



Full wwPDB NMR Structure Validation Report ⓘ

May 30, 2017 – 02:00 PM EDT

PDB ID : 5KBO
Title : Structural characterization of melanoregulin (mreg): the protein involved in regulation of cell pigmentation
Authors : Rout, A.K.; Bermejo, G.; Marie-Paule, S.; Hammer III, J.A.; Tjandra, N.
Deposited on : 2016-06-03

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
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : rb-20029077
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20029077

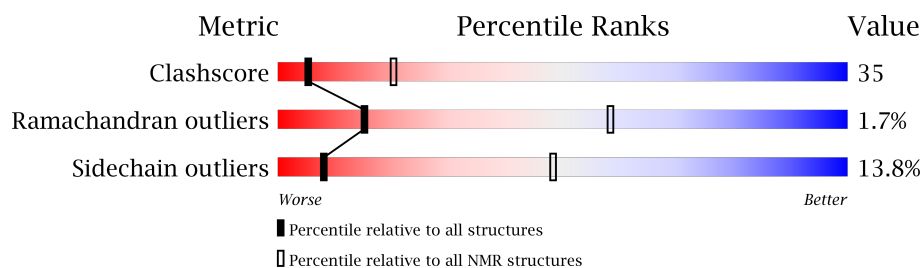
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 60%.

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	125131	11601
Ramachandran outliers	121729	10391
Sidechain outliers	121581	10367

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	214	

2 Ensemble composition and analysis

This entry contains 20 models. Model 16 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:59-A:197 (139)	0.31	16

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 5 clusters and 3 single-model clusters were found.

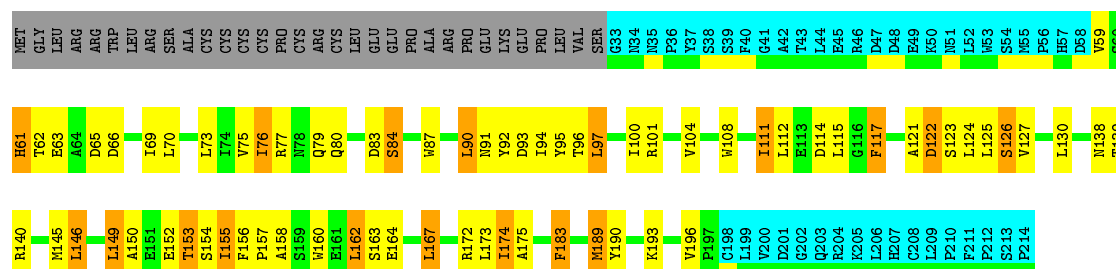
Cluster number	Models
1	2, 3, 8, 10, 11, 16, 17, 18
2	9, 13, 15
3	1, 14
4	5, 6
5	19, 20
Single-model clusters	4; 7; 12

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 2991 atoms, of which 1489 are hydrogens and 0 are deuteriums.

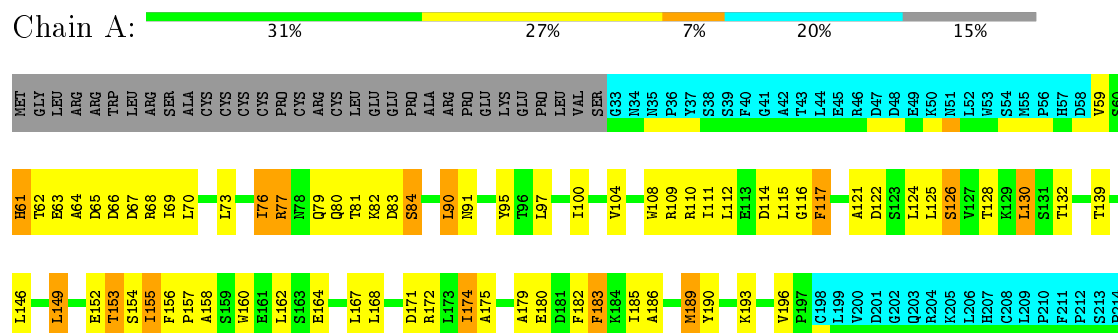
- Molecule 1 is a protein called Melanoregulin.

Mol	Chain	Residues	Atoms						Trace
1	A	182	Total	C	H	N	O	S	0
			2991	943	1489	268	285	6	



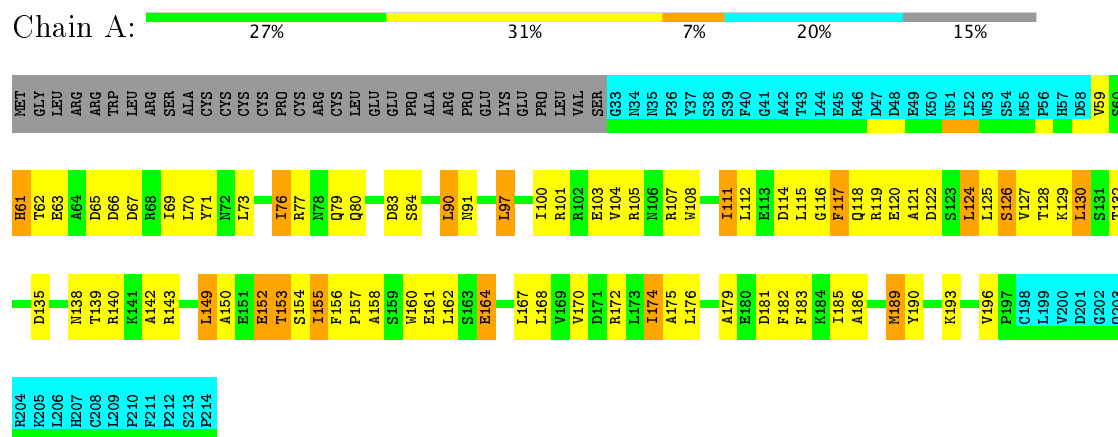
4.2.11 Score per residue for model 11

- Molecule 1: Melanoregulin



4.2.12 Score per residue for model 12

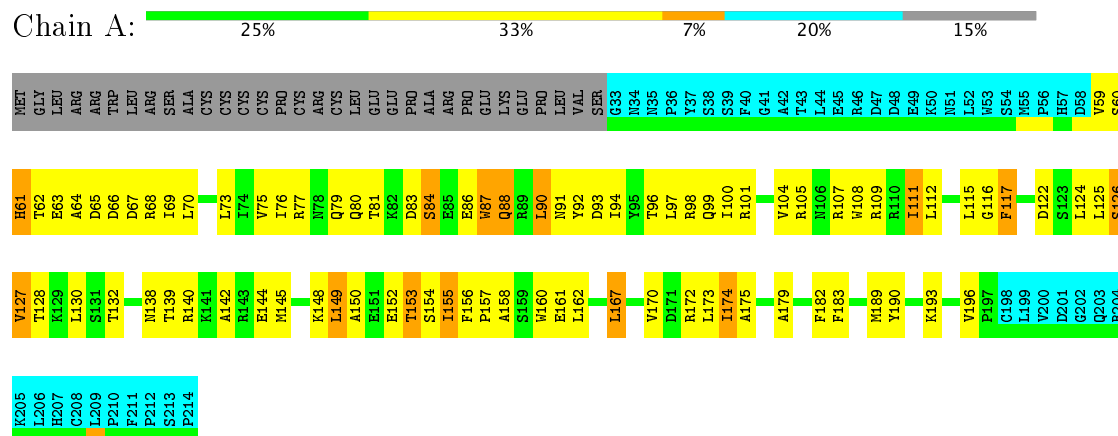
- Molecule 1: Melanoregulin





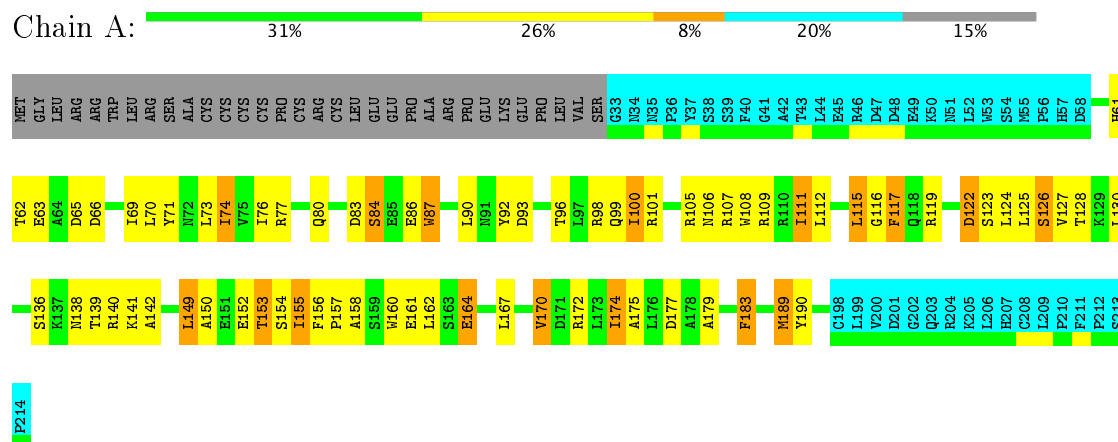
4.2.14 Score per residue for model 14

- Molecule 1: Melanoregulin



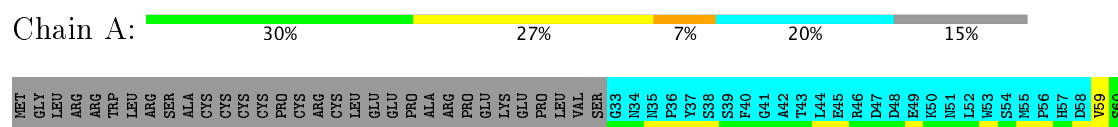
4.2.15 Score per residue for model 15

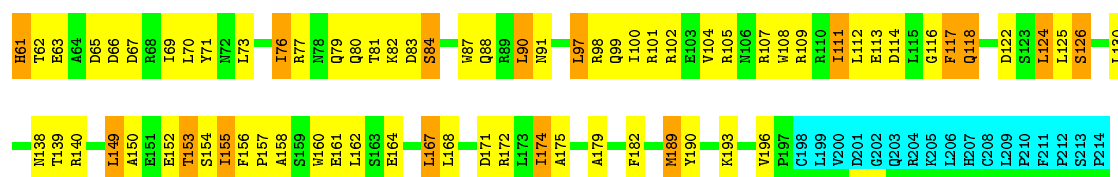
- Molecule 1: Melanoregulin



4.2.16 Score per residue for model 16 (medoid)

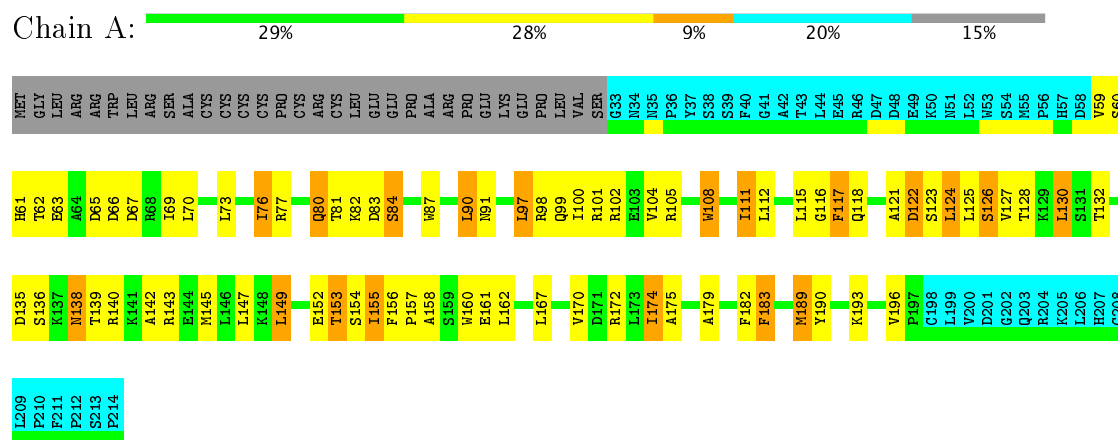
- Molecule 1: Melanoregulin





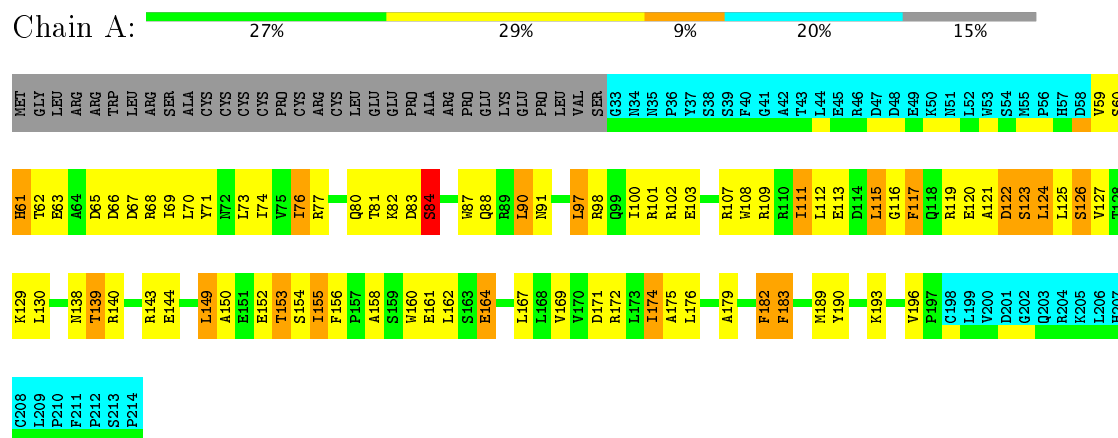
4.2.17 Score per residue for model 17

- Molecule 1: Melanoregulin



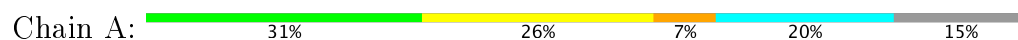
4.2.18 Score per residue for model 18

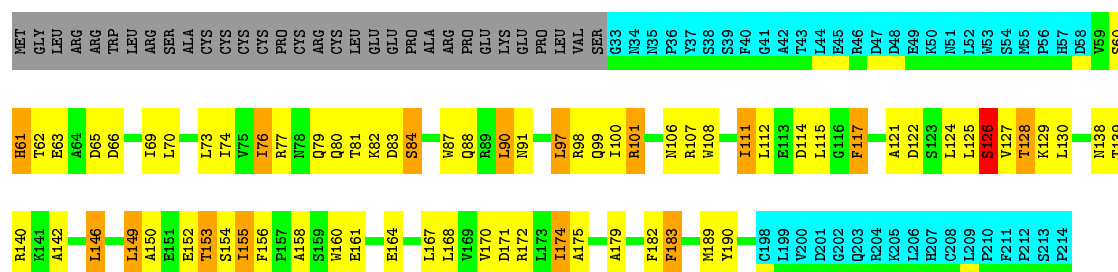
- Molecule 1: Melanoregulin



4.2.19 Score per residue for model 19

- Molecule 1: Melanoregulin

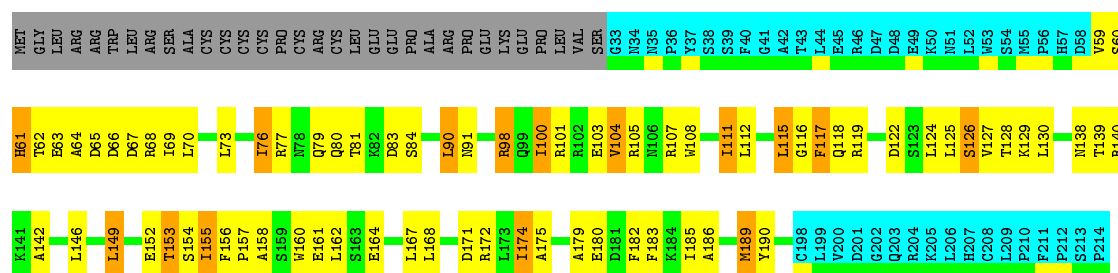




4.2.20 Score per residue for model 20

- Molecule 1: Melanoregulin

Chain A: 29% 29% 7% 20% 15%



5 Refinement protocol and experimental data overview

The models were refined using the following method: *simulated annealing*.

Of the 100 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
XPLOR	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)	5kbo_cs.cif
Number of chemical shift lists	1
Total number of shifts	1360
Number of shifts mapped to atoms	1360
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	60%

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](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the (average) root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.75±0.01	0±0/1180 (0.0±0.0%)	0.92±0.01	1±1/1593 (0.0±0.0%)
All	All	0.75	0/23600 (0.0%)	0.92	10/31860 (0.0%)

There are no bond-length outliers.

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	117	PHE	CB-CG-CD1	-6.18	116.47	120.80	8	5
1	A	182	PHE	CB-CG-CD1	-5.95	116.64	120.80	18	3
1	A	108	TRP	CA-CB-CG	-5.83	102.62	113.70	17	1
1	A	183	PHE	CB-CG-CD2	-5.13	117.21	120.80	20	1

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	1160	1171	1170	82±9
All	All	23200	23420	23400	1633

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 35.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:108:TRP:CZ2	1:A:167:LEU:HD21	0.95	1.95	14	1
1:A:124:LEU:HD22	1:A:153:THR:OG1	0.92	1.65	3	6
1:A:90:LEU:HD13	1:A:91:ASN:N	0.90	1.80	19	10
1:A:149:LEU:HD13	1:A:150:ALA:N	0.90	1.80	9	2
1:A:149:LEU:HD23	1:A:150:ALA:N	0.87	1.83	19	14
1:A:100:ILE:HD12	1:A:101:ARG:N	0.87	1.83	18	4
1:A:112:LEU:HD21	1:A:121:ALA:HB3	0.86	1.45	10	1
1:A:124:LEU:HD12	1:A:125:LEU:N	0.86	1.86	10	8
1:A:149:LEU:HD11	1:A:162:LEU:HD11	0.85	1.48	14	2
1:A:149:LEU:HD11	1:A:162:LEU:HD21	0.85	1.47	9	2
1:A:171:ASP:O	1:A:174:ILE:HG23	0.84	1.71	7	6
1:A:108:TRP:HE1	1:A:167:LEU:HD13	0.84	1.29	7	3
1:A:171:ASP:O	1:A:174:ILE:HG22	0.84	1.72	19	1
1:A:158:ALA:HB2	1:A:189:MET:SD	0.84	2.13	10	20
1:A:124:LEU:HD13	1:A:149:LEU:HD12	0.83	1.48	20	5
1:A:101:ARG:NE	1:A:146:LEU:HD23	0.83	1.88	19	1
1:A:130:LEU:O	1:A:130:LEU:HD23	0.83	1.74	7	6
1:A:174:ILE:O	1:A:174:ILE:HD12	0.82	1.74	18	8
1:A:130:LEU:HD23	1:A:130:LEU:O	0.81	1.74	1	3
1:A:162:LEU:HD12	1:A:167:LEU:HD11	0.81	1.51	11	3
1:A:107:ARG:NH2	1:A:168:LEU:HD21	0.81	1.90	16	1
1:A:130:LEU:HD22	1:A:130:LEU:O	0.81	1.74	8	1
1:A:90:LEU:HD22	1:A:90:LEU:O	0.81	1.76	3	7
1:A:108:TRP:NE1	1:A:167:LEU:HD11	0.81	1.90	14	4
1:A:108:TRP:HE1	1:A:167:LEU:HD11	0.79	1.37	10	4
1:A:66:ASP:O	1:A:70:LEU:HD13	0.78	1.77	20	17
1:A:90:LEU:HD23	1:A:91:ASN:N	0.78	1.94	1	9
1:A:108:TRP:CZ3	1:A:121:ALA:HB1	0.78	2.13	2	3
1:A:90:LEU:O	1:A:90:LEU:HD22	0.77	1.80	17	1
1:A:105:ARG:CZ	1:A:127:VAL:HG21	0.76	2.10	7	1
1:A:130:LEU:HD21	1:A:132:THR:OG1	0.76	1.80	1	9
1:A:108:TRP:CZ3	1:A:124:LEU:HD11	0.76	2.16	10	3
1:A:162:LEU:HD23	1:A:162:LEU:N	0.76	1.96	11	9
1:A:149:LEU:HD21	1:A:162:LEU:HD21	0.76	1.57	4	5
1:A:174:ILE:O	1:A:174:ILE:HD13	0.75	1.81	19	1
1:A:107:ARG:O	1:A:111:ILE:HG22	0.75	1.81	1	7
1:A:124:LEU:N	1:A:124:LEU:HD23	0.75	1.97	18	5
1:A:179:ALA:HB1	1:A:182:PHE:CZ	0.74	2.18	12	1
1:A:162:LEU:H	1:A:162:LEU:HD23	0.74	1.42	6	5
1:A:149:LEU:HD22	1:A:149:LEU:C	0.74	2.03	9	1
1:A:101:ARG:NH2	1:A:146:LEU:HD12	0.73	1.97	1	1
1:A:149:LEU:C	1:A:149:LEU:HD22	0.73	2.04	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:162:LEU:HD23	1:A:162:LEU:H	0.73	1.42	16	7
1:A:90:LEU:HD22	1:A:90:LEU:C	0.73	2.03	3	4
1:A:193:LYS:O	1:A:196:VAL:HG13	0.73	1.84	4	10
1:A:124:LEU:HD23	1:A:124:LEU:N	0.73	1.99	3	1
1:A:90:LEU:C	1:A:90:LEU:HD22	0.72	2.05	7	4
1:A:162:LEU:HD23	1:A:167:LEU:HD11	0.71	1.61	17	3
1:A:122:ASP:OD1	1:A:123:SER:N	0.71	2.24	13	6
1:A:100:ILE:HD12	1:A:164:GLU:OE2	0.70	1.87	15	1
1:A:124:LEU:HD23	1:A:149:LEU:HD23	0.70	1.61	9	2
1:A:108:TRP:CZ3	1:A:125:LEU:HD12	0.70	2.21	4	5
1:A:101:ARG:HH22	1:A:146:LEU:HD12	0.70	1.45	1	1
1:A:100:ILE:O	1:A:104:VAL:HG23	0.69	1.87	7	1
1:A:108:TRP:CE3	1:A:121:ALA:HB1	0.69	2.22	19	5
1:A:149:LEU:O	1:A:149:LEU:HD22	0.69	1.87	6	2
1:A:174:ILE:HD13	1:A:175:ALA:N	0.69	2.03	20	1
1:A:108:TRP:NE1	1:A:167:LEU:HD13	0.69	2.03	7	3
1:A:127:VAL:HG12	1:A:127:VAL:O	0.68	1.89	9	2
1:A:149:LEU:HD11	1:A:162:LEU:HD22	0.68	1.66	7	4
1:A:77:ARG:O	1:A:80:GLN:O	0.68	2.12	1	20
1:A:117:PHE:CE2	1:A:183:PHE:CE2	0.68	2.82	5	1
1:A:146:LEU:CD2	1:A:149:LEU:HD22	0.67	2.19	10	3
1:A:127:VAL:O	1:A:127:VAL:HG12	0.67	1.88	20	1
1:A:152:GLU:O	1:A:190:TYR:CG	0.67	2.48	12	20
1:A:104:VAL:HG13	1:A:167:LEU:CD1	0.67	2.20	14	4
1:A:117:PHE:CD1	1:A:183:PHE:CD1	0.66	2.83	10	6
1:A:90:LEU:C	1:A:90:LEU:HD13	0.66	2.11	13	2
1:A:90:LEU:HD13	1:A:90:LEU:C	0.66	2.10	9	8
1:A:162:LEU:HD12	1:A:167:LEU:CD1	0.66	2.21	11	2
1:A:115:LEU:HD12	1:A:117:PHE:CZ	0.66	2.25	18	6
1:A:128:THR:O	1:A:128:THR:HG23	0.66	1.90	17	2
1:A:174:ILE:C	1:A:174:ILE:HD13	0.66	2.11	20	1
1:A:76:ILE:O	1:A:80:GLN:N	0.65	2.29	8	20
1:A:64:ALA:HB3	1:A:143:ARG:HH12	0.65	1.50	13	1
1:A:80:GLN:NE2	1:A:87:TRP:NE1	0.65	2.45	14	2
1:A:172:ARG:O	1:A:175:ALA:HB3	0.65	1.91	12	19
1:A:128:THR:HG23	1:A:128:THR:O	0.65	1.91	15	1
1:A:107:ARG:O	1:A:111:ILE:HG23	0.65	1.92	15	5
1:A:117:PHE:CZ	1:A:183:PHE:CE2	0.65	2.84	5	1
1:A:117:PHE:CE1	1:A:183:PHE:CD1	0.64	2.85	17	6
1:A:124:LEU:HD12	1:A:125:LEU:H	0.64	1.50	17	8
1:A:92:TYR:O	1:A:96:THR:HG23	0.64	1.93	10	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:87:TRP:CZ2	1:A:88:GLN:NE2	0.64	2.66	16	1
1:A:97:LEU:O	1:A:100:ILE:HG13	0.64	1.93	11	2
1:A:152:GLU:O	1:A:190:TYR:CD1	0.64	2.51	8	20
1:A:100:ILE:HG22	1:A:164:GLU:CD	0.63	2.14	6	2
1:A:169:VAL:HG13	1:A:172:ARG:NH1	0.63	2.08	18	1
1:A:117:PHE:CE1	1:A:183:PHE:CD2	0.63	2.86	5	1
1:A:183:PHE:CD2	1:A:183:PHE:N	0.63	2.66	5	1
1:A:130:LEU:HD12	1:A:130:LEU:O	0.63	1.94	10	2
1:A:124:LEU:HD22	1:A:153:THR:HG1	0.63	1.52	16	1
1:A:130:LEU:O	1:A:130:LEU:HD12	0.63	1.94	3	4
1:A:111:ILE:HG23	1:A:112:LEU:HD12	0.63	1.69	9	7
1:A:125:LEU:HD23	1:A:126:SER:OG	0.62	1.94	18	5
1:A:108:TRP:HE1	1:A:167:LEU:HD22	0.62	1.54	17	3
1:A:149:LEU:O	1:A:153:THR:O	0.62	2.18	4	19
1:A:80:GLN:CB	1:A:87:TRP:HE1	0.62	2.07	15	5
1:A:130:LEU:HD13	1:A:130:LEU:H	0.62	1.53	8	1
1:A:98:ARG:NH1	1:A:102:ARG:NH1	0.62	2.48	1	1
1:A:98:ARG:NH1	1:A:102:ARG:NE	0.62	2.46	4	1
1:A:160:TRP:CD1	1:A:161:GLU:O	0.62	2.52	7	18
1:A:98:ARG:NH1	1:A:99:GLN:NE2	0.62	2.47	19	3
1:A:62:THR:HG22	1:A:63:GLU:N	0.62	2.10	9	20
1:A:124:LEU:N	1:A:124:LEU:HD12	0.62	2.08	9	1
1:A:105:ARG:HH11	1:A:109:ARG:NH1	0.61	1.93	14	1
1:A:104:VAL:HG13	1:A:167:LEU:HD13	0.61	1.72	17	8
1:A:120:GLU:O	1:A:124:LEU:HD21	0.61	1.95	18	3
1:A:101:ARG:NH2	1:A:102:ARG:NE	0.61	2.48	9	2
1:A:101:ARG:HH22	1:A:102:ARG:NE	0.61	1.94	9	1
1:A:70:LEU:HB3	1:A:90:LEU:HD23	0.61	1.73	3	4
1:A:189:MET:O	1:A:189:MET:SD	0.61	2.59	13	11
1:A:80:GLN:NE2	1:A:81:THR:H	0.61	1.93	2	1
1:A:189:MET:SD	1:A:189:MET:O	0.61	2.59	18	9
1:A:87:TRP:N	1:A:87:TRP:CD2	0.60	2.69	4	4
1:A:67:ASP:OD1	1:A:68:ARG:N	0.60	2.34	14	5
1:A:169:VAL:HG22	1:A:172:ARG:HH11	0.60	1.57	7	2
1:A:104:VAL:CG1	1:A:108:TRP:CE2	0.60	2.85	7	2
1:A:101:ARG:NH2	1:A:145:MET:SD	0.60	2.74	5	1
1:A:119:ARG:HH21	1:A:129:LYS:NZ	0.60	1.95	9	1
1:A:145:MET:SD	1:A:145:MET:N	0.60	2.75	3	1
1:A:105:ARG:NE	1:A:127:VAL:HG22	0.60	2.11	5	1
1:A:193:LYS:O	1:A:196:VAL:HG23	0.60	1.97	10	4
1:A:117:PHE:CD2	1:A:117:PHE:N	0.60	2.70	12	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:98:ARG:NH2	1:A:102:ARG:NH2	0.60	2.50	18	1
1:A:111:ILE:HD12	1:A:182:PHE:CE1	0.60	2.31	3	2
1:A:174:ILE:HD12	1:A:174:ILE:C	0.59	2.17	7	5
1:A:66:ASP:O	1:A:70:LEU:HD23	0.59	1.97	8	1
1:A:105:ARG:HE	1:A:109:ARG:NH1	0.59	1.95	14	1
1:A:117:PHE:N	1:A:117:PHE:CD2	0.59	2.68	14	3
1:A:101:ARG:NE	1:A:125:LEU:HD21	0.59	2.12	5	2
1:A:122:ASP:O	1:A:126:SER:O	0.59	2.21	11	2
1:A:87:TRP:CD2	1:A:87:TRP:N	0.59	2.70	13	1
1:A:124:LEU:HD11	1:A:153:THR:OG1	0.58	1.97	6	2
1:A:117:PHE:CZ	1:A:179:ALA:HB1	0.58	2.33	2	1
1:A:77:ARG:NH2	1:A:82:LYS:NZ	0.58	2.51	4	1
1:A:124:LEU:N	1:A:124:LEU:CD2	0.58	2.62	18	6
1:A:176:LEU:N	1:A:176:LEU:HD12	0.58	2.12	18	5
1:A:127:VAL:O	1:A:130:LEU:N	0.58	2.36	6	4
1:A:102:ARG:HH11	1:A:138:ASN:HD21	0.58	1.42	17	1
1:A:130:LEU:HD21	1:A:132:THR:CB	0.58	2.28	1	9
1:A:70:LEU:O	1:A:73:LEU:N	0.57	2.37	11	18
1:A:162:LEU:CD2	1:A:162:LEU:N	0.57	2.67	11	5
1:A:80:GLN:NE2	1:A:87:TRP:HE1	0.57	1.98	1	2
1:A:111:ILE:HD12	1:A:174:ILE:HG21	0.57	1.74	2	6
1:A:124:LEU:N	1:A:124:LEU:CD1	0.57	2.67	9	1
1:A:77:ARG:NH1	1:A:87:TRP:CZ3	0.57	2.73	18	1
1:A:162:LEU:N	1:A:162:LEU:CD2	0.57	2.68	14	4
1:A:61:HIS:ND1	1:A:62:THR:O	0.57	2.37	7	1
1:A:101:ARG:NH2	1:A:146:LEU:CD1	0.57	2.68	1	1
1:A:107:ARG:HE	1:A:168:LEU:CD1	0.57	2.13	12	2
1:A:108:TRP:HE1	1:A:167:LEU:CD1	0.57	2.13	2	3
1:A:107:ARG:NE	1:A:168:LEU:CD1	0.57	2.67	12	1
1:A:81:THR:O	1:A:83:ASP:N	0.56	2.38	3	7
1:A:108:TRP:CD1	1:A:108:TRP:N	0.56	2.70	13	2
1:A:174:ILE:HG22	1:A:182:PHE:CZ	0.56	2.35	1	3
1:A:101:ARG:NE	1:A:125:LEU:CD2	0.56	2.68	3	2
1:A:98:ARG:NH1	1:A:102:ARG:NH2	0.56	2.53	18	1
1:A:62:THR:CG2	1:A:63:GLU:N	0.56	2.69	7	20
1:A:121:ALA:O	1:A:124:LEU:CD1	0.56	2.53	7	3
1:A:160:TRP:NE1	1:A:161:GLU:O	0.56	2.38	4	15
1:A:107:ARG:HE	1:A:168:LEU:HD21	0.56	1.60	9	2
1:A:169:VAL:HG22	1:A:172:ARG:NH1	0.56	2.15	5	2
1:A:122:ASP:OD1	1:A:122:ASP:C	0.56	2.44	15	1
1:A:101:ARG:HH12	1:A:138:ASN:HD22	0.56	1.44	7	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:102:ARG:HH21	1:A:105:ARG:NH1	0.56	1.99	16	1
1:A:102:ARG:NH2	1:A:105:ARG:NH1	0.56	2.52	16	2
1:A:176:LEU:N	1:A:176:LEU:CD1	0.56	2.68	12	5
1:A:105:ARG:CZ	1:A:127:VAL:HG22	0.56	2.30	5	3
1:A:117:PHE:CD1	1:A:117:PHE:O	0.56	2.58	5	1
1:A:98:ARG:NH2	1:A:138:ASN:H	0.56	1.98	20	1
1:A:106:ASN:OD1	1:A:109:ARG:NH1	0.56	2.39	15	2
1:A:80:GLN:NE2	1:A:84:SER:OG	0.56	2.39	7	2
1:A:102:ARG:NH2	1:A:105:ARG:HH11	0.56	1.98	16	1
1:A:87:TRP:CZ3	1:A:88:GLN:NE2	0.56	2.74	19	1
1:A:77:ARG:HH11	1:A:87:TRP:HE1	0.56	1.44	3	2
1:A:111:ILE:HG23	1:A:112:LEU:CD1	0.56	2.31	10	1
1:A:125:LEU:HD23	1:A:126:SER:HG	0.56	1.61	16	2
1:A:154:SER:OG	1:A:156:PHE:O	0.55	2.23	8	20
1:A:139:THR:OG1	1:A:140:ARG:N	0.55	2.39	17	17
1:A:174:ILE:C	1:A:174:ILE:HD12	0.55	2.22	3	4
1:A:124:LEU:HD12	1:A:124:LEU:N	0.55	2.16	6	1
1:A:130:LEU:CD1	1:A:130:LEU:H	0.55	2.13	8	1
1:A:98:ARG:NH1	1:A:102:ARG:HH11	0.55	1.98	13	1
1:A:80:GLN:NE2	1:A:81:THR:N	0.55	2.54	2	1
1:A:107:ARG:HE	1:A:168:LEU:CD2	0.55	2.14	8	2
1:A:103:GLU:OE2	1:A:107:ARG:NH2	0.55	2.40	18	1
1:A:74:ILE:CD1	1:A:77:ARG:HH11	0.55	2.15	18	3
1:A:98:ARG:HH22	1:A:102:ARG:NH1	0.55	2.00	8	1
1:A:122:ASP:CG	1:A:123:SER:N	0.55	2.60	15	1
1:A:118:GLN:OE1	1:A:118:GLN:N	0.55	2.40	16	1
1:A:61:HIS:O	1:A:61:HIS:ND1	0.55	2.39	11	5
1:A:112:LEU:O	1:A:116:GLY:N	0.55	2.40	13	14
1:A:73:LEU:HB3	1:A:90:LEU:HD22	0.55	1.78	15	1
1:A:127:VAL:O	1:A:129:LYS:N	0.55	2.40	5	3
1:A:74:ILE:CD1	1:A:77:ARG:NH1	0.55	2.70	18	3
1:A:76:ILE:O	1:A:79:GLN:N	0.54	2.39	1	14
1:A:122:ASP:OD1	1:A:127:VAL:HG21	0.54	2.03	2	1
1:A:98:ARG:HH11	1:A:99:GLN:NE2	0.54	2.00	5	4
1:A:104:VAL:CG1	1:A:108:TRP:CZ2	0.54	2.91	7	1
1:A:125:LEU:O	1:A:126:SER:CB	0.54	2.55	20	19
1:A:124:LEU:CD1	1:A:153:THR:OG1	0.54	2.56	6	2
1:A:119:ARG:HH21	1:A:129:LYS:HZ2	0.54	1.45	9	1
1:A:119:ARG:HH11	1:A:129:LYS:CE	0.54	2.16	18	1
1:A:173:LEU:HD23	1:A:173:LEU:O	0.54	2.02	14	4
1:A:66:ASP:OD1	1:A:67:ASP:N	0.54	2.41	6	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:117:PHE:CZ	1:A:180:GLU:OE2	0.54	2.60	11	2
1:A:91:ASN:OD1	1:A:95:TYR:CE1	0.54	2.61	11	1
1:A:119:ARG:O	1:A:122:ASP:OD1	0.54	2.26	13	3
1:A:146:LEU:HD22	1:A:149:LEU:HD22	0.54	1.78	2	1
1:A:87:TRP:CZ3	1:A:88:GLN:OE1	0.54	2.61	3	2
1:A:146:LEU:HD13	1:A:149:LEU:HD22	0.54	1.78	19	2
1:A:103:GLU:OE1	1:A:107:ARG:NH2	0.54	2.41	12	1
1:A:124:LEU:HD23	1:A:153:THR:HB	0.53	1.79	7	10
1:A:87:TRP:CH2	1:A:88:GLN:OE1	0.53	2.61	2	2
1:A:144:GLU:OE2	1:A:148:LYS:NZ	0.53	2.41	14	1
1:A:67:ASP:OD2	1:A:71:TYR:CZ	0.53	2.62	12	2
1:A:148:LYS:NZ	1:A:152:GLU:OE1	0.53	2.41	4	1
1:A:111:ILE:CD1	1:A:182:PHE:CE2	0.53	2.91	20	3
1:A:156:PHE:HB2	1:A:160:TRP:CG	0.53	2.39	14	20
1:A:146:LEU:HD23	1:A:149:LEU:HD22	0.53	1.81	10	1
1:A:88:GLN:OE1	1:A:92:TYR:CD1	0.53	2.62	14	1
1:A:124:LEU:CD2	1:A:153:THR:OG1	0.53	2.48	18	1
1:A:117:PHE:CD1	1:A:183:PHE:CE1	0.53	2.96	17	6
1:A:130:LEU:HD23	1:A:130:LEU:C	0.53	2.24	1	5
1:A:61:HIS:ND1	1:A:61:HIS:O	0.53	2.38	14	3
1:A:143:ARG:NH2	1:A:147:LEU:HD11	0.53	2.19	17	1
1:A:77:ARG:NH2	1:A:82:LYS:HZ3	0.53	2.02	4	1
1:A:65:ASP:OD1	1:A:66:ASP:N	0.52	2.42	20	19
1:A:155:ILE:HG22	1:A:156:PHE:N	0.52	2.20	18	19
1:A:179:ALA:O	1:A:182:PHE:N	0.52	2.42	11	12
1:A:117:PHE:O	1:A:117:PHE:CG	0.52	2.61	5	1
1:A:80:GLN:HE21	1:A:84:SER:CB	0.52	2.18	17	2
1:A:87:TRP:CE2	1:A:88:GLN:NE2	0.52	2.78	16	1
1:A:108:TRP:CE3	1:A:125:LEU:HD12	0.52	2.40	4	3
1:A:125:LEU:HD23	1:A:125:LEU:C	0.52	2.25	11	1
1:A:108:TRP:N	1:A:108:TRP:CD1	0.52	2.75	4	2
1:A:174:ILE:O	1:A:177:ASP:N	0.52	2.40	4	3
1:A:108:TRP:NE1	1:A:167:LEU:HD22	0.52	2.20	17	1
1:A:98:ARG:HH22	1:A:138:ASN:H	0.52	1.45	20	1
1:A:116:GLY:O	1:A:118:GLN:NE2	0.52	2.42	16	1
1:A:89:ARG:NH2	1:A:93:ASP:OD2	0.51	2.43	9	1
1:A:166:TYR:O	1:A:169:VAL:N	0.51	2.43	4	1
1:A:117:PHE:O	1:A:183:PHE:CE1	0.51	2.64	15	4
1:A:130:LEU:CD1	1:A:130:LEU:N	0.51	2.74	8	1
1:A:61:HIS:CD2	1:A:61:HIS:N	0.51	2.78	18	1
1:A:87:TRP:CE3	1:A:87:TRP:N	0.51	2.78	14	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:70:LEU:O	1:A:90:LEU:CD1	0.51	2.59	11	9
1:A:140:ARG:HH11	1:A:143:ARG:HH12	0.51	1.48	8	1
1:A:110:ARG:NH1	1:A:171:ASP:OD2	0.51	2.43	11	1
1:A:80:GLN:NE2	1:A:81:THR:O	0.51	2.44	2	1
1:A:71:TYR:OH	1:A:140:ARG:NH2	0.51	2.44	5	1
1:A:173:LEU:O	1:A:173:LEU:HD23	0.51	2.04	8	1
1:A:102:ARG:HH11	1:A:138:ASN:ND2	0.51	2.03	17	1
1:A:98:ARG:NH1	1:A:102:ARG:HH12	0.51	2.04	1	1
1:A:111:ILE:HB	1:A:174:ILE:HG21	0.51	1.82	15	4
1:A:167:LEU:O	1:A:170:VAL:N	0.51	2.44	4	3
1:A:149:LEU:HD12	1:A:150:ALA:N	0.51	2.21	12	1
1:A:74:ILE:HD13	1:A:87:TRP:CD1	0.51	2.41	2	3
1:A:141:LYS:O	1:A:145:MET:SD	0.51	2.69	3	1
1:A:124:LEU:CD1	1:A:124:LEU:N	0.51	2.74	6	1
1:A:69:ILE:CD1	1:A:69:ILE:N	0.51	2.74	8	2
1:A:98:ARG:HH22	1:A:102:ARG:NH2	0.51	2.02	18	1
1:A:154:SER:CB	1:A:156:PHE:O	0.50	2.58	6	20
1:A:101:ARG:HH12	1:A:138:ASN:CB	0.50	2.19	7	1
1:A:75:VAL:O	1:A:79:GLN:NE2	0.50	2.44	10	1
1:A:122:ASP:O	1:A:127:VAL:O	0.50	2.29	19	1
1:A:126:SER:O	1:A:128:THR:N	0.50	2.42	14	2
1:A:130:LEU:C	1:A:130:LEU:HD23	0.50	2.27	4	3
1:A:102:ARG:NH2	1:A:133:MET:CE	0.50	2.74	7	1
1:A:122:ASP:OD1	1:A:127:VAL:O	0.50	2.29	15	1
1:A:98:ARG:NH2	1:A:99:GLN:OE1	0.50	2.43	17	1
1:A:127:VAL:O	1:A:127:VAL:CG1	0.50	2.60	20	2
1:A:101:ARG:CD	1:A:125:LEU:HD21	0.50	2.37	3	2
1:A:61:HIS:N	1:A:61:HIS:CD2	0.50	2.80	20	3
1:A:108:TRP:CZ3	1:A:111:ILE:HD13	0.50	2.42	17	1
1:A:81:THR:C	1:A:83:ASP:N	0.49	2.65	17	8
1:A:167:LEU:HD23	1:A:170:VAL:HB	0.49	1.84	14	1
1:A:83:ASP:O	1:A:84:SER:C	0.49	2.50	4	16
1:A:98:ARG:HH11	1:A:102:ARG:NE	0.49	2.05	4	2
1:A:112:LEU:CD1	1:A:121:ALA:HB3	0.49	2.37	18	4
1:A:87:TRP:CG	1:A:88:GLN:N	0.49	2.79	18	2
1:A:67:ASP:OD2	1:A:143:ARG:NH2	0.49	2.44	12	2
1:A:112:LEU:HD23	1:A:117:PHE:O	0.49	2.07	20	2
1:A:173:LEU:HD23	1:A:173:LEU:C	0.49	2.26	14	1
1:A:98:ARG:HH12	1:A:102:ARG:NH2	0.49	2.05	18	1
1:A:111:ILE:CG1	1:A:112:LEU:N	0.49	2.76	15	5
1:A:160:TRP:CD1	1:A:160:TRP:C	0.49	2.85	6	10

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:111:ILE:HD12	1:A:174:ILE:CG2	0.49	2.37	14	5
1:A:124:LEU:HD21	1:A:153:THR:HB	0.49	1.83	6	1
1:A:160:TRP:HE1	1:A:162:LEU:HB3	0.49	1.67	11	2
1:A:108:TRP:CE2	1:A:167:LEU:HD11	0.49	2.42	14	1
1:A:75:VAL:O	1:A:79:GLN:OE1	0.49	2.31	14	1
1:A:149:LEU:CD2	1:A:149:LEU:C	0.49	2.76	9	1
1:A:101:ARG:HE	1:A:125:LEU:HD21	0.49	1.68	12	1
1:A:101:ARG:HH21	1:A:142:ALA:C	0.49	2.10	19	1
1:A:104:VAL:HG11	1:A:108:TRP:CZ2	0.49	2.43	7	1
1:A:62:THR:OG1	1:A:68:ARG:NH1	0.49	2.46	18	1
1:A:121:ALA:O	1:A:124:LEU:HG	0.49	2.07	17	2
1:A:73:LEU:CB	1:A:90:LEU:HD22	0.49	2.38	15	1
1:A:100:ILE:C	1:A:100:ILE:HD12	0.49	2.29	16	3
1:A:87:TRP:N	1:A:87:TRP:CE3	0.48	2.81	15	2
1:A:138:ASN:O	1:A:139:THR:OG1	0.48	2.31	16	8
1:A:164:GLU:CD	1:A:164:GLU:H	0.48	2.09	15	2
1:A:105:ARG:NH1	1:A:109:ARG:NH1	0.48	2.61	14	1
1:A:108:TRP:CE2	1:A:167:LEU:HD21	0.48	2.42	14	1
1:A:154:SER:O	1:A:186:ALA:HA	0.48	2.08	6	3
1:A:119:ARG:HH11	1:A:129:LYS:NZ	0.48	2.07	18	2
1:A:104:VAL:O	1:A:107:ARG:N	0.48	2.45	7	5
1:A:107:ARG:NE	1:A:168:LEU:CD2	0.48	2.77	5	1
1:A:196:VAL:O	1:A:196:VAL:HG23	0.48	2.08	7	1
1:A:112:LEU:HD11	1:A:121:ALA:HB3	0.48	1.84	17	1
1:A:80:GLN:NE2	1:A:87:TRP:CE2	0.48	2.81	14	2
1:A:130:LEU:O	1:A:130:LEU:CD1	0.48	2.62	3	1
1:A:108:TRP:CZ3	1:A:121:ALA:O	0.48	2.67	12	1
1:A:101:ARG:CZ	1:A:146:LEU:HD23	0.48	2.38	19	1
1:A:160:TRP:C	1:A:160:TRP:CD1	0.48	2.87	9	8
1:A:119:ARG:NH1	1:A:129:LYS:CE	0.48	2.76	18	1
1:A:115:LEU:HG	1:A:179:ALA:HB3	0.48	1.84	15	2
1:A:126:SER:O	1:A:130:LEU:HD21	0.48	2.08	5	1
1:A:130:LEU:HD13	1:A:130:LEU:N	0.48	2.22	8	1
1:A:108:TRP:CH2	1:A:167:LEU:HD21	0.48	2.43	14	1
1:A:67:ASP:OD2	1:A:71:TYR:CE1	0.48	2.66	1	2
1:A:155:ILE:CG2	1:A:156:PHE:N	0.48	2.77	18	5
1:A:170:VAL:CG1	1:A:182:PHE:CZ	0.48	2.97	4	1
1:A:124:LEU:HD23	1:A:149:LEU:CD2	0.48	2.37	6	1
1:A:174:ILE:CD1	1:A:174:ILE:C	0.48	2.78	20	4
1:A:115:LEU:HD13	1:A:179:ALA:CB	0.48	2.39	20	3
1:A:105:ARG:HH11	1:A:109:ARG:HH12	0.48	1.51	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:157:PRO:O	1:A:160:TRP:HB3	0.47	2.09	4	17
1:A:130:LEU:CD1	1:A:130:LEU:O	0.47	2.61	10	1
1:A:64:ALA:O	1:A:67:ASP:OD1	0.47	2.32	7	6
1:A:98:ARG:HH11	1:A:102:ARG:CZ	0.47	2.22	4	1
1:A:117:PHE:O	1:A:183:PHE:CZ	0.47	2.67	15	4
1:A:124:LEU:HD13	1:A:149:LEU:CG	0.47	2.39	10	1
1:A:90:LEU:CD2	1:A:90:LEU:C	0.47	2.77	7	4
1:A:121:ALA:O	1:A:124:LEU:HD12	0.47	2.10	7	1
1:A:64:ALA:HB3	1:A:143:ARG:NH1	0.47	2.23	13	1
1:A:67:ASP:CG	1:A:143:ARG:NE	0.47	2.68	18	2
1:A:81:THR:O	1:A:84:SER:OG	0.47	2.32	3	4
1:A:112:LEU:HD22	1:A:118:GLN:HA	0.47	1.84	17	1
1:A:98:ARG:CZ	1:A:102:ARG:NH2	0.47	2.78	18	1
1:A:120:GLU:O	1:A:124:LEU:CD2	0.47	2.61	18	1
1:A:105:ARG:NE	1:A:109:ARG:NH1	0.47	2.63	14	1
1:A:74:ILE:HD13	1:A:87:TRP:NE1	0.47	2.24	6	2
1:A:121:ALA:O	1:A:122:ASP:C	0.47	2.51	17	4
1:A:101:ARG:HH22	1:A:102:ARG:CZ	0.47	2.22	7	1
1:A:122:ASP:OD2	1:A:127:VAL:O	0.47	2.32	10	3
1:A:90:LEU:HD23	1:A:90:LEU:C	0.47	2.29	11	2
1:A:107:ARG:CZ	1:A:110:ARG:NH1	0.47	2.78	8	1
1:A:93:ASP:O	1:A:96:THR:OG1	0.47	2.32	8	6
1:A:156:PHE:CB	1:A:160:TRP:CG	0.47	2.98	15	6
1:A:61:HIS:HD1	1:A:61:HIS:C	0.46	2.12	14	4
1:A:86:GLU:CB	1:A:87:TRP:CZ3	0.46	2.99	14	4
1:A:66:ASP:O	1:A:70:LEU:CG	0.46	2.63	8	1
1:A:189:MET:C	1:A:189:MET:SD	0.46	2.94	15	13
1:A:67:ASP:CG	1:A:143:ARG:CD	0.46	2.84	18	3
1:A:90:LEU:C	1:A:90:LEU:HD23	0.46	2.30	5	4
1:A:160:TRP:HE1	1:A:162:LEU:CB	0.46	2.23	18	2
1:A:127:VAL:O	1:A:128:THR:C	0.46	2.53	14	4
1:A:107:ARG:NH2	1:A:168:LEU:CD2	0.46	2.73	16	1
1:A:61:HIS:ND1	1:A:61:HIS:C	0.46	2.69	14	4
1:A:125:LEU:O	1:A:126:SER:OG	0.46	2.34	20	9
1:A:118:GLN:OE1	1:A:122:ASP:OD2	0.46	2.33	6	3
1:A:109:ARG:HH11	1:A:127:VAL:CG1	0.46	2.23	14	1
1:A:117:PHE:CD2	1:A:183:PHE:CZ	0.46	3.04	5	1
1:A:108:TRP:CE3	1:A:121:ALA:O	0.46	2.68	12	1
1:A:158:ALA:C	1:A:160:TRP:H	0.46	2.13	12	1
1:A:106:ASN:ND2	1:A:107:ARG:NH1	0.46	2.63	19	1
1:A:61:HIS:C	1:A:61:HIS:HD1	0.46	2.13	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:185:ILE:HG13	1:A:186:ALA:N	0.46	2.26	9	8
1:A:111:ILE:HD11	1:A:182:PHE:CD1	0.46	2.45	16	2
1:A:128:THR:O	1:A:128:THR:CG2	0.46	2.63	17	2
1:A:90:LEU:C	1:A:90:LEU:CD1	0.46	2.83	9	1
1:A:108:TRP:O	1:A:109:ARG:C	0.46	2.54	11	4
1:A:105:ARG:NH2	1:A:127:VAL:HG21	0.46	2.26	7	1
1:A:117:PHE:CE2	1:A:180:GLU:OE2	0.46	2.68	11	1
1:A:97:LEU:CD1	1:A:100:ILE:HD11	0.46	2.41	18	1
1:A:189:MET:SD	1:A:189:MET:C	0.45	2.94	2	7
1:A:128:THR:C	1:A:130:LEU:N	0.45	2.68	11	1
1:A:158:ALA:C	1:A:160:TRP:N	0.45	2.69	12	1
1:A:122:ASP:C	1:A:127:VAL:O	0.45	2.54	19	1
1:A:61:HIS:C	1:A:61:HIS:ND1	0.45	2.70	10	2
1:A:140:ARG:O	1:A:144:GLU:OE1	0.45	2.34	18	1
1:A:103:GLU:OE1	1:A:164:GLU:OE2	0.45	2.35	20	1
1:A:59:VAL:HG13	1:A:60:SER:N	0.45	2.27	8	4
1:A:66:ASP:O	1:A:70:LEU:CD2	0.45	2.63	8	1
1:A:69:ILE:N	1:A:69:ILE:HD12	0.45	2.26	8	2
1:A:101:ARG:HH12	1:A:138:ASN:ND2	0.45	2.09	7	1
1:A:124:LEU:HD13	1:A:153:THR:OG1	0.45	2.10	18	1
1:A:67:ASP:OD1	1:A:143:ARG:NE	0.45	2.50	18	1
1:A:118:GLN:O	1:A:122:ASP:CG	0.45	2.55	16	6
1:A:118:GLN:CD	1:A:119:ARG:N	0.45	2.70	6	3
1:A:86:GLU:CG	1:A:87:TRP:CZ3	0.45	2.99	1	1
1:A:114:ASP:OD1	1:A:114:ASP:O	0.45	2.35	8	7
1:A:62:THR:CG2	1:A:63:GLU:H	0.45	2.25	17	8
1:A:164:GLU:CD	1:A:164:GLU:N	0.45	2.70	12	1
1:A:167:LEU:O	1:A:170:VAL:HG22	0.45	2.12	15	1
1:A:90:LEU:C	1:A:90:LEU:CD2	0.45	2.79	8	2
1:A:95:TYR:CE1	1:A:139:THR:CG2	0.44	2.99	10	1
1:A:179:ALA:C	1:A:181:ASP:N	0.44	2.67	12	1
1:A:179:ALA:CB	1:A:182:PHE:CZ	0.44	2.98	12	1
1:A:61:HIS:CB	1:A:65:ASP:OD1	0.44	2.65	12	1
1:A:146:LEU:O	1:A:149:LEU:HD23	0.44	2.12	20	1
1:A:101:ARG:HE	1:A:142:ALA:C	0.44	2.15	1	1
1:A:83:ASP:O	1:A:84:SER:O	0.44	2.35	15	2
1:A:119:ARG:O	1:A:122:ASP:OD2	0.44	2.35	15	1
1:A:62:THR:HG22	1:A:63:GLU:H	0.44	1.73	17	1
1:A:101:ARG:HB2	1:A:142:ALA:HB1	0.44	1.89	19	13
1:A:135:ASP:OD1	1:A:135:ASP:O	0.44	2.36	12	2
1:A:101:ARG:NH2	1:A:142:ALA:O	0.44	2.47	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:125:LEU:C	1:A:125:LEU:HD23	0.44	2.33	1	1
1:A:64:ALA:HB3	1:A:143:ARG:NH2	0.44	2.28	2	1
1:A:115:LEU:HD13	1:A:179:ALA:HB3	0.44	1.89	14	2
1:A:127:VAL:HG13	1:A:130:LEU:O	0.44	2.13	7	1
1:A:115:LEU:HD21	1:A:177:ASP:OD1	0.44	2.13	15	1
1:A:101:ARG:NH1	1:A:126:SER:OG	0.44	2.51	3	1
1:A:174:ILE:C	1:A:174:ILE:CD1	0.44	2.86	3	2
1:A:144:GLU:CG	1:A:148:LYS:NZ	0.44	2.81	13	1
1:A:71:TYR:OH	1:A:140:ARG:CD	0.44	2.66	16	1
1:A:104:VAL:CG1	1:A:105:ARG:N	0.44	2.81	1	2
1:A:70:LEU:HD21	1:A:93:ASP:HB3	0.44	1.90	9	1
1:A:97:LEU:O	1:A:100:ILE:CG1	0.43	2.65	11	5
1:A:94:ILE:O	1:A:97:LEU:CB	0.43	2.66	8	4
1:A:105:ARG:HE	1:A:127:VAL:CG2	0.43	2.26	12	1
1:A:81:THR:HG22	1:A:83:ASP:H	0.43	1.73	14	1
1:A:97:LEU:HD13	1:A:100:ILE:HD11	0.43	1.88	18	1
1:A:98:ARG:HH11	1:A:102:ARG:NH1	0.43	2.11	4	1
1:A:157:PRO:O	1:A:160:TRP:CB	0.43	2.66	12	1
1:A:95:TYR:OH	1:A:98:ARG:NH1	0.43	2.52	2	1
1:A:73:LEU:O	1:A:76:ILE:HG12	0.43	2.13	10	5
1:A:128:THR:OG1	1:A:128:THR:O	0.43	2.37	4	1
1:A:100:ILE:HG12	1:A:101:ARG:N	0.43	2.29	9	5
1:A:138:ASN:C	1:A:139:THR:HG23	0.43	2.32	18	1
1:A:106:ASN:ND2	1:A:107:ARG:HH12	0.43	2.12	19	1
1:A:174:ILE:HD12	1:A:174:ILE:O	0.43	2.13	2	1
1:A:107:ARG:HE	1:A:168:LEU:HD23	0.43	1.73	8	1
1:A:124:LEU:CD1	1:A:124:LEU:H	0.43	2.27	9	1
1:A:122:ASP:OD1	1:A:127:VAL:CG2	0.43	2.66	2	1
1:A:97:LEU:O	1:A:97:LEU:HD13	0.43	2.13	10	2
1:A:124:LEU:HD22	1:A:149:LEU:HD12	0.43	1.90	17	1
1:A:115:LEU:HD22	1:A:179:ALA:HB3	0.43	1.91	19	1
1:A:126:SER:C	1:A:128:THR:H	0.43	2.16	1	1
1:A:108:TRP:O	1:A:112:LEU:HD12	0.43	2.14	14	1
1:A:164:GLU:H	1:A:164:GLU:CD	0.43	2.13	18	1
1:A:98:ARG:NH1	1:A:102:ARG:HH21	0.43	2.12	18	1
1:A:112:LEU:HD13	1:A:121:ALA:HB3	0.42	1.91	4	2
1:A:107:ARG:HE	1:A:168:LEU:CG	0.42	2.26	4	1
1:A:114:ASP:O	1:A:114:ASP:OD1	0.42	2.37	19	3
1:A:125:LEU:HD23	1:A:125:LEU:O	0.42	2.13	20	1
1:A:130:LEU:O	1:A:130:LEU:CG	0.42	2.68	3	1
1:A:67:ASP:OD2	1:A:71:TYR:OH	0.42	2.36	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:109:ARG:O	1:A:113:GLU:CB	0.42	2.68	16	6
1:A:154:SER:HB2	1:A:156:PHE:O	0.42	2.13	6	1
1:A:124:LEU:HD13	1:A:149:LEU:HG	0.42	1.91	10	1
1:A:128:THR:O	1:A:129:LYS:CB	0.42	2.65	19	1
1:A:98:ARG:HH21	1:A:99:GLN:NE2	0.42	2.12	16	1
1:A:149:LEU:CD1	1:A:150:ALA:N	0.42	2.69	9	1
1:A:84:SER:O	1:A:87:TRP:CD1	0.42	2.73	8	1
1:A:164:GLU:OE1	1:A:164:GLU:O	0.42	2.37	19	1
1:A:124:LEU:HB3	1:A:153:THR:OG1	0.42	2.13	2	1
1:A:116:GLY:O	1:A:118:GLN:OE1	0.42	2.37	16	1
1:A:130:LEU:CG	1:A:130:LEU:O	0.42	2.68	10	1
1:A:67:ASP:O	1:A:67:ASP:OD1	0.42	2.37	16	1
1:A:115:LEU:HD12	1:A:179:ALA:HB3	0.42	1.91	17	1
1:A:117:PHE:CZ	1:A:183:PHE:CD2	0.42	3.07	5	1
1:A:104:VAL:CG1	1:A:167:LEU:HD13	0.42	2.43	17	1
1:A:86:GLU:OE1	1:A:86:GLU:N	0.42	2.53	4	3
1:A:126:SER:OG	1:A:145:MET:CE	0.42	2.68	10	1
1:A:108:TRP:CH2	1:A:155:ILE:HG21	0.42	2.50	14	1
1:A:127:VAL:C	1:A:128:THR:HG1	0.42	2.17	19	1
1:A:100:ILE:CG1	1:A:101:ARG:N	0.42	2.82	9	3
1:A:61:HIS:ND1	1:A:69:ILE:HD12	0.41	2.29	9	1
1:A:98:ARG:NH1	1:A:99:GLN:HE22	0.41	2.12	14	1
1:A:81:THR:O	1:A:82:LYS:C	0.41	2.59	11	1
1:A:100:ILE:CD1	1:A:101:ARG:N	0.41	2.71	18	1
1:A:124:LEU:HD13	1:A:153:THR:CB	0.41	2.46	18	1
1:A:149:LEU:CD2	1:A:150:ALA:N	0.41	2.75	8	1
1:A:100:ILE:HD13	1:A:164:GLU:CD	0.41	2.36	18	1
1:A:108:TRP:CZ3	1:A:124:LEU:CD1	0.41	3.03	7	2
1:A:101:ARG:NH1	1:A:138:ASN:CB	0.41	2.83	7	1
1:A:67:ASP:CG	1:A:68:ARG:N	0.41	2.73	2	1
1:A:135:ASP:OD1	1:A:136:SER:N	0.41	2.54	7	2
1:A:80:GLN:CD	1:A:84:SER:OG	0.41	2.59	10	1
1:A:117:PHE:HB3	1:A:183:PHE:CZ	0.41	2.51	13	1
1:A:105:ARG:NE	1:A:109:ARG:CZ	0.41	2.84	14	1
1:A:105:ARG:NH1	1:A:109:ARG:CZ	0.41	2.83	14	1
1:A:80:GLN:CD	1:A:81:THR:H	0.41	2.17	2	2
1:A:154:SER:OG	1:A:189:MET:CB	0.41	2.69	4	2
1:A:104:VAL:HG12	1:A:108:TRP:CE2	0.41	2.49	7	1
1:A:61:HIS:ND1	1:A:65:ASP:OD1	0.41	2.54	12	1
1:A:87:TRP:O	1:A:88:GLN:C	0.41	2.57	13	1
1:A:74:ILE:HG12	1:A:90:LEU:HD23	0.41	1.91	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:91:ASN:ND2	1:A:95:TYR:CE1	0.41	2.89	1	1
1:A:105:ARG:HH11	1:A:109:ARG:HH11	0.41	1.59	4	1
1:A:127:VAL:C	1:A:129:LYS:N	0.41	2.74	5	1
1:A:75:VAL:O	1:A:78:ASN:N	0.41	2.53	5	1
1:A:100:ILE:HG22	1:A:164:GLU:OE2	0.41	2.15	6	1
1:A:101:ARG:NH2	1:A:102:ARG:CZ	0.41	2.84	7	1
1:A:122:ASP:HB3	1:A:127:VAL:O	0.41	2.16	12	1
1:A:130:LEU:CD1	1:A:132:THR:OG1	0.41	2.68	14	1
1:A:124:LEU:H	1:A:124:LEU:CD2	0.41	2.29	16	1
1:A:143:ARG:CZ	1:A:147:LEU:HD11	0.41	2.46	17	1
1:A:108:TRP:CZ3	1:A:124:LEU:HD13	0.41	2.51	7	1
1:A:81:THR:O	1:A:84:SER:N	0.41	2.52	11	1
1:A:70:LEU:HB3	1:A:90:LEU:HD11	0.41	1.92	15	1
1:A:107:ARG:CD	1:A:171:ASP:OD2	0.40	2.69	3	1
1:A:125:LEU:O	1:A:126:SER:HB3	0.40	2.17	11	1
1:A:108:TRP:CZ2	1:A:162:LEU:HD21	0.40	2.51	12	1
1:A:162:LEU:N	1:A:162:LEU:HD23	0.40	2.31	13	1
1:A:141:LYS:NZ	1:A:145:MET:CE	0.40	2.85	1	1
1:A:98:ARG:NH1	1:A:102:ARG:HE	0.40	2.14	4	1
1:A:95:TYR:CE1	1:A:137:LYS:NZ	0.40	2.89	13	1
1:A:69:ILE:O	1:A:70:LEU:C	0.40	2.60	15	1
1:A:100:ILE:HG22	1:A:164:GLU:OE1	0.40	2.17	4	1
1:A:105:ARG:CG	1:A:105:ARG:NH2	0.40	2.82	7	1
1:A:103:GLU:OE2	1:A:107:ARG:CZ	0.40	2.68	18	1
1:A:146:LEU:O	1:A:149:LEU:CD2	0.40	2.70	20	1
1:A:101:ARG:NH2	1:A:146:LEU:CG	0.40	2.85	1	1
1:A:130:LEU:O	1:A:130:LEU:CD2	0.40	2.61	8	1
1:A:90:LEU:HD13	1:A:91:ASN:CA	0.40	2.46	16	1
1:A:70:LEU:O	1:A:71:TYR:C	0.40	2.60	18	1
1:A:166:TYR:O	1:A:167:LEU:C	0.40	2.58	4	1
1:A:101:ARG:NE	1:A:101:ARG:HA	0.40	2.31	19	1

6.3 Torsion angles ⓘ

6.3.1 Protein backbone ⓘ

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	139/214 (65%)	133±1 (95±1%)	4±1 (3±1%)	2±1 (2±1%)	15	58
All	All	2780/4280 (65%)	2651 (95%)	82 (3%)	47 (2%)	15	58

All 6 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	126	SER	20
1	A	84	SER	11
1	A	82	LYS	7
1	A	128	THR	5
1	A	139	THR	2
1	A	127	VAL	2

6.3.2 Protein sidechains ⓘ

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	128/196 (65%)	110±2 (86±2%)	18±2 (14±2%)	8	48
All	All	2560/3920 (65%)	2206 (86%)	354 (14%)	8	48

All 53 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	149	LEU	20
1	A	111	ILE	20
1	A	174	ILE	20
1	A	155	ILE	20
1	A	153	THR	20
1	A	90	LEU	19
1	A	183	PHE	17
1	A	117	PHE	16
1	A	61	HIS	16
1	A	76	ILE	15
1	A	130	LEU	12
1	A	60	SER	11

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Mol	Chain	Res	Type	Models (Total)
1	A	124	LEU	11
1	A	189	MET	11
1	A	97	LEU	10
1	A	100	ILE	9
1	A	136	SER	9
1	A	164	GLU	9
1	A	125	LEU	7
1	A	87	TRP	7
1	A	84	SER	7
1	A	146	LEU	6
1	A	167	LEU	6
1	A	115	LEU	5
1	A	145	MET	4
1	A	122	ASP	4
1	A	107	ARG	3
1	A	170	VAL	3
1	A	71	TYR	3
1	A	123	SER	2
1	A	141	LYS	2
1	A	74	ILE	2
1	A	128	THR	2
1	A	138	ASN	2
1	A	80	GLN	2
1	A	168	LEU	2
1	A	70	LEU	2
1	A	104	VAL	2
1	A	152	GLU	2
1	A	77	ARG	1
1	A	194	PRO	1
1	A	140	ARG	1
1	A	118	GLN	1
1	A	162	LEU	1
1	A	105	ARG	1
1	A	190	TYR	1
1	A	173	LEU	1
1	A	101	ARG	1
1	A	163	SER	1
1	A	67	ASP	1
1	A	88	GLN	1
1	A	98	ARG	1
1	A	126	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 60% for the well-defined parts and 55% for the entire structure.

7.1 Chemical shift list 1

File name: 5kbo_cs.cif

Chemical shift list name: *MregChemicalShiftBmrbl.tbl*

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	1360
Number of shifts mapped to atoms	1360
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	165	-0.29 ± 0.15	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	161	1.34 ± 0.09	Should be applied
$^{13}\text{C}'$	153	-0.44 ± 0.13	None needed (< 0.5 ppm)
^{15}N	151	0.72 ± 0.20	Should be applied

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 60%, i.e. 1118 atoms were assigned a chemical shift out of a possible 1858. 6 out of 24 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	660/687 (96%)	265/274 (97%)	266/278 (96%)	129/135 (96%)
Sidechain	455/1051 (43%)	271/616 (44%)	184/371 (50%)	0/64 (0%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	3/120 (2%)	3/62 (5%)	0/53 (0%)	0/5 (0%)
Overall	1118/1858 (60%)	539/952 (57%)	450/702 (64%)	129/204 (63%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 55%, i.e. 1318 atoms were assigned a chemical shift out of a possible 2386. 7 out of 30 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	784/892 (88%)	315/355 (89%)	318/364 (87%)	151/173 (87%)
Sidechain	531/1320 (40%)	316/778 (41%)	215/466 (46%)	0/76 (0%)
Aromatic	3/174 (2%)	3/90 (3%)	0/74 (0%)	0/10 (0%)
Overall	1318/2386 (55%)	634/1223 (52%)	533/904 (59%)	151/259 (58%)

7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

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:

