Full wwPDB NMR Structure Validation Report (i)

Apr 26, 2016 – 07:56 PM BST

PDB ID	:	2E4J
Title	:	Solution Structure of mouse Lipocalin-type Prostaglandin D Synthase
Authors	:	Shimamoto, S.; Ohkubo, T.
Deposited on	:	2006-12-11

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

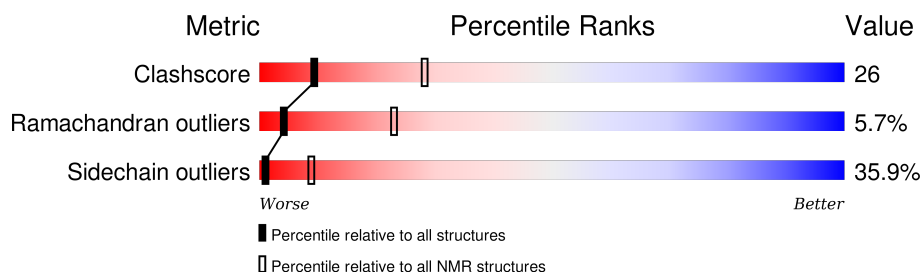|		
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	rb-20027457
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027457

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
SOLUTION NMR

The overall completeness of chemical shifts assignment is 54%.

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	Percentile Ranks	Value
Clashscore		26
Ramachandran outliers		5.7%
Sidechain outliers		35.9%

Worse   *Better*

▮ Percentile relative to all structures

❑ Percentile relative to all NMR structures

Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	114402	11133
Ramachandran outliers	111179	9975
Sidechain outliers	111093	9958

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	A	167	28% 47% 10% 15%

2 Ensemble composition and analysis (i)

This entry contains 15 models. Model 1 is the overall representative, medoid model (most similar to other models).

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:30-A:84, A:88-A:108, A:114-A:137, A:142-A:183 (142)	0.53	1

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 5 single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 2592 atoms, of which 1282 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Prostaglandin-H2 D-isomerase.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	167	2592	828	1282	223	255	4	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	23	GLY	-	EXPRESSION TAG	UNP O09114
A	24	SER	-	EXPRESSION TAG	UNP O09114
A	89	ALA	CYS	ENGINEERED	UNP O09114
A	186	ALA	CYS	ENGINEERED	UNP O09114

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: Prostaglandin-H2 D-isomerase
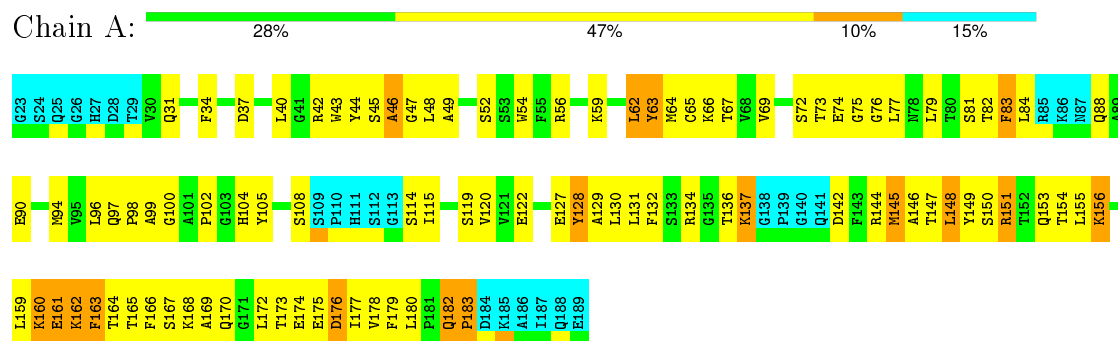
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1 (medoid)

• Molecule 1: Prostaglandin-H2 D-isomerase
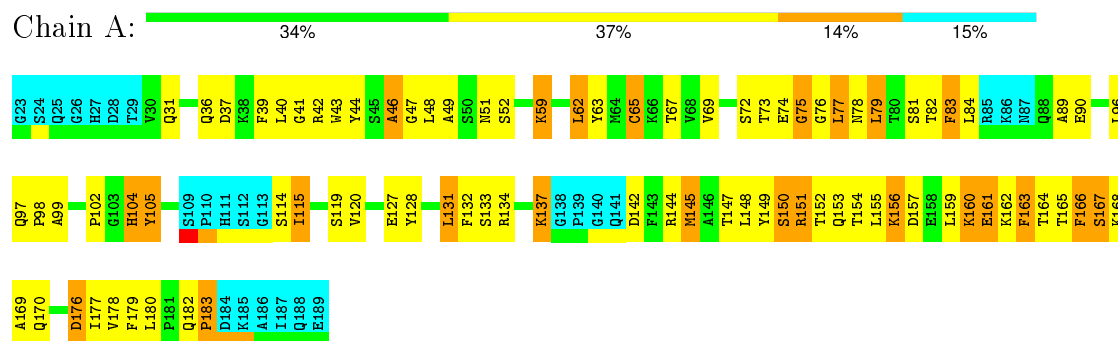
4.2.2 Score per residue for model 2

• Molecule 1: Prostaglandin-H2 D-isomerase

4.2.3 Score per residue for model 3

• Molecule 1: Prostaglandin-H2 D-isomerase

4.2.4 Score per residue for model 4

• Molecule 1: Prostaglandin-H2 D-isomerase
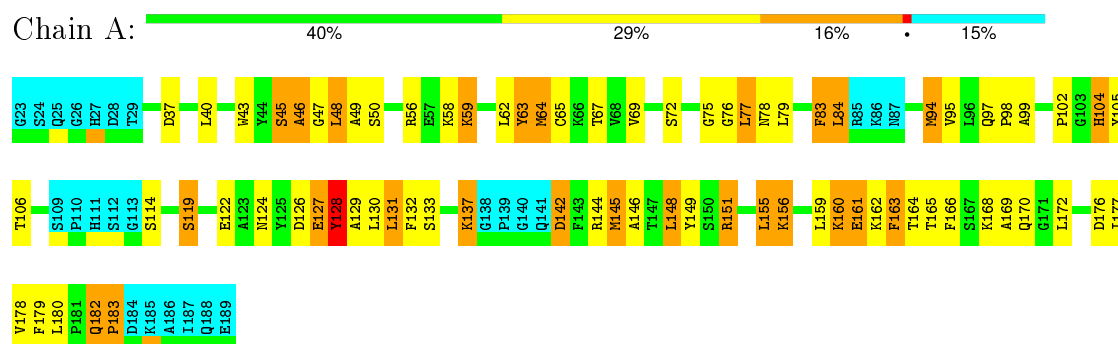
4.2.5   Score per residue for model 5

• Molecule 1: Prostaglandin-H2 D-isomerase
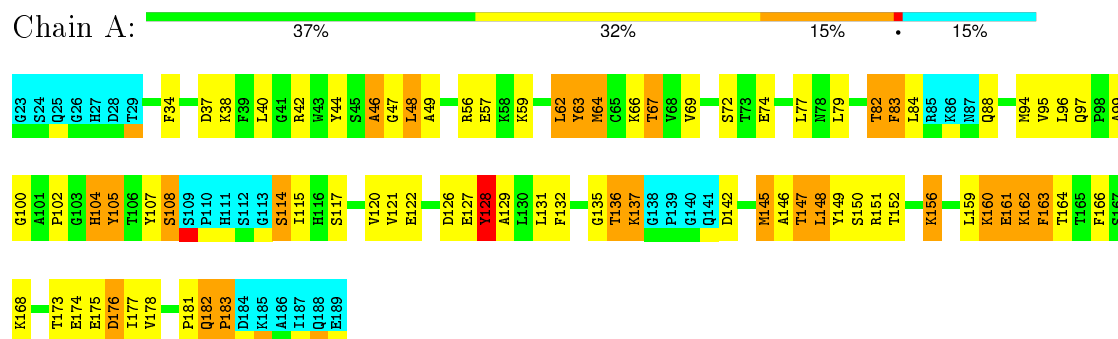
4.2.6   Score per residue for model 6

• Molecule 1: Prostaglandin-H2 D-isomerase

4.2.7   Score per residue for model 7

• Molecule 1: Prostaglandin-H2 D-isomerase
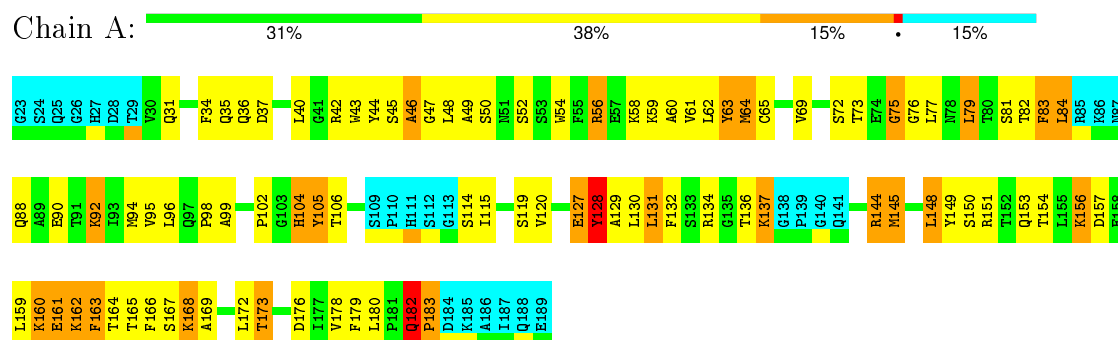
4.2.8　Score per residue for model 8

• Molecule 1: Prostaglandin-H2 D-isomerase
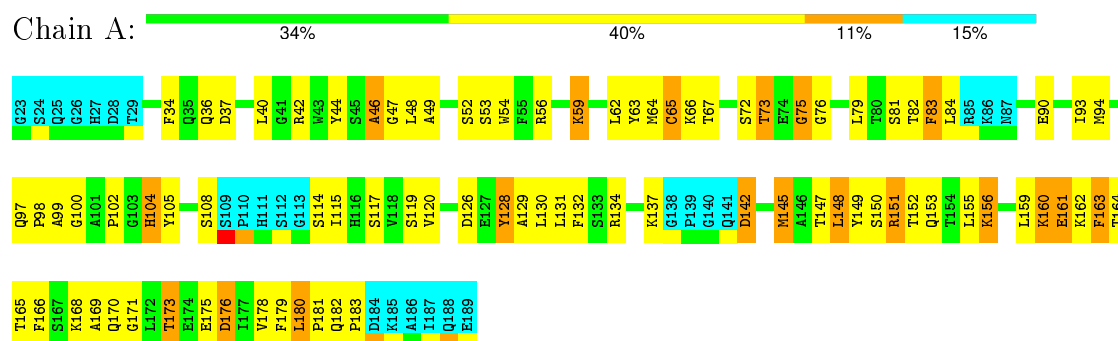
4.2.9　Score per residue for model 9
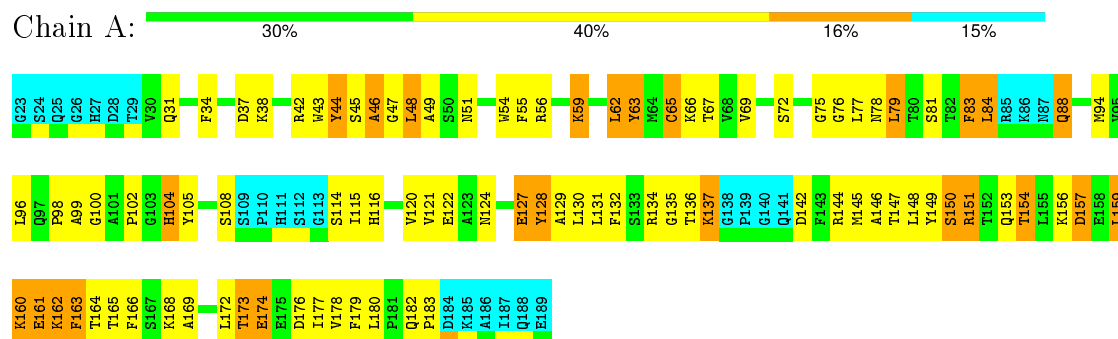
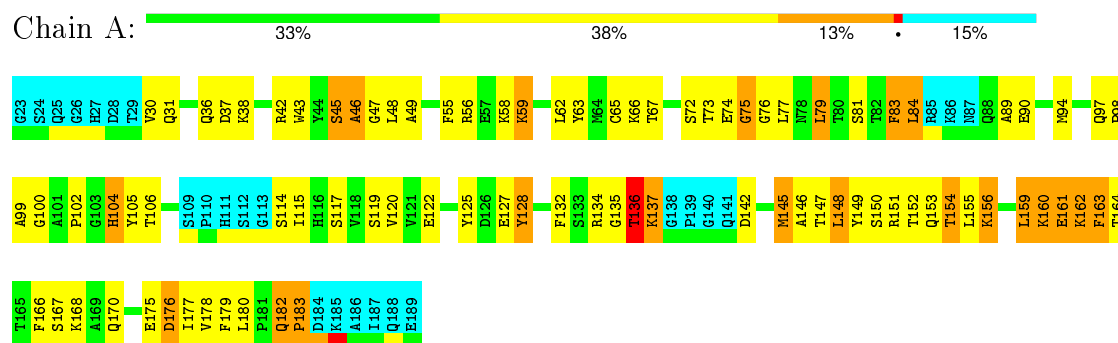• Molecule 1: Prostaglandin-H2 D-isomerase
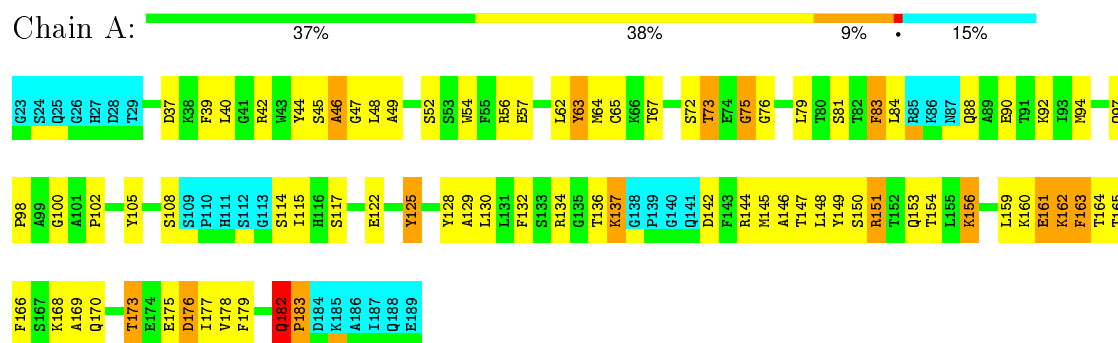
4.2.10　Score per residue for model 10

• Molecule 1: Prostaglandin-H2 D-isomerase
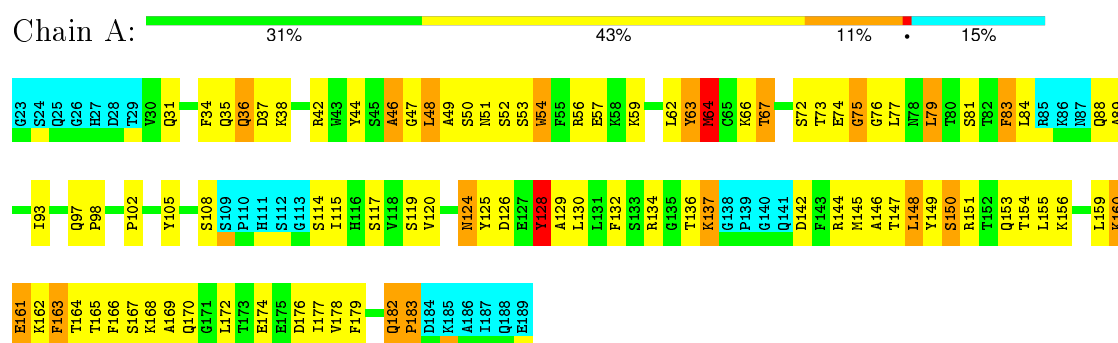
4.2.11 Score per residue for model 11

● Molecule 1: Prostaglandin-H2 D-isomerase

Chain A:

41%   34%   10%   15%
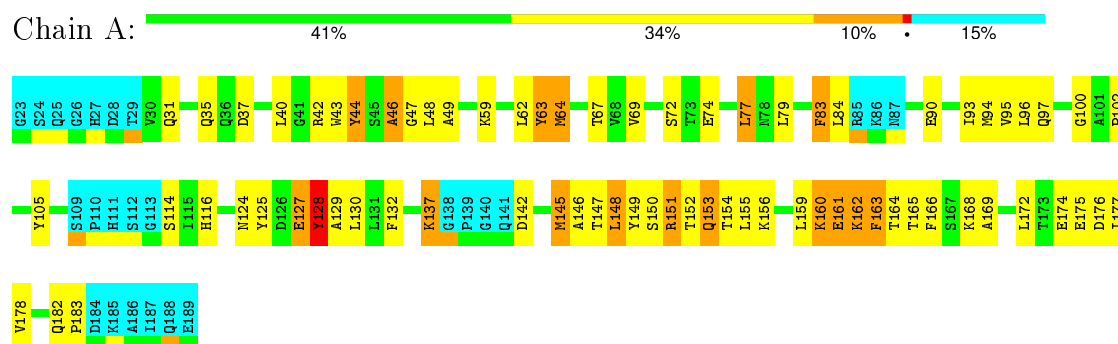
4.2.12 Score per residue for model 12

● Molecule 1: Prostaglandin-H2 D-isomerase

Chain A:

33%   38%   13%   15%
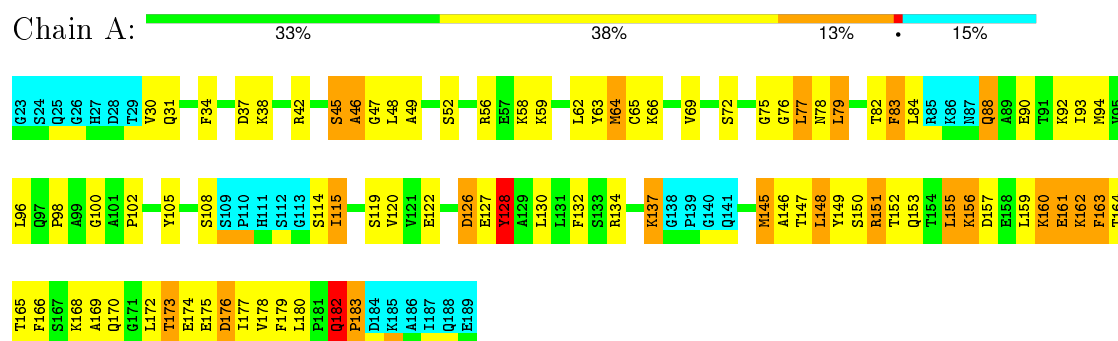
4.2.13 Score per residue for model 13

● Molecule 1: Prostaglandin-H2 D-isomerase

Chain A:

41%   33%   11%   15%
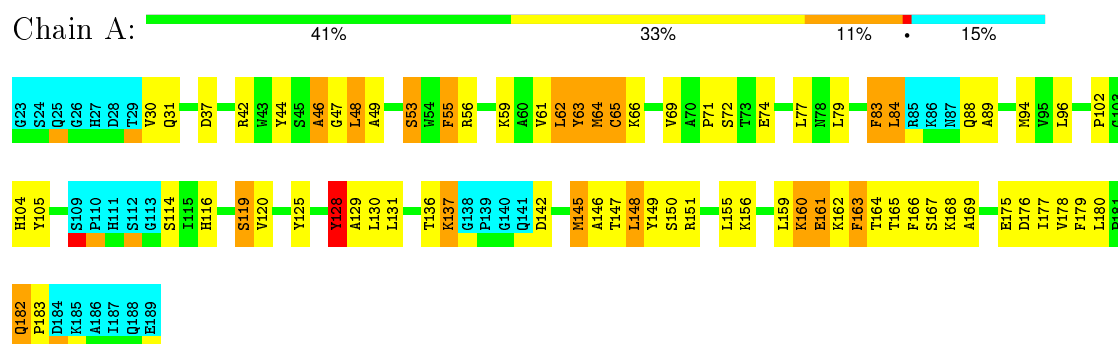
4.2.14 Score per residue for model 14

• Molecule 1: Prostaglandin-H2 D-isomerase

Chain A:

37% 38% 11% 15%
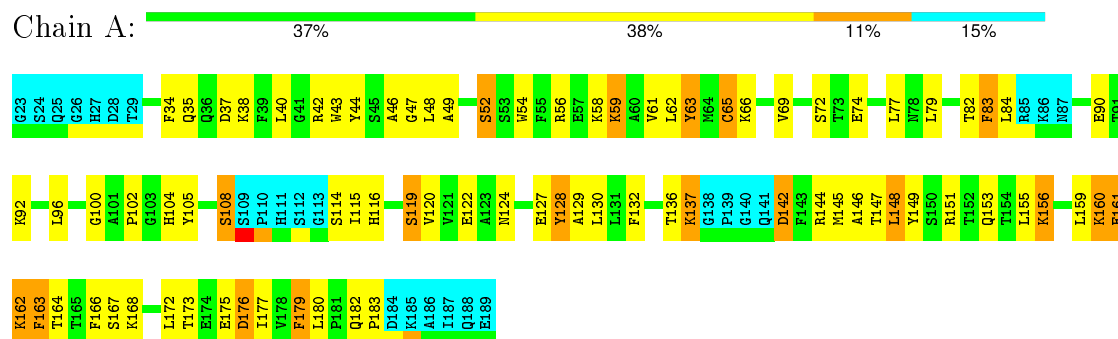
4.2.15 Score per residue for model 15

• Molecule 1: Prostaglandin-H2 D-isomerase

Chain A:

32% 38% 15% • 15%
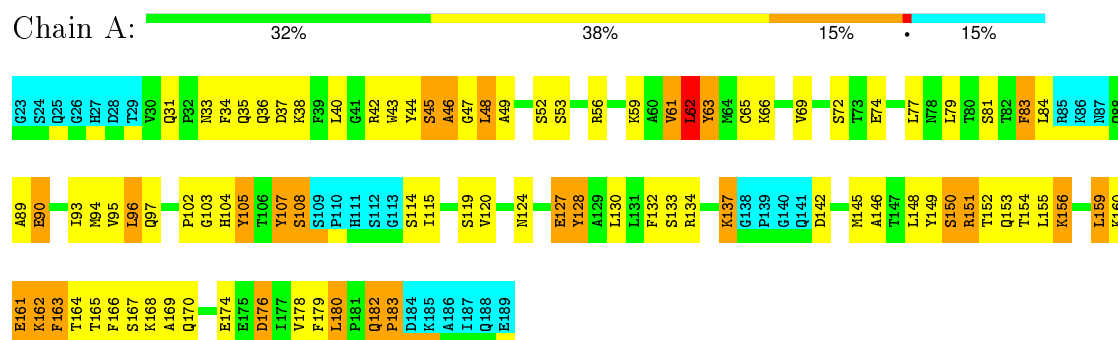
5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *DISTANCE GEOMETRY, SIMULATED ANNEALING, TORSION ANGLE DYNAMICS*.

Of the 30 calculated structures, 15 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	1.1

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

Chemical shift file(s)	BMRB entry 10137
Number of chemical shift lists	1
Total number of shifts	1132
Number of shifts mapped to atoms	1120
Number of unparsed shifts	0
Number of shifts with mapping errors	12
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	54%

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

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	1128	1114	1112	59±4
All	All	16920	16710	16680	888

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 26.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Models Total
1:A:148:LEU:HD21	1:A:159:LEU:HD13	1.09	1.20	5	13
1:A:148:LEU:HD11	1:A:159:LEU:HD22	0.94	1.36	12	8
1:A:159:LEU:HD12	1:A:160:LYS:N	0.93	1.79	13	10
1:A:84:LEU:HD13	1:A:89:ALA:HB2	0.85	1.48	15	3
1:A:164:THR:HG22	1:A:177:ILE:HD13	0.84	1.49	13	1
1:A:148:LEU:HD11	1:A:159:LEU:HD13	0.82	1.47	14	2
1:A:148:LEU:HD12	1:A:149:TYR:N	0.80	1.91	13	15
1:A:69:VAL:HG13	1:A:77:LEU:HD21	0.80	1.52	4	7
1:A:46:ALA:HB3	1:A:150:SER:OG	0.79	1.78	3	12
1:A:163:PHE:CE1	1:A:177:ILE:HD12	0.79	2.13	9	3
1:A:128:TYR:HB3	1:A:159:LEU:HD23	0.78	1.54	12	9
1:A:30:VAL:HG11	1:A:119:SER:OG	0.76	1.80	13	1
1:A:62:LEU:CD2	1:A:180:LEU:HD23	0.76	2.11	1	1
1:A:59:LYS:O	1:A:62:LEU:HD23	0.74	1.82	13	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:65:CYS:SG	1:A:180:LEU:HD13	0.73	2.23	12	2
1:A:108:SER:OG	1:A:115:ILE:HG23	0.73	1.82	14	2
1:A:148:LEU:CD2	1:A:159:LEU:HD13	0.72	2.12	12	6
1:A:59:LYS:HB2	1:A:62:LEU:HD12	0.71	1.61	3	3
1:A:62:LEU:O	1:A:62:LEU:HD12	0.70	1.84	8	2
1:A:148:LEU:HD21	1:A:159:LEU:CD1	0.70	2.17	8	7
1:A:108:SER:CB	1:A:115:ILE:HG23	0.70	2.16	14	4
1:A:129:ALA:C	1:A:130:LEU:HD22	0.70	2.07	9	9
1:A:148:LEU:CD1	1:A:159:LEU:HD13	0.69	2.17	14	2
1:A:179:PHE:CD1	1:A:179:PHE:N	0.69	2.58	14	1
1:A:34:PHE:CE2	1:A:120:VAL:HG11	0.69	2.22	14	6
1:A:82:THR:HG23	1:A:90:GLU:O	0.69	1.87	14	3
1:A:69:VAL:CG1	1:A:77:LEU:HD11	0.69	2.18	15	2
1:A:48:LEU:HD23	1:A:146:ALA:O	0.68	1.88	5	4
1:A:164:THR:HG23	1:A:177:ILE:HD11	0.68	1.65	10	2
1:A:156:LYS:HD2	1:A:159:LEU:HD21	0.68	1.66	3	5
1:A:168:LYS:NZ	1:A:173:THR:HG23	0.68	2.03	6	1
1:A:65:CYS:HB2	1:A:180:LEU:HD22	0.68	1.64	2	8
1:A:114:SER:HA	1:A:137:LYS:CB	0.67	2.19	13	3
1:A:83:PHE:N	1:A:83:PHE:CD1	0.67	2.62	6	6
1:A:129:ALA:C	1:A:130:LEU:HD12	0.67	2.10	6	1
1:A:120:VAL:HA	1:A:131:LEU:HD23	0.67	1.67	8	2
1:A:108:SER:HA	1:A:115:ILE:HG23	0.67	1.64	9	1
1:A:67:THR:CG2	1:A:79:LEU:HD21	0.67	2.19	5	4
1:A:36:GLN:OE1	1:A:77:LEU:HD13	0.66	1.90	10	1
1:A:79:LEU:HD21	1:A:96:LEU:HD23	0.66	1.67	6	1
1:A:84:LEU:HD22	1:A:89:ALA:HB2	0.66	1.64	13	1
1:A:108:SER:HB2	1:A:115:ILE:HG22	0.66	1.67	2	1
1:A:96:LEU:HD12	1:A:105:TYR:CD2	0.66	2.25	1	1
1:A:49:ALA:HB1	1:A:176:ASP:O	0.66	1.91	11	15
1:A:176:ASP:O	1:A:177:ILE:HD13	0.66	1.90	3	4
1:A:131:LEU:HD22	1:A:131:LEU:N	0.66	2.06	6	2
1:A:148:LEU:CD1	1:A:159:LEU:HD22	0.66	2.18	12	1
1:A:130:LEU:HD11	1:A:163:PHE:HB2	0.65	1.67	10	3
1:A:114:SER:HA	1:A:137:LYS:HB2	0.65	1.69	13	3
1:A:67:THR:CG2	1:A:79:LEU:HD22	0.64	2.22	11	1
1:A:83:PHE:CD1	1:A:83:PHE:N	0.64	2.63	15	9
1:A:160:LYS:O	1:A:164:THR:HG22	0.64	1.92	12	4
1:A:135:GLY:O	1:A:136:THR:HG23	0.64	1.93	3	3
1:A:48:LEU:HD23	1:A:49:ALA:N	0.64	2.08	9	1
1:A:182:GLN:HB2	1:A:183:PRO:HD2	0.64	1.68	6	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:69:VAL:HG12	1:A:77:LEU:HD11	0.63	1.68	15	1
1:A:48:LEU:O	1:A:178:VAL:N	0.63	2.32	11	5
1:A:65:CYS:SG	1:A:180:LEU:HD22	0.62	2.34	8	2
1:A:84:LEU:CD1	1:A:89:ALA:HB2	0.62	2.22	15	2
1:A:159:LEU:O	1:A:163:PHE:HB3	0.62	1.95	7	15
1:A:62:LEU:HD13	1:A:181:PRO:HD3	0.62	1.70	8	1
1:A:148:LEU:C	1:A:148:LEU:HD12	0.62	2.14	4	4
1:A:151:ARG:HD3	1:A:152:THR:HG23	0.62	1.71	8	1
1:A:65:CYS:HB2	1:A:180:LEU:HD13	0.62	1.72	14	1
1:A:67:THR:HG21	1:A:79:LEU:HD11	0.61	1.72	7	2
1:A:168:LYS:HZ2	1:A:173:THR:HG23	0.61	1.56	6	1
1:A:129:ALA:O	1:A:130:LEU:HD22	0.61	1.95	10	3
1:A:67:THR:CG2	1:A:79:LEU:HD11	0.61	2.25	7	2
1:A:67:THR:HG22	1:A:79:LEU:HD22	0.61	1.73	11	2
1:A:166:PHE:CD1	1:A:167:SER:N	0.61	2.68	1	1
1:A:84:LEU:HD13	1:A:89:ALA:CB	0.60	2.25	15	1
1:A:166:PHE:C	1:A:166:PHE:CD1	0.59	2.76	1	9
1:A:148:LEU:HD11	1:A:159:LEU:CD1	0.59	2.26	14	1
1:A:156:LYS:CE	1:A:159:LEU:HD21	0.59	2.28	2	2
1:A:76:GLY:HA2	1:A:98:PRO:CD	0.59	2.27	8	9
1:A:55:PHE:CE1	1:A:178:VAL:HG23	0.58	2.34	13	1
1:A:104:HIS:CD2	1:A:119:SER:HG	0.57	2.17	14	1
1:A:114:SER:HA	1:A:137:LYS:HA	0.57	1.76	15	10
1:A:115:ILE:HD13	1:A:115:ILE:N	0.57	2.15	1	1
1:A:108:SER:HB3	1:A:115:ILE:HG23	0.57	1.76	14	2
1:A:115:ILE:N	1:A:115:ILE:HD13	0.57	2.15	12	1
1:A:163:PHE:HE1	1:A:177:ILE:HD12	0.57	1.58	3	3
1:A:172:LEU:HD21	1:A:176:ASP:CG	0.57	2.21	2	6
1:A:131:LEU:HB2	1:A:147:THR:HG23	0.57	1.77	7	2
1:A:173:THR:O	1:A:177:ILE:HD12	0.56	1.99	2	2
1:A:45:SER:OG	1:A:180:LEU:HD13	0.56	2.00	15	2
1:A:45:SER:CB	1:A:180:LEU:HD13	0.56	2.29	15	1
1:A:128:TYR:CB	1:A:159:LEU:HD23	0.56	2.30	4	3
1:A:163:PHE:CD1	1:A:163:PHE:C	0.56	2.79	13	9
1:A:108:SER:HB2	1:A:115:ILE:HG23	0.56	1.77	10	1
1:A:156:LYS:HZ1	1:A:159:LEU:HD23	0.56	1.61	13	2
1:A:47:GLY:HA3	1:A:148:LEU:HD23	0.56	1.78	14	13
1:A:154:THR:O	1:A:156:LYS:NZ	0.55	2.39	15	5
1:A:65:CYS:CB	1:A:180:LEU:HD22	0.55	2.31	15	1
1:A:62:LEU:HD12	1:A:62:LEU:O	0.55	2.01	5	3
1:A:84:LEU:HD22	1:A:89:ALA:CB	0.55	2.32	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:93:ILE:HD12	1:A:93:ILE:N	0.54	2.16	7	1
1:A:182:GLN:HB3	1:A:183:PRO:HD2	0.54	1.79	12	3
1:A:96:LEU:HD23	1:A:96:LEU:O	0.54	2.03	15	1
1:A:161:GLU:HG2	1:A:162:LYS:N	0.54	2.18	1	15
1:A:67:THR:HG23	1:A:79:LEU:HD21	0.54	1.78	7	2
1:A:30:VAL:HG11	1:A:119:SER:CB	0.54	2.32	13	1
1:A:84:LEU:CD2	1:A:89:ALA:HB2	0.54	2.31	13	1
1:A:69:VAL:HG22	1:A:79:LEU:HD21	0.54	1.78	11	1
1:A:96:LEU:HD12	1:A:105:TYR:HB2	0.54	1.79	6	2
1:A:150:SER:HA	1:A:156:LYS:HE3	0.53	1.78	10	3
1:A:67:THR:HG21	1:A:79:LEU:HD21	0.53	1.78	4	3
1:A:155:LEU:HD13	1:A:179:PHE:CE2	0.53	2.38	12	2
1:A:154:THR:O	1:A:156:LYS:HE2	0.53	2.03	3	1
1:A:64:MET:HB3	1:A:182:GLN:O	0.53	2.04	12	4
1:A:49:ALA:O	1:A:145:MET:HA	0.53	2.03	14	15
1:A:77:LEU:O	1:A:95:VAL:HG23	0.53	2.04	6	4
1:A:47:GLY:HA3	1:A:148:LEU:CD2	0.53	2.34	4	5
1:A:163:PHE:C	1:A:163:PHE:CD1	0.52	2.82	10	6
1:A:159:LEU:C	1:A:159:LEU:HD12	0.52	2.24	14	4
1:A:56:ARG:O	1:A:60:ALA:HB2	0.52	2.04	6	1
1:A:128:TYR:CD1	1:A:128:TYR:N	0.52	2.78	14	3
1:A:164:THR:CG2	1:A:177:ILE:HD13	0.52	2.29	13	1
1:A:96:LEU:HD11	1:A:105:TYR:CD2	0.52	2.40	15	1
1:A:84:LEU:C	1:A:84:LEU:HD23	0.52	2.25	5	1
1:A:115:ILE:H	1:A:115:ILE:HD13	0.52	1.63	1	1
1:A:65:CYS:CB	1:A:180:LEU:HD13	0.52	2.33	14	1
1:A:120:VAL:HA	1:A:131:LEU:HD12	0.52	1.81	6	2
1:A:96:LEU:HD23	1:A:96:LEU:C	0.52	2.24	15	1
1:A:49:ALA:HB3	1:A:146:ALA:HB3	0.52	1.82	10	9
1:A:49:ALA:HB2	1:A:163:PHE:CZ	0.52	2.40	9	12
1:A:182:GLN:O	1:A:183:PRO:O	0.51	2.27	15	1
1:A:114:SER:C	1:A:137:LYS:HG3	0.51	2.26	1	2
1:A:163:PHE:HA	1:A:166:PHE:CD2	0.51	2.40	1	1
1:A:163:PHE:CD1	1:A:164:THR:N	0.51	2.78	1	15
1:A:182:GLN:CB	1:A:183:PRO:HD2	0.51	2.35	15	3
1:A:79:LEU:HD22	1:A:96:LEU:HD12	0.51	1.82	12	1
1:A:45:SER:HB3	1:A:180:LEU:HD13	0.51	1.82	15	2
1:A:151:ARG:H	1:A:156:LYS:CD	0.51	2.18	1	2
1:A:61:VAL:HG21	1:A:63:TYR:CE2	0.51	2.41	15	1
1:A:150:SER:CA	1:A:156:LYS:HE3	0.50	2.36	10	3
1:A:149:TYR:O	1:A:159:LEU:HD22	0.50	2.06	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Total
1:A:129:ALA:HB3	1:A:149:TYR:HB2	0.50	1.83	6	5
1:A:96:LEU:CD1	1:A:105:TYR:CD2	0.50	2.93	15	1
1:A:182:GLN:CB	1:A:183:PRO:CD	0.50	2.88	5	4
1:A:156:LYS:CE	1:A:159:LEU:HD23	0.50	2.37	11	2
1:A:95:VAL:O	1:A:96:LEU:HD22	0.50	2.06	5	1
1:A:164:THR:HG23	1:A:177:ILE:CD1	0.50	2.36	10	3
1:A:43:TRP:CZ3	1:A:127:GLU:O	0.50	2.65	14	3
1:A:59:LYS:CB	1:A:62:LEU:HD12	0.50	2.34	3	1
1:A:114:SER:HA	1:A:137:LYS:CA	0.49	2.37	11	5
1:A:63:TYR:CD1	1:A:83:PHE:CB	0.49	2.96	4	3
1:A:128:TYR:CD1	1:A:156:LYS:HD2	0.49	2.43	2	3
1:A:61:VAL:O	1:A:63:TYR:CD2	0.49	2.65	13	4
1:A:152:THR:OG1	1:A:156:LYS:HG3	0.49	2.07	15	2
1:A:156:LYS:N	1:A:156:LYS:HE2	0.49	2.23	1	1
1:A:148:LEU:HD11	1:A:159:LEU:CD2	0.49	2.25	12	1
1:A:115:ILE:HD13	1:A:115:ILE:H	0.49	1.67	12	1
1:A:67:THR:HG23	1:A:79:LEU:HD12	0.49	1.84	2	1
1:A:59:LYS:HE3	1:A:178:VAL:HG23	0.49	1.84	3	1
1:A:69:VAL:CG1	1:A:77:LEU:HD21	0.48	2.33	4	1
1:A:167:SER:OG	1:A:172:LEU:HD23	0.48	2.08	14	1
1:A:148:LEU:HD21	1:A:159:LEU:HB2	0.48	1.85	3	2
1:A:156:LYS:HE2	1:A:156:LYS:H	0.48	1.67	10	2
1:A:49:ALA:CB	1:A:176:ASP:O	0.48	2.62	1	13
1:A:48:LEU:HA	1:A:146:ALA:O	0.48	2.09	10	7
1:A:156:LYS:O	1:A:159:LEU:CD1	0.48	2.62	4	8
1:A:148:LEU:HD12	1:A:148:LEU:C	0.48	2.28	8	4
1:A:30:VAL:HG12	1:A:120:VAL:O	0.48	2.09	3	2
1:A:61:VAL:CG2	1:A:63:TYR:CE2	0.47	2.97	15	1
1:A:99:ALA:HB3	1:A:104:HIS:O	0.47	2.09	3	8
1:A:62:LEU:HD12	1:A:62:LEU:C	0.47	2.30	12	2
1:A:114:SER:CA	1:A:137:LYS:HA	0.47	2.40	5	5
1:A:114:SER:HA	1:A:137:LYS:HG3	0.47	1.85	14	8
1:A:34:PHE:CE2	1:A:120:VAL:HG21	0.47	2.44	12	1
1:A:128:TYR:N	1:A:128:TYR:CD1	0.47	2.82	15	2
1:A:76:GLY:HA2	1:A:98:PRO:HD2	0.47	1.86	8	2
1:A:83:PHE:CD2	1:A:90:GLU:CB	0.47	2.98	15	2
1:A:108:SER:CA	1:A:115:ILE:HG23	0.46	2.37	9	1
1:A:174:GLU:HA	1:A:177:ILE:HD12	0.46	1.87	12	2
1:A:181:PRO:O	1:A:182:GLN:O	0.46	2.33	5	1
1:A:156:LYS:HE2	1:A:156:LYS:N	0.46	2.25	3	2
1:A:64:MET:HB2	1:A:84:LEU:CB	0.46	2.40	6	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:156:LYS:HE2	1:A:159:LEU:HD21	0.46	1.87	10	1
1:A:46:ALA:O	1:A:179:PHE:CD2	0.46	2.68	3	12
1:A:47:GLY:O	1:A:148:LEU:N	0.46	2.48	15	12
1:A:128:TYR:CD1	1:A:156:LYS:NZ	0.46	2.83	11	2
1:A:43:TRP:CH2	1:A:127:GLU:HA	0.46	2.46	6	5
1:A:34:PHE:CE2	1:A:120:VAL:CG1	0.46	2.99	14	1
1:A:44:TYR:CZ	1:A:183:PRO:HG3	0.46	2.45	10	2
1:A:77:LEU:N	1:A:96:LEU:O	0.46	2.49	5	7
1:A:45:SER:O	1:A:46:ALA:HB2	0.46	2.11	12	3
1:A:178:VAL:O	1:A:178:VAL:HG13	0.45	2.11	10	9
1:A:150:SER:HB3	1:A:156:LYS:CE	0.45	2.40	3	1
1:A:156:LYS:CE	1:A:156:LYS:N	0.45	2.79	1	2
1:A:150:SER:CB	1:A:156:LYS:NZ	0.45	2.79	5	1
1:A:114:SER:OG	1:A:137:LYS:HD3	0.45	2.11	11	3
1:A:44:TYR:CZ	1:A:183:PRO:CG	0.45	3.00	10	1
1:A:130:LEU:N	1:A:130:LEU:HD22	0.45	2.25	14	1
1:A:178:VAL:HG13	1:A:178:VAL:O	0.45	2.11	15	3
1:A:151:ARG:H	1:A:156:LYS:HD3	0.45	1.71	1	2
1:A:48:LEU:HB3	1:A:178:VAL:HG13	0.45	1.87	9	1
1:A:128:TYR:CD2	1:A:151:ARG:CB	0.45	3.00	4	2
1:A:151:ARG:CB	1:A:156:LYS:HD3	0.45	2.41	6	3
1:A:44:TYR:N	1:A:44:TYR:CD1	0.45	2.84	11	3
1:A:156:LYS:NZ	1:A:159:LEU:HD23	0.45	2.27	13	2
1:A:44:TYR:CE2	1:A:183:PRO:CG	0.45	2.99	9	1
1:A:40:LEU:HD23	1:A:41:GLY:N	0.45	2.27	1	1
1:A:64:MET:O	1:A:83:PHE:HA	0.45	2.11	7	2
1:A:157:ASP:HA	1:A:160:LYS:HB3	0.45	1.87	12	4
1:A:124:ASN:O	1:A:128:TYR:CD1	0.45	2.70	4	1
1:A:156:LYS:H	1:A:156:LYS:HE2	0.45	1.72	15	1
1:A:130:LEU:HD22	1:A:130:LEU:N	0.45	2.27	7	1
1:A:67:THR:HG23	1:A:79:LEU:CD2	0.45	2.41	7	2
1:A:108:SER:CB	1:A:115:ILE:HG22	0.45	2.42	5	2
1:A:63:TYR:CE1	1:A:83:PHE:CD2	0.44	3.05	4	2
1:A:49:ALA:O	1:A:145:MET:CA	0.44	2.65	13	3
1:A:173:THR:HG22	1:A:174:GLU:H	0.44	1.72	2	2
1:A:159:LEU:HD12	1:A:160:LYS:H	0.44	1.67	13	2
1:A:119:SER:O	1:A:131:LEU:HD23	0.44	2.12	4	1
1:A:121:VAL:HG23	1:A:131:LEU:CA	0.44	2.42	2	1
1:A:64:MET:HG3	1:A:182:GLN:O	0.44	2.13	11	2
1:A:64:MET:HB2	1:A:84:LEU:HB3	0.44	1.88	10	1
1:A:128:TYR:CD2	1:A:156:LYS:HG2	0.44	2.46	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:148:LEU:HD13	1:A:159:LEU:HD13	0.44	1.90	4	1
1:A:154:THR:O	1:A:156:LYS:CE	0.44	2.65	3	1
1:A:47:GLY:HA3	1:A:148:LEU:CG	0.44	2.42	9	4
1:A:83:PHE:CD2	1:A:90:GLU:HB3	0.44	2.48	15	2
1:A:152:THR:OG1	1:A:156:LYS:CE	0.44	2.66	1	2
1:A:42:ARG:NH1	1:A:44:TYR:CE1	0.44	2.85	10	1
1:A:103:GLY:CA	1:A:120:VAL:HG12	0.44	2.43	15	1
1:A:83:PHE:O	1:A:89:ALA:HA	0.43	2.13	10	2
1:A:166:PHE:CD1	1:A:166:PHE:C	0.43	2.91	8	6
1:A:124:ASN:O	1:A:128:TYR:CD2	0.43	2.71	14	1
1:A:64:MET:HG3	1:A:84:LEU:HD23	0.43	1.89	9	1
1:A:99:ALA:CB	1:A:104:HIS:O	0.43	2.67	3	5
1:A:67:THR:CG2	1:A:79:LEU:HD12	0.43	2.42	2	1
1:A:96:LEU:HD11	1:A:105:TYR:CE2	0.43	2.49	15	1
1:A:152:THR:CG2	1:A:156:LYS:CG	0.43	2.96	1	1
1:A:64:MET:O	1:A:83:PHE:HB3	0.43	2.14	12	2
