



Full wwPDB NMR Structure Validation Report ⓘ

Mar 8, 2026 – 02:56 AM UTC

PDB ID : 1R3B / pdb_00001r3b
Title : Solution structure of xenopus laevis Mob1
Authors : Ponchon, L.; Dumas, C.; Kajava, A.V.; Fesquet, D.; Padilla, A.
Deposited on : 2003-10-01

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
wwPDB-ShiftChecker : v1.2
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

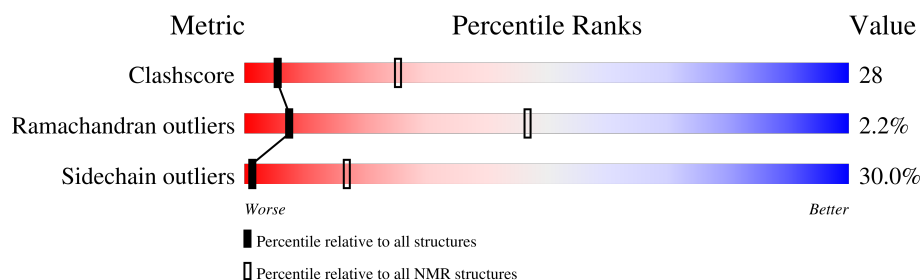
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment was not calculated.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

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	202	20% 38% . 39%

2 Ensemble composition and analysis

This entry contains 20 models. Model 2 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:40-A:78, A:111-A:131, A:142-A:193, A:199-A:210 (124)	1.19	2

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 3 clusters and 2 single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 3233 atoms, of which 1592 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called MOB1.

Mol	Chain	Residues	Atoms						Trace
1	A	202	Total	C	H	N	O	S	0
			3233	1050	1592	282	299	10	

There are 18 discrepancies between the modelled and reference sequences:

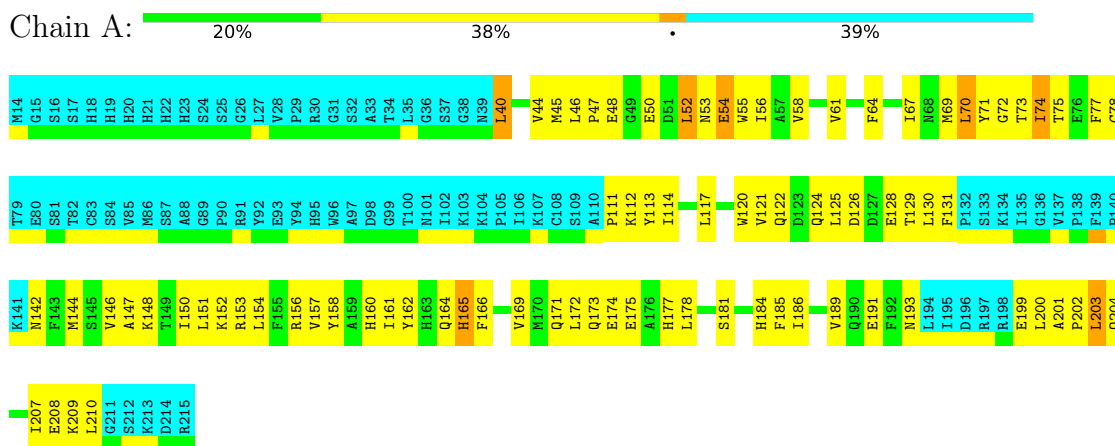
Chain	Residue	Modelled	Actual	Comment	Reference
A	14	MET	-	cloning artifact	UNP Q7T1M9
A	15	GLY	-	cloning artifact	UNP Q7T1M9
A	16	SER	-	cloning artifact	UNP Q7T1M9
A	17	SER	-	cloning artifact	UNP Q7T1M9
A	18	HIS	-	expression tag	UNP Q7T1M9
A	19	HIS	-	expression tag	UNP Q7T1M9
A	20	HIS	-	expression tag	UNP Q7T1M9
A	21	HIS	-	expression tag	UNP Q7T1M9
A	22	HIS	-	expression tag	UNP Q7T1M9
A	23	HIS	-	expression tag	UNP Q7T1M9
A	24	SER	-	cloning artifact	UNP Q7T1M9
A	25	SER	-	cloning artifact	UNP Q7T1M9
A	26	GLY	-	cloning artifact	UNP Q7T1M9
A	28	VAL	-	cloning artifact	UNP Q7T1M9
A	29	PRO	-	cloning artifact	UNP Q7T1M9
A	30	ARG	-	cloning artifact	UNP Q7T1M9
A	31	GLY	-	cloning artifact	UNP Q7T1M9
A	32	SER	-	cloning artifact	UNP Q7T1M9

4 Residue-property plots [i](#)

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

- Molecule 1: MOB1

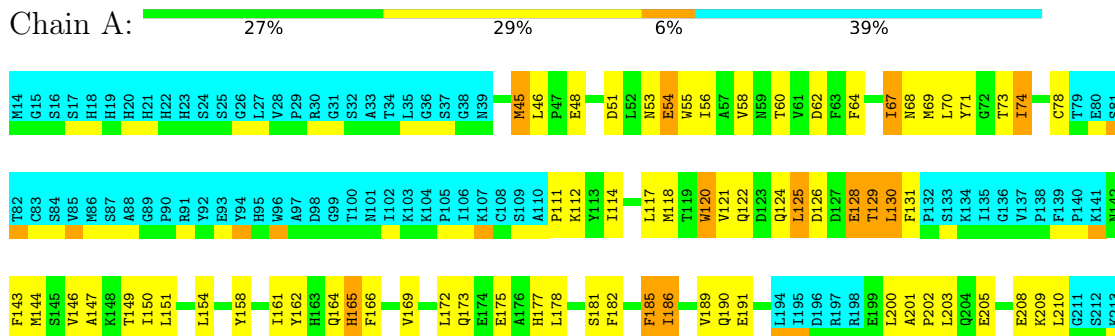


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

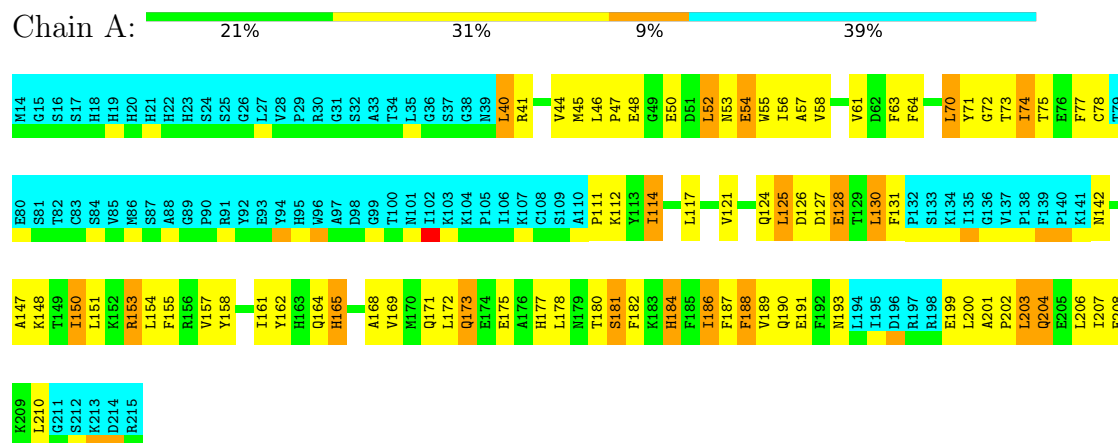
- Molecule 1: MOB1



D214
R215

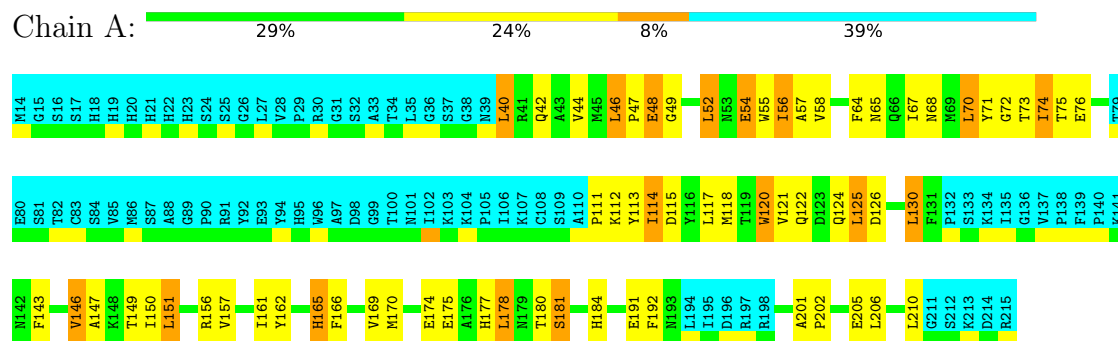
4.2.2 Score per residue for model 2 (medoid)

- Molecule 1: MOB1



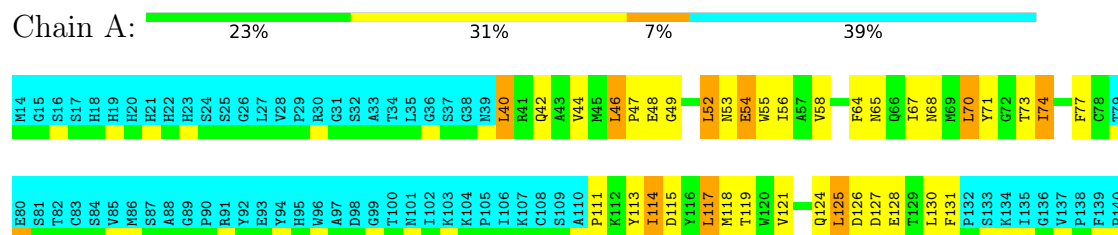
4.2.3 Score per residue for model 3

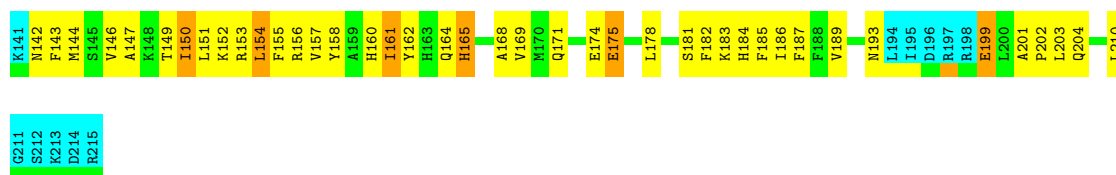
- Molecule 1: MOB1



4.2.4 Score per residue for model 4

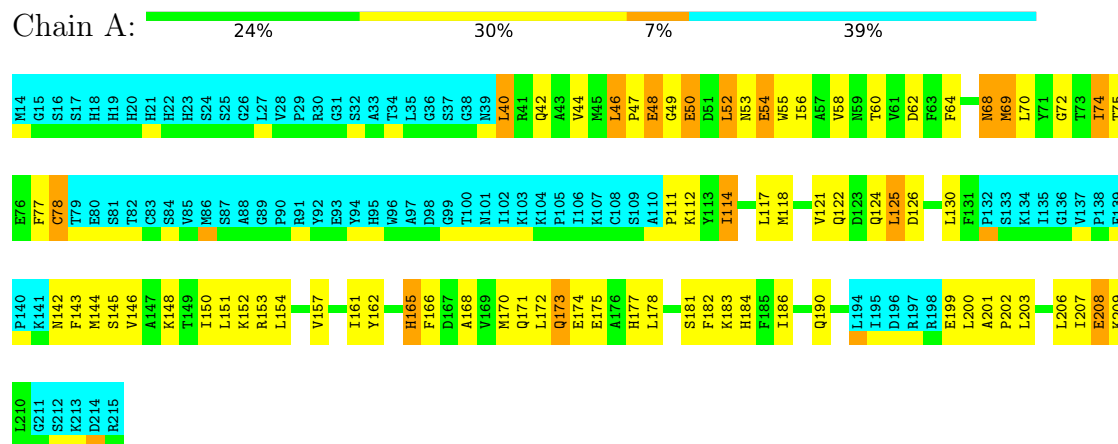
- Molecule 1: MOB1





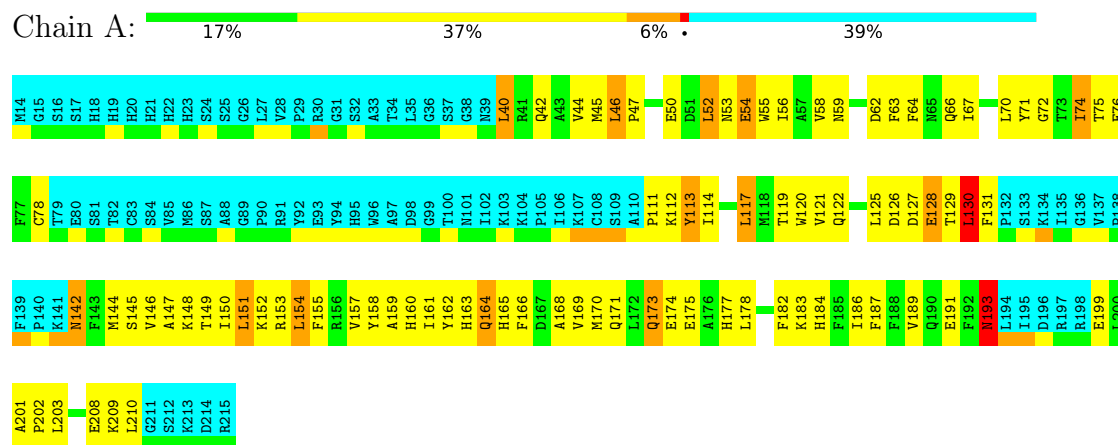
4.2.5 Score per residue for model 5

- Molecule 1: MOB1



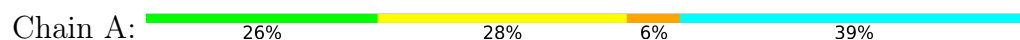
4.2.6 Score per residue for model 6

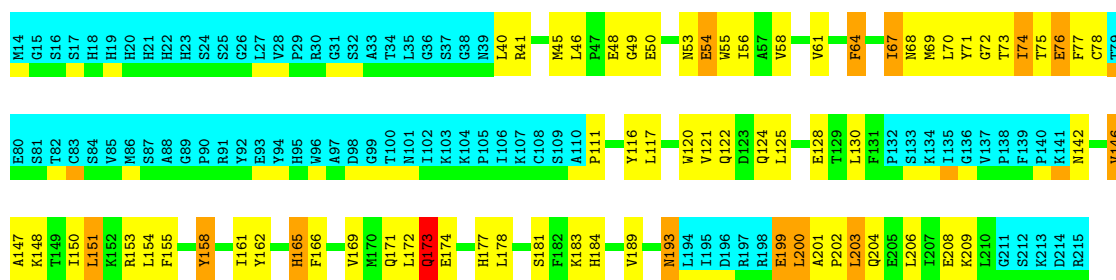
- Molecule 1: MOB1



4.2.7 Score per residue for model 7

- Molecule 1: MOB1

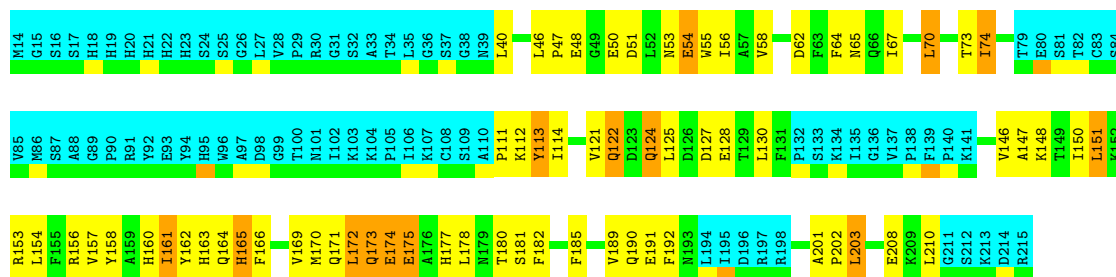




4.2.8 Score per residue for model 8

- Molecule 1: MOB1

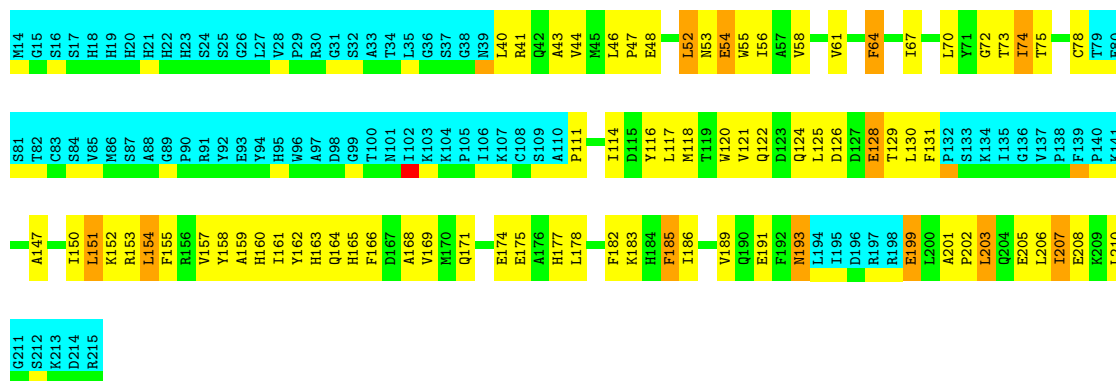
Chain A: 28% 27% 7% 39%



4.2.9 Score per residue for model 9

- Molecule 1: MOB1

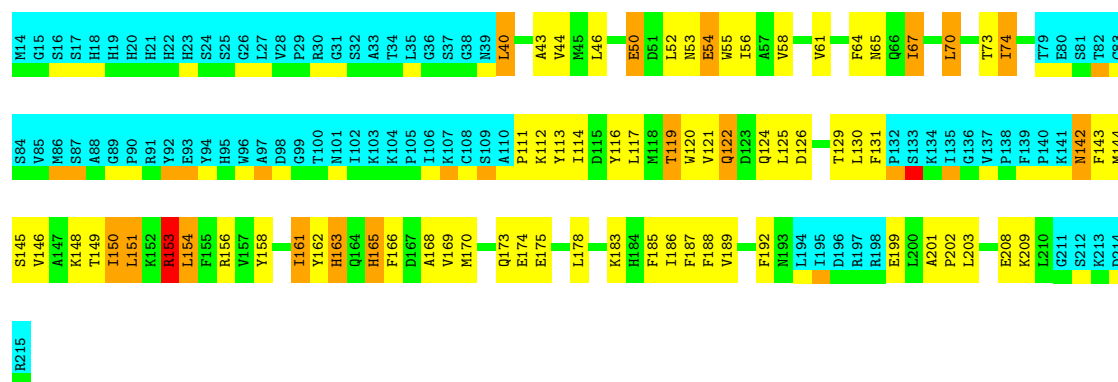
Chain A: 23% 32% 6% 39%



4.2.10 Score per residue for model 10

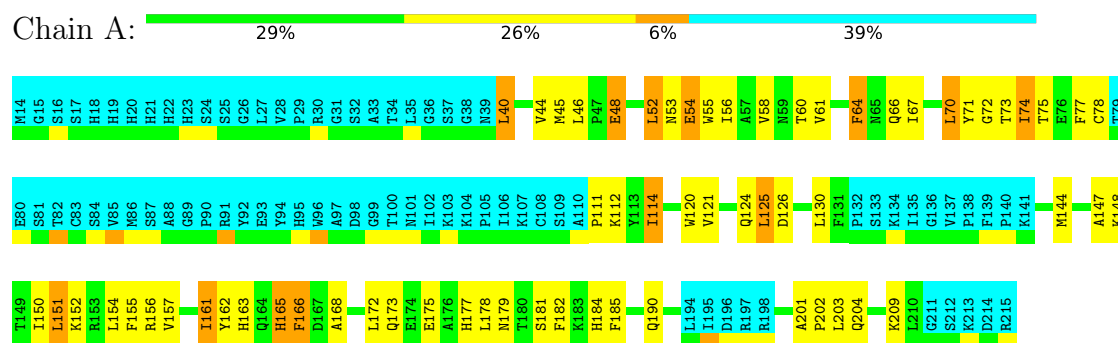
- Molecule 1: MOB1

Chain A: 26% 28% 7% 39%



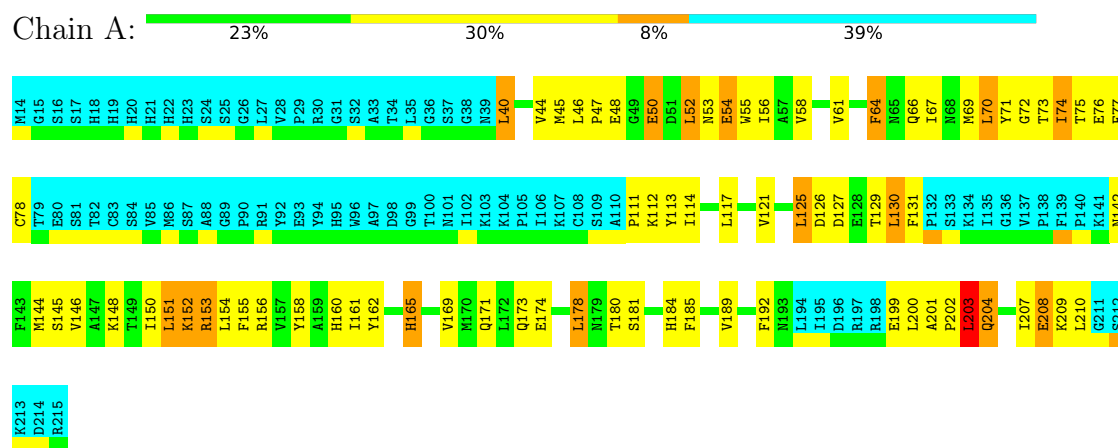
4.2.11 Score per residue for model 11

- Molecule 1: MOB1



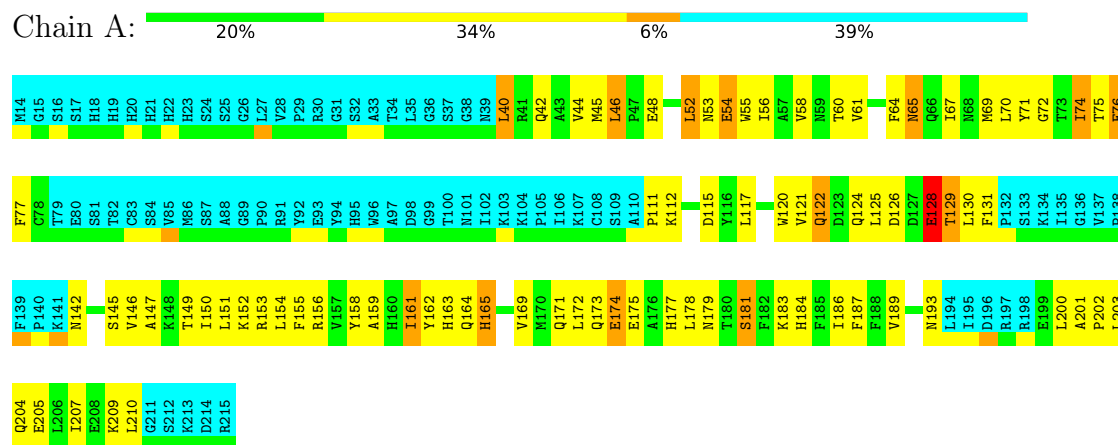
4.2.12 Score per residue for model 12

- Molecule 1: MOB1



4.2.13 Score per residue for model 13

- Molecule 1: MOB1



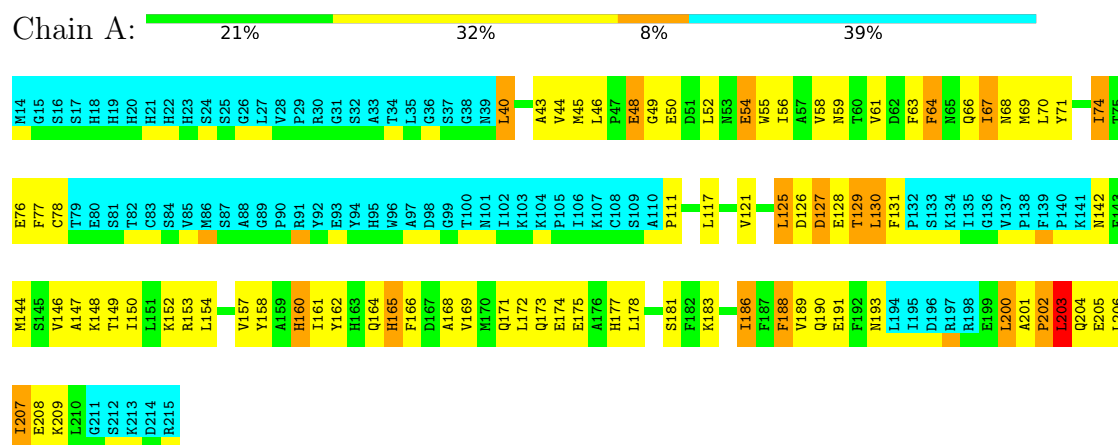
4.2.14 Score per residue for model 14

- Molecule 1: MOB1



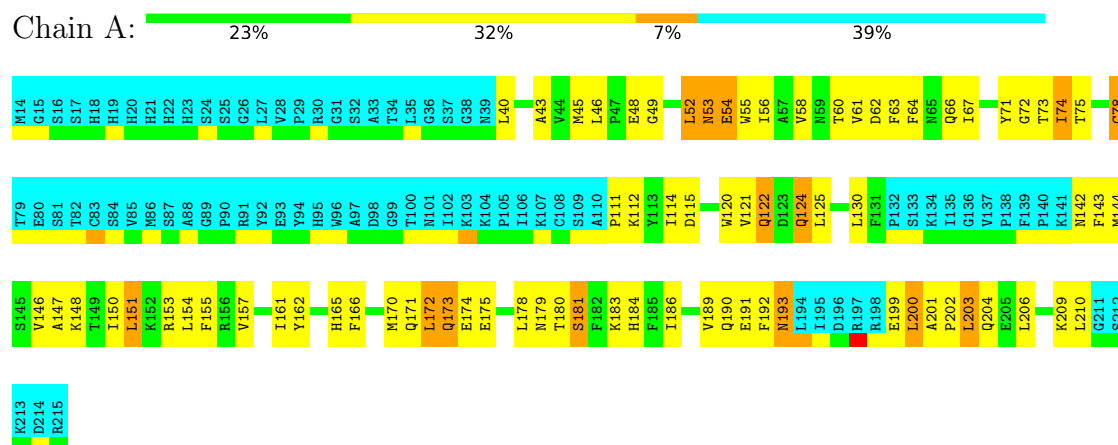
4.2.15 Score per residue for model 15

- Molecule 1: MOB1



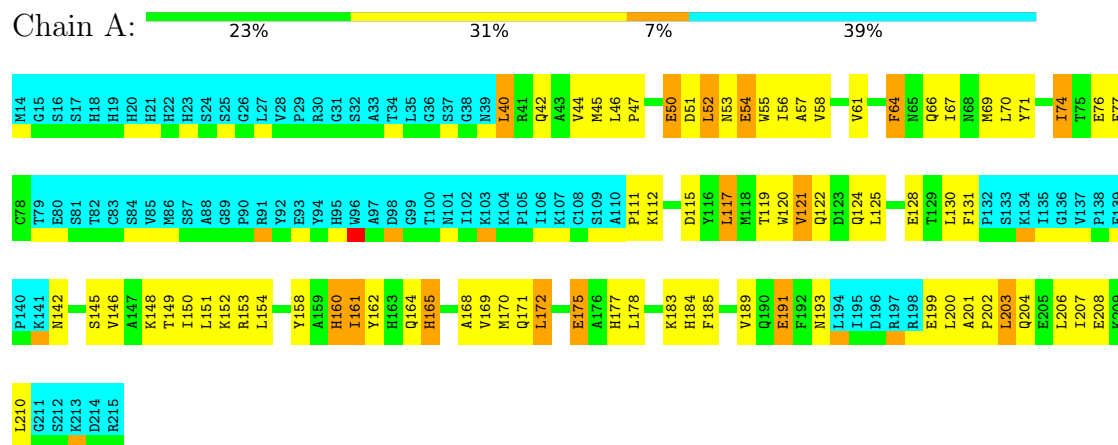
4.2.16 Score per residue for model 16

• Molecule 1: MOB1



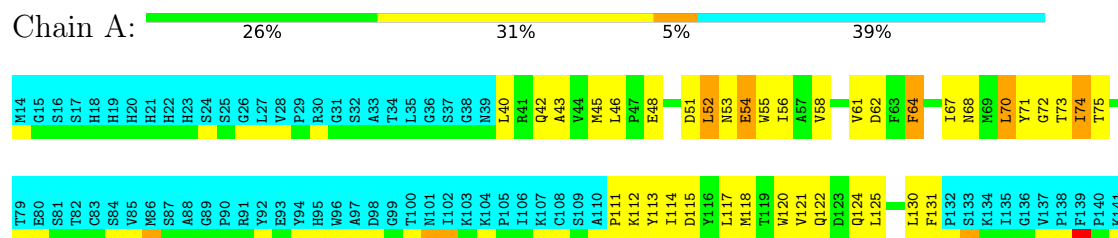
4.2.17 Score per residue for model 17

• Molecule 1: MOB1



4.2.18 Score per residue for model 18

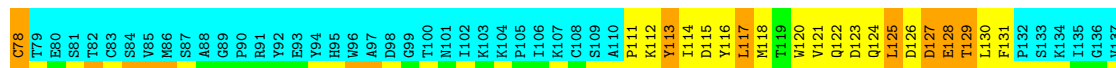
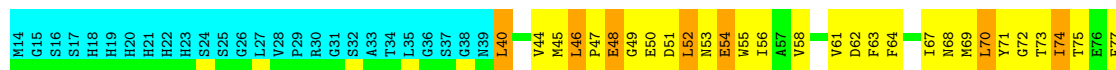
• Molecule 1: MOB1





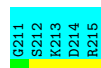
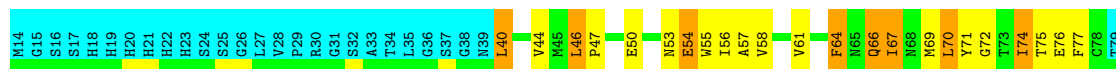
4.2.19 Score per residue for model 19

- Molecule 1: MOB1



4.2.20 Score per residue for model 20

- Molecule 1: MOB1



5 Refinement protocol and experimental data overview ⓘ

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

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *target function*.

The following table shows the software used for structure solution, optimisation and refinement.

Software name	Classification	Version
DYANA	structure solution	1.5
CNS	refinement	1.0

No chemical shift data was provided.

6 Model quality [i](#)

6.1 Standard geometry [i](#)

There are no covalent bond-length or bond-angle outliers.

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	0.1±0.2
All	All	0	1

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

All unique planar outliers are listed below.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	153	ARG	Sidechain	1

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	1051	1016	1016	57±6
All	All	21020	20320	20320	1148

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 28.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:61:VAL:HG22	1:A:125:LEU:HD22	1.05	1.14	14	8
1:A:121:VAL:HG13	1:A:150:ILE:HD11	0.98	1.32	11	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:67:ILE:HD11	1:A:154:LEU:HD22	0.96	1.33	14	2
1:A:52:LEU:HD22	1:A:53:ASN:N	0.95	1.77	14	1
1:A:54:GLU:O	1:A:58:VAL:HG23	0.90	1.67	4	20
1:A:52:LEU:O	1:A:56:ILE:HD12	0.90	1.67	15	3
1:A:52:LEU:HD12	1:A:56:ILE:HD11	0.88	1.44	11	6
1:A:114:ILE:HD11	1:A:157:VAL:HG13	0.87	1.45	11	4
1:A:169:VAL:HG21	1:A:178:LEU:HD12	0.87	1.44	7	4
1:A:52:LEU:HD13	1:A:56:ILE:HD11	0.86	1.43	3	5
1:A:122:GLN:HA	1:A:125:LEU:HD12	0.82	1.51	13	14
1:A:46:LEU:HD13	1:A:55:TRP:HB2	0.81	1.53	12	11
1:A:121:VAL:HG21	1:A:154:LEU:HD21	0.81	1.53	5	4
1:A:72:GLY:O	1:A:75:THR:HG22	0.80	1.77	19	13
1:A:162:TYR:CE2	1:A:178:LEU:HD12	0.80	2.12	12	1
1:A:158:TYR:CZ	1:A:178:LEU:HD12	0.79	2.12	15	7
1:A:73:THR:HG23	1:A:172:LEU:HD22	0.78	1.52	2	2
1:A:121:VAL:CG1	1:A:150:ILE:HD11	0.78	2.08	11	3
1:A:70:LEU:O	1:A:73:THR:HG22	0.77	1.78	4	12
1:A:64:PHE:CD1	1:A:154:LEU:HD21	0.77	2.15	16	1
1:A:40:LEU:O	1:A:44:VAL:HG23	0.77	1.79	6	13
1:A:61:VAL:HG22	1:A:125:LEU:CD2	0.76	2.10	20	6
1:A:117:LEU:O	1:A:121:VAL:HG23	0.76	1.80	5	8
1:A:146:VAL:O	1:A:149:THR:HG22	0.76	1.81	14	8
1:A:206:LEU:HD12	1:A:207:ILE:N	0.75	1.96	9	4
1:A:52:LEU:C	1:A:56:ILE:HD12	0.75	2.06	16	3
1:A:162:TYR:CD2	1:A:178:LEU:HD21	0.75	2.17	13	4
1:A:147:ALA:O	1:A:151:LEU:HD22	0.75	1.80	6	6
1:A:161:ILE:C	1:A:161:ILE:HD13	0.75	2.07	18	3
1:A:71:TYR:CE2	1:A:161:ILE:HG21	0.74	2.17	15	6
1:A:70:LEU:HD22	1:A:71:TYR:N	0.74	1.98	20	1
1:A:117:LEU:HD23	1:A:157:VAL:CG2	0.74	2.13	3	2
1:A:77:PHE:CD2	1:A:168:ALA:HB1	0.73	2.18	11	2
1:A:74:ILE:HD13	1:A:74:ILE:O	0.73	1.82	17	15
1:A:60:THR:HG23	1:A:150:ILE:HD11	0.73	1.60	13	1
1:A:120:TRP:CZ3	1:A:150:ILE:HG22	0.72	2.19	16	3
1:A:68:ASN:OD1	1:A:118:MET:HE2	0.72	1.84	19	2
1:A:66:GLN:O	1:A:70:LEU:HD12	0.72	1.85	11	2
1:A:67:ILE:CD1	1:A:154:LEU:HD22	0.72	2.14	14	4
1:A:74:ILE:HD11	1:A:168:ALA:HB3	0.71	1.63	17	1
1:A:70:LEU:HD13	1:A:70:LEU:H	0.71	1.46	20	1
1:A:74:ILE:HD11	1:A:165:HIS:CG	0.71	2.20	15	14
1:A:162:TYR:CE1	1:A:178:LEU:HD21	0.71	2.21	10	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:203:LEU:HD12	1:A:204:GLN:N	0.71	2.01	20	6
1:A:157:VAL:O	1:A:161:ILE:HG23	0.70	1.86	9	2
1:A:52:LEU:CD1	1:A:56:ILE:HD11	0.70	2.16	3	8
1:A:127:ASP:HB2	1:A:130:LEU:HD11	0.70	1.62	12	3
1:A:161:ILE:HD13	1:A:161:ILE:O	0.70	1.87	18	3
1:A:120:TRP:O	1:A:120:TRP:HE3	0.70	1.70	3	2
1:A:67:ILE:HG23	1:A:158:TYR:CE1	0.70	2.22	12	1
1:A:67:ILE:HD12	1:A:154:LEU:HD22	0.69	1.64	16	4
1:A:165:HIS:O	1:A:169:VAL:HG23	0.69	1.87	15	7
1:A:210:LEU:HD23	1:A:210:LEU:O	0.69	1.88	2	1
1:A:61:VAL:CG2	1:A:125:LEU:HD22	0.69	2.07	14	2
1:A:186:ILE:O	1:A:189:VAL:HG22	0.69	1.86	15	2
1:A:46:LEU:HD22	1:A:50:GLU:HB3	0.69	1.64	10	1
1:A:124:GLN:HB2	1:A:130:LEU:HD11	0.69	1.64	8	4
1:A:70:LEU:HD22	1:A:177:HIS:CG	0.68	2.22	5	1
1:A:162:TYR:CD2	1:A:178:LEU:HD22	0.68	2.23	9	2
1:A:71:TYR:CD1	1:A:161:ILE:HG21	0.68	2.22	3	2
1:A:160:HIS:NE2	1:A:161:ILE:HG23	0.68	2.04	12	1
1:A:64:PHE:CE1	1:A:125:LEU:HD23	0.68	2.24	11	3
1:A:162:TYR:CZ	1:A:178:LEU:HD21	0.68	2.24	17	4
1:A:124:GLN:CB	1:A:130:LEU:HD11	0.68	2.19	16	6
1:A:189:VAL:HG11	1:A:200:LEU:HD11	0.68	1.65	7	1
1:A:162:TYR:CZ	1:A:178:LEU:HD12	0.68	2.23	12	1
1:A:124:GLN:HB3	1:A:130:LEU:HD11	0.67	1.67	4	8
1:A:52:LEU:H	1:A:52:LEU:HD13	0.67	1.49	18	2
1:A:189:VAL:O	1:A:193:ASN:N	0.67	2.27	19	10
1:A:73:THR:HG23	1:A:172:LEU:CD2	0.67	2.19	2	1
1:A:118:MET:HE2	1:A:157:VAL:HG11	0.67	1.65	3	1
1:A:169:VAL:HG21	1:A:178:LEU:CD1	0.67	2.19	7	2
1:A:201:ALA:HB3	1:A:202:PRO:HD3	0.67	1.65	6	19
1:A:77:PHE:CE1	1:A:168:ALA:HB1	0.66	2.24	19	2
1:A:160:HIS:CD2	1:A:161:ILE:HG23	0.66	2.25	12	1
1:A:162:TYR:CD1	1:A:178:LEU:HD13	0.66	2.26	11	3
1:A:150:ILE:HG22	1:A:154:LEU:CD1	0.66	2.20	18	5
1:A:71:TYR:CG	1:A:161:ILE:HD11	0.66	2.25	1	1
1:A:188:PHE:CE2	1:A:189:VAL:HG13	0.65	2.27	2	1
1:A:128:GLU:O	1:A:129:THR:HG22	0.65	1.91	19	1
1:A:53:ASN:HA	1:A:56:ILE:HD12	0.65	1.68	2	15
1:A:73:THR:CG2	1:A:172:LEU:HD22	0.65	2.22	2	1
1:A:169:VAL:HG21	1:A:178:LEU:HD22	0.65	1.69	15	1
1:A:64:PHE:CD2	1:A:125:LEU:HD11	0.64	2.27	4	7

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:46:LEU:HD11	1:A:50:GLU:HB3	0.64	1.68	12	3
1:A:67:ILE:CD1	1:A:154:LEU:HD13	0.64	2.21	11	3
1:A:67:ILE:HD11	1:A:154:LEU:HD13	0.64	1.68	11	2
1:A:46:LEU:HD13	1:A:55:TRP:CE3	0.64	2.27	18	6
1:A:46:LEU:HD21	1:A:55:TRP:HB2	0.64	1.68	7	4
1:A:70:LEU:HD21	1:A:177:HIS:HB3	0.64	1.67	2	2
1:A:169:VAL:HG13	1:A:178:LEU:HD23	0.64	1.70	12	1
1:A:64:PHE:CD1	1:A:125:LEU:HD11	0.64	2.28	19	2
1:A:124:GLN:CB	1:A:130:LEU:HD21	0.63	2.22	1	1
1:A:172:LEU:HD12	1:A:173:GLN:CG	0.63	2.23	8	1
1:A:74:ILE:HD12	1:A:165:HIS:CE1	0.63	2.29	6	2
1:A:203:LEU:HD23	1:A:206:LEU:HD11	0.63	1.70	9	1
1:A:117:LEU:HD22	1:A:153:ARG:HD3	0.62	1.68	10	1
1:A:61:VAL:HG13	1:A:125:LEU:HG	0.62	1.69	12	3
1:A:71:TYR:CE1	1:A:161:ILE:HG21	0.62	2.29	20	3
1:A:169:VAL:HG13	1:A:175:GLU:HB2	0.62	1.70	10	1
1:A:60:THR:HG22	1:A:125:LEU:HD21	0.62	1.70	16	1
1:A:153:ARG:O	1:A:157:VAL:HG23	0.61	1.95	16	1
1:A:61:VAL:HA	1:A:125:LEU:HD22	0.61	1.72	10	1
1:A:64:PHE:CE2	1:A:150:ILE:HD12	0.61	2.31	16	1
1:A:71:TYR:CD2	1:A:118:MET:HE3	0.61	2.31	20	2
1:A:64:PHE:CE1	1:A:154:LEU:HD11	0.61	2.30	16	1
1:A:185:PHE:O	1:A:189:VAL:HG23	0.61	1.96	20	3
1:A:127:ASP:CB	1:A:130:LEU:HD11	0.61	2.26	20	2
1:A:117:LEU:HD12	1:A:153:ARG:NH1	0.61	2.11	12	1
1:A:73:THR:O	1:A:172:LEU:HD11	0.61	1.96	1	1
1:A:124:GLN:O	1:A:130:LEU:HD21	0.60	1.96	2	2
1:A:142:ASN:O	1:A:146:VAL:HG23	0.60	1.96	6	6
1:A:189:VAL:HG21	1:A:200:LEU:HD11	0.60	1.72	13	1
1:A:52:LEU:HD13	1:A:52:LEU:N	0.60	2.11	18	2
1:A:162:TYR:CE2	1:A:178:LEU:HD21	0.60	2.31	17	2
1:A:165:HIS:CD2	1:A:165:HIS:N	0.60	2.70	10	5
1:A:161:ILE:HB	1:A:165:HIS:NE2	0.60	2.12	9	2
1:A:70:LEU:HD12	1:A:71:TYR:N	0.60	2.12	6	1
1:A:121:VAL:HG13	1:A:150:ILE:HD13	0.59	1.74	12	1
1:A:172:LEU:HD12	1:A:172:LEU:O	0.59	1.96	17	2
1:A:64:PHE:CZ	1:A:150:ILE:HD12	0.59	2.32	16	1
1:A:121:VAL:HG12	1:A:150:ILE:CG1	0.59	2.27	4	2
1:A:207:ILE:O	1:A:207:ILE:HD13	0.59	1.97	15	1
1:A:158:TYR:CZ	1:A:178:LEU:HD23	0.59	2.33	2	1
1:A:46:LEU:HD13	1:A:55:TRP:CD2	0.59	2.33	18	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:151:LEU:HD12	1:A:154:LEU:HD12	0.59	1.73	16	1
1:A:77:PHE:CZ	1:A:168:ALA:HB1	0.58	2.33	19	2
1:A:154:LEU:HD12	1:A:155:PHE:N	0.58	2.13	6	3
1:A:121:VAL:HG21	1:A:154:LEU:CD2	0.58	2.26	20	2
1:A:64:PHE:CD2	1:A:121:VAL:HG11	0.58	2.34	10	1
1:A:151:LEU:HD12	1:A:152:LYS:N	0.58	2.14	20	3
1:A:155:PHE:CE2	1:A:203:LEU:HD23	0.58	2.33	20	1
1:A:200:LEU:HD23	1:A:200:LEU:N	0.58	2.14	15	3
1:A:162:TYR:CG	1:A:178:LEU:HD21	0.57	2.34	15	1
1:A:67:ILE:HA	1:A:70:LEU:HD11	0.57	1.76	20	1
1:A:172:LEU:HD12	1:A:173:GLN:HG2	0.57	1.77	8	1
1:A:153:ARG:NH2	1:A:154:LEU:HD23	0.57	2.14	14	1
1:A:71:TYR:CE1	1:A:74:ILE:HD11	0.57	2.34	16	1
1:A:169:VAL:HG12	1:A:175:GLU:HA	0.57	1.76	4	5
1:A:117:LEU:HD11	1:A:153:ARG:HB3	0.57	1.74	7	1
1:A:56:ILE:HD13	1:A:56:ILE:N	0.57	2.15	3	1
1:A:117:LEU:HD22	1:A:153:ARG:CD	0.57	2.30	10	1
1:A:60:THR:HG23	1:A:151:LEU:HD21	0.57	1.77	5	1
1:A:64:PHE:CD1	1:A:154:LEU:HD11	0.56	2.35	16	1
1:A:128:GLU:O	1:A:129:THR:HG23	0.56	2.00	1	1
1:A:71:TYR:CG	1:A:118:MET:HE1	0.56	2.36	4	1
1:A:200:LEU:O	1:A:203:LEU:HD21	0.56	2.01	15	3
1:A:117:LEU:HD12	1:A:153:ARG:CZ	0.56	2.29	12	1
1:A:46:LEU:HD13	1:A:55:TRP:CB	0.56	2.29	17	5
1:A:128:GLU:C	1:A:129:THR:HG23	0.56	2.26	13	2
1:A:60:THR:CG2	1:A:150:ILE:HD11	0.56	2.29	13	1
1:A:204:GLN:HA	1:A:207:ILE:HD12	0.56	1.78	2	1
1:A:158:TYR:CE1	1:A:185:PHE:CE1	0.56	2.94	12	1
1:A:130:LEU:HD12	1:A:131:PHE:CD1	0.56	2.36	1	3
1:A:161:ILE:C	1:A:161:ILE:CD1	0.56	2.77	18	3
1:A:127:ASP:O	1:A:128:GLU:O	0.56	2.24	6	1
1:A:67:ILE:HG21	1:A:185:PHE:CE2	0.56	2.35	4	2
1:A:154:LEU:O	1:A:157:VAL:HG23	0.56	2.01	5	3
1:A:64:PHE:CE1	1:A:125:LEU:HD13	0.56	2.36	14	4
1:A:46:LEU:HD11	1:A:55:TRP:HB2	0.56	1.78	1	4
1:A:147:ALA:O	1:A:150:ILE:HG22	0.56	2.01	1	7
1:A:77:PHE:HD2	1:A:168:ALA:HB1	0.56	1.60	11	2
1:A:155:PHE:HE2	1:A:203:LEU:HD23	0.55	1.62	20	1
1:A:64:PHE:O	1:A:68:ASN:HB2	0.55	2.01	14	7
1:A:186:ILE:HD11	1:A:203:LEU:CD2	0.55	2.31	19	4
1:A:121:VAL:HG12	1:A:150:ILE:HG13	0.55	1.78	3	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:70:LEU:HD11	1:A:181:SER:CB	0.55	2.31	13	2
1:A:124:GLN:OE1	1:A:150:ILE:HD12	0.55	2.00	1	2
1:A:169:VAL:HG11	1:A:178:LEU:HD22	0.55	1.78	8	1
1:A:46:LEU:HG	1:A:55:TRP:CG	0.55	2.36	16	4
1:A:161:ILE:HD12	1:A:162:TYR:N	0.55	2.16	15	1
1:A:70:LEU:HD13	1:A:158:TYR:OH	0.55	2.01	2	3
1:A:124:GLN:HA	1:A:130:LEU:HD11	0.55	1.78	18	2
1:A:206:LEU:HD12	1:A:206:LEU:C	0.55	2.27	2	9
1:A:121:VAL:HG13	1:A:150:ILE:HD12	0.55	1.78	5	1
1:A:117:LEU:HD13	1:A:157:VAL:CG1	0.55	2.32	20	1
1:A:127:ASP:O	1:A:130:LEU:HD22	0.55	2.02	2	1
1:A:201:ALA:HB3	1:A:202:PRO:CD	0.54	2.32	11	11
1:A:200:LEU:HB3	1:A:203:LEU:HD21	0.54	1.78	20	1
1:A:71:TYR:CB	1:A:118:MET:HE1	0.54	2.32	4	1
1:A:158:TYR:O	1:A:161:ILE:HG22	0.54	2.03	17	3
1:A:169:VAL:HG11	1:A:178:LEU:HD12	0.54	1.79	19	1
1:A:70:LEU:HD11	1:A:181:SER:OG	0.54	2.02	13	1
1:A:121:VAL:O	1:A:125:LEU:HG	0.54	2.02	1	1
1:A:60:THR:CG2	1:A:150:ILE:HD13	0.54	2.33	1	1
1:A:64:PHE:CD1	1:A:121:VAL:HG11	0.54	2.38	8	3
1:A:46:LEU:HD22	1:A:55:TRP:CG	0.54	2.38	1	3
1:A:46:LEU:HD12	1:A:47:PRO:HD2	0.54	1.80	12	4
1:A:147:ALA:O	1:A:151:LEU:HG	0.54	2.02	19	2
1:A:169:VAL:HG21	1:A:178:LEU:CD2	0.54	2.33	18	2
1:A:130:LEU:HD12	1:A:130:LEU:C	0.54	2.27	18	1
1:A:167:ASP:HA	1:A:170:MET:HE3	0.54	1.80	20	1
1:A:127:ASP:O	1:A:130:LEU:CD2	0.54	2.56	2	2
1:A:64:PHE:CD2	1:A:125:LEU:CD1	0.53	2.92	6	2
1:A:170:MET:HE3	1:A:175:GLU:OE1	0.53	2.03	17	1
1:A:121:VAL:HG11	1:A:154:LEU:HD11	0.53	1.81	5	1
1:A:127:ASP:O	1:A:128:GLU:C	0.53	2.52	6	1
1:A:121:VAL:CG1	1:A:150:ILE:HG23	0.53	2.33	17	1
1:A:155:PHE:CZ	1:A:203:LEU:HD11	0.53	2.39	4	1
1:A:162:TYR:CD2	1:A:178:LEU:CD2	0.53	2.91	15	3
1:A:61:VAL:HG13	1:A:125:LEU:HB3	0.53	1.81	19	2
1:A:64:PHE:CZ	1:A:125:LEU:HD23	0.53	2.39	15	2
1:A:120:TRP:CE3	1:A:121:VAL:HG13	0.53	2.39	7	1
1:A:118:MET:HE1	1:A:157:VAL:HG21	0.53	1.79	9	1
1:A:151:LEU:HA	1:A:154:LEU:HD21	0.53	1.81	6	3
1:A:203:LEU:CD2	1:A:207:ILE:HD11	0.53	2.34	18	1
1:A:74:ILE:HD11	1:A:168:ALA:CB	0.52	2.32	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:203:LEU:HD23	1:A:206:LEU:HD21	0.52	1.79	17	1
1:A:172:LEU:HD12	1:A:174:GLU:HB2	0.52	1.80	19	1
1:A:64:PHE:CE1	1:A:121:VAL:CG2	0.52	2.93	4	2
1:A:172:LEU:HD13	1:A:175:GLU:OE2	0.52	2.04	5	1
1:A:117:LEU:HD21	1:A:153:ARG:HG2	0.52	1.82	19	1
1:A:150:ILE:HG23	1:A:151:LEU:N	0.52	2.20	7	4
1:A:64:PHE:CE2	1:A:125:LEU:HD11	0.52	2.39	5	4
1:A:74:ILE:CD1	1:A:165:HIS:CG	0.52	2.93	6	4
1:A:165:HIS:HB2	1:A:168:ALA:HB3	0.52	1.80	9	2
1:A:64:PHE:CE1	1:A:154:LEU:HD21	0.52	2.38	16	1
1:A:67:ILE:HG21	1:A:185:PHE:CE1	0.52	2.39	1	1
1:A:158:TYR:CE1	1:A:185:PHE:CE2	0.52	2.97	9	1
1:A:169:VAL:HG13	1:A:175:GLU:CB	0.52	2.33	10	1
1:A:162:TYR:CG	1:A:178:LEU:HD13	0.52	2.39	2	1
1:A:40:LEU:O	1:A:40:LEU:HD13	0.52	2.05	4	1
1:A:46:LEU:HG	1:A:55:TRP:CD2	0.52	2.39	7	4
1:A:64:PHE:HA	1:A:154:LEU:HD13	0.52	1.81	7	2
1:A:121:VAL:HG13	1:A:150:ILE:CD1	0.52	2.30	8	1
1:A:67:ILE:HG23	1:A:158:TYR:CZ	0.52	2.39	12	2
1:A:120:TRP:O	1:A:120:TRP:CE3	0.51	2.57	1	2
1:A:121:VAL:HG22	1:A:150:ILE:HG22	0.51	1.80	6	1
1:A:117:LEU:O	1:A:121:VAL:HG22	0.51	2.05	7	2
1:A:71:TYR:CE2	1:A:160:HIS:CE1	0.51	2.98	17	1
1:A:46:LEU:HD21	1:A:50:GLU:O	0.51	2.06	19	2
1:A:66:GLN:O	1:A:70:LEU:HD13	0.51	2.05	20	1
1:A:71:TYR:HD1	1:A:161:ILE:HG21	0.51	1.62	3	1
1:A:46:LEU:CD2	1:A:55:TRP:CG	0.51	2.94	1	3
1:A:71:TYR:CE2	1:A:114:ILE:HG21	0.51	2.40	6	1
1:A:77:PHE:CE1	1:A:168:ALA:CB	0.51	2.94	19	1
1:A:57:ALA:O	1:A:61:VAL:HG23	0.51	2.06	2	2
1:A:64:PHE:CE1	1:A:121:VAL:HG23	0.51	2.41	4	2
1:A:74:ILE:HD13	1:A:74:ILE:C	0.51	2.30	17	5
1:A:74:ILE:CD1	1:A:165:HIS:ND1	0.51	2.74	17	2
1:A:162:TYR:CE1	1:A:166:PHE:CE2	0.50	2.99	3	1
1:A:182:PHE:CZ	1:A:203:LEU:HD23	0.50	2.41	5	1
1:A:203:LEU:CD2	1:A:206:LEU:HD11	0.50	2.36	9	1
1:A:130:LEU:H	1:A:130:LEU:HD13	0.50	1.66	15	3
1:A:161:ILE:HG22	1:A:165:HIS:NE2	0.50	2.21	5	2
1:A:67:ILE:HG21	1:A:154:LEU:HD13	0.50	1.82	7	1
1:A:155:PHE:CD2	1:A:185:PHE:CE2	0.50	2.99	9	1
1:A:162:TYR:CD1	1:A:166:PHE:CE2	0.50	3.00	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:57:ALA:HB1	1:A:131:PHE:CE2	0.50	2.41	17	1
1:A:55:TRP:CD1	1:A:192:PHE:CZ	0.50	2.99	3	4
1:A:57:ALA:HB2	1:A:143:PHE:CE2	0.50	2.42	3	1
1:A:117:LEU:HD23	1:A:157:VAL:HG23	0.50	1.79	3	1
1:A:169:VAL:CG2	1:A:178:LEU:HD12	0.50	2.28	7	2
1:A:67:ILE:HD13	1:A:154:LEU:HB3	0.50	1.84	9	5
1:A:77:PHE:CG	1:A:168:ALA:HB1	0.50	2.40	15	2
1:A:162:TYR:CD2	1:A:166:PHE:CE2	0.50	3.00	5	1
1:A:162:TYR:CZ	1:A:166:PHE:CZ	0.50	2.99	11	2
1:A:68:ASN:CG	1:A:118:MET:HE2	0.50	2.31	1	1
1:A:71:TYR:CD1	1:A:161:ILE:HD11	0.50	2.42	1	1
1:A:161:ILE:HA	1:A:165:HIS:CD2	0.50	2.41	1	3
1:A:71:TYR:OH	1:A:114:ILE:HD13	0.50	2.06	19	2
1:A:64:PHE:CE1	1:A:125:LEU:CD1	0.50	2.94	14	4
1:A:52:LEU:N	1:A:52:LEU:HD13	0.50	2.22	14	1
1:A:158:TYR:CZ	1:A:178:LEU:CD1	0.50	2.94	4	6
1:A:64:PHE:CE1	1:A:121:VAL:HB	0.50	2.42	6	1
1:A:70:LEU:HD11	1:A:158:TYR:CE1	0.50	2.42	1	1
1:A:161:ILE:O	1:A:165:HIS:CD2	0.50	2.65	6	2
1:A:63:PHE:CZ	1:A:188:PHE:CD2	0.50	3.00	15	1
1:A:161:ILE:HD12	1:A:161:ILE:N	0.49	2.22	1	1
1:A:64:PHE:CD1	1:A:125:LEU:HD13	0.49	2.41	9	2
1:A:74:ILE:HG13	1:A:77:PHE:CE1	0.49	2.42	4	1
1:A:130:LEU:HD12	1:A:131:PHE:HD1	0.49	1.67	14	2
1:A:64:PHE:C	1:A:64:PHE:CD1	0.49	2.90	11	3
1:A:150:ILE:HG22	1:A:154:LEU:HD11	0.49	1.84	18	4
1:A:150:ILE:HG22	1:A:154:LEU:HD12	0.49	1.85	17	2
1:A:70:LEU:HD11	1:A:177:HIS:HB3	0.49	1.82	3	1
1:A:162:TYR:CE2	1:A:178:LEU:HD22	0.49	2.42	9	1
1:A:160:HIS:O	1:A:164:GLN:HB2	0.49	2.08	9	3
1:A:201:ALA:N	1:A:202:PRO:HD2	0.49	2.22	7	4
1:A:64:PHE:CE2	1:A:121:VAL:HB	0.49	2.43	19	2
1:A:74:ILE:HD12	1:A:161:ILE:HD11	0.49	1.85	17	1
1:A:203:LEU:HD23	1:A:207:ILE:HD11	0.49	1.85	18	1
1:A:47:PRO:CD	1:A:55:TRP:CZ3	0.48	2.96	4	5
1:A:160:HIS:CD2	1:A:161:ILE:N	0.48	2.80	15	2
1:A:172:LEU:HD12	1:A:173:GLN:HB2	0.48	1.84	2	2
1:A:161:ILE:O	1:A:165:HIS:CE1	0.48	2.66	6	2
1:A:189:VAL:HG11	1:A:200:LEU:HD21	0.48	1.86	17	1
1:A:158:TYR:CE2	1:A:182:PHE:CD1	0.48	3.01	6	1
1:A:146:VAL:O	1:A:150:ILE:HG22	0.48	2.09	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:71:TYR:CZ	1:A:161:ILE:HG21	0.48	2.43	15	1
1:A:73:THR:HB	1:A:172:LEU:HD13	0.48	1.85	16	1
1:A:74:ILE:HG13	1:A:77:PHE:CZ	0.48	2.44	4	1
1:A:64:PHE:CE2	1:A:121:VAL:CG1	0.48	2.97	19	2
1:A:67:ILE:CD1	1:A:154:LEU:HB2	0.48	2.39	10	1
1:A:150:ILE:CG2	1:A:151:LEU:N	0.48	2.76	4	9
1:A:70:LEU:HD22	1:A:177:HIS:HB3	0.48	1.84	5	1
1:A:159:ALA:O	1:A:163:HIS:CD2	0.48	2.67	6	3
1:A:64:PHE:CD1	1:A:125:LEU:HD23	0.48	2.43	11	1
1:A:61:VAL:O	1:A:65:ASN:HB2	0.48	2.09	14	1
1:A:64:PHE:CG	1:A:121:VAL:HG11	0.48	2.44	1	1
1:A:74:ILE:CD1	1:A:165:HIS:CD2	0.48	2.97	19	4
1:A:71:TYR:CD2	1:A:161:ILE:HG21	0.48	2.43	13	1
1:A:67:ILE:HD11	1:A:154:LEU:CD2	0.48	2.23	14	1
1:A:160:HIS:CG	1:A:161:ILE:N	0.48	2.82	15	1
1:A:61:VAL:HG22	1:A:125:LEU:CD1	0.47	2.39	11	1
1:A:46:LEU:HD21	1:A:51:ASP:H	0.47	1.69	18	1
1:A:70:LEU:HD22	1:A:177:HIS:CB	0.47	2.39	5	1
1:A:70:LEU:HD13	1:A:158:TYR:HE1	0.47	1.68	13	1
1:A:162:TYR:HD2	1:A:178:LEU:HD21	0.47	1.64	13	1
1:A:155:PHE:CZ	1:A:203:LEU:HD23	0.47	2.43	7	1
1:A:158:TYR:CE2	1:A:185:PHE:CD2	0.47	3.02	9	1
1:A:64:PHE:CD1	1:A:125:LEU:CD1	0.47	2.98	10	3
1:A:158:TYR:OH	1:A:178:LEU:HD12	0.47	2.08	15	4
1:A:150:ILE:CG2	1:A:154:LEU:HD11	0.47	2.39	18	1
1:A:64:PHE:CE1	1:A:121:VAL:CG1	0.47	2.97	6	1
1:A:67:ILE:HD13	1:A:154:LEU:HB2	0.47	1.84	11	1
1:A:70:LEU:HD13	1:A:177:HIS:HB3	0.47	1.87	5	1
1:A:67:ILE:HG23	1:A:158:TYR:OH	0.47	2.09	10	1
1:A:71:TYR:CE1	1:A:161:ILE:CG2	0.47	2.97	16	1
1:A:71:TYR:CZ	1:A:160:HIS:CE1	0.47	3.02	17	1
1:A:169:VAL:HG21	1:A:178:LEU:HD23	0.47	1.86	18	1
1:A:71:TYR:OH	1:A:114:ILE:HG21	0.47	2.10	20	1
1:A:130:LEU:HD23	1:A:131:PHE:CD2	0.47	2.45	2	1
1:A:162:TYR:CD2	1:A:178:LEU:HD13	0.47	2.45	2	1
1:A:69:MET:HA	1:A:69:MET:HE3	0.47	1.86	19	1
1:A:189:VAL:HG21	1:A:200:LEU:HD21	0.47	1.87	14	1
1:A:52:LEU:HD22	1:A:52:LEU:C	0.46	2.32	14	4
1:A:162:TYR:CD1	1:A:178:LEU:CD1	0.46	2.98	6	3
1:A:67:ILE:HG23	1:A:68:ASN:N	0.46	2.24	15	2
1:A:200:LEU:HA	1:A:203:LEU:HD21	0.46	1.87	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:130:LEU:N	1:A:130:LEU:HD22	0.46	2.25	12	3
1:A:67:ILE:HG21	1:A:154:LEU:HD22	0.46	1.87	15	1
1:A:124:GLN:CA	1:A:130:LEU:HD11	0.46	2.41	3	1
1:A:169:VAL:HG13	1:A:175:GLU:CG	0.46	2.39	10	1
1:A:200:LEU:CB	1:A:203:LEU:HD21	0.46	2.40	16	1
1:A:130:LEU:N	1:A:130:LEU:HD13	0.46	2.25	2	1
1:A:172:LEU:HD12	1:A:173:GLN:N	0.46	2.24	2	1
1:A:158:TYR:O	1:A:162:TYR:HB2	0.46	2.10	19	2
1:A:182:PHE:CZ	1:A:206:LEU:HD21	0.46	2.45	18	1
1:A:120:TRP:HE3	1:A:120:TRP:C	0.46	2.19	3	2
1:A:64:PHE:CE1	1:A:154:LEU:CG	0.46	2.99	16	1
1:A:74:ILE:CG1	1:A:77:PHE:CE1	0.46	2.99	4	1
1:A:121:VAL:HG13	1:A:153:ARG:NH1	0.46	2.26	14	1
1:A:124:GLN:HG3	1:A:130:LEU:HD21	0.46	1.88	14	1
1:A:161:ILE:O	1:A:165:HIS:N	0.46	2.46	14	1
1:A:64:PHE:HE2	1:A:121:VAL:HG23	0.46	1.71	17	1
1:A:117:LEU:HD11	1:A:153:ARG:HG2	0.46	1.88	19	1
1:A:124:GLN:HG2	1:A:130:LEU:HD21	0.46	1.87	5	1
1:A:71:TYR:CG	1:A:118:MET:CE	0.46	2.99	4	1
1:A:127:ASP:O	1:A:129:THR:N	0.46	2.49	20	3
1:A:186:ILE:HD11	1:A:203:LEU:HD22	0.45	1.87	4	1
1:A:207:ILE:CG2	1:A:208:GLU:N	0.45	2.80	9	5
1:A:200:LEU:CA	1:A:203:LEU:HD21	0.45	2.41	12	1
1:A:63:PHE:CE1	1:A:184:HIS:CD2	0.45	3.04	16	1
1:A:70:LEU:HD22	1:A:70:LEU:C	0.45	2.36	20	1
1:A:64:PHE:CD2	1:A:121:VAL:CG1	0.45	3.00	15	5
1:A:207:ILE:HD13	1:A:207:ILE:C	0.45	2.37	15	1
1:A:158:TYR:C	1:A:158:TYR:CD1	0.45	2.94	7	1
1:A:119:THR:HA	1:A:122:GLN:HG2	0.45	1.86	17	1
1:A:64:PHE:CD1	1:A:121:VAL:CG1	0.45	2.99	8	1
1:A:64:PHE:HD1	1:A:154:LEU:HD21	0.45	1.64	16	1
1:A:120:TRP:CE3	1:A:120:TRP:C	0.45	2.94	1	1
1:A:159:ALA:HB2	1:A:202:PRO:HB2	0.45	1.87	6	1
1:A:130:LEU:O	1:A:131:PHE:CD1	0.45	2.69	6	1
1:A:76:GLU:CG	1:A:77:PHE:CE1	0.45	2.99	20	4
1:A:188:PHE:CG	1:A:189:VAL:N	0.45	2.84	10	1
1:A:200:LEU:O	1:A:203:LEU:HD11	0.45	2.12	15	1
1:A:121:VAL:CG1	1:A:150:ILE:HD12	0.45	2.41	5	1
1:A:182:PHE:CZ	1:A:203:LEU:HD12	0.45	2.46	6	1
1:A:165:HIS:N	1:A:165:HIS:CD2	0.45	2.84	14	1
1:A:74:ILE:HA	1:A:77:PHE:CD2	0.45	2.47	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:63:PHE:O	1:A:67:ILE:HG23	0.45	2.12	19	1
1:A:46:LEU:HD22	1:A:55:TRP:CD2	0.45	2.47	1	1
1:A:124:GLN:CA	1:A:130:LEU:HD21	0.45	2.42	2	1
1:A:64:PHE:CE2	1:A:125:LEU:CD1	0.45	3.00	8	1
1:A:128:GLU:O	1:A:129:THR:CG2	0.44	2.65	19	1
1:A:70:LEU:C	1:A:70:LEU:CD2	0.44	2.90	20	1
1:A:52:LEU:HD22	1:A:52:LEU:O	0.44	2.12	2	2
1:A:47:PRO:HD3	1:A:55:TRP:CZ3	0.44	2.47	3	5
1:A:150:ILE:HG13	1:A:151:LEU:N	0.44	2.27	13	5
1:A:46:LEU:HD22	1:A:50:GLU:HB2	0.44	1.88	7	1
1:A:157:VAL:HG23	1:A:160:HIS:CE1	0.44	2.46	15	1
1:A:71:TYR:C	1:A:71:TYR:CD1	0.44	2.95	19	1
1:A:52:LEU:HD13	1:A:56:ILE:CD1	0.44	2.30	3	5
1:A:71:TYR:CE2	1:A:161:ILE:CG2	0.44	3.00	11	2
1:A:169:VAL:CG1	1:A:178:LEU:HD23	0.44	2.40	12	1
1:A:158:TYR:O	1:A:161:ILE:HG12	0.44	2.12	14	1
1:A:64:PHE:HB2	1:A:154:LEU:HD11	0.44	1.89	14	1
1:A:143:PHE:CE1	1:A:147:ALA:HB2	0.44	2.47	3	1
1:A:120:TRP:CZ3	1:A:121:VAL:CG1	0.44	3.01	7	1
1:A:153:ARG:HD2	1:A:153:ARG:C	0.44	2.38	10	1
1:A:53:ASN:ND2	1:A:143:PHE:CD2	0.44	2.85	16	1
1:A:146:VAL:CG1	1:A:147:ALA:N	0.44	2.81	14	7
1:A:114:ILE:HG12	1:A:157:VAL:HG13	0.44	1.90	6	1
1:A:158:TYR:CE2	1:A:178:LEU:CD2	0.44	3.00	7	3
1:A:64:PHE:CZ	1:A:121:VAL:HB	0.44	2.48	16	1
1:A:124:GLN:HB3	1:A:130:LEU:HD21	0.44	1.89	1	1
1:A:74:ILE:HD12	1:A:165:HIS:CD2	0.44	2.47	6	1
1:A:162:TYR:CE1	1:A:166:PHE:CE1	0.44	3.06	11	3
1:A:60:THR:HG23	1:A:150:ILE:HD13	0.44	1.89	11	1
1:A:78:CYS:SG	1:A:165:HIS:CE1	0.43	3.11	5	1
1:A:162:TYR:CZ	1:A:178:LEU:HD13	0.43	2.47	9	1
1:A:43:ALA:O	1:A:55:TRP:CZ2	0.43	2.71	16	4
1:A:46:LEU:CD2	1:A:55:TRP:HB2	0.43	2.43	10	1
1:A:64:PHE:CE2	1:A:121:VAL:HG11	0.43	2.48	10	1
1:A:124:GLN:CG	1:A:130:LEU:HD11	0.43	2.43	11	1
1:A:64:PHE:CE2	1:A:121:VAL:HG23	0.43	2.49	17	1
1:A:169:VAL:HG11	1:A:178:LEU:CB	0.43	2.43	18	1
1:A:67:ILE:HG21	1:A:185:PHE:HE2	0.43	1.73	20	1
1:A:45:MET:O	1:A:46:LEU:C	0.43	2.61	1	2
1:A:180:THR:CG2	1:A:181:SER:N	0.43	2.82	2	7
1:A:52:LEU:HD21	1:A:192:PHE:HE2	0.43	1.74	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:120:TRP:CZ3	1:A:150:ILE:CG2	0.43	3.02	9	1
1:A:64:PHE:HB2	1:A:154:LEU:CD1	0.43	2.44	18	1
1:A:207:ILE:HG23	1:A:208:GLU:N	0.43	2.29	12	5
1:A:175:GLU:HG2	1:A:178:LEU:HD23	0.43	1.91	8	1
1:A:162:TYR:CE1	1:A:166:PHE:CZ	0.43	3.07	11	1
1:A:121:VAL:HG12	1:A:150:ILE:HG23	0.43	1.89	14	1
1:A:76:GLU:CG	1:A:77:PHE:CD1	0.43	3.01	20	3
1:A:154:LEU:O	1:A:157:VAL:HG22	0.43	2.13	14	1
1:A:189:VAL:HG21	1:A:200:LEU:HD13	0.43	1.90	15	1
1:A:67:ILE:HG23	1:A:158:TYR:HE1	0.43	1.74	9	1
1:A:203:LEU:HG	1:A:207:ILE:HD11	0.43	1.90	13	1
1:A:64:PHE:HD1	1:A:154:LEU:HD22	0.43	1.74	5	1
1:A:161:ILE:HD12	1:A:165:HIS:CE1	0.43	2.49	6	1
1:A:129:THR:OG1	1:A:130:LEU:HD23	0.43	2.13	6	1
1:A:158:TYR:CE1	1:A:185:PHE:CZ	0.43	3.07	9	1
1:A:125:LEU:CD1	1:A:125:LEU:N	0.43	2.82	11	1
1:A:130:LEU:HD12	1:A:130:LEU:O	0.43	2.14	16	1
1:A:156:ARG:O	1:A:160:HIS:CD2	0.43	2.71	20	2
1:A:70:LEU:H	1:A:70:LEU:CD1	0.43	2.23	20	1
1:A:148:LYS:HA	1:A:151:LEU:HD21	0.43	1.91	10	1
1:A:52:LEU:N	1:A:52:LEU:CD1	0.43	2.82	14	1
1:A:64:PHE:CE1	1:A:154:LEU:CD1	0.43	3.00	16	1
1:A:189:VAL:O	1:A:193:ASN:CB	0.43	2.66	16	1
1:A:46:LEU:CD1	1:A:55:TRP:CE3	0.43	3.00	18	1
1:A:130:LEU:CD2	1:A:131:PHE:CD2	0.42	3.02	2	1
1:A:63:PHE:CD1	1:A:185:PHE:CE1	0.42	3.07	14	1
1:A:44:VAL:HG12	1:A:191:GLU:CD	0.42	2.39	17	1
1:A:46:LEU:HD13	1:A:55:TRP:CG	0.42	2.49	18	3
1:A:124:GLN:C	1:A:130:LEU:HD21	0.42	2.38	2	1
1:A:47:PRO:HD2	1:A:55:TRP:CZ3	0.42	2.48	19	3
1:A:52:LEU:HD13	1:A:192:PHE:CE2	0.42	2.48	10	1
1:A:46:LEU:HD22	1:A:55:TRP:HB2	0.42	1.91	14	1
1:A:162:TYR:CE2	1:A:178:LEU:CD2	0.42	3.02	17	1
1:A:64:PHE:CD1	1:A:154:LEU:HD22	0.42	2.49	5	2
1:A:155:PHE:CA	1:A:185:PHE:CE2	0.42	3.01	12	1
1:A:121:VAL:CG1	1:A:153:ARG:NH1	0.42	2.83	14	1
1:A:155:PHE:CD1	1:A:155:PHE:C	0.42	2.97	2	3
1:A:71:TYR:CD2	1:A:118:MET:CE	0.42	3.03	3	1
1:A:59:ASN:HD22	1:A:59:ASN:N	0.42	2.13	14	1
1:A:71:TYR:CD2	1:A:161:ILE:HD11	0.42	2.49	1	1
1:A:160:HIS:CD2	1:A:160:HIS:C	0.42	2.97	15	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:70:LEU:HD22	1:A:178:LEU:HA	0.42	1.90	13	1
1:A:74:ILE:HD12	1:A:165:HIS:CG	0.42	2.49	6	1
1:A:159:ALA:O	1:A:163:HIS:CG	0.42	2.73	6	1
1:A:163:HIS:N	1:A:163:HIS:CD2	0.42	2.86	11	1
1:A:130:LEU:HD22	1:A:131:PHE:N	0.42	2.29	15	1
1:A:191:GLU:OE1	1:A:192:PHE:CE2	0.42	2.72	16	1
1:A:122:GLN:HA	1:A:125:LEU:CD1	0.42	2.41	1	1
1:A:64:PHE:CD1	1:A:64:PHE:C	0.42	2.98	9	1
1:A:67:ILE:HA	1:A:70:LEU:HD23	0.42	1.91	10	1
1:A:161:ILE:CG2	1:A:162:TYR:N	0.42	2.83	17	1
1:A:46:LEU:CD1	1:A:55:TRP:HB2	0.42	2.43	1	2
1:A:70:LEU:CD2	1:A:177:HIS:CG	0.42	2.98	5	1
1:A:44:VAL:HG12	1:A:191:GLU:OE1	0.42	2.15	9	1
1:A:64:PHE:CB	1:A:154:LEU:HD11	0.42	2.45	14	1
1:A:203:LEU:HD12	1:A:203:LEU:C	0.42	2.39	16	1
1:A:121:VAL:HG11	1:A:154:LEU:HD21	0.42	1.91	18	1
1:A:70:LEU:HD21	1:A:158:TYR:CE1	0.42	2.49	20	1
1:A:130:LEU:HD12	1:A:131:PHE:CE2	0.42	2.50	6	1
1:A:114:ILE:CG2	1:A:115:ASP:N	0.42	2.83	3	1
1:A:169:VAL:O	1:A:172:LEU:CD2	0.42	2.68	17	1
1:A:124:GLN:O	1:A:131:PHE:CD2	0.41	2.73	4	1
1:A:158:TYR:CD1	1:A:185:PHE:CE2	0.41	3.08	9	1
1:A:161:ILE:HD12	1:A:161:ILE:H	0.41	1.75	1	1
1:A:162:TYR:O	1:A:166:PHE:HB2	0.41	2.15	1	1
1:A:63:PHE:CZ	1:A:184:HIS:CG	0.41	3.09	2	1
1:A:173:GLN:O	1:A:174:GLU:CB	0.41	2.68	5	1
1:A:158:TYR:CE2	1:A:178:LEU:HD21	0.41	2.50	20	1
1:A:143:PHE:C	1:A:143:PHE:CD1	0.41	2.99	3	1
1:A:64:PHE:O	1:A:68:ASN:CB	0.41	2.68	4	1
1:A:120:TRP:CE3	1:A:121:VAL:CG2	0.41	3.03	19	1
1:A:76:GLU:HG3	1:A:77:PHE:CD1	0.41	2.51	20	1
1:A:143:PHE:CD1	1:A:143:PHE:C	0.41	2.98	5	1
1:A:148:LYS:HA	1:A:151:LEU:HD12	0.41	1.91	5	1
1:A:67:ILE:CG2	1:A:68:ASN:N	0.41	2.84	7	2
1:A:76:GLU:HG2	1:A:77:PHE:CD1	0.41	2.50	13	2
1:A:201:ALA:N	1:A:202:PRO:CD	0.41	2.83	14	2
1:A:158:TYR:CE1	1:A:178:LEU:CD1	0.41	3.04	4	1
1:A:59:ASN:O	1:A:63:PHE:HB2	0.41	2.14	6	1
1:A:163:HIS:ND1	1:A:163:HIS:C	0.41	2.79	10	1
1:A:52:LEU:H	1:A:52:LEU:CD1	0.41	2.19	18	1
1:A:71:TYR:CD1	1:A:71:TYR:O	0.41	2.74	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:74:ILE:HD11	1:A:165:HIS:CD2	0.41	2.50	19	1
1:A:123:ASP:O	1:A:127:ASP:N	0.41	2.53	19	1
1:A:66:GLN:O	1:A:70:LEU:CD1	0.41	2.68	20	1
1:A:120:TRP:C	1:A:120:TRP:CE3	0.41	2.98	3	1
1:A:160:HIS:HA	1:A:163:HIS:CE1	0.41	2.50	8	1
1:A:182:PHE:CE2	1:A:203:LEU:HD21	0.41	2.51	8	1
1:A:161:ILE:HG13	1:A:162:TYR:N	0.41	2.30	16	1
1:A:151:LEU:HD12	1:A:154:LEU:HD21	0.41	1.92	6	1
1:A:63:PHE:CZ	1:A:184:HIS:CD2	0.41	3.09	16	1
1:A:162:TYR:CE1	1:A:178:LEU:HD13	0.41	2.51	3	1
1:A:161:ILE:CG1	1:A:162:TYR:N	0.41	2.83	6	2
1:A:74:ILE:HG12	1:A:168:ALA:HB1	0.41	1.92	10	1
1:A:130:LEU:CD2	1:A:131:PHE:N	0.41	2.84	12	1
1:A:73:THR:C	1:A:172:LEU:HD11	0.41	2.40	1	1
1:A:130:LEU:HD13	1:A:130:LEU:H	0.41	1.74	2	1
1:A:76:GLU:HG3	1:A:77:PHE:CE1	0.41	2.51	13	1
1:A:128:GLU:C	1:A:129:THR:CG2	0.41	2.93	13	1
1:A:162:TYR:C	1:A:162:TYR:CD1	0.41	2.99	13	1
1:A:158:TYR:O	1:A:161:ILE:HG13	0.41	2.15	15	1
1:A:64:PHE:CG	1:A:125:LEU:HD11	0.41	2.51	17	1
1:A:71:TYR:HA	1:A:74:ILE:HG22	0.41	1.92	17	1
1:A:201:ALA:CB	1:A:202:PRO:CD	0.41	2.99	19	1
1:A:46:LEU:CD2	1:A:55:TRP:CD1	0.41	3.04	1	1
1:A:186:ILE:HD11	1:A:203:LEU:HD13	0.41	1.92	6	1
1:A:74:ILE:CD1	1:A:165:HIS:CE1	0.41	3.04	14	1
1:A:161:ILE:HG23	1:A:162:TYR:N	0.41	2.31	18	1
1:A:130:LEU:CD2	1:A:130:LEU:C	0.40	2.94	12	1
1:A:74:ILE:HD11	1:A:165:HIS:CB	0.40	2.46	13	1
1:A:60:THR:CG2	1:A:125:LEU:HD21	0.40	2.44	16	1
1:A:155:PHE:CE2	1:A:203:LEU:HD11	0.40	2.51	4	1
1:A:169:VAL:CG2	1:A:178:LEU:HD22	0.40	2.46	10	1
1:A:65:ASN:ND2	1:A:69:MET:HE3	0.40	2.31	13	1
1:A:169:VAL:CG1	1:A:175:GLU:CG	0.40	2.99	17	1
1:A:71:TYR:O	1:A:71:TYR:CD1	0.40	2.73	18	1
1:A:130:LEU:O	1:A:143:PHE:CD1	0.40	2.74	1	1
1:A:186:ILE:O	1:A:189:VAL:HG12	0.40	2.17	1	1
1:A:121:VAL:HG12	1:A:150:ILE:HG12	0.40	1.92	4	1
1:A:118:MET:SD	1:A:118:MET:N	0.40	2.95	9	1
1:A:71:TYR:O	1:A:75:THR:N	0.40	2.54	11	2
1:A:161:ILE:HG12	1:A:165:HIS:CD2	0.40	2.52	18	1
1:A:44:VAL:HG11	1:A:187:PHE:CD1	0.40	2.51	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:166:PHE:CZ	1:A:175:GLU:CD	0.40	3.00	8	1
1:A:121:VAL:HG12	1:A:125:LEU:HD11	0.40	1.94	9	1
1:A:200:LEU:N	1:A:200:LEU:CD2	0.40	2.81	16	1
1:A:163:HIS:CD2	1:A:163:HIS:C	0.40	2.99	18	1
1:A:143:PHE:O	1:A:147:ALA:CB	0.40	2.69	19	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	124/202 (61%)	114±2 (92±2%)	8±2 (6±2%)	3±2 (2±1%)	7	47
All	All	2480/4040 (61%)	2275 (92%)	150 (6%)	55 (2%)	7	47

All 12 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	173	GLN	8
1	A	203	LEU	8
1	A	48	GLU	8
1	A	128	GLU	7
1	A	49	GLY	7
1	A	174	GLU	7
1	A	142	ASN	3
1	A	78	CYS	3
1	A	129	THR	1
1	A	130	LEU	1
1	A	193	ASN	1
1	A	202	PRO	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	115/180 (64%)	81±4 (70±4%)	34±4 (30±4%)	1	17
All	All	2300/3600 (64%)	1611 (70%)	689 (30%)	1	17

All 91 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	54	GLU	20
1	A	74	ILE	20
1	A	40	LEU	19
1	A	165	HIS	18
1	A	112	LYS	15
1	A	126	ASP	15
1	A	153	ARG	15
1	A	114	ILE	14
1	A	52	LEU	14
1	A	48	GLU	13
1	A	209	LYS	13
1	A	210	LEU	13
1	A	171	GLN	13
1	A	78	CYS	12
1	A	144	MET	12
1	A	70	LEU	12
1	A	184	HIS	12
1	A	45	MET	11
1	A	181	SER	11
1	A	208	GLU	11
1	A	148	LYS	11
1	A	152	LYS	11
1	A	164	GLN	10
1	A	177	HIS	10
1	A	203	LEU	10
1	A	151	LEU	10
1	A	156	ARG	10
1	A	174	GLU	10
1	A	183	LYS	10
1	A	173	GLN	10
1	A	125	LEU	9
1	A	175	GLU	9
1	A	204	GLN	9

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Mol	Chain	Res	Type	Models (Total)
1	A	199	GLU	9
1	A	50	GLU	9
1	A	64	PHE	9
1	A	62	ASP	8
1	A	69	MET	8
1	A	191	GLU	8
1	A	128	GLU	8
1	A	161	ILE	8
1	A	145	SER	8
1	A	67	ILE	7
1	A	130	LEU	7
1	A	186	ILE	7
1	A	190	GLN	7
1	A	205	GLU	7
1	A	42	GLN	7
1	A	46	LEU	7
1	A	170	MET	7
1	A	172	LEU	7
1	A	117	LEU	6
1	A	185	PHE	6
1	A	154	LEU	6
1	A	187	PHE	6
1	A	193	ASN	6
1	A	65	ASN	6
1	A	115	ASP	6
1	A	182	PHE	5
1	A	76	GLU	5
1	A	122	GLN	5
1	A	66	GLN	5
1	A	166	PHE	5
1	A	129	THR	5
1	A	179	ASN	5
1	A	51	ASP	4
1	A	41	ARG	4
1	A	150	ILE	4
1	A	178	LEU	4
1	A	127	ASP	4
1	A	142	ASN	4
1	A	200	LEU	4
1	A	146	VAL	3
1	A	119	THR	3
1	A	160	HIS	3

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Mol	Chain	Res	Type	Models (Total)
1	A	113	TYR	3
1	A	131	PHE	3
1	A	120	TRP	2
1	A	188	PHE	2
1	A	116	TYR	2
1	A	124	GLN	2
1	A	207	ILE	2
1	A	56	ILE	1
1	A	68	ASN	1
1	A	118	MET	1
1	A	158	TYR	1
1	A	163	HIS	1
1	A	59	ASN	1
1	A	53	ASN	1
1	A	121	VAL	1
1	A	149	THR	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.6 Ligand geometry ⓘ

There are no ligands in this entry.

6.7 Other polymers ⓘ

There are no such molecules in this entry.

6.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided