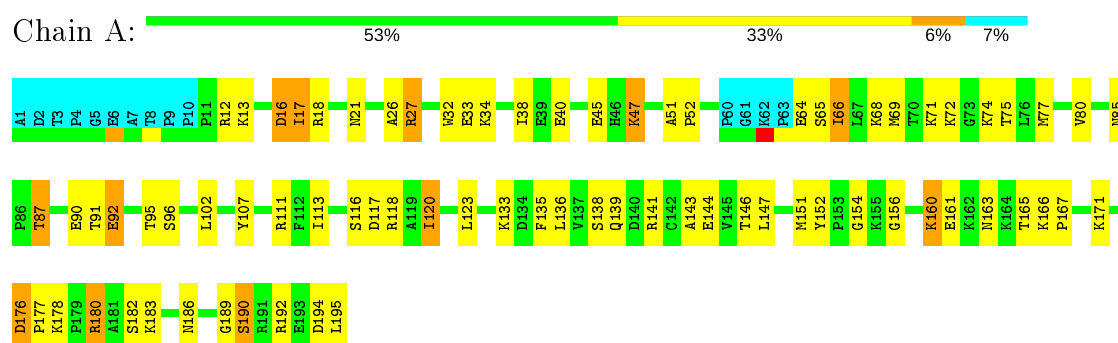
4.2.15 Score per residue for model 15

- Molecule 1: Mesoderm development candidate 2



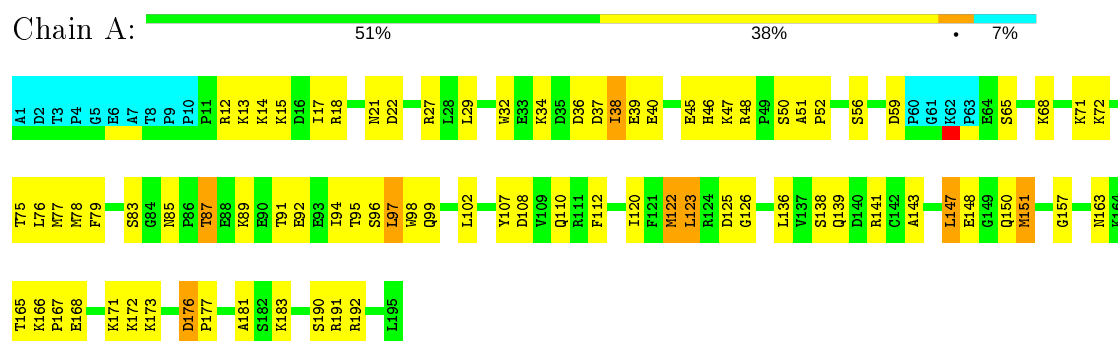
4.2.16 Score per residue for model 16

- Molecule 1: Mesoderm development candidate 2



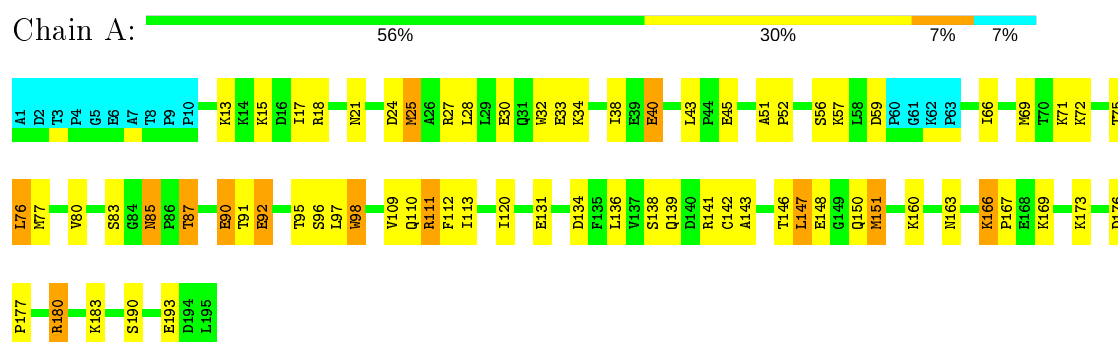
4.2.17 Score per residue for model 17

- Molecule 1: Mesoderm development candidate 2



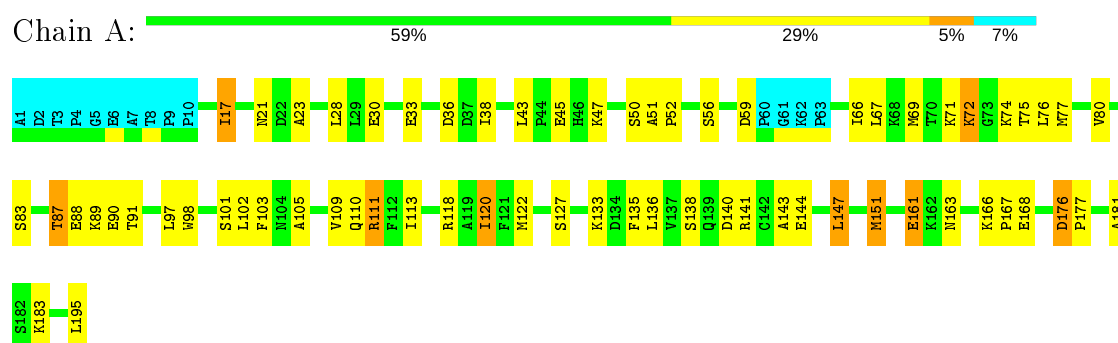
4.2.18 Score per residue for model 18

- Molecule 1: Mesoderm development candidate 2



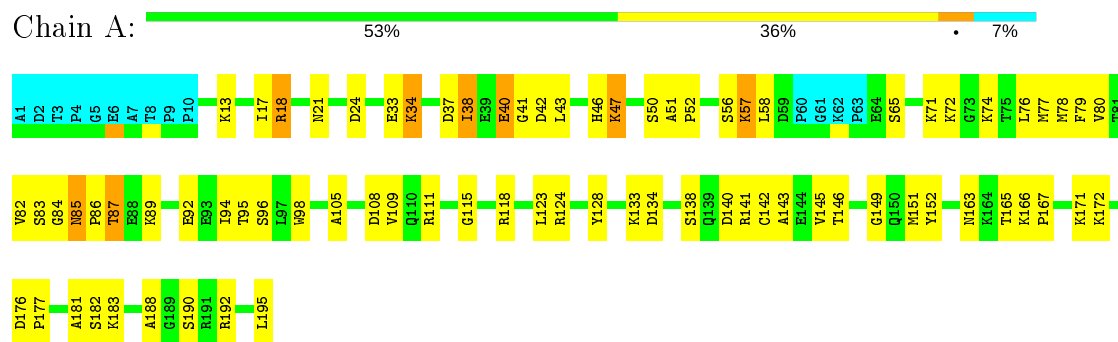
4.2.19 Score per residue for model 19

- Molecule 1: Mesoderm development candidate 2



4.2.20 Score per residue for model 20

- Molecule 1: Mesoderm development candidate 2



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
CNS	refinement	1.2

No chemical shift data was provided. No validations of the models with respect to experimental NMR restraints is performed at this time.

6 Model quality

6.1 Standard geometry

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	1453	1439	1439	21±3
All	All	29060	28780	28780	425

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 7.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:76:LEU:HD23	1:A:97:LEU:HD13	0.86	1.46	11	3
1:A:97:LEU:HD13	1:A:147:LEU:HD21	0.81	1.52	17	1
1:A:123:LEU:HD23	1:A:129:ALA:HB2	0.81	1.52	12	1
1:A:76:LEU:HD23	1:A:97:LEU:HD12	0.77	1.56	19	1
1:A:76:LEU:C	1:A:76:LEU:HD22	0.72	2.05	12	1
1:A:76:LEU:HD22	1:A:76:LEU:C	0.70	2.06	18	1
1:A:97:LEU:HD11	1:A:147:LEU:HD23	0.69	1.64	15	1
1:A:147:LEU:C	1:A:147:LEU:HD22	0.68	2.10	19	2
1:A:147:LEU:HD22	1:A:147:LEU:C	0.67	2.10	13	2
1:A:27:ARG:HB3	1:A:91:THR:HG21	0.67	1.67	14	5
1:A:87:THR:O	1:A:91:THR:HG23	0.65	1.92	4	7
1:A:76:LEU:HD11	1:A:122:MET:CG	0.64	2.22	8	1
1:A:41:GLY:O	1:A:145:VAL:HG12	0.64	1.93	20	2
1:A:87:THR:HG21	1:A:145:VAL:HG21	0.63	1.68	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:76:LEU:CD2	1:A:97:LEU:HD13	0.63	2.24	9	1
1:A:87:THR:HG22	1:A:90:GLU:HB2	0.62	1.71	14	6
1:A:40:GLU:HB3	1:A:143:ALA:HB3	0.61	1.71	15	4
1:A:87:THR:HG22	1:A:90:GLU:CG	0.61	2.25	12	1
1:A:98:TRP:CZ2	1:A:109:VAL:HG21	0.61	2.30	14	3
1:A:78:MET:CG	1:A:145:VAL:HG13	0.61	2.26	7	1
1:A:147:LEU:HD13	1:A:147:LEU:N	0.61	2.11	12	1
1:A:76:LEU:HD13	1:A:77:MET:N	0.60	2.12	19	4
1:A:29:LEU:HD22	1:A:192:ARG:HA	0.60	1.73	8	2
1:A:97:LEU:HD21	1:A:147:LEU:HD11	0.60	1.72	17	1
1:A:23:ALA:HB1	1:A:111:ARG:NE	0.60	2.12	9	1
1:A:76:LEU:HD11	1:A:122:MET:HG3	0.59	1.74	8	1
1:A:27:ARG:CB	1:A:91:THR:HG21	0.59	2.27	14	4
1:A:85:ASN:OD1	1:A:143:ALA:HB1	0.59	1.98	20	3
1:A:92:GLU:O	1:A:95:THR:HG22	0.58	1.98	13	15
1:A:98:TRP:NE1	1:A:102:LEU:HD23	0.58	2.14	3	2
1:A:132:ILE:HG22	1:A:136:LEU:HD23	0.58	1.73	5	1
1:A:79:PHE:CE1	1:A:123:LEU:HD12	0.58	2.34	17	1
1:A:80:VAL:HG23	1:A:143:ALA:HA	0.57	1.75	1	15
1:A:76:LEU:HD13	1:A:122:MET:CE	0.57	2.29	7	1
1:A:67:LEU:HD13	1:A:163:ASN:HB2	0.57	1.76	8	1
1:A:40:GLU:CB	1:A:143:ALA:HB3	0.57	2.30	17	3
1:A:93:GLU:HB3	1:A:147:LEU:HD11	0.57	1.77	10	1
1:A:87:THR:HG22	1:A:90:GLU:HG3	0.57	1.77	12	1
1:A:78:MET:CG	1:A:145:VAL:HG23	0.56	2.29	1	3
1:A:75:THR:O	1:A:97:LEU:HD22	0.56	2.01	13	1
1:A:97:LEU:HD11	1:A:147:LEU:HD21	0.56	1.77	14	2
1:A:68:LYS:O	1:A:70:THR:HG23	0.56	2.00	3	1
1:A:98:TRP:CZ2	1:A:102:LEU:HD12	0.56	2.36	17	2
1:A:45:GLU:HG2	1:A:146:THR:HG23	0.56	1.76	8	1
1:A:17:ILE:HD11	1:A:109:VAL:O	0.56	2.01	14	2
1:A:56:SER:OG	1:A:105:ALA:HB3	0.56	1.99	15	1
1:A:80:VAL:HG21	1:A:85:ASN:CG	0.56	2.20	10	3
1:A:59:ASP:CB	1:A:105:ALA:HB1	0.56	2.30	4	1
1:A:67:LEU:HD22	1:A:159:SER:CB	0.56	2.30	7	1
1:A:29:LEU:HD12	1:A:192:ARG:HG2	0.56	1.76	17	1
1:A:81:THR:HG21	1:A:139:GLN:HB2	0.56	1.77	10	1
1:A:74:LYS:O	1:A:97:LEU:HD22	0.55	2.00	19	2
1:A:67:LEU:HD22	1:A:161:GLU:HG3	0.55	1.79	3	2
1:A:23:ALA:HB1	1:A:111:ARG:CD	0.55	2.32	2	4
1:A:90:GLU:OE2	1:A:147:LEU:HD21	0.55	2.02	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:98:TRP:CH2	1:A:109:VAL:HG21	0.55	2.36	14	2
1:A:97:LEU:CD1	1:A:147:LEU:HD23	0.54	2.32	15	1
1:A:27:ARG:CZ	1:A:120:ILE:HG21	0.54	2.32	16	1
1:A:25:MET:HG3	1:A:28:LEU:HD12	0.54	1.80	18	1
1:A:76:LEU:HD21	1:A:122:MET:HB2	0.54	1.79	13	1
1:A:75:THR:HG22	1:A:154:GLY:CA	0.54	2.33	15	1
1:A:94:ILE:HD12	1:A:122:MET:CE	0.54	2.33	3	2
1:A:76:LEU:HD22	1:A:97:LEU:CB	0.54	2.32	2	1
1:A:43:LEU:HD11	1:A:144:GLU:CG	0.54	2.31	14	1
1:A:48:ARG:CZ	1:A:146:THR:HG21	0.53	2.33	12	1
1:A:70:THR:HG23	1:A:162:LYS:HB3	0.53	1.78	13	1
1:A:78:MET:HG3	1:A:145:VAL:HG13	0.53	1.79	7	1
1:A:58:LEU:HD23	1:A:105:ALA:O	0.53	2.03	14	1
1:A:26:ALA:HB2	1:A:190:SER:CB	0.53	2.34	16	1
1:A:29:LEU:HD13	1:A:192:ARG:HB3	0.53	1.81	8	1
1:A:121:PHE:CE1	1:A:129:ALA:HB1	0.53	2.37	13	2
1:A:147:LEU:HD22	1:A:148:GLU:N	0.53	2.19	11	2
1:A:67:LEU:HD13	1:A:163:ASN:CB	0.53	2.34	8	1
1:A:146:THR:C	1:A:147:LEU:HD13	0.52	2.24	12	1
1:A:39:GLU:HG2	1:A:82:VAL:HG21	0.52	1.80	6	3
1:A:102:LEU:HD23	1:A:102:LEU:O	0.52	2.04	16	1
1:A:97:LEU:CD2	1:A:147:LEU:HD11	0.52	2.34	17	1
1:A:166:LYS:CB	1:A:167:PRO:CD	0.52	2.87	15	17
1:A:70:THR:HG23	1:A:162:LYS:CB	0.52	2.34	13	2
1:A:147:LEU:HD22	1:A:147:LEU:O	0.52	2.05	13	2
1:A:29:LEU:HD13	1:A:192:ARG:CB	0.52	2.35	8	1
1:A:113:ILE:HG22	1:A:118:ARG:CZ	0.52	2.35	7	1
1:A:26:ALA:HB2	1:A:190:SER:HB3	0.52	1.82	16	1
1:A:147:LEU:O	1:A:147:LEU:HD22	0.51	2.05	6	2
1:A:76:LEU:CD2	1:A:76:LEU:C	0.51	2.79	18	1
1:A:102:LEU:O	1:A:102:LEU:HD13	0.51	2.05	12	2
1:A:45:GLU:HG3	1:A:146:THR:HG22	0.51	1.82	13	1
1:A:70:THR:HG23	1:A:162:LYS:HB2	0.51	1.83	4	2
1:A:27:ARG:NE	1:A:120:ILE:HD13	0.51	2.21	6	1
1:A:166:LYS:N	1:A:167:PRO:HD2	0.51	2.21	19	15
1:A:76:LEU:O	1:A:76:LEU:HD22	0.51	2.06	18	2
1:A:102:LEU:HD11	1:A:176:ASP:OD2	0.51	2.06	11	1
1:A:109:VAL:HG22	1:A:122:MET:CB	0.51	2.36	19	2
1:A:28:LEU:HG	1:A:91:THR:HG21	0.51	1.83	19	3
1:A:67:LEU:HD13	1:A:161:GLU:HG2	0.50	1.82	9	1
1:A:109:VAL:HG22	1:A:122:MET:HB2	0.50	1.82	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:17:ILE:HG23	1:A:23:ALA:HB2	0.49	1.84	4	1
1:A:97:LEU:HD21	1:A:147:LEU:HD21	0.49	1.83	18	2
1:A:111:ARG:HA	1:A:120:ILE:HD12	0.49	1.84	19	2
1:A:39:GLU:CG	1:A:82:VAL:HG21	0.49	2.37	8	1
1:A:87:THR:HG21	1:A:145:VAL:HG11	0.49	1.84	14	2
1:A:75:THR:HG21	1:A:124:ARG:NH2	0.49	2.23	10	1
1:A:109:VAL:HG13	1:A:122:MET:HB3	0.49	1.83	19	2
1:A:51:ALA:HB1	1:A:52:PRO:HD2	0.49	1.85	15	20
1:A:78:MET:SD	1:A:145:VAL:HG23	0.49	2.48	10	2
1:A:16:ASP:C	1:A:17:ILE:HD12	0.49	2.28	16	2
1:A:108:ASP:OD2	1:A:129:ALA:HB3	0.49	2.07	2	1
1:A:43:LEU:HB3	1:A:145:VAL:HG13	0.49	1.85	12	1
1:A:29:LEU:HD13	1:A:192:ARG:HB2	0.48	1.84	13	1
1:A:147:LEU:C	1:A:147:LEU:CD2	0.48	2.82	6	2
1:A:80:VAL:CG2	1:A:82:VAL:HG12	0.48	2.38	20	1
1:A:27:ARG:HD3	1:A:120:ILE:HD12	0.48	1.84	3	1
1:A:147:LEU:HD13	1:A:148:GLU:N	0.48	2.24	17	1
1:A:18:ARG:NH1	1:A:188:ALA:HB1	0.48	2.24	20	1
1:A:102:LEU:HD13	1:A:102:LEU:O	0.48	2.08	3	1
1:A:76:LEU:C	1:A:76:LEU:CD2	0.48	2.78	12	1
1:A:17:ILE:HG23	1:A:23:ALA:CB	0.48	2.38	4	2
1:A:23:ALA:HB1	1:A:111:ARG:HG2	0.48	1.85	11	1
1:A:97:LEU:HD21	1:A:147:LEU:CD2	0.48	2.39	15	1
1:A:39:GLU:HG2	1:A:82:VAL:HG11	0.47	1.85	1	3
1:A:98:TRP:CE2	1:A:102:LEU:HD23	0.47	2.44	2	1
1:A:27:ARG:CD	1:A:120:ILE:HD12	0.47	2.38	3	1
1:A:86:PRO:O	1:A:87:THR:HG23	0.47	2.09	12	3
1:A:58:LEU:HD23	1:A:106:ASN:OD1	0.47	2.09	8	1
1:A:27:ARG:HB2	1:A:91:THR:HG21	0.47	1.86	9	1
1:A:78:MET:SD	1:A:94:ILE:HD11	0.47	2.49	4	2
1:A:50:SER:HB3	1:A:75:THR:HG21	0.47	1.86	13	1
1:A:27:ARG:NE	1:A:120:ILE:HG21	0.47	2.23	16	2
1:A:27:ARG:CZ	1:A:120:ILE:HD13	0.47	2.39	6	1
1:A:67:LEU:HD22	1:A:159:SER:HB3	0.47	1.87	7	1
1:A:147:LEU:CD2	1:A:147:LEU:C	0.47	2.82	19	2
1:A:23:ALA:HB1	1:A:111:ARG:HD2	0.47	1.86	2	1
1:A:176:ASP:N	1:A:177:PRO:HD2	0.47	2.25	16	20
1:A:34:LYS:CE	1:A:38:ILE:HD12	0.47	2.40	20	1
1:A:65:SER:HA	1:A:165:THR:HG21	0.47	1.87	9	1
1:A:79:PHE:HB3	1:A:136:LEU:HD13	0.47	1.87	11	4
1:A:97:LEU:HD11	1:A:147:LEU:CD2	0.47	2.40	14	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:176:ASP:CB	1:A:177:PRO:CD	0.46	2.94	13	20
1:A:109:VAL:HG23	1:A:122:MET:HB3	0.46	1.84	9	1
1:A:66:ILE:HG12	1:A:102:LEU:HD23	0.46	1.86	4	1
1:A:111:ARG:NH1	1:A:113:ILE:HD12	0.46	2.26	18	1
1:A:147:LEU:HD13	1:A:147:LEU:C	0.46	2.32	11	5
1:A:17:ILE:HG12	1:A:109:VAL:HG23	0.46	1.86	10	1
1:A:30:GLU:OE2	1:A:113:ILE:HG23	0.46	2.11	11	1
1:A:24:ASP:O	1:A:91:THR:HG23	0.46	2.11	3	1
1:A:66:ILE:HD11	1:A:99:GLN:O	0.46	2.11	7	1
1:A:76:LEU:HD13	1:A:94:ILE:HD12	0.46	1.87	10	1
1:A:165:THR:HG22	1:A:167:PRO:HD2	0.45	1.88	4	1
1:A:147:LEU:HD13	1:A:147:LEU:O	0.45	2.11	11	1
1:A:17:ILE:HD13	1:A:109:VAL:CG1	0.45	2.42	6	1
1:A:76:LEU:HD23	1:A:147:LEU:HD23	0.45	1.89	5	1
1:A:136:LEU:HD23	1:A:137:VAL:N	0.44	2.26	2	1
1:A:75:THR:HG22	1:A:154:GLY:N	0.44	2.27	4	3
1:A:43:LEU:N	1:A:43:LEU:HD22	0.44	2.27	19	1
1:A:80:VAL:HG21	1:A:85:ASN:OD1	0.44	2.12	18	1
1:A:34:LYS:HE3	1:A:38:ILE:HD12	0.44	1.89	20	1
1:A:27:ARG:CD	1:A:120:ILE:HG21	0.44	2.42	10	2
1:A:21:ASN:OD1	1:A:95:THR:HG23	0.44	2.13	7	1
1:A:98:TRP:CZ2	1:A:102:LEU:HD13	0.44	2.48	11	1
1:A:94:ILE:HD12	1:A:122:MET:HE2	0.43	1.90	3	1
1:A:43:LEU:HD12	1:A:144:GLU:HA	0.43	1.89	13	1
1:A:45:GLU:CG	1:A:146:THR:HG23	0.43	2.43	8	1
1:A:126:GLY:O	1:A:129:ALA:HB3	0.43	2.13	6	1
1:A:98:TRP:CH2	1:A:109:VAL:HG11	0.43	2.49	14	2
1:A:75:THR:HG21	1:A:124:ARG:CD	0.43	2.43	9	1
1:A:78:MET:HG2	1:A:145:VAL:HG23	0.43	1.90	1	1
1:A:76:LEU:C	1:A:76:LEU:HD13	0.43	2.34	11	2
1:A:147:LEU:CD1	1:A:147:LEU:N	0.43	2.82	13	5
1:A:29:LEU:HD22	1:A:192:ARG:CA	0.43	2.43	13	1
1:A:147:LEU:C	1:A:147:LEU:HD13	0.42	2.34	1	3
1:A:76:LEU:HD12	1:A:94:ILE:HG23	0.42	1.91	14	1
1:A:82:VAL:HG13	1:A:84:GLY:O	0.42	2.14	20	1
1:A:121:PHE:HE1	1:A:129:ALA:HB1	0.42	1.73	13	1
1:A:79:PHE:CZ	1:A:123:LEU:HD13	0.42	2.49	9	1
1:A:76:LEU:HD12	1:A:77:MET:N	0.42	2.30	8	1
1:A:66:ILE:HD13	1:A:103:PHE:CE2	0.42	2.50	19	1
1:A:76:LEU:HD13	1:A:122:MET:HE3	0.42	1.88	7	1
1:A:39:GLU:CG	1:A:82:VAL:HG11	0.42	2.44	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:76:LEU:HD22	1:A:97:LEU:C	0.42	2.35	17	1
1:A:98:TRP:CZ3	1:A:102:LEU:HD23	0.42	2.49	15	1
1:A:40:GLU:HB2	1:A:143:ALA:HB3	0.42	1.90	17	1
1:A:37:ASP:O	1:A:38:ILE:C	0.42	2.58	3	6
1:A:98:TRP:CZ2	1:A:109:VAL:HG11	0.42	2.49	15	1
1:A:78:MET:CE	1:A:94:ILE:HD11	0.42	2.44	10	2
1:A:26:ALA:HB3	1:A:27:ARG:NH2	0.41	2.30	8	1
1:A:17:ILE:HG13	1:A:109:VAL:HG23	0.41	1.91	1	1
1:A:166:LYS:CB	1:A:167:PRO:HD3	0.41	2.45	15	2
1:A:193:GLU:OE2	1:A:195:LEU:HD23	0.41	2.14	2	1
1:A:166:LYS:N	1:A:167:PRO:CD	0.41	2.84	11	1
1:A:87:THR:HG22	1:A:90:GLU:CB	0.41	2.46	16	1
1:A:185:ASP:O	1:A:188:ALA:HB3	0.41	2.15	13	1
1:A:80:VAL:HG23	1:A:143:ALA:CB	0.41	2.46	4	2
1:A:76:LEU:HD11	1:A:122:MET:HG2	0.41	1.90	8	1
1:A:27:ARG:HH22	1:A:119:ALA:N	0.41	2.14	9	1
1:A:136:LEU:HD13	1:A:136:LEU:C	0.40	2.36	4	1
1:A:69:MET:O	1:A:70:THR:C	0.40	2.59	5	3
1:A:78:MET:HE2	1:A:147:LEU:HB2	0.40	1.92	17	1
1:A:39:GLU:HG3	1:A:82:VAL:HG21	0.40	1.94	5	1
1:A:195:LEU:O	1:A:195:LEU:HD23	0.40	2.15	6	1
1:A:67:LEU:HD22	1:A:161:GLU:CB	0.40	2.46	19	1
1:A:58:LEU:HD22	1:A:105:ALA:O	0.40	2.15	20	1
1:A:43:LEU:HD23	1:A:44:PRO:HD2	0.40	1.92	4	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	180/195 (92%)	131±4 (73±2%)	37±4 (20±2%)	12±2 (7±1%)	2	17
All	All	3600/3900 (92%)	2620 (73%)	735 (20%)	245 (7%)	2	17

All 38 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	21	ASN	20
1	A	17	ILE	20
1	A	38	ILE	20
1	A	71	LYS	20
1	A	141	ARG	20
1	A	47	LYS	15
1	A	151	MET	15
1	A	181	ALA	13
1	A	160	LYS	9
1	A	75	THR	8
1	A	45	GLU	8
1	A	56	SER	7
1	A	180	ARG	7
1	A	189	GLY	7
1	A	57	LYS	6
1	A	150	GLN	4
1	A	115	GLY	4
1	A	53	ILE	3
1	A	41	GLY	3
1	A	73	GLY	3
1	A	156	GLY	3
1	A	194	ASP	3
1	A	72	LYS	3
1	A	126	GLY	3
1	A	107	TYR	3
1	A	42	ASP	3
1	A	159	SER	2
1	A	162	LYS	2
1	A	158	GLY	2
1	A	157	GLY	1
1	A	83	SER	1
1	A	55	PHE	1
1	A	191	ARG	1
1	A	149	GLY	1
1	A	87	THR	1
1	A	58	LEU	1
1	A	84	GLY	1
1	A	13	LYS	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	158/168 (94%)	108±5 (68±3%)	50±5 (32±3%)	1	14
All	All	3160/3360 (94%)	2163 (68%)	997 (32%)	1	14

All 130 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	85	ASN	19
1	A	183	LYS	18
1	A	138	SER	18
1	A	72	LYS	15
1	A	18	ARG	15
1	A	146	THR	15
1	A	172	LYS	14
1	A	34	LYS	14
1	A	133	LYS	14
1	A	165	THR	14
1	A	15	LYS	13
1	A	83	SER	13
1	A	168	GLU	13
1	A	176	ASP	13
1	A	195	LEU	13
1	A	190	SER	13
1	A	59	ASP	13
1	A	87	THR	13
1	A	111	ARG	13
1	A	96	SER	12
1	A	151	MET	12
1	A	140	ASP	12
1	A	36	ASP	11
1	A	173	LYS	11
1	A	65	SER	11
1	A	124	ARG	11
1	A	32	TRP	11
1	A	27	ARG	11
1	A	13	LYS	11
1	A	43	LEU	11
1	A	136	LEU	11
1	A	180	ARG	11
1	A	33	GLU	11

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Mol	Chain	Res	Type	Models (Total)
1	A	118	ARG	10
1	A	40	GLU	10
1	A	163	ASN	10
1	A	77	MET	10
1	A	171	LYS	10
1	A	68	LYS	10
1	A	127	SER	10
1	A	69	MET	10
1	A	74	LYS	10
1	A	12	ARG	10
1	A	89	LYS	10
1	A	155	LYS	9
1	A	134	ASP	9
1	A	148	GLU	9
1	A	50	SER	9
1	A	162	LYS	9
1	A	24	ASP	9
1	A	112	PHE	9
1	A	123	LEU	9
1	A	110	GLN	9
1	A	128	TYR	9
1	A	47	LYS	9
1	A	108	ASP	9
1	A	120	ILE	8
1	A	142	CYS	8
1	A	150	GLN	8
1	A	116	SER	8
1	A	166	LYS	8
1	A	102	LEU	8
1	A	93	GLU	8
1	A	57	LYS	8
1	A	147	LEU	8
1	A	64	GLU	8
1	A	125	ASP	8
1	A	178	LYS	7
1	A	139	GLN	7
1	A	169	LYS	7
1	A	25	MET	7
1	A	191	ARG	7
1	A	99	GLN	7
1	A	135	PHE	7
1	A	122	MET	7

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Mol	Chain	Res	Type	Models (Total)
1	A	131	GLU	6
1	A	106	ASN	6
1	A	90	GLU	6
1	A	193	GLU	6
1	A	30	GLU	6
1	A	161	GLU	6
1	A	192	ARG	6
1	A	35	ASP	6
1	A	92	GLU	5
1	A	46	HIS	5
1	A	174	GLU	5
1	A	76	LEU	5
1	A	48	ARG	5
1	A	45	GLU	5
1	A	101	SER	5
1	A	14	LYS	5
1	A	159	SER	5
1	A	144	GLU	5
1	A	182	SER	5
1	A	39	GLU	5
1	A	97	LEU	5
1	A	56	SER	5
1	A	152	TYR	5
1	A	113	ILE	4
1	A	141	ARG	4
1	A	88	GLU	4
1	A	16	ASP	4
1	A	37	ASP	4
1	A	187	ARG	4
1	A	58	LEU	4
1	A	42	ASP	4
1	A	31	GLN	3
1	A	21	ASN	3
1	A	54	ASP	3
1	A	66	ILE	3
1	A	20	TYR	3
1	A	19	ASP	3
1	A	117	ASP	3
1	A	71	LYS	3
1	A	130	TRP	3
1	A	164	LYS	3
1	A	22	ASP	2

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Mol	Chain	Res	Type	Models (Total)
1	A	78	MET	2
1	A	98	TRP	2
1	A	91	THR	2
1	A	194	ASP	2
1	A	160	LYS	2
1	A	53	ILE	1
1	A	79	PHE	1
1	A	28	LEU	1
1	A	186	ASN	1
1	A	103	PHE	1
1	A	38	ILE	1
1	A	81	THR	1
1	A	121	PHE	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 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

No chemical shift data were provided