1:A:69:VAL:HG13	1:A:77:LEU:CD2	0.43	2.42	15	1
1:A:127:GLU:O	1:A:129:ALA:N	0.43	2.52	5	1
1:A:156:LYS:HB2	1:A:159:LEU:CD2	0.43	2.44	8	3
1:A:44:TYR:CD2	1:A:151:ARG:O	0.43	2.71	8	1
1:A:155:LEU:HD12	1:A:155:LEU:O	0.43	2.13	11	1
1:A:73:THR:O	1:A:75:GLY:N	0.43	2.52	6	6
1:A:177:ILE:HG22	1:A:179:PHE:CE1	0.43	2.49	14	1
1:A:150:SER:CB	1:A:156:LYS:HZ1	0.43	2.27	5	1
1:A:121:VAL:HG12	1:A:122:GLU:HG2	0.43	1.91	5	1
1:A:128:TYR:CE1	1:A:151:ARG:HB3	0.43	2.48	1	2
1:A:44:TYR:CE2	1:A:183:PRO:HG3	0.43	2.49	6	2
1:A:79:LEU:N	1:A:94:MET:O	0.43	2.51	4	1
1:A:130:LEU:HD12	1:A:163:PHE:HB2	0.43	1.89	14	1
1:A:155:LEU:HD13	1:A:179:PHE:HE2	0.43	1.74	12	1
1:A:44:TYR:CD2	1:A:183:PRO:HG3	0.43	2.48	14	1
1:A:150:SER:OG	1:A:156:LYS:HE3	0.42	2.14	1	2
1:A:46:ALA:CB	1:A:150:SER:OG	0.42	2.67	7	1
1:A:155:LEU:C	1:A:155:LEU:HD12	0.42	2.35	7	1
1:A:44:TYR:O	1:A:150:SER:N	0.42	2.48	2	3
1:A:63:TYR:CD1	1:A:83:PHE:HB3	0.42	2.49	11	2
1:A:165:THR:O	1:A:169:ALA:CB	0.42	2.67	4	11
1:A:156:LYS:H	1:A:156:LYS:HZ1	0.42	1.56	9	2
1:A:115:ILE:HD12	1:A:115:ILE:O	0.42	2.14	2	1
1:A:121:VAL:HG23	1:A:131:LEU:C	0.42	2.34	2	1
1:A:156:LYS:HB2	1:A:159:LEU:HD21	0.42	1.91	9	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:69:VAL:HG22	1:A:79:LEU:CD1	0.42	2.45	4	1
1:A:161:GLU:CG	1:A:162:LYS:N	0.42	2.82	1	2
1:A:152:THR:OG1	1:A:156:LYS:NZ	0.42	2.53	12	1
1:A:64:MET:CG	1:A:182:GLN:O	0.42	2.68	4	2
1:A:173:THR:HG23	1:A:175:GLU:H	0.42	1.73	8	3
1:A:115:ILE:CD1	1:A:115:ILE:N	0.42	2.82	1	1
1:A:34:PHE:CD2	1:A:120:VAL:HG21	0.42	2.48	14	1
1:A:67:THR:HG22	1:A:79:LEU:CD2	0.42	2.44	10	1
1:A:128:TYR:CE1	1:A:156:LYS:CD	0.42	3.02	15	1
1:A:83:PHE:CD2	1:A:90:GLU:HB2	0.42	2.50	7	1
1:A:159:LEU:HD12	1:A:159:LEU:C	0.42	2.32	12	2
1:A:54:TRP:CD1	1:A:57:GLU:OE2	0.42	2.73	10	1
1:A:128:TYR:CG	1:A:159:LEU:HD23	0.42	2.50	15	2
1:A:150:SER:OG	1:A:156:LYS:NZ	0.42	2.52	5	1
1:A:44:TYR:CD1	1:A:44:TYR:N	0.42	2.87	5	2
1:A:46:ALA:O	1:A:179:PHE:CE2	0.42	2.73	8	1
1:A:182:GLN:HB2	1:A:183:PRO:CD	0.42	2.44	10	1
1:A:152:THR:HG22	1:A:153:GLN:N	0.42	2.30	11	2
1:A:160:LYS:HG2	1:A:179:PHE:CE2	0.42	2.50	3	1
1:A:95:VAL:O	1:A:107:TYR:CE1	0.42	2.72	15	1
1:A:59:LYS:HD2	1:A:62:LEU:HD23	0.42	1.92	8	1
1:A:34:PHE:CD1	1:A:35:GLN:N	0.41	2.88	15	1
1:A:93:ILE:N	1:A:93:ILE:HD12	0.41	2.30	12	1
1:A:156:LYS:O	1:A:159:LEU:HG	0.41	2.16	11	1
1:A:34:PHE:HE2	1:A:120:VAL:HG21	0.41	1.75	12	1
1:A:62:LEU:CD1	1:A:181:PRO:CG	0.41	2.97	8	1
1:A:173:THR:O	1:A:177:ILE:CD1	0.41	2.68	5	2
1:A:39:PHE:CZ	1:A:125:TYR:O	0.41	2.74	9	1
1:A:71:PRO:HA	1:A:77:LEU:HD12	0.41	1.91	13	1
1:A:83:PHE:CE2	1:A:90:GLU:HB3	0.41	2.51	7	2
1:A:115:ILE:N	1:A:115:ILE:CD1	0.41	2.84	12	1
1:A:128:TYR:CE1	1:A:156:LYS:HD2	0.41	2.50	11	1
1:A:83:PHE:CE1	1:A:92:LYS:HB2	0.41	2.51	6	1
1:A:120:VAL:O	1:A:120:VAL:HG23	0.41	2.14	13	1
1:A:64:MET:CE	1:A:66:LYS:CB	0.41	2.98	13	1
1:A:114:SER:N	1:A:137:LYS:HA	0.41	2.31	11	2
1:A:133:SER:OG	1:A:145:MET:HB2	0.41	2.16	1	1
1:A:67:THR:HG23	1:A:79:LEU:HD13	0.41	1.93	8	1
1:A:69:VAL:HA	1:A:79:LEU:HD23	0.41	1.92	11	1
1:A:130:LEU:N	1:A:130:LEU:HD12	0.41	2.30	6	1
1:A:115:ILE:HG22	1:A:136:THR:O	0.41	2.16	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:128:TYR:O	1:A:130:LEU:HD12	0.41	2.16	15	1
1:A:151:ARG:O	1:A:151:ARG:HG3	0.41	2.15	5	1
1:A:67:THR:CG2	1:A:79:LEU:CD1	0.41	2.99	1	1
1:A:172:LEU:CD2	1:A:176:ASP:CB	0.41	2.99	12	1
1:A:126:ASP:O	1:A:128:TYR:CZ	0.41	2.74	8	1
1:A:163:PHE:CE1	1:A:177:ILE:HG23	0.40	2.51	9	2
1:A:36:GLN:NE2	1:A:77:LEU:CD1	0.40	2.84	1	1
1:A:39:PHE:CD1	1:A:39:PHE:N	0.40	2.89	7	1
1:A:63:TYR:HA	1:A:84:LEU:O	0.40	2.16	5	1
1:A:67:THR:HG22	1:A:79:LEU:HD11	0.40	1.93	4	1
1:A:128:TYR:CD2	1:A:151:ARG:HB2	0.40	2.51	4	1
1:A:46:ALA:HB3	1:A:155:LEU:HB3	0.40	1.93	4	1
1:A:64:MET:CB	1:A:84:LEU:O	0.40	2.70	8	1
1:A:39:PHE:N	1:A:39:PHE:CD1	0.40	2.89	1	1
1:A:49:ALA:O	1:A:146:ALA:N	0.40	2.53	13	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	142/167 (85%)	115±3 (81±2%)	18±3 (13±2%)	8±2 (6±1%)	4	23
All	All	2130/2505 (85%)	1732 (81%)	276 (13%)	122 (6%)	4	23

All 24 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	PRO	15
1	A	46	ALA	15
1	A	183	PRO	11
1	A	128	TYR	10
1	A	75	GLY	9
1	A	74	GLU	9
1	A	100	GLY	8

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Mol	Chain	Res	Type	Models (Total)
1	A	151	ARG	6
1	A	182	GLN	5
1	A	142	ASP	4
1	A	52	SER	4
1	A	136	THR	4
1	A	126	ASP	3
1	A	88	GLN	3
1	A	62	LEU	3
1	A	127	GLU	2
1	A	173	THR	2
1	A	153	GLN	2
1	A	64	MET	2
1	A	144	ARG	1
1	A	33	ASN	1
1	A	124	ASN	1
1	A	171	GLY	1
1	A	53	SER	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	123/142 (87%)	79±5 (64±4%)	44±5 (36±4%)	1	9
All	All	1845/2130 (87%)	1183 (64%)	662 (36%)	1	9

All 94 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	160	LYS	15
1	A	168	LYS	15
1	A	63	TYR	15
1	A	163	PHE	15
1	A	72	SER	15
1	A	105	TYR	15
1	A	83	PHE	15
1	A	37	ASP	15

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Mol	Chain	Res	Type	Models (Total)
1	A	161	GLU	15
1	A	137	LYS	14
1	A	132	PHE	13
1	A	56	ARG	13
1	A	42	ARG	13
1	A	48	LEU	12
1	A	142	ASP	12
1	A	147	THR	12
1	A	94	MET	12
1	A	128	TYR	12
1	A	119	SER	11
1	A	156	LYS	11
1	A	134	ARG	10
1	A	148	LEU	10
1	A	162	LYS	10
1	A	151	ARG	10
1	A	104	HIS	10
1	A	59	LYS	10
1	A	31	GLN	10
1	A	97	GLN	9
1	A	66	LYS	9
1	A	79	LEU	9
1	A	155	LEU	9
1	A	145	MET	9
1	A	170	GLN	9
1	A	153	GLN	8
1	A	40	LEU	8
1	A	81	SER	8
1	A	176	ASP	8
1	A	90	GLU	8
1	A	144	ARG	8
1	A	122	GLU	7
1	A	62	LEU	7
1	A	167	SER	7
1	A	182	GLN	7
1	A	54	TRP	7
1	A	88	GLN	7
1	A	38	LYS	7
1	A	65	CYS	6
1	A	77	LEU	6
1	A	45	SER	6
1	A	154	THR	6

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Mol	Chain	Res	Type	Models (Total)
1	A	64	MET	6
1	A	92	LYS	5
1	A	84	LEU	5
1	A	174	GLU	5
1	A	125	TYR	5
1	A	52	SER	5
1	A	36	GLN	5
1	A	58	LYS	5
1	A	175	GLU	5
1	A	117	SER	5
1	A	116	HIS	4
1	A	93	ILE	4
1	A	44	TYR	4
1	A	127	GLU	4
1	A	78	ASN	4
1	A	136	THR	4
1	A	124	ASN	4
1	A	35	GLN	4
1	A	159	LEU	4
1	A	173	THR	4
1	A	53	SER	4
1	A	150	SER	4
1	A	82	THR	4
1	A	55	PHE	3
1	A	51	ASN	3
1	A	108	SER	3
1	A	50	SER	3
1	A	180	LEU	3
1	A	131	LEU	3
1	A	126	ASP	3
1	A	106	THR	3
1	A	107	TYR	2
1	A	69	VAL	2
1	A	115	ILE	2
1	A	133	SER	2
1	A	73	THR	2
1	A	67	THR	2
1	A	57	GLU	2
1	A	166	PHE	1
1	A	179	PHE	1
1	A	96	LEU	1
1	A	61	VAL	1

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Mol	Chain	Res	Type	Models (Total)
1	A	157	ASP	1
1	A	114	SER	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 ⓘ

The completeness of assignment taking into account all chemical shift lists is 54% for the well-defined parts and 51% for the entire structure.

7.1 Chemical shift list 1

File name: BMRB entry 10137

Chemical shift list name: *assigned_ chem_ shift_ list_ 1*

7.1.1 Bookkeeping ⓘ

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

Total number of shifts	1132
Number of shifts mapped to atoms	1120
Number of unparsed shifts	0
Number of shifts with mapping errors	12
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	3

The following assigned chemical shifts were not mapped to the molecules present in the coordinate file.

- Residue not found in structure. All 12 occurences are reported below.

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	67	CYS	N	125.995	-1.0	1
A	164	CYS	HB2	1.356	-1.0	1
A	67	CYS	HA	4.758	-1.0	1
A	164	CYS	H	8.218	-1.0	1
A	67	CYS	CA	52.272	-1.0	1
A	164	CYS	HA	4.285	-1.0	1
A	67	CYS	CB	19.615	-1.0	1
A	164	CYS	CB	19.117	-1.0	1
A	164	CYS	CA	52.799	-1.0	1
A	67	CYS	H	8.477	-1.0	1
A	67	CYS	HB2	1.301	-1.0	1
A	164	CYS	N	123.944	-1.0	1

7.1.2 Chemical shift referencing ⓘ

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_\alpha$	119	-0.03 ± 0.13	None needed (< 0.5 ppm)
$^{13}C_\beta$	110	0.01 ± 0.26	None needed (< 0.5 ppm)
$^{13}C'$	0	—	—
^{15}N	107	-0.64 ± 0.52	None needed (imprecise)

7.1.3 Completeness of resonance assignments ⓘ

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 54%, i.e. 936 atoms were assigned a chemical shift out of a possible 1747. 10 out of 23 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	399/698 (57%)	199/278 (72%)	105/284 (37%)	95/136 (70%)
Sidechain	509/872 (58%)	309/513 (60%)	200/322 (62%)	0/37 (0%)
Aromatic	28/177 (16%)	28/93 (30%)	0/78 (0%)	0/6 (0%)
Overall	936/1747 (54%)	536/884 (61%)	305/684 (45%)	95/179 (53%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 51%, i.e. 1029 atoms were assigned a chemical shift out of a possible 2028. 10 out of 23 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	443/819 (54%)	221/326 (68%)	117/334 (35%)	105/159 (66%)
Sidechain	558/1016 (55%)	340/600 (57%)	218/370 (59%)	0/46 (0%)
Aromatic	28/193 (15%)	28/101 (28%)	0/82 (0%)	0/10 (0%)
Overall	1029/2028 (51%)	589/1027 (57%)	335/786 (43%)	105/215 (49%)

7.1.4 Statistically unusual chemical shifts ⓘ

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

Mol	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	152	THR	CG2	36.73	27.15 − 15.95	13.5
1	A	88	GLN	CG	27.40	39.38 − 28.18	-5.7
1	A	140	GLY	CA	38.46	51.81 − 38.91	-5.4

7.1.5 Random Coil Index (RCI) plots (i)

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

Random coil index (RCI) for chain A: