



Full wwPDB NMR Structure Validation Report ⓘ

Apr 27, 2016 – 12:36 AM BST

PDB ID : 2L9N
Title : Structure of the human Shwachman-Bodian-Diamond syndrome (SBDS) protein
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Deposited on : 2011-02-21

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
<http://wwpdb.org/validation/2016/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
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

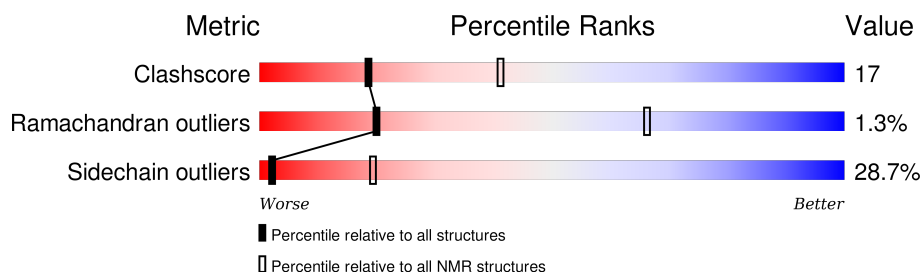
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 81%.

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	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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	252	

2 Ensemble composition and analysis

This entry contains 20 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:15-A:40, A:46-A:94 (75)	0.27	1
2	A:95-A:169 (75)	0.59	16
3	A:171-A:238 (68)	0.50	17

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 4 clusters. No single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 4129 atoms, of which 2114 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Ribosome maturation protein SBDS.

Mol	Chain	Residues	Atoms						Trace
1	A	250	Total	C	H	N	O	S	0
			4129	1272	2114	352	380	11	

There are 2 discrepancies between the modelled and reference sequences:

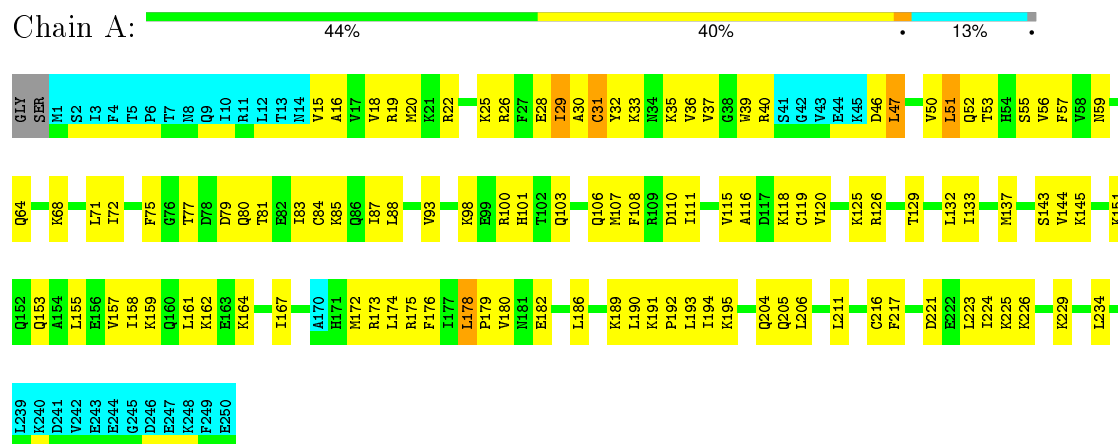
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	EXPRESSION TAG	UNP Q9Y3A5
A	0	SER	-	EXPRESSION TAG	UNP Q9Y3A5

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: Ribosome maturation protein SBDS

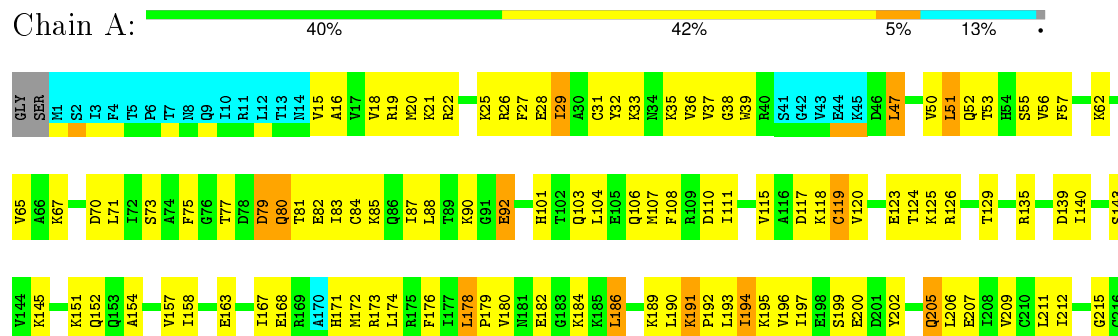


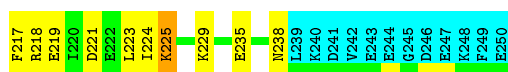
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1 (medoid)

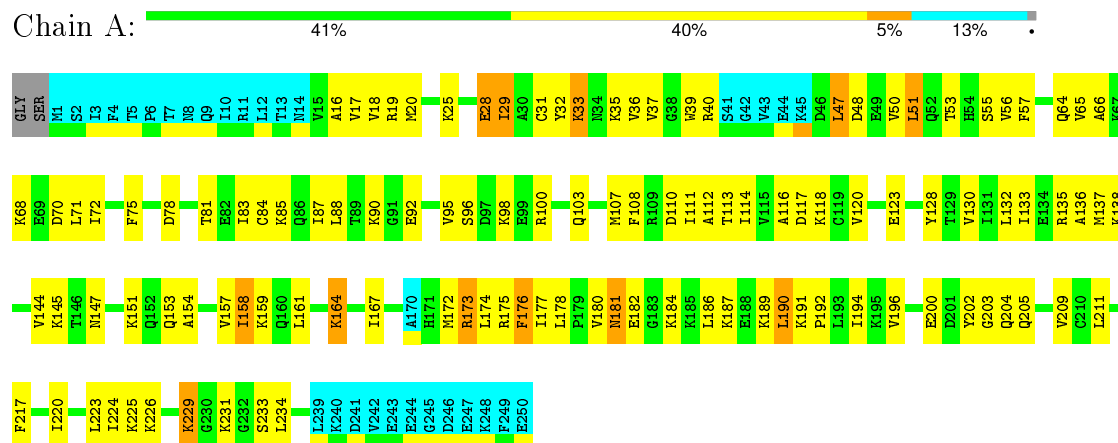
- Molecule 1: Ribosome maturation protein SBDS

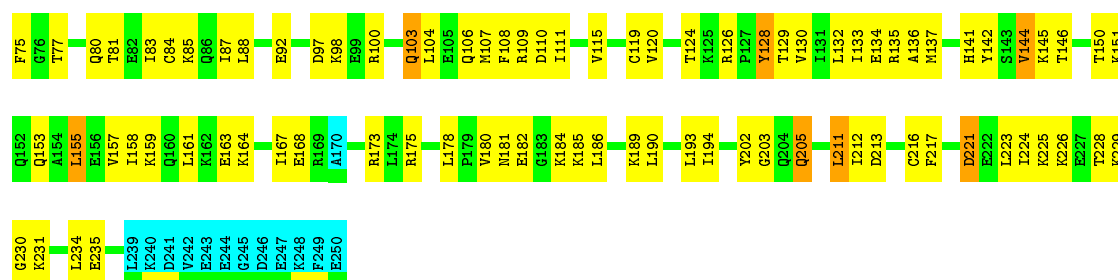




4.2.2 Score per residue for model 2

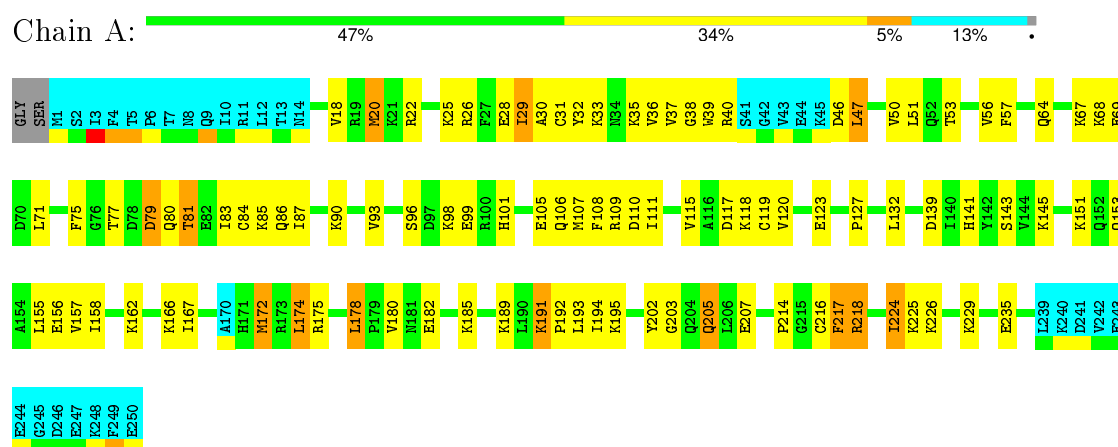
- Molecule 1: Ribosome maturation protein SBDS





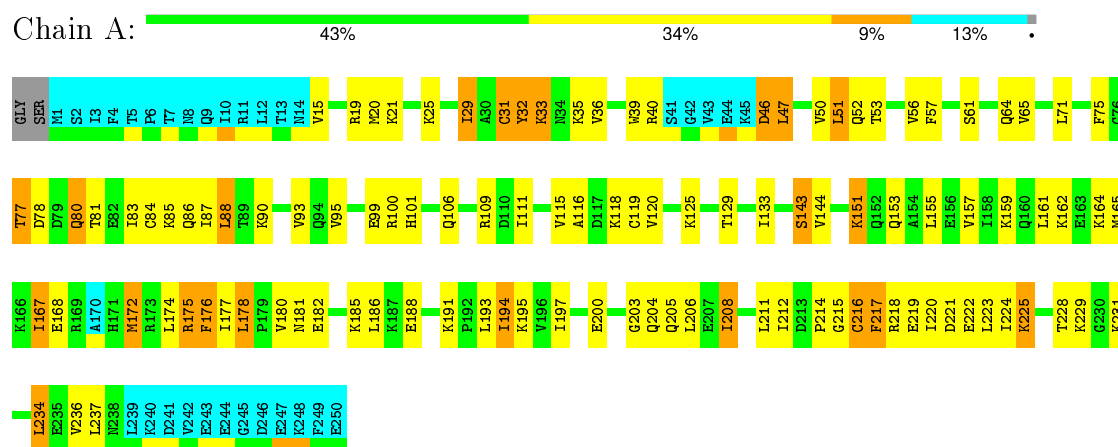
4.2.5 Score per residue for model 5

- Molecule 1: Ribosome maturation protein SBDS



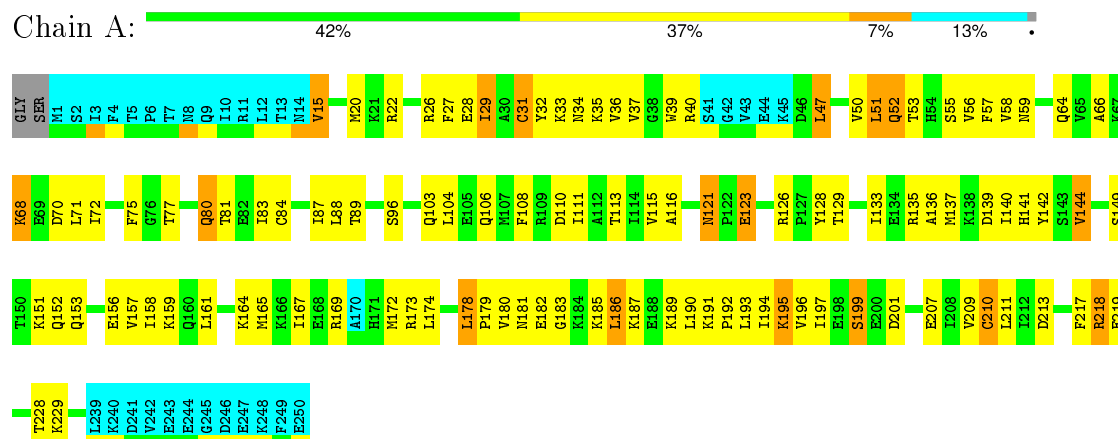
4.2.6 Score per residue for model 6

- Molecule 1: Ribosome maturation protein SBDS



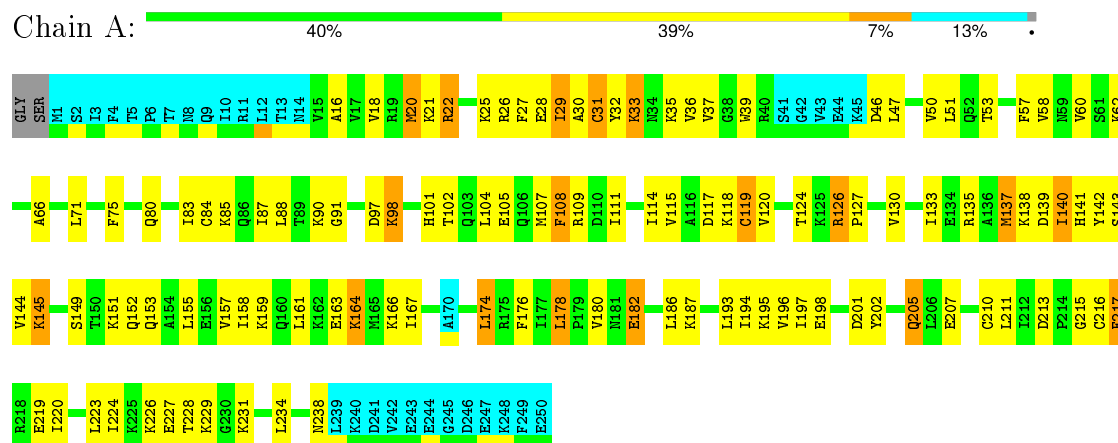
4.2.7 Score per residue for model 7

- Molecule 1: Ribosome maturation protein SBDS



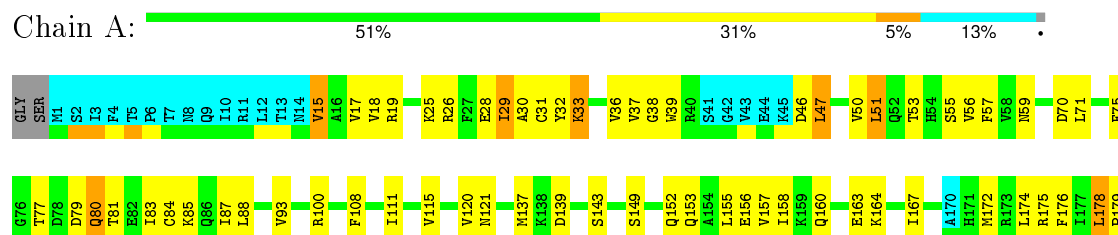
4.2.8 Score per residue for model 8

- Molecule 1: Ribosome maturation protein SBDS



4.2.9 Score per residue for model 9

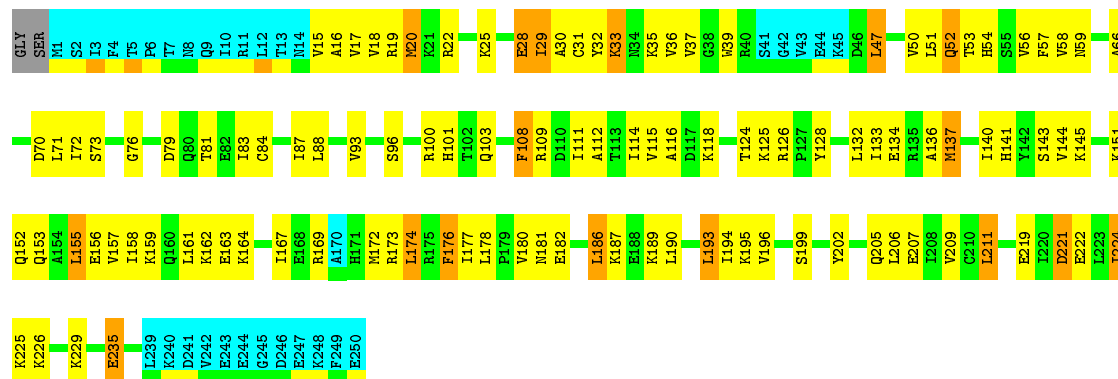
- Molecule 1: Ribosome maturation protein SBDS





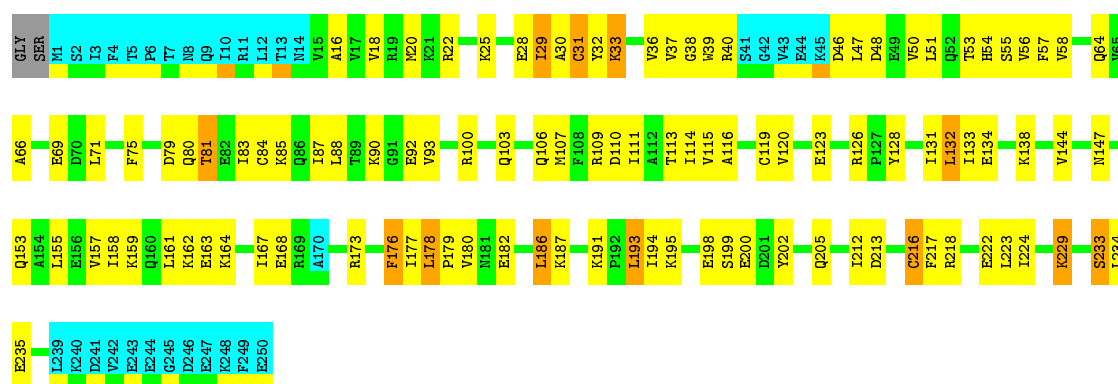
4.2.10 Score per residue for model 10

- Molecule 1: Ribosome maturation protein SBDS



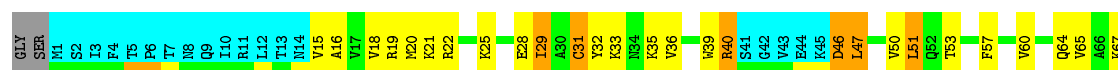
4.2.11 Score per residue for model 11

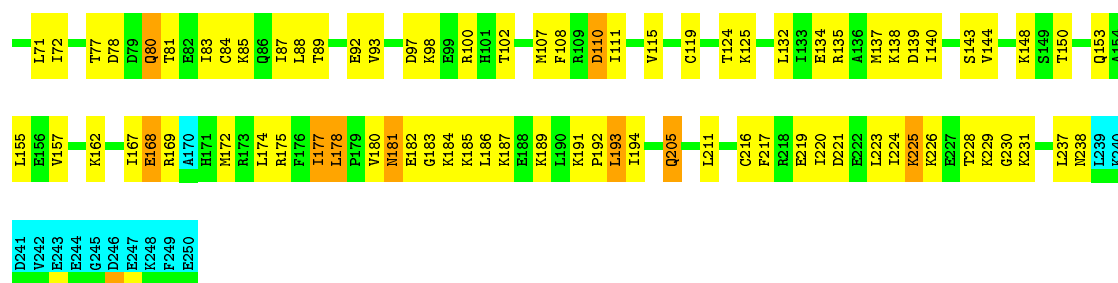
- Molecule 1: Ribosome maturation protein SBDS



4.2.12 Score per residue for model 12

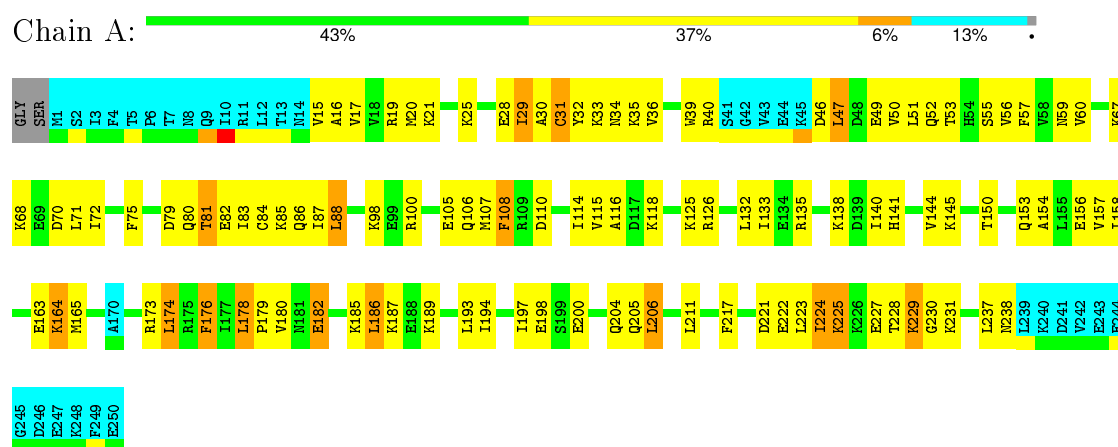
- Molecule 1: Ribosome maturation protein SBDS





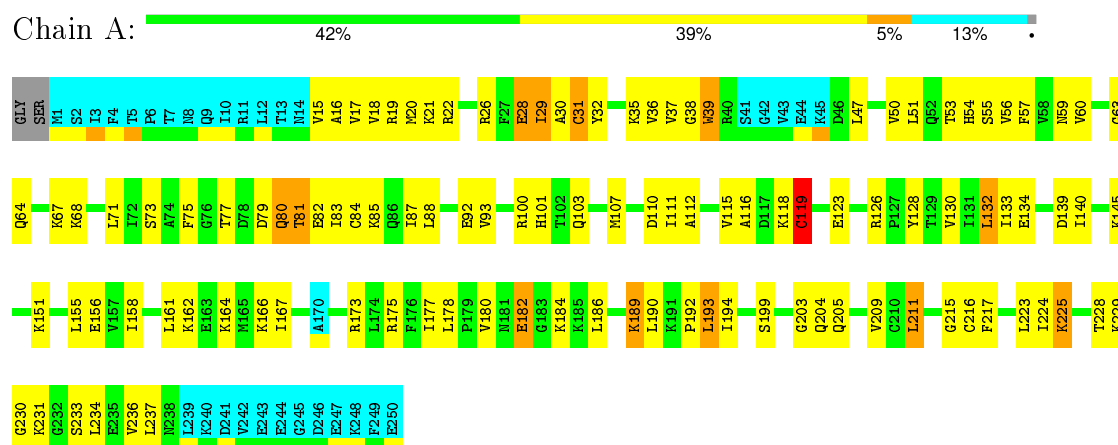
4.2.13 Score per residue for model 13

- Molecule 1: Ribosome maturation protein SBDS



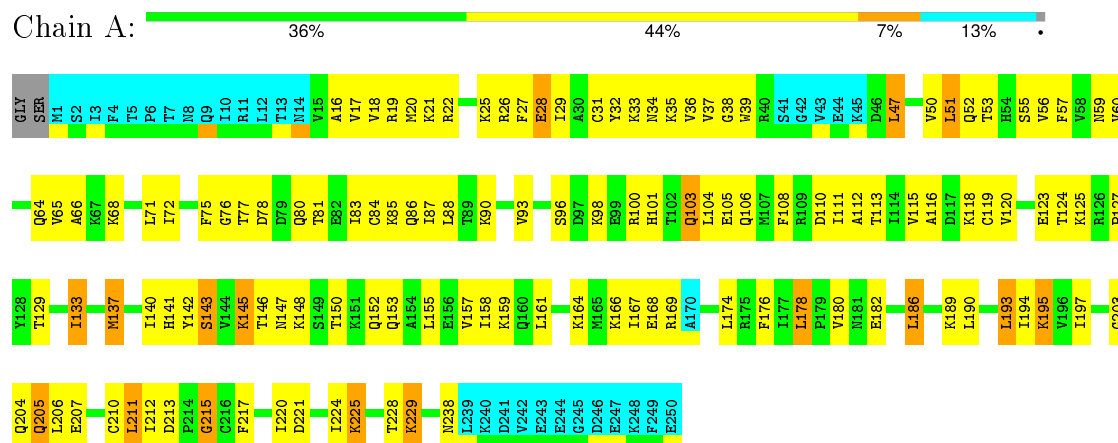
4.2.14 Score per residue for model 14

- Molecule 1: Ribosome maturation protein SBDS



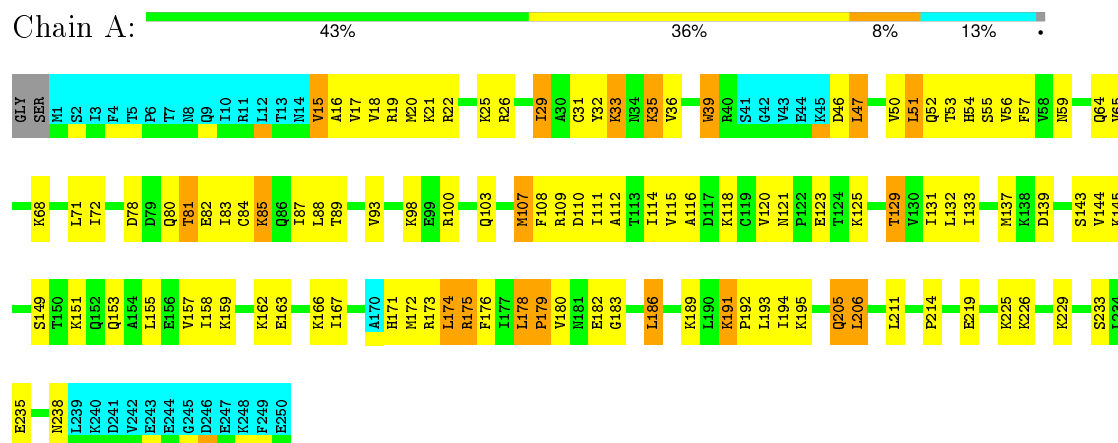
4.2.15 Score per residue for model 15

- Molecule 1: Ribosome maturation protein SBDS



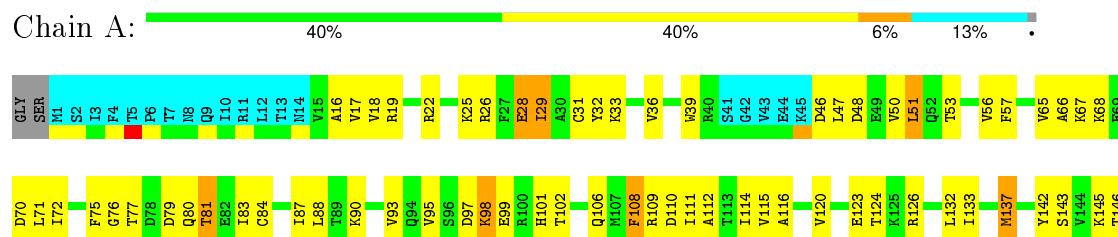
4.2.16 Score per residue for model 16

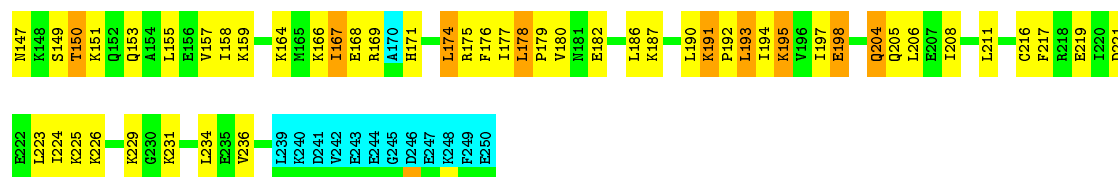
- Molecule 1: Ribosome maturation protein SBDS



4.2.17 Score per residue for model 17

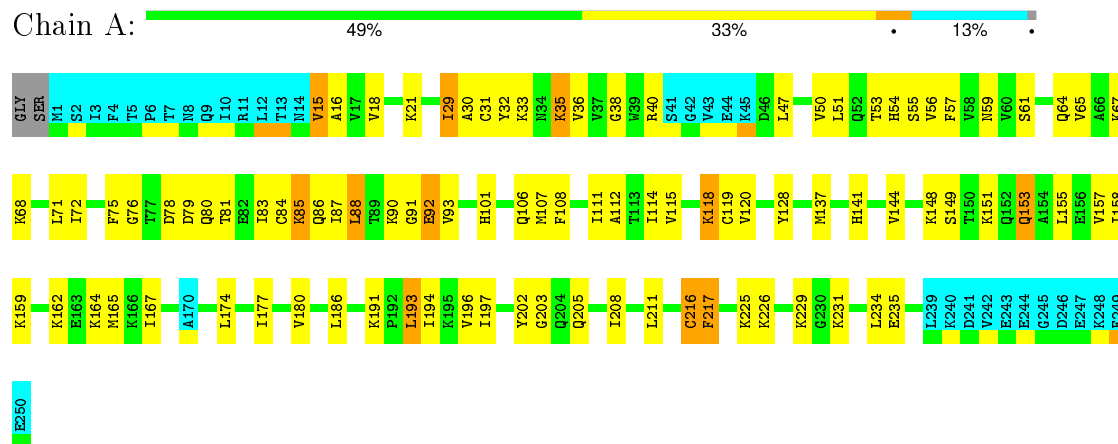
- Molecule 1: Ribosome maturation protein SBDS





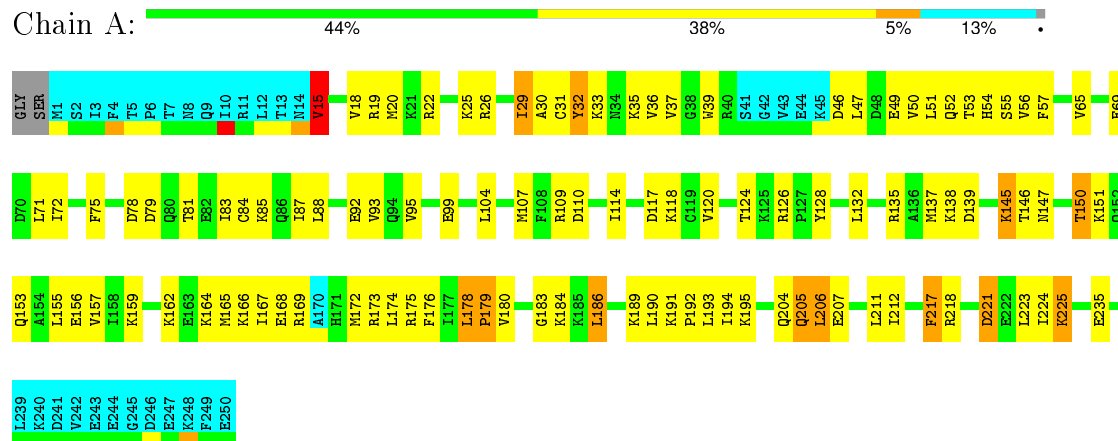
4.2.18 Score per residue for model 18

- Molecule 1: Ribosome maturation protein SBDS



4.2.19 Score per residue for model 19

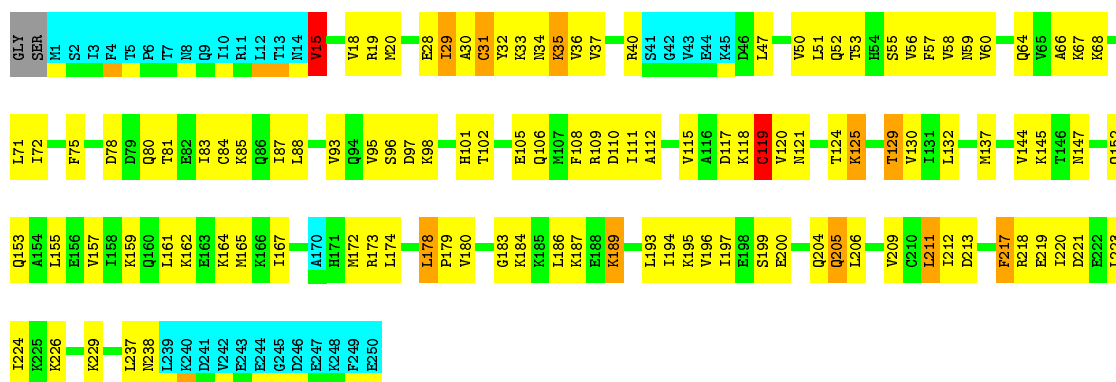
- Molecule 1: Ribosome maturation protein SBDS



4.2.20 Score per residue for model 20

- Molecule 1: Ribosome maturation protein SBDS





5 Refinement protocol and experimental data overview

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

Of the 50 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	

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)	2l9n_cs.str
Number of chemical shift lists	1
Total number of shifts	2843
Number of shifts mapped to atoms	2843
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	81%

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	1761	1866	1862	62±7
All	All	35220	37320	37240	1230

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 17.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:71:LEU:HD22	1:A:83:ILE:HD13	1.03	1.26	6	20
1:A:136:ALA:HB1	1:A:161:LEU:HD21	1.00	1.29	4	1
1:A:56:VAL:HG21	1:A:71:LEU:HD21	0.96	1.31	3	14
1:A:186:LEU:HD11	1:A:190:LEU:HD23	0.93	1.41	2	1
1:A:193:LEU:HD23	1:A:194:ILE:HG23	0.92	1.41	4	4
1:A:196:VAL:HG12	1:A:211:LEU:HD22	0.89	1.40	18	1
1:A:32:TYR:O	1:A:36:VAL:HG23	0.87	1.70	19	20
1:A:30:ALA:HB3	1:A:53:THR:HG22	0.85	1.45	14	9
1:A:51:LEU:HD11	1:A:84:CYS:CB	0.83	2.02	18	17
1:A:196:VAL:HG12	1:A:211:LEU:CD2	0.83	2.04	18	1
1:A:190:LEU:HD13	1:A:211:LEU:HD21	0.82	1.47	19	2
1:A:177:ILE:HD12	1:A:208:ILE:HG22	0.80	1.53	18	1
1:A:153:GLN:O	1:A:157:VAL:HG23	0.80	1.77	20	14
1:A:158:ILE:HG23	1:A:167:ILE:HG23	0.79	1.53	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:31:CYS:SG	1:A:50:VAL:HG22	0.78	2.19	20	5
1:A:47:LEU:HD12	1:A:51:LEU:HD12	0.78	1.52	14	4
1:A:33:LYS:O	1:A:37:VAL:HG23	0.78	1.78	15	1
1:A:29:ILE:HG21	1:A:84:CYS:SG	0.77	2.19	13	18
1:A:56:VAL:CG2	1:A:71:LEU:HD21	0.77	2.10	15	10
1:A:36:VAL:HG11	1:A:93:VAL:HG11	0.76	1.57	17	1
1:A:16:ALA:HB2	1:A:33:LYS:HG3	0.76	1.58	15	6
1:A:116:ALA:HB2	1:A:133:ILE:CD1	0.76	2.11	17	8
1:A:178:LEU:CD2	1:A:186:LEU:HD13	0.76	2.11	6	1
1:A:194:ILE:HD11	1:A:211:LEU:HB3	0.75	1.59	1	2
1:A:20:MET:HB2	1:A:87:ILE:HG23	0.75	1.59	1	16
1:A:178:LEU:CD2	1:A:186:LEU:HD22	0.74	2.12	8	2
1:A:111:ILE:O	1:A:115:VAL:HG23	0.74	1.83	6	16
1:A:39:TRP:CE3	1:A:50:VAL:HG11	0.73	2.18	16	2
1:A:20:MET:CB	1:A:87:ILE:HG23	0.73	2.13	14	9
1:A:30:ALA:HB3	1:A:53:THR:CB	0.73	2.13	19	2
1:A:116:ALA:HB2	1:A:133:ILE:HD11	0.73	1.58	2	1
1:A:18:VAL:HG22	1:A:93:VAL:HG12	0.73	1.61	17	1
1:A:186:LEU:HD12	1:A:190:LEU:HD11	0.73	1.60	14	1
1:A:187:LYS:CG	1:A:209:VAL:HG21	0.72	2.13	10	1
1:A:190:LEU:HD22	1:A:211:LEU:CD2	0.72	2.14	9	1
1:A:31:CYS:HB3	1:A:51:LEU:HD23	0.72	1.60	14	6
1:A:31:CYS:SG	1:A:36:VAL:HG21	0.72	2.24	17	10
1:A:114:ILE:HG23	1:A:118:LYS:HD2	0.72	1.59	16	2
1:A:35:LYS:CB	1:A:50:VAL:HG23	0.71	2.15	7	8
1:A:47:LEU:HG	1:A:81:THR:HG22	0.71	1.62	17	6
1:A:51:LEU:HD11	1:A:84:CYS:SG	0.71	2.26	6	13
1:A:18:VAL:HG22	1:A:93:VAL:HG23	0.70	1.60	11	3
1:A:56:VAL:HG21	1:A:71:LEU:CD2	0.70	2.16	5	11
1:A:112:ALA:HA	1:A:133:ILE:HG21	0.70	1.64	10	2
1:A:31:CYS:SG	1:A:88:LEU:HD21	0.70	2.27	4	4
1:A:115:VAL:HG13	1:A:167:ILE:HG21	0.69	1.63	18	2
1:A:47:LEU:HD21	1:A:85:LYS:HE3	0.69	1.64	4	4
1:A:30:ALA:HB3	1:A:53:THR:HB	0.69	1.63	19	1
1:A:196:VAL:HG13	1:A:209:VAL:HG23	0.69	1.63	2	1
1:A:210:CYS:C	1:A:211:LEU:HD12	0.69	2.08	7	2
1:A:119:CYS:SG	1:A:167:ILE:HD13	0.69	2.28	20	2
1:A:177:ILE:C	1:A:178:LEU:HD13	0.69	2.08	11	1
1:A:51:LEU:HD13	1:A:54:HIS:HA	0.68	1.63	19	4
1:A:186:LEU:CD1	1:A:190:LEU:HD23	0.68	2.17	2	1
1:A:178:LEU:HD11	1:A:186:LEU:CD2	0.68	2.18	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:80:GLN:HA	1:A:83:ILE:HD12	0.68	1.65	12	10
1:A:178:LEU:HD11	1:A:209:VAL:HG12	0.68	1.66	9	1
1:A:39:TRP:CH2	1:A:47:LEU:HD23	0.68	2.24	7	6
1:A:130:VAL:HA	1:A:133:ILE:HD12	0.68	1.65	4	3
1:A:31:CYS:SG	1:A:88:LEU:HD11	0.68	2.28	1	7
1:A:178:LEU:HD22	1:A:186:LEU:HB2	0.67	1.64	10	1
1:A:39:TRP:CZ3	1:A:50:VAL:HG11	0.67	2.24	13	3
1:A:158:ILE:HG23	1:A:167:ILE:CG2	0.67	2.20	14	2
1:A:112:ALA:O	1:A:133:ILE:HD13	0.67	1.88	2	2
1:A:15:VAL:HG23	1:A:32:TYR:CD1	0.67	2.24	19	1
1:A:194:ILE:HB	1:A:211:LEU:HD23	0.67	1.65	7	1
1:A:186:LEU:HD11	1:A:229:LYS:HG3	0.67	1.66	11	1
1:A:177:ILE:CG2	1:A:206:LEU:HD12	0.66	2.19	10	2
1:A:47:LEU:HD12	1:A:51:LEU:CD1	0.66	2.19	14	2
1:A:47:LEU:HD12	1:A:81:THR:HG22	0.66	1.65	16	1
1:A:220:ILE:O	1:A:224:ILE:HG22	0.66	1.90	20	5
1:A:111:ILE:CD1	1:A:144:VAL:HG11	0.66	2.21	6	1
1:A:193:LEU:HD11	1:A:224:ILE:HG21	0.66	1.68	17	4
1:A:178:LEU:HD23	1:A:229:LYS:HD2	0.66	1.67	2	1
1:A:51:LEU:HD11	1:A:84:CYS:HB3	0.66	1.66	18	1
1:A:33:LYS:O	1:A:37:VAL:HG22	0.66	1.91	5	2
1:A:35:LYS:HB2	1:A:50:VAL:HG23	0.65	1.66	7	4
1:A:197:ILE:HG21	1:A:212:ILE:CD1	0.65	2.21	15	1
1:A:83:ILE:HG22	1:A:87:ILE:HD11	0.65	1.69	18	8
1:A:140:ILE:HD13	1:A:140:ILE:O	0.65	1.91	8	1
1:A:71:LEU:HD22	1:A:83:ILE:CD1	0.65	2.22	16	5
1:A:224:ILE:HD12	1:A:225:LYS:N	0.65	2.06	9	5
1:A:158:ILE:HG23	1:A:167:ILE:HB	0.65	1.69	18	2
1:A:189:LYS:HD3	1:A:224:ILE:HD11	0.65	1.67	10	2
1:A:178:LEU:HD11	1:A:186:LEU:HD22	0.65	1.69	1	3
1:A:47:LEU:CD1	1:A:81:THR:HG22	0.65	2.22	16	1
1:A:72:ILE:HD11	1:A:78:ASP:OD1	0.65	1.91	20	7
1:A:217:PHE:CD1	1:A:220:ILE:HD13	0.65	2.26	3	1
1:A:57:PHE:CZ	1:A:65:VAL:HG22	0.64	2.27	1	10
1:A:111:ILE:HA	1:A:114:ILE:HD12	0.64	1.70	2	3
1:A:178:LEU:HD12	1:A:183:GLY:HA2	0.64	1.68	19	1
1:A:178:LEU:HB3	1:A:186:LEU:HD11	0.64	1.69	20	1
1:A:186:LEU:HD12	1:A:190:LEU:CD1	0.64	2.23	14	1
1:A:47:LEU:HD13	1:A:51:LEU:HB2	0.64	1.68	15	5
1:A:29:ILE:HG23	1:A:56:VAL:HA	0.64	1.69	4	6
1:A:193:LEU:HD23	1:A:194:ILE:HD11	0.64	1.70	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:194:ILE:HB	1:A:211:LEU:HD22	0.64	1.68	15	2
1:A:75:PHE:CE2	1:A:83:ILE:HG23	0.64	2.28	11	4
1:A:176:PHE:HB2	1:A:211:LEU:HD11	0.64	1.69	6	1
1:A:190:LEU:HD13	1:A:211:LEU:CD2	0.64	2.20	19	2
1:A:185:LYS:HE2	1:A:228:THR:HG23	0.64	1.67	7	1
1:A:178:LEU:HD12	1:A:207:GLU:O	0.64	1.92	7	1
1:A:18:VAL:HG11	1:A:88:LEU:HA	0.63	1.70	18	1
1:A:16:ALA:HB3	1:A:31:CYS:O	0.63	1.92	8	10
1:A:187:LYS:HG2	1:A:209:VAL:HG21	0.63	1.71	10	1
1:A:186:LEU:HD12	1:A:187:LYS:N	0.63	2.08	12	1
1:A:186:LEU:HD11	1:A:225:LYS:HA	0.63	1.68	16	1
1:A:35:LYS:HB3	1:A:50:VAL:HG23	0.63	1.70	4	10
1:A:178:LEU:N	1:A:178:LEU:HD12	0.63	2.09	2	2
1:A:158:ILE:HG22	1:A:167:ILE:CG1	0.63	2.24	17	1
1:A:180:VAL:HG22	1:A:205:GLN:HA	0.63	1.69	20	11
1:A:174:LEU:O	1:A:211:LEU:HD12	0.63	1.94	15	2
1:A:15:VAL:HG22	1:A:31:CYS:O	0.63	1.94	20	2
1:A:186:LEU:HD21	1:A:229:LYS:CD	0.63	2.24	11	1
1:A:194:ILE:HG13	1:A:211:LEU:HD22	0.62	1.71	20	1
1:A:120:VAL:HG12	1:A:127:PRO:N	0.62	2.10	8	1
1:A:84:CYS:O	1:A:88:LEU:HD13	0.62	1.94	12	5
1:A:211:LEU:HD11	1:A:221:ASP:OD2	0.62	1.94	4	1
1:A:51:LEU:HD21	1:A:84:CYS:HB3	0.62	1.70	9	1
1:A:154:ALA:O	1:A:158:ILE:HG23	0.62	1.94	1	1
1:A:158:ILE:HA	1:A:167:ILE:HG21	0.62	1.71	4	1
1:A:33:LYS:HG3	1:A:95:VAL:HG11	0.62	1.71	6	1
1:A:178:LEU:HD13	1:A:186:LEU:HB3	0.62	1.70	19	1
1:A:194:ILE:CD1	1:A:211:LEU:HD13	0.62	2.25	14	1
1:A:178:LEU:HD13	1:A:186:LEU:CB	0.61	2.25	19	1
1:A:179:PRO:HA	1:A:206:LEU:HD23	0.61	1.73	16	2
1:A:53:THR:HG21	1:A:57:PHE:CE1	0.61	2.29	14	17
1:A:37:VAL:HG22	1:A:147:ASN:O	0.61	1.95	19	1
1:A:112:ALA:HB1	1:A:133:ILE:CD1	0.61	2.25	15	1
1:A:31:CYS:HG	1:A:50:VAL:HG22	0.61	1.54	6	2
1:A:193:LEU:HD13	1:A:224:ILE:HD13	0.61	1.72	6	2
1:A:36:VAL:HG13	1:A:88:LEU:HG	0.61	1.73	14	3
1:A:112:ALA:HB1	1:A:130:VAL:HG12	0.60	1.70	20	1
1:A:180:VAL:HG12	1:A:205:GLN:C	0.60	2.16	11	3
1:A:211:LEU:HD11	1:A:225:LYS:HE3	0.60	1.73	10	1
1:A:47:LEU:HD21	1:A:85:LYS:CE	0.60	2.27	14	4
1:A:158:ILE:HG22	1:A:167:ILE:HD12	0.60	1.72	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:128:TYR:CD1	1:A:132:LEU:HD13	0.60	2.32	14	4
1:A:47:LEU:HD13	1:A:51:LEU:CB	0.60	2.26	15	1
1:A:158:ILE:HA	1:A:167:ILE:HD13	0.60	1.74	10	1
1:A:33:LYS:O	1:A:37:VAL:HG13	0.60	1.97	9	3
1:A:190:LEU:HD12	1:A:211:LEU:HD22	0.60	1.73	10	1
1:A:116:ALA:HB2	1:A:133:ILE:HD13	0.60	1.74	13	1
1:A:173:ARG:HG2	1:A:212:ILE:HD12	0.59	1.73	19	2
1:A:211:LEU:O	1:A:212:ILE:HD13	0.59	1.96	4	1
1:A:56:VAL:O	1:A:66:ALA:HB3	0.59	1.97	10	4
1:A:120:VAL:HG12	1:A:127:PRO:HA	0.59	1.72	15	2
1:A:144:VAL:HG13	1:A:153:GLN:HG2	0.59	1.74	12	1
1:A:37:VAL:HG23	1:A:147:ASN:HA	0.59	1.75	20	1
1:A:194:ILE:HD11	1:A:211:LEU:HD22	0.59	1.74	16	1
1:A:194:ILE:HD13	1:A:211:LEU:HB3	0.59	1.74	18	1
1:A:71:LEU:CD2	1:A:83:ILE:HD13	0.59	2.16	6	1
1:A:211:LEU:N	1:A:211:LEU:HD12	0.59	2.13	6	1
1:A:31:CYS:SG	1:A:36:VAL:HG22	0.59	2.38	19	2
1:A:18:VAL:HG22	1:A:93:VAL:HA	0.58	1.74	18	3
1:A:114:ILE:HG23	1:A:118:LYS:HG3	0.58	1.74	19	1
1:A:178:LEU:HD22	1:A:183:GLY:HA2	0.58	1.74	7	2
1:A:180:VAL:HG12	1:A:205:GLN:CA	0.58	2.28	11	3
1:A:197:ILE:HG22	1:A:210:CYS:O	0.58	1.98	15	1
1:A:142:TYR:CD2	1:A:144:VAL:HG22	0.58	2.33	7	1
1:A:30:ALA:HB3	1:A:53:THR:OG1	0.58	1.98	18	2
1:A:18:VAL:CG2	1:A:93:VAL:HG23	0.58	2.28	11	1
1:A:110:ASP:HB3	1:A:150:THR:HG21	0.58	1.76	12	1
1:A:233:SER:O	1:A:234:LEU:HD12	0.58	1.98	2	1
1:A:167:ILE:HD13	1:A:167:ILE:N	0.58	2.13	17	2
1:A:161:LEU:CB	1:A:167:ILE:HD11	0.58	2.28	10	1
1:A:157:VAL:HG12	1:A:161:LEU:HD12	0.58	1.75	10	3
1:A:29:ILE:HG22	1:A:56:VAL:HA	0.58	1.76	19	1
1:A:18:VAL:HG21	1:A:88:LEU:HD12	0.58	1.76	20	2
1:A:173:ARG:C	1:A:174:LEU:HD22	0.58	2.19	2	1
1:A:186:LEU:HD23	1:A:229:LYS:CD	0.58	2.29	3	1
1:A:129:THR:O	1:A:133:ILE:HD12	0.58	1.99	16	1
1:A:29:ILE:HG23	1:A:56:VAL:HG13	0.57	1.73	19	1
1:A:158:ILE:HG22	1:A:167:ILE:HG13	0.57	1.74	17	1
1:A:173:ARG:HG3	1:A:212:ILE:HG23	0.57	1.75	11	1
1:A:211:LEU:HD12	1:A:211:LEU:N	0.57	2.14	9	1
1:A:120:VAL:HG21	1:A:216:CYS:HB2	0.57	1.74	4	3
1:A:31:CYS:SG	1:A:51:LEU:HD23	0.57	2.39	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:196:VAL:HG13	1:A:209:VAL:CG1	0.57	2.29	20	1
1:A:186:LEU:HD22	1:A:229:LYS:HG3	0.57	1.75	2	1
1:A:137:MET:CE	1:A:161:LEU:HD11	0.57	2.29	15	1
1:A:37:VAL:HG21	1:A:146:THR:O	0.57	1.99	19	1
1:A:158:ILE:HA	1:A:167:ILE:HD11	0.57	1.76	17	2
1:A:30:ALA:HB3	1:A:53:THR:CG2	0.57	2.28	11	4
1:A:18:VAL:HG22	1:A:93:VAL:CG2	0.57	2.30	11	1
1:A:186:LEU:HD21	1:A:229:LYS:HD3	0.57	1.77	11	1
1:A:224:ILE:O	1:A:228:THR:HG23	0.57	2.00	8	3
1:A:120:VAL:HG11	1:A:216:CYS:HB2	0.57	1.76	18	2
1:A:18:VAL:HG11	1:A:87:ILE:O	0.57	2.00	17	1
1:A:178:LEU:HD21	1:A:207:GLU:OE1	0.57	2.00	15	1
1:A:178:LEU:N	1:A:178:LEU:HD22	0.57	2.15	1	1
1:A:114:ILE:HG23	1:A:118:LYS:HD3	0.56	1.76	18	1
1:A:194:ILE:CD1	1:A:211:LEU:HD23	0.56	2.30	2	1
1:A:16:ALA:HB2	1:A:33:LYS:CG	0.56	2.30	12	4
1:A:47:LEU:HA	1:A:50:VAL:HG12	0.56	1.78	10	10
1:A:111:ILE:HD11	1:A:153:GLN:OE1	0.56	1.99	11	1
1:A:93:VAL:O	1:A:93:VAL:HG13	0.56	2.00	9	5
1:A:186:LEU:HD23	1:A:190:LEU:HD11	0.56	1.76	1	2
1:A:118:LYS:O	1:A:120:VAL:HG13	0.56	2.00	15	1
1:A:47:LEU:HD21	1:A:85:LYS:HD2	0.56	1.78	18	2
1:A:120:VAL:HG21	1:A:216:CYS:HB3	0.56	1.76	5	1
1:A:111:ILE:HD13	1:A:137:MET:HE1	0.56	1.76	8	1
1:A:174:LEU:N	1:A:211:LEU:O	0.56	2.39	16	6
1:A:136:ALA:O	1:A:140:ILE:HG22	0.56	2.00	7	2
1:A:75:PHE:CD1	1:A:83:ILE:HG23	0.56	2.36	19	2
1:A:58:VAL:HG23	1:A:66:ALA:N	0.56	2.16	8	1
1:A:17:VAL:HG12	1:A:28:GLU:HG2	0.55	1.76	17	4
1:A:110:ASP:OD1	1:A:114:ILE:HD11	0.55	2.01	11	1
1:A:186:LEU:HD21	1:A:225:LYS:HG2	0.55	1.77	15	1
1:A:190:LEU:HD23	1:A:224:ILE:HD11	0.55	1.78	14	1
1:A:180:VAL:HG22	1:A:205:GLN:CA	0.55	2.32	20	10
1:A:56:VAL:CB	1:A:71:LEU:HD21	0.55	2.31	16	5
1:A:18:VAL:HG21	1:A:88:LEU:CD1	0.55	2.32	20	2
1:A:120:VAL:HG21	1:A:125:LYS:HE2	0.55	1.78	20	1
1:A:137:MET:HE1	1:A:157:VAL:HG13	0.55	1.79	10	1
1:A:178:LEU:HD23	1:A:186:LEU:HB3	0.55	1.79	17	2
1:A:178:LEU:HD12	1:A:183:GLY:CA	0.55	2.32	12	1
1:A:107:MET:HB3	1:A:144:VAL:HG11	0.55	1.77	16	1
1:A:172:MET:SD	1:A:174:LEU:HD21	0.55	2.42	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:177:ILE:N	1:A:177:ILE:HD13	0.55	2.16	12	1
1:A:196:VAL:HG13	1:A:209:VAL:CG2	0.55	2.29	2	1
1:A:178:LEU:HD13	1:A:178:LEU:N	0.55	2.15	11	1
1:A:186:LEU:HD23	1:A:190:LEU:CD1	0.55	2.31	15	1
1:A:144:VAL:HG13	1:A:153:GLN:OE1	0.55	2.01	4	1
1:A:75:PHE:CZ	1:A:83:ILE:HG23	0.55	2.37	14	5
1:A:110:ASP:OD2	1:A:150:THR:HG21	0.55	2.01	4	1
1:A:154:ALA:O	1:A:158:ILE:HG22	0.55	2.01	13	2
1:A:47:LEU:HD12	1:A:81:THR:CG2	0.55	2.32	16	1
1:A:75:PHE:CE1	1:A:83:ILE:HG23	0.54	2.37	19	4
1:A:167:ILE:O	1:A:167:ILE:HD12	0.54	2.02	19	2
1:A:36:VAL:HG11	1:A:93:VAL:HG21	0.54	1.79	20	1
1:A:176:PHE:CE2	1:A:190:LEU:HD11	0.54	2.37	17	1
1:A:189:LYS:HG3	1:A:228:THR:HG21	0.54	1.79	14	2
1:A:167:ILE:H	1:A:167:ILE:HD13	0.54	1.61	6	2
1:A:178:LEU:N	1:A:178:LEU:HD23	0.54	2.17	19	2
1:A:189:LYS:HD3	1:A:228:THR:HG21	0.54	1.79	12	1
1:A:47:LEU:HD21	1:A:85:LYS:HE2	0.54	1.79	19	4
1:A:33:LYS:O	1:A:37:VAL:HG12	0.54	2.03	10	2
1:A:119:CYS:HB3	1:A:167:ILE:HD11	0.54	1.79	14	2
1:A:51:LEU:HD11	1:A:84:CYS:HB2	0.54	1.79	18	1
1:A:29:ILE:HD11	1:A:88:LEU:CD1	0.54	2.33	16	1
1:A:140:ILE:O	1:A:140:ILE:HG22	0.54	2.03	13	2
1:A:193:LEU:HD21	1:A:220:ILE:HG22	0.54	1.80	12	2
1:A:53:THR:CG2	1:A:57:PHE:CE1	0.53	2.91	19	4
1:A:186:LEU:HD21	1:A:225:LYS:CG	0.53	2.33	15	1
1:A:18:VAL:HG13	1:A:92:GLU:C	0.53	2.24	11	4
1:A:98:LYS:O	1:A:102:THR:HG23	0.53	2.03	8	1
1:A:193:LEU:HD13	1:A:224:ILE:CD1	0.53	2.34	15	1
1:A:83:ILE:HG22	1:A:87:ILE:CD1	0.53	2.32	3	4
1:A:18:VAL:HG23	1:A:31:CYS:SG	0.53	2.44	10	8
1:A:178:LEU:HD12	1:A:183:GLY:HA3	0.53	1.80	20	2
1:A:140:ILE:HG22	1:A:140:ILE:O	0.53	2.03	14	1
1:A:29:ILE:HD11	1:A:87:ILE:CG2	0.52	2.33	5	1
1:A:18:VAL:HG22	1:A:93:VAL:HG13	0.52	1.81	14	1
1:A:32:TYR:O	1:A:36:VAL:CG2	0.52	2.57	15	14
1:A:116:ALA:HB2	1:A:133:ILE:CG1	0.52	2.35	10	1
1:A:98:LYS:O	1:A:102:THR:HG22	0.52	2.05	17	3
1:A:217:PHE:CE1	1:A:220:ILE:HD11	0.52	2.39	8	1
1:A:172:MET:HE2	1:A:218:ARG:HB2	0.52	1.81	5	1
1:A:174:LEU:HD11	1:A:218:ARG:HD3	0.52	1.81	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:174:LEU:HB3	1:A:211:LEU:HD13	0.52	1.81	17	1
1:A:211:LEU:C	1:A:212:ILE:HD12	0.52	2.24	15	1
1:A:15:VAL:HG23	1:A:32:TYR:CE1	0.52	2.39	19	1
1:A:34:ASN:O	1:A:37:VAL:HG12	0.52	2.03	20	2
1:A:178:LEU:CD1	1:A:186:LEU:HD22	0.52	2.34	11	2
1:A:174:LEU:HD22	1:A:211:LEU:HD22	0.52	1.81	12	1
1:A:180:VAL:HG12	1:A:205:GLN:HA	0.52	1.80	4	1
1:A:189:LYS:CE	1:A:224:ILE:HD11	0.52	2.34	20	1
1:A:112:ALA:CB	1:A:130:VAL:HG12	0.52	2.34	20	1
1:A:217:PHE:CD1	1:A:220:ILE:HD11	0.52	2.40	8	1
1:A:47:LEU:HD21	1:A:85:LYS:HG2	0.52	1.81	12	5
1:A:15:VAL:HG22	1:A:52:GLN:NE2	0.52	2.20	6	2
1:A:190:LEU:HD23	1:A:224:ILE:CD1	0.52	2.34	14	1
1:A:137:MET:CE	1:A:157:VAL:HG13	0.52	2.34	10	1
1:A:47:LEU:CD1	1:A:51:LEU:HD12	0.52	2.35	5	3
1:A:93:VAL:HG13	1:A:93:VAL:O	0.52	2.04	16	3
1:A:196:VAL:CG1	1:A:209:VAL:HG11	0.51	2.36	1	1
1:A:200:GLU:HB2	1:A:208:ILE:HD11	0.51	1.82	6	1
1:A:71:LEU:HD22	1:A:83:ILE:HD12	0.51	1.81	16	1
1:A:120:VAL:HG12	1:A:126:ARG:C	0.51	2.25	8	1
1:A:27:PHE:CD2	1:A:75:PHE:CE2	0.51	2.99	15	3
1:A:211:LEU:HD22	1:A:211:LEU:N	0.51	2.21	1	1
1:A:155:LEU:HA	1:A:158:ILE:HD12	0.51	1.82	5	3
1:A:196:VAL:C	1:A:197:ILE:HD12	0.51	2.25	20	1
1:A:158:ILE:HA	1:A:167:ILE:HD12	0.51	1.82	16	2
1:A:103:GLN:HB3	1:A:146:THR:HG21	0.51	1.83	15	2
1:A:174:LEU:CG	1:A:237:LEU:HD23	0.51	2.36	6	1
1:A:180:VAL:HG23	1:A:205:GLN:O	0.51	2.06	2	2
1:A:193:LEU:HD22	1:A:224:ILE:HG21	0.51	1.81	15	4
1:A:111:ILE:O	1:A:115:VAL:HG12	0.51	2.04	15	1
1:A:173:ARG:CG	1:A:212:ILE:HD12	0.51	2.36	1	1
1:A:211:LEU:HD23	1:A:221:ASP:OD2	0.50	2.05	6	1
1:A:29:ILE:CG2	1:A:56:VAL:HG13	0.50	2.36	19	1
1:A:193:LEU:CD1	1:A:224:ILE:HG21	0.50	2.36	4	3
1:A:84:CYS:O	1:A:88:LEU:HD23	0.50	2.06	18	1
1:A:186:LEU:HD23	1:A:229:LYS:HD2	0.50	1.83	3	1
1:A:111:ILE:HD13	1:A:144:VAL:HG11	0.50	1.83	6	1
1:A:190:LEU:HD21	1:A:221:ASP:OD1	0.50	2.06	17	2
1:A:196:VAL:CG1	1:A:209:VAL:HG21	0.50	2.36	9	1
1:A:113:THR:HG22	1:A:117:ASP:OD2	0.50	2.07	2	1
1:A:68:LYS:O	1:A:72:ILE:HD12	0.50	2.06	4	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:172:MET:HE3	1:A:174:LEU:HD11	0.50	1.82	5	1
1:A:199:SER:CB	1:A:209:VAL:HG22	0.50	2.37	14	1
1:A:178:LEU:HD22	1:A:178:LEU:H	0.50	1.67	11	1
1:A:186:LEU:HD12	1:A:228:THR:HG23	0.50	1.83	6	1
1:A:115:VAL:CG1	1:A:167:ILE:HG21	0.49	2.34	18	1
1:A:193:LEU:O	1:A:194:ILE:HG23	0.49	2.07	1	2
1:A:29:ILE:HD13	1:A:29:ILE:H	0.49	1.67	12	1
1:A:175:ARG:HD3	1:A:236:VAL:HG13	0.49	1.85	6	1
1:A:28:GLU:OE2	1:A:60:VAL:HG23	0.49	2.07	20	5
1:A:194:ILE:HD13	1:A:221:ASP:OD1	0.49	2.07	12	1
1:A:158:ILE:HG22	1:A:167:ILE:CD1	0.49	2.37	15	1
1:A:158:ILE:HD11	1:A:167:ILE:O	0.49	2.07	2	1
1:A:182:GLU:O	1:A:186:LEU:HD23	0.49	2.07	14	1
1:A:186:LEU:HD21	1:A:229:LYS:HG3	0.49	1.84	18	1
1:A:58:VAL:HG23	1:A:66:ALA:HB2	0.49	1.83	10	2
1:A:39:TRP:CH2	1:A:85:LYS:HD3	0.49	2.42	16	1
1:A:15:VAL:HG21	1:A:52:GLN:HG2	0.49	1.84	16	2
1:A:174:LEU:O	1:A:211:LEU:N	0.49	2.46	3	4
1:A:36:VAL:HG22	1:A:88:LEU:CD1	0.49	2.38	18	1
1:A:39:TRP:CH2	1:A:47:LEU:CD2	0.49	2.96	10	10
1:A:178:LEU:HD22	1:A:178:LEU:N	0.49	2.22	11	2
1:A:186:LEU:HD21	1:A:229:LYS:HB3	0.49	1.84	13	1
1:A:178:LEU:HG	1:A:186:LEU:HD13	0.49	1.84	11	1
1:A:17:VAL:HG11	1:A:28:GLU:OE2	0.49	2.08	9	1
1:A:178:LEU:HD11	1:A:207:GLU:HB3	0.49	1.85	5	1
1:A:108:PHE:CE1	1:A:144:VAL:HG23	0.48	2.43	18	1
1:A:194:ILE:HD11	1:A:221:ASP:CG	0.48	2.29	15	1
1:A:95:VAL:HG11	1:A:99:GLU:OE2	0.48	2.07	19	1
1:A:18:VAL:CG2	1:A:93:VAL:HG12	0.48	2.35	17	1
1:A:196:VAL:O	1:A:197:ILE:HG23	0.48	2.08	8	2
1:A:120:VAL:HG11	1:A:125:LYS:HE2	0.48	1.84	20	1
1:A:39:TRP:C	1:A:39:TRP:CD1	0.48	2.87	14	3
1:A:194:ILE:HG22	1:A:217:PHE:CD1	0.48	2.44	5	1
1:A:157:VAL:HG22	1:A:161:LEU:HD12	0.48	1.84	3	2
1:A:137:MET:HE1	1:A:161:LEU:HD11	0.48	1.86	15	1
1:A:115:VAL:HG13	1:A:133:ILE:CD1	0.48	2.39	13	1
1:A:129:THR:OG1	1:A:132:LEU:HD23	0.48	2.08	20	1
1:A:47:LEU:CG	1:A:81:THR:HG22	0.48	2.38	17	2
1:A:109:ARG:O	1:A:113:THR:HG23	0.48	2.07	11	1
1:A:142:TYR:CE2	1:A:144:VAL:HG22	0.48	2.44	8	1
1:A:190:LEU:HD12	1:A:194:ILE:CG2	0.48	2.39	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:177:ILE:HD11	1:A:236:VAL:HG23	0.48	1.85	17	1
1:A:18:VAL:HG22	1:A:93:VAL:CB	0.48	2.39	11	1
1:A:142:TYR:HE2	1:A:144:VAL:HG22	0.48	1.68	8	1
1:A:15:VAL:CG2	1:A:32:TYR:CD1	0.47	2.97	19	1
1:A:133:ILE:HG22	1:A:137:MET:HE2	0.47	1.86	2	1
1:A:186:LEU:HD11	1:A:229:LYS:HA	0.47	1.86	13	1
1:A:29:ILE:HD11	1:A:88:LEU:HD12	0.47	1.86	2	5
1:A:178:LEU:O	1:A:178:LEU:HD12	0.47	2.09	5	1
1:A:174:LEU:HD12	1:A:211:LEU:HB2	0.47	1.86	18	1
1:A:120:VAL:HG11	1:A:216:CYS:CB	0.47	2.39	9	1
1:A:194:ILE:HD11	1:A:211:LEU:HD13	0.47	1.85	20	1
1:A:178:LEU:HD11	1:A:186:LEU:HD23	0.47	1.86	4	1
1:A:180:VAL:HG13	1:A:204:GLN:C	0.47	2.30	13	5
1:A:180:VAL:HG22	1:A:205:GLN:C	0.47	2.30	16	3
1:A:110:ASP:O	1:A:113:THR:HG22	0.47	2.10	7	2
1:A:180:VAL:HG23	1:A:181:ASN:N	0.47	2.24	12	2
1:A:178:LEU:HD22	1:A:186:LEU:HD22	0.47	1.85	8	1
1:A:193:LEU:HD13	1:A:224:ILE:HG21	0.47	1.86	13	2
1:A:197:ILE:CD1	1:A:212:ILE:HD11	0.47	2.39	6	1
1:A:16:ALA:HB2	1:A:33:LYS:HB3	0.47	1.87	10	2
1:A:115:VAL:CG1	1:A:133:ILE:HD12	0.47	2.40	13	1
1:A:206:LEU:CD2	1:A:206:LEU:O	0.47	2.63	13	1
1:A:32:TYR:C	1:A:36:VAL:HG23	0.47	2.29	4	2
1:A:197:ILE:HD12	1:A:197:ILE:N	0.47	2.25	20	1
1:A:75:PHE:CE2	1:A:83:ILE:CG2	0.47	2.98	1	5
1:A:176:PHE:CE1	1:A:235:GLU:CB	0.47	2.98	10	1
1:A:189:LYS:CD	1:A:224:ILE:HD11	0.47	2.39	20	1
1:A:186:LEU:C	1:A:186:LEU:HD12	0.47	2.29	12	1
1:A:28:GLU:O	1:A:57:PHE:N	0.47	2.47	20	8
1:A:178:LEU:HD11	1:A:209:VAL:CG1	0.47	2.40	9	1
1:A:108:PHE:HA	1:A:111:ILE:HD12	0.47	1.85	8	2
1:A:199:SER:OG	1:A:209:VAL:HG22	0.47	2.09	7	1
1:A:39:TRP:CZ3	1:A:47:LEU:CD2	0.46	2.98	6	1
1:A:191:LYS:N	1:A:192:PRO:CD	0.46	2.78	9	5
1:A:161:LEU:HD12	1:A:167:ILE:HD11	0.46	1.86	7	2
1:A:18:VAL:HG13	1:A:92:GLU:O	0.46	2.10	18	1
1:A:112:ALA:HB1	1:A:130:VAL:CG1	0.46	2.41	20	1
1:A:56:VAL:HG11	1:A:71:LEU:HD21	0.46	1.86	18	3
1:A:57:PHE:CE2	1:A:65:VAL:HG22	0.46	2.45	19	2
1:A:29:ILE:HD13	1:A:88:LEU:CD1	0.46	2.40	9	1
1:A:161:LEU:HD23	1:A:164:LYS:NZ	0.46	2.25	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:161:LEU:HB2	1:A:167:ILE:HD11	0.46	1.86	10	1
1:A:224:ILE:HG23	1:A:225:LYS:N	0.46	2.26	6	3
1:A:107:MET:CE	1:A:150:THR:HG22	0.46	2.41	13	1
1:A:29:ILE:HD13	1:A:88:LEU:HD13	0.46	1.88	9	1
1:A:129:THR:OG1	1:A:132:LEU:HD12	0.46	2.11	3	1
1:A:85:LYS:CA	1:A:85:LYS:CE	0.46	2.94	16	1
1:A:197:ILE:HG21	1:A:212:ILE:HD11	0.46	1.87	15	1
1:A:185:LYS:HD3	1:A:228:THR:HG23	0.46	1.87	4	1
1:A:114:ILE:HG23	1:A:118:LYS:CG	0.45	2.40	19	1
1:A:36:VAL:HG22	1:A:88:LEU:HD21	0.45	1.88	14	2
1:A:33:LYS:HB2	1:A:95:VAL:HG11	0.45	1.89	20	1
1:A:50:VAL:HG13	1:A:51:LEU:N	0.45	2.27	14	9
1:A:178:LEU:HD23	1:A:182:GLU:HB3	0.45	1.89	10	1
1:A:15:VAL:HG12	1:A:16:ALA:N	0.45	2.26	1	2
1:A:115:VAL:HG13	1:A:133:ILE:HG21	0.45	1.87	15	1
1:A:75:PHE:CE1	1:A:83:ILE:CG2	0.45	3.00	4	2
1:A:136:ALA:HB1	1:A:164:LYS:CE	0.45	2.42	2	1
1:A:115:VAL:HG13	1:A:116:ALA:N	0.45	2.27	15	1
1:A:194:ILE:CG2	1:A:217:PHE:CD1	0.45	3.00	5	3
1:A:196:VAL:CG1	1:A:209:VAL:CG1	0.45	2.95	1	1
1:A:100:ARG:O	1:A:104:LEU:HD13	0.45	2.12	15	1
1:A:174:LEU:HD22	1:A:211:LEU:HD13	0.45	1.89	13	1
1:A:194:ILE:HG22	1:A:195:LYS:N	0.45	2.27	11	5
1:A:40:ARG:HA	1:A:89:THR:HG22	0.45	1.89	12	1
1:A:197:ILE:HD12	1:A:198:GLU:HB2	0.45	1.89	17	1
1:A:46:ASP:O	1:A:50:VAL:HG12	0.45	2.11	12	2
1:A:189:LYS:HE2	1:A:224:ILE:HD11	0.45	1.87	20	1
1:A:18:VAL:HB	1:A:29:ILE:HD11	0.45	1.89	19	1
1:A:120:VAL:HG22	1:A:215:GLY:HA3	0.45	1.88	15	1
1:A:178:LEU:HD22	1:A:186:LEU:HD13	0.45	1.89	13	1
1:A:194:ILE:HD13	1:A:211:LEU:HD13	0.45	1.89	14	1
1:A:22:ARG:CD	1:A:75:PHE:CZ	0.45	3.00	8	1
1:A:111:ILE:CG2	1:A:112:ALA:N	0.44	2.79	17	2
1:A:190:LEU:HD22	1:A:211:LEU:HD21	0.44	1.88	9	1
1:A:36:VAL:HG22	1:A:88:LEU:CD2	0.44	2.42	17	1
1:A:37:VAL:HG12	1:A:146:THR:O	0.44	2.12	15	1
1:A:180:VAL:HG13	1:A:181:ASN:N	0.44	2.27	7	3
1:A:196:VAL:HG12	1:A:211:LEU:HB3	0.44	1.88	10	1
1:A:18:VAL:HG12	1:A:87:ILE:HG22	0.44	1.90	19	1
1:A:196:VAL:HG13	1:A:209:VAL:HG11	0.44	1.89	20	1
1:A:72:ILE:HD11	1:A:78:ASP:CG	0.44	2.32	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:176:PHE:CD2	1:A:190:LEU:CD1	0.44	3.01	15	1
1:A:39:TRP:CD1	1:A:39:TRP:C	0.44	2.90	3	6
1:A:191:LYS:CB	1:A:192:PRO:CD	0.44	2.96	3	5
1:A:128:TYR:CE1	1:A:132:LEU:HD13	0.44	2.47	14	1
1:A:112:ALA:HB1	1:A:130:VAL:HG13	0.44	1.88	14	1
1:A:18:VAL:HG22	1:A:93:VAL:CA	0.44	2.43	11	3
1:A:154:ALA:O	1:A:158:ILE:HD12	0.44	2.13	3	1
1:A:177:ILE:CD1	1:A:208:ILE:HG22	0.44	2.36	18	1
1:A:190:LEU:CD1	1:A:194:ILE:HG22	0.44	2.43	10	1
1:A:18:VAL:HB	1:A:29:ILE:HD12	0.44	1.88	9	1
1:A:53:THR:HG23	1:A:53:THR:O	0.44	2.13	5	2
1:A:29:ILE:N	1:A:29:ILE:HD13	0.44	2.28	12	1
1:A:186:LEU:HD22	1:A:228:THR:CG2	0.44	2.42	3	1
1:A:151:LYS:HG2	1:A:220:ILE:HD11	0.43	1.89	6	1
1:A:161:LEU:HB3	1:A:167:ILE:HD11	0.43	1.90	10	1
1:A:182:GLU:O	1:A:186:LEU:HD12	0.43	2.13	8	2
1:A:225:LYS:HG3	1:A:226:LYS:N	0.43	2.28	17	1
1:A:158:ILE:HG23	1:A:159:LYS:N	0.43	2.28	2	1
1:A:161:LEU:HD22	1:A:164:LYS:HZ1	0.43	1.73	2	1
1:A:194:ILE:HD11	1:A:221:ASP:CB	0.43	2.42	15	1
1:A:72:ILE:O	1:A:76:GLY:N	0.43	2.51	10	4
1:A:120:VAL:HG11	1:A:215:GLY:O	0.43	2.13	1	1
1:A:116:ALA:HB2	1:A:133:ILE:HD12	0.43	1.89	3	1
1:A:133:ILE:CG2	1:A:137:MET:HE1	0.43	2.43	17	1
1:A:145:LYS:HD2	1:A:150:THR:HG23	0.43	1.90	17	1
1:A:211:LEU:HD13	1:A:221:ASP:OD2	0.43	2.13	19	1
1:A:157:VAL:HG13	1:A:158:ILE:N	0.43	2.29	8	5
1:A:186:LEU:HD13	1:A:228:THR:HB	0.43	1.90	4	1
1:A:140:ILE:O	1:A:141:HIS:CG	0.43	2.71	13	1
1:A:196:VAL:CG1	1:A:209:VAL:CG2	0.43	2.96	9	1
1:A:58:VAL:CG2	1:A:66:ALA:HB2	0.43	2.43	20	2
1:A:17:VAL:HG13	1:A:60:VAL:HG21	0.43	1.90	14	3
1:A:140:ILE:HD11	1:A:161:LEU:HD23	0.43	1.91	14	1
1:A:191:LYS:HA	1:A:196:VAL:HG21	0.43	1.90	1	1
1:A:196:VAL:CG1	1:A:209:VAL:HG23	0.43	2.41	2	1
1:A:178:LEU:HD12	1:A:233:SER:HB3	0.43	1.90	11	1
1:A:31:CYS:CB	1:A:36:VAL:CG2	0.43	2.96	18	1
1:A:194:ILE:HD11	1:A:211:LEU:HD23	0.43	1.91	13	1
1:A:47:LEU:CD1	1:A:51:LEU:CD1	0.43	2.96	5	1
1:A:111:ILE:HD11	1:A:144:VAL:HG11	0.43	1.91	12	1
1:A:53:THR:O	1:A:54:HIS:HB2	0.43	2.14	18	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:111:ILE:HG23	1:A:112:ALA:N	0.43	2.29	18	2
1:A:174:LEU:HD21	1:A:237:LEU:CD2	0.43	2.43	6	1
1:A:116:ALA:HB1	1:A:128:TYR:O	0.43	2.14	10	1
1:A:213:ASP:CB	1:A:214:PRO:CD	0.43	2.97	3	1
1:A:85:LYS:HA	1:A:85:LYS:CE	0.43	2.42	16	1
1:A:33:LYS:CG	1:A:95:VAL:HG11	0.43	2.41	6	2
1:A:15:VAL:HG22	1:A:32:TYR:HA	0.43	1.91	9	2
1:A:167:ILE:HG22	1:A:168:GLU:N	0.43	2.29	11	2
1:A:33:LYS:HD3	1:A:95:VAL:HG12	0.43	1.89	17	1
1:A:111:ILE:CG2	1:A:157:VAL:HG11	0.42	2.44	20	2
1:A:173:ARG:HG2	1:A:212:ILE:HG23	0.42	1.91	20	1
1:A:115:VAL:HG13	1:A:167:ILE:HG12	0.42	1.91	1	1
1:A:178:LEU:HD13	1:A:186:LEU:HD11	0.42	1.91	12	1
1:A:31:CYS:SG	1:A:51:LEU:HD22	0.42	2.54	9	1
1:A:37:VAL:HG23	1:A:38:GLY:N	0.42	2.28	11	2
1:A:33:LYS:CB	1:A:95:VAL:HG12	0.42	2.44	2	1
1:A:77:THR:O	1:A:78:ASP:CB	0.42	2.67	6	1
1:A:121:ASN:O	1:A:125:LYS:N	0.42	2.52	20	1
1:A:116:ALA:HB2	1:A:133:ILE:HG13	0.42	1.90	10	1
1:A:54:HIS:CD2	1:A:54:HIS:N	0.42	2.86	14	1
1:A:176:PHE:CD1	1:A:234:LEU:O	0.42	2.72	6	1
1:A:180:VAL:CG1	1:A:181:ASN:N	0.42	2.83	7	3
1:A:190:LEU:HB3	1:A:211:LEU:HD21	0.42	1.91	7	1
1:A:33:LYS:HB2	1:A:95:VAL:HG12	0.42	1.92	2	1
1:A:31:CYS:HB2	1:A:36:VAL:CG2	0.42	2.45	18	1
1:A:176:PHE:CE1	1:A:225:LYS:CE	0.42	3.02	13	1
1:A:114:ILE:HG13	1:A:150:THR:HG22	0.42	1.92	19	1
1:A:225:LYS:O	1:A:229:LYS:N	0.42	2.53	12	1
1:A:18:VAL:O	1:A:28:GLU:HA	0.42	2.15	17	2
1:A:177:ILE:O	1:A:177:ILE:HG23	0.42	2.14	2	1
1:A:158:ILE:HD13	1:A:167:ILE:CD1	0.42	2.45	8	1
1:A:36:VAL:HG22	1:A:88:LEU:HD13	0.42	1.91	18	1
1:A:18:VAL:CG2	1:A:31:CYS:SG	0.42	3.08	17	1
1:A:16:ALA:HB2	1:A:33:LYS:HG2	0.42	1.92	17	1
1:A:178:LEU:H	1:A:178:LEU:HD22	0.42	1.73	1	1
1:A:197:ILE:HD11	1:A:212:ILE:HD11	0.42	1.90	1	1
1:A:111:ILE:HD13	1:A:137:MET:CE	0.42	2.44	8	1
1:A:140:ILE:HD11	1:A:164:LYS:HB2	0.42	1.91	13	1
1:A:178:LEU:CD1	1:A:209:VAL:HG12	0.42	2.43	9	1
1:A:186:LEU:HD12	1:A:190:LEU:HG	0.42	1.91	3	1
1:A:87:ILE:O	1:A:91:GLY:N	0.41	2.53	18	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:108:PHE:HD1	1:A:144:VAL:HG21	0.41	1.75	13	1
1:A:201:ASP:CB	1:A:207:GLU:CG	0.41	2.98	8	2
1:A:178:LEU:CG	1:A:186:LEU:HD22	0.41	2.45	11	1
1:A:18:VAL:HG22	1:A:93:VAL:HG22	0.41	1.92	20	1
1:A:83:ILE:O	1:A:86:GLN:HG2	0.41	2.15	15	1
1:A:178:LEU:CD2	1:A:178:LEU:N	0.41	2.83	4	1
1:A:189:LYS:HD2	1:A:228:THR:HG21	0.41	1.92	9	1
1:A:210:CYS:O	1:A:211:LEU:HD12	0.41	2.15	7	1
1:A:75:PHE:CZ	1:A:83:ILE:CG2	0.41	3.03	14	1
1:A:194:ILE:C	1:A:194:ILE:HD12	0.41	2.35	18	1
1:A:174:LEU:HD21	1:A:237:LEU:HD23	0.41	1.91	6	1
1:A:211:LEU:HD22	1:A:221:ASP:OD1	0.41	2.16	13	1
1:A:107:MET:HE1	1:A:145:LYS:O	0.41	2.15	19	1
1:A:144:VAL:HG12	1:A:145:LYS:N	0.41	2.30	2	1
1:A:15:VAL:HG21	1:A:52:GLN:HG3	0.41	1.92	7	1
1:A:57:PHE:CE1	1:A:65:VAL:HG22	0.41	2.49	1	1
1:A:18:VAL:O	1:A:29:ILE:HD13	0.41	2.15	16	1
1:A:108:PHE:CE2	1:A:144:VAL:HG21	0.41	2.51	20	1
1:A:37:VAL:HG13	1:A:38:GLY:N	0.41	2.31	14	2
1:A:194:ILE:CD1	1:A:211:LEU:HD22	0.41	2.44	16	1
1:A:233:SER:O	1:A:234:LEU:HD22	0.41	2.15	14	1
1:A:193:LEU:O	1:A:217:PHE:CE1	0.41	2.74	6	1
1:A:194:ILE:HG21	1:A:211:LEU:HD13	0.41	1.93	10	1
1:A:121:ASN:O	1:A:123:GLU:N	0.41	2.54	7	1
1:A:177:ILE:HD11	1:A:236:VAL:CG2	0.41	2.46	14	1
1:A:196:VAL:HG12	1:A:211:LEU:HG	0.41	1.92	7	1
1:A:29:ILE:CD1	1:A:88:LEU:CD1	0.41	2.98	10	1
1:A:108:PHE:CD2	1:A:144:VAL:HG21	0.41	2.51	10	1
1:A:193:LEU:O	1:A:194:ILE:CG2	0.41	2.68	1	1
1:A:174:LEU:HD13	1:A:175:ARG:H	0.41	1.75	16	1
1:A:176:PHE:CZ	1:A:229:LYS:HD3	0.41	2.49	11	1
1:A:178:LEU:HG	1:A:186:LEU:HD22	0.41	1.93	11	1
1:A:53:THR:O	1:A:53:THR:HG23	0.41	2.16	8	1
1:A:26:ARG:O	1:A:27:PHE:CD1	0.41	2.74	8	1
1:A:212:ILE:HG22	1:A:213:ASP:N	0.41	2.31	9	1
1:A:31:CYS:HB3	1:A:36:VAL:HG21	0.41	1.93	7	1
1:A:193:LEU:O	1:A:217:PHE:CZ	0.40	2.75	20	1
1:A:75:PHE:CE2	1:A:83:ILE:HG21	0.40	2.51	1	1
1:A:177:ILE:HD13	1:A:177:ILE:H	0.40	1.76	12	1
1:A:16:ALA:HB2	1:A:33:LYS:HD2	0.40	1.91	11	1
1:A:178:LEU:HD21	1:A:186:LEU:HD22	0.40	1.91	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:211:LEU:N	1:A:211:LEU:CD1	0.40	2.84	6	1
1:A:191:LYS:N	1:A:192:PRO:HD2	0.40	2.30	12	1
1:A:108:PHE:CE1	1:A:143:SER:O	0.40	2.74	17	1
1:A:193:LEU:HD23	1:A:194:ILE:CD1	0.40	2.45	8	1
1:A:212:ILE:N	1:A:212:ILE:HD12	0.40	2.31	15	1
1:A:193:LEU:HD23	1:A:221:ASP:OD1	0.40	2.16	10	1
1:A:15:VAL:HG12	1:A:31:CYS:O	0.40	2.17	1	1
1:A:120:VAL:HG11	1:A:216:CYS:H	0.40	1.77	17	1
1:A:176:PHE:HD2	1:A:211:LEU:HD11	0.40	1.77	2	1
1:A:178:LEU:HD22	1:A:186:LEU:CB	0.40	2.45	8	1
1:A:27:PHE:CD2	1:A:75:PHE:CZ	0.40	3.10	15	1
1:A:194:ILE:HD12	1:A:194:ILE:C	0.40	2.37	13	1
1:A:133:ILE:CG2	1:A:137:MET:CE	0.40	2.99	17	1
1:A:167:ILE:N	1:A:167:ILE:CD1	0.40	2.83	17	1
1:A:168:GLU:O	1:A:215:GLY:HA2	0.40	2.16	15	1
1:A:32:TYR:O	1:A:36:VAL:N	0.40	2.54	4	1
1:A:214:PRO:O	1:A:216:CYS:N	0.40	2.54	6	1
1:A:176:PHE:CZ	1:A:235:GLU:HB3	0.40	2.52	1	1
1:A:171:HIS:HA	1:A:214:PRO:HA	0.40	1.92	16	1
1:A:174:LEU:O	1:A:211:LEU:HB2	0.40	2.17	15	1
1:A:128:TYR:CE1	1:A:132:LEU:HD22	0.40	2.52	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	218/252 (87%)	195±4 (90±2%)	20±4 (9±2%)	3±1 (1±1%)	20	66
All	All	4360/5040 (87%)	3905 (90%)	398 (9%)	57 (1%)	20	66

All 20 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	179	PRO	9

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Mol	Chain	Res	Type	Models (Total)
1	A	203	GLY	8
1	A	79	ASP	6
1	A	230	GLY	6
1	A	15	VAL	4
1	A	144	VAL	3
1	A	119	CYS	3
1	A	214	PRO	2
1	A	143	SER	2
1	A	145	LYS	2
1	A	215	GLY	2
1	A	238	ASN	2
1	A	54	HIS	1
1	A	124	THR	1
1	A	123	GLU	1
1	A	166	LYS	1
1	A	192	PRO	1
1	A	229	LYS	1
1	A	194	ILE	1
1	A	231	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	199/229 (87%)	142±6 (71±3%)	57±6 (29±3%)	2	19
All	All	3980/4580 (87%)	2837 (71%)	1143 (29%)	2	19

All 154 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	29	ILE	20
1	A	81	THR	19
1	A	217	PHE	18
1	A	229	LYS	16
1	A	25	LYS	16
1	A	178	LEU	15

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Mol	Chain	Res	Type	Models (Total)
1	A	164	LYS	15
1	A	182	GLU	15
1	A	151	LYS	14
1	A	155	LEU	14
1	A	223	LEU	13
1	A	33	LYS	13
1	A	108	PHE	13
1	A	55	SER	13
1	A	19	ARG	13
1	A	189	LYS	12
1	A	46	ASP	12
1	A	47	LEU	12
1	A	195	LYS	12
1	A	64	GLN	12
1	A	22	ARG	12
1	A	193	LEU	12
1	A	106	GLN	12
1	A	137	MET	12
1	A	80	GLN	12
1	A	159	LYS	12
1	A	205	GLN	12
1	A	172	MET	11
1	A	100	ARG	11
1	A	101	HIS	11
1	A	162	LYS	11
1	A	59	ASN	11
1	A	110	ASP	11
1	A	107	MET	11
1	A	145	LYS	11
1	A	119	CYS	11
1	A	143	SER	10
1	A	40	ARG	10
1	A	225	LYS	10
1	A	226	LYS	10
1	A	21	LYS	10
1	A	68	LYS	10
1	A	126	ARG	10
1	A	77	THR	10
1	A	31	CYS	10
1	A	26	ARG	10
1	A	51	LEU	10
1	A	139	ASP	10

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Mol	Chain	Res	Type	Models (Total)
1	A	175	ARG	10
1	A	90	LYS	9
1	A	125	LYS	9
1	A	191	LYS	9
1	A	109	ARG	9
1	A	184	LYS	9
1	A	135	ARG	9
1	A	231	LYS	9
1	A	219	GLU	9
1	A	176	PHE	9
1	A	132	LEU	9
1	A	103	GLN	9
1	A	118	LYS	9
1	A	186	LEU	9
1	A	152	GLN	8
1	A	213	ASP	8
1	A	123	GLU	8
1	A	124	THR	8
1	A	67	LYS	8
1	A	202	TYR	8
1	A	234	LEU	8
1	A	98	LYS	8
1	A	129	THR	8
1	A	173	ARG	8
1	A	218	ARG	8
1	A	206	LEU	8
1	A	163	GLU	8
1	A	166	LYS	7
1	A	187	LYS	7
1	A	235	GLU	7
1	A	204	GLN	7
1	A	156	GLU	7
1	A	28	GLU	7
1	A	79	ASP	7
1	A	149	SER	7
1	A	141	HIS	7
1	A	52	GLN	7
1	A	174	LEU	7
1	A	216	CYS	7
1	A	70	ASP	7
1	A	117	ASP	6
1	A	134	GLU	6

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Mol	Chain	Res	Type	Models (Total)
1	A	92	GLU	6
1	A	199	SER	6
1	A	165	MET	6
1	A	35	LYS	6
1	A	200	GLU	6
1	A	96	SER	6
1	A	168	GLU	6
1	A	15	VAL	6
1	A	169	ARG	6
1	A	138	LYS	6
1	A	153	GLN	5
1	A	198	GLU	5
1	A	238	ASN	5
1	A	221	ASP	5
1	A	97	ASP	5
1	A	105	GLU	5
1	A	128	TYR	5
1	A	211	LEU	5
1	A	104	LEU	5
1	A	237	LEU	4
1	A	69	GLU	4
1	A	147	ASN	4
1	A	20	MET	4
1	A	222	GLU	4
1	A	86	GLN	4
1	A	82	GLU	4
1	A	121	ASN	4
1	A	185	LYS	4
1	A	48	ASP	3
1	A	148	LYS	3
1	A	88	LEU	3
1	A	207	GLU	3
1	A	140	ILE	3
1	A	224	ILE	3
1	A	62	LYS	3
1	A	73	SER	3
1	A	34	ASN	3
1	A	99	GLU	3
1	A	32	TYR	3
1	A	142	TYR	3
1	A	181	ASN	3
1	A	150	THR	3

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Mol	Chain	Res	Type	Models (Total)
1	A	208	ILE	2
1	A	89	THR	2
1	A	39	TRP	2
1	A	167	ILE	2
1	A	131	ILE	2
1	A	61	SER	2
1	A	197	ILE	2
1	A	85	LYS	2
1	A	160	GLN	2
1	A	233	SER	2
1	A	49	GLU	2
1	A	171	HIS	2
1	A	210	CYS	2
1	A	227	GLU	2
1	A	146	THR	1
1	A	190	LEU	1
1	A	158	ILE	1
1	A	177	ILE	1
1	A	188	GLU	1
1	A	133	ILE	1
1	A	114	ILE	1
1	A	194	ILE	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 81% for the well-defined parts and 81% for the entire structure.

7.1 Chemical shift list 1

File name: 2l9n_cs.str

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	2843
Number of shifts mapped to atoms	2843
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	7

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	243	-0.01 ± 0.09	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	225	0.00 ± 0.09	None needed (< 0.5 ppm)
$^{13}\text{C}'$	214	-0.00 ± 0.05	None needed (< 0.5 ppm)
^{15}N	237	0.04 ± 0.24	None needed (< 0.5 ppm)

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 81%, i.e. 2315 atoms were assigned a chemical shift out of a possible 2854. 32 out of 39 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	1029/1080 (95%)	423/431 (98%)	399/436 (92%)	207/213 (97%)
Sidechain	1234/1644 (75%)	799/961 (83%)	427/599 (71%)	8/84 (10%)

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	Total	¹H	¹³C	¹⁵N
Aromatic	52/130 (40%)	51/68 (75%)	0/53 (0%)	1/9 (11%)
Overall	2315/2854 (81%)	1273/1460 (87%)	826/1088 (76%)	216/306 (71%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 81%, i.e. 2643 atoms were assigned a chemical shift out of a possible 3245. 35 out of 43 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	1178/1238 (95%)	484/494 (98%)	457/500 (91%)	237/244 (97%)
Sidechain	1404/1859 (76%)	909/1086 (84%)	485/680 (71%)	10/93 (11%)
Aromatic	61/148 (41%)	60/78 (77%)	0/61 (0%)	1/9 (11%)
Overall	2643/3245 (81%)	1453/1658 (88%)	942/1241 (76%)	248/346 (72%)

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	83	ILE	HG23	-0.61	2.13 – -0.57	-5.2
1	A	83	ILE	HG22	-0.61	2.13 – -0.57	-5.2
1	A	83	ILE	HG21	-0.61	2.13 – -0.57	-5.2
1	A	52	GLN	HG2	0.93	3.67 – 0.97	-5.2
1	A	77	THR	CG2	15.78	27.15 – 15.95	-5.2
1	A	72	ILE	CG2	10.27	24.63 – 10.43	-5.1
1	A	109	ARG	CD	38.70	47.57 – 38.77	-5.1

7.1.5 Random Coil Index (RCI) plots ⓘ

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:

