



Full wwPDB NMR Structure Validation Report ⓘ

Mar 5, 2026 – 01:37 PM UTC

PDB ID : 1S79 / pdb_00001s79
Title : Solution structure of the central RRM of human La protein
Authors : Alfano, C.; Sanfelice, D.; Babon, J.; Kelly, G.; Jacks, A.; Curry, S.; Conte, M.R.
Deposited on : 2004-01-29

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

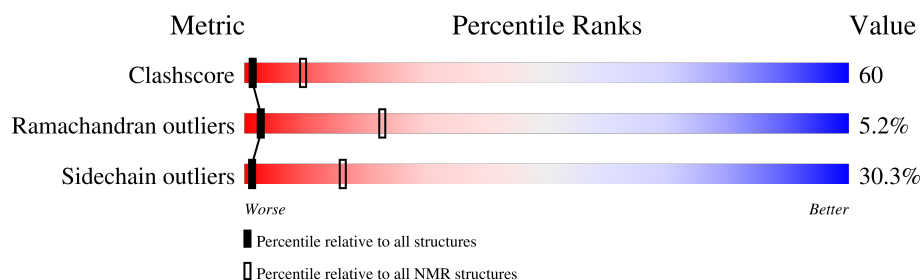
1 Overall quality at a glance

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	103	

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: *closest to the average*.

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:109-A:192 (84)	0.85	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 2 clusters and 1 single-model cluster was found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1740 atoms, of which 879 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Lupus La protein.

Mol	Chain	Residues	Atoms						Trace
1	A	103	Total	C	H	N	O	S	0
			1740	554	879	147	159	1	

There are 5 discrepancies between the modelled and reference sequences:

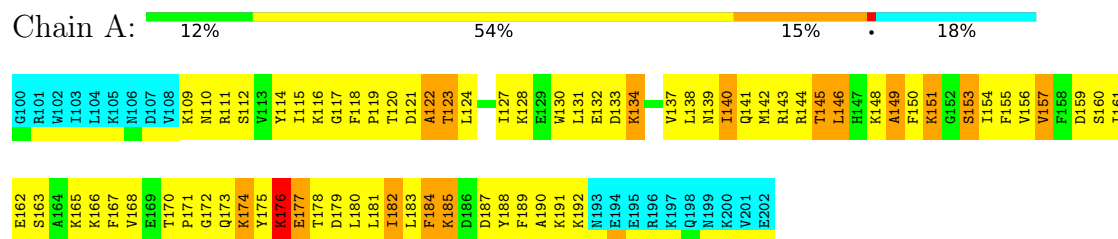
Chain	Residue	Modelled	Actual	Comment	Reference
A	100	GLY	-	cloning artifact	UNP P05455
A	101	ARG	-	cloning artifact	UNP P05455
A	102	TRP	-	cloning artifact	UNP P05455
A	103	ILE	-	cloning artifact	UNP P05455
A	104	LEU	-	cloning artifact	UNP P05455

4 Residue-property plots

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: Lupus La protein

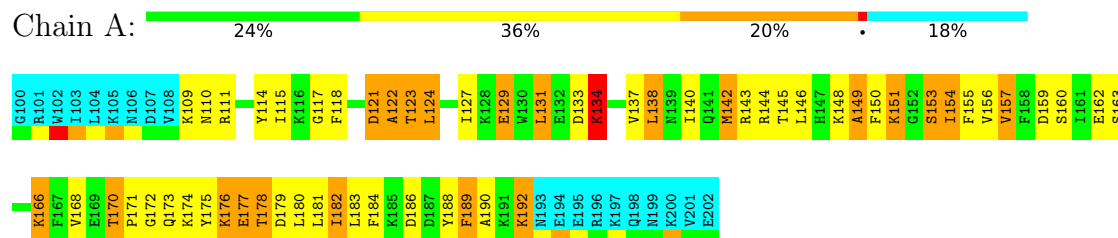


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

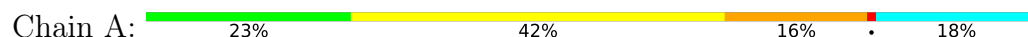
4.2.1 Score per residue for model 1

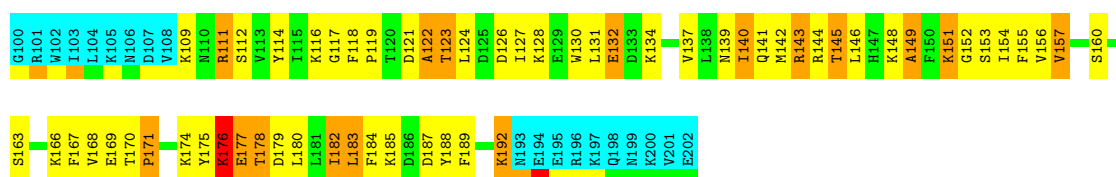
- Molecule 1: Lupus La protein



4.2.2 Score per residue for model 2 (medoid)

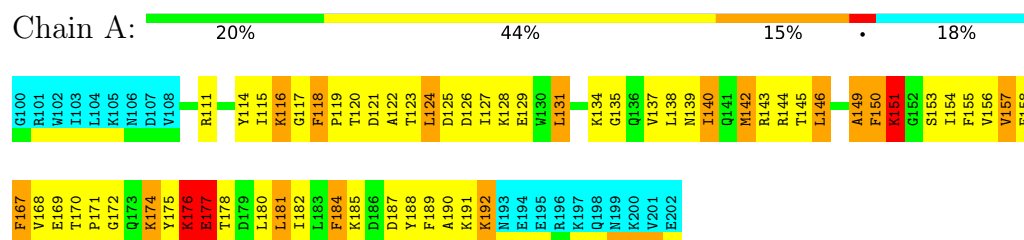
- Molecule 1: Lupus La protein





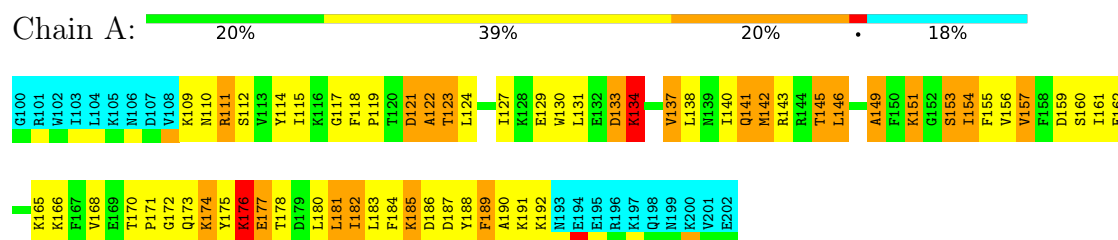
4.2.3 Score per residue for model 3

- Molecule 1: Lupus La protein



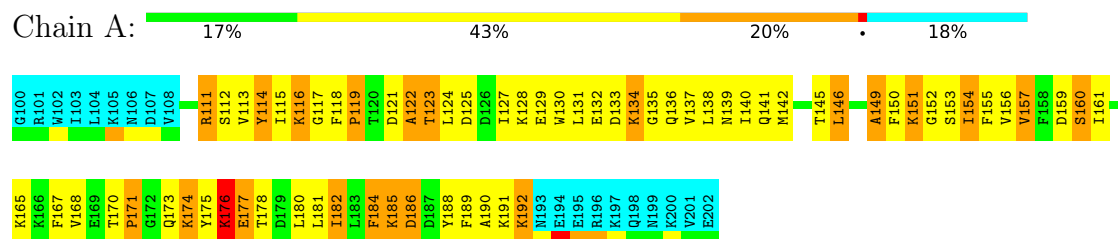
4.2.4 Score per residue for model 4

- Molecule 1: Lupus La protein



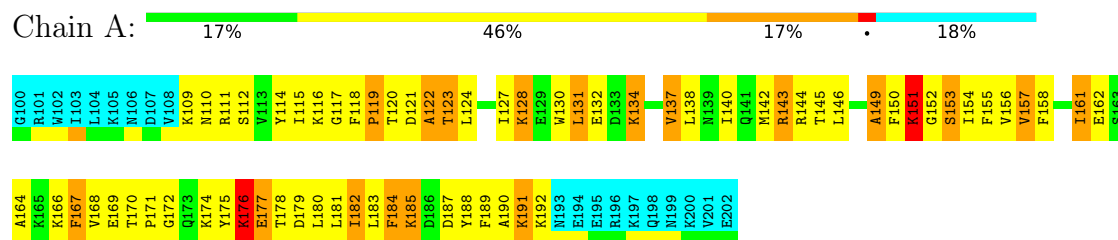
4.2.5 Score per residue for model 5

- Molecule 1: Lupus La protein



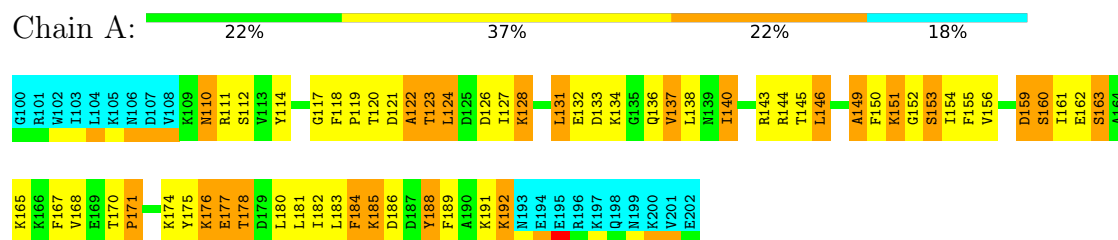
4.2.6 Score per residue for model 6

- Molecule 1: Lupus La protein



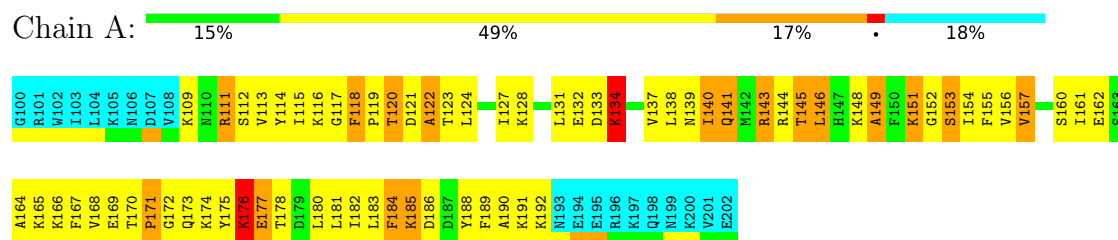
4.2.7 Score per residue for model 7

- Molecule 1: Lupus La protein



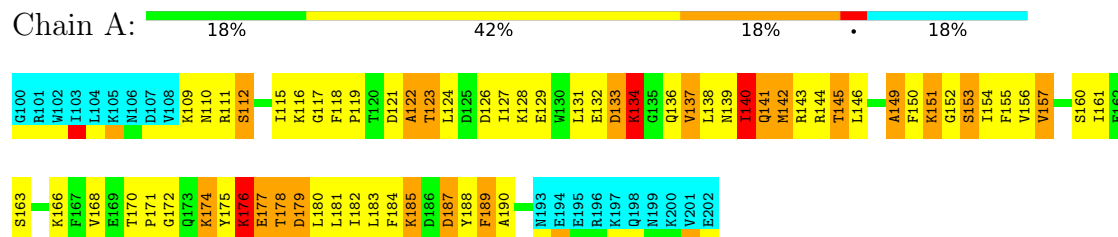
4.2.8 Score per residue for model 8

- Molecule 1: Lupus La protein



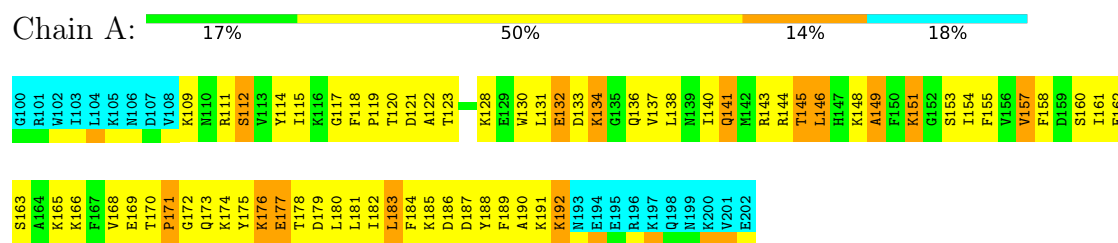
4.2.9 Score per residue for model 9

- Molecule 1: Lupus La protein



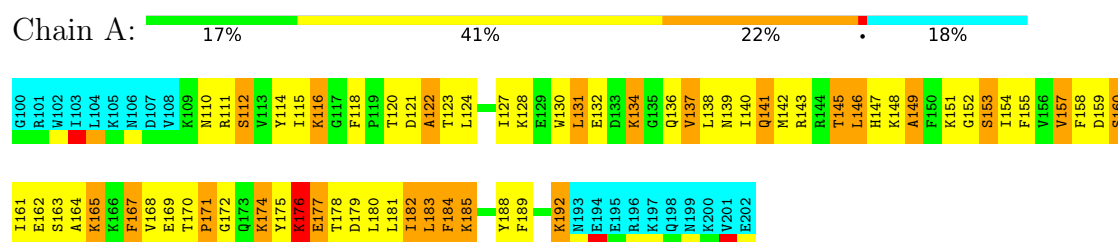
4.2.10 Score per residue for model 10

- Molecule 1: Lupus La protein



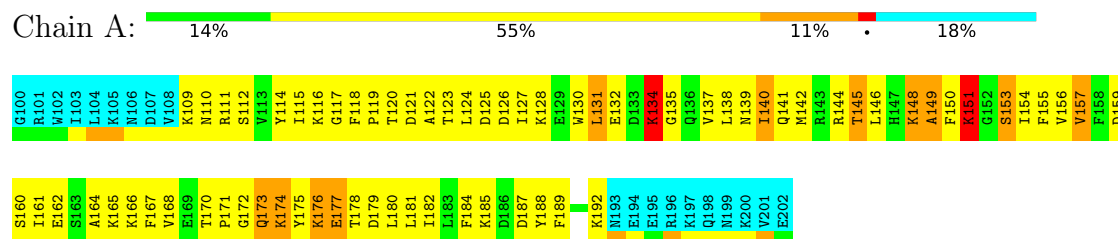
4.2.11 Score per residue for model 11

- Molecule 1: Lupus La protein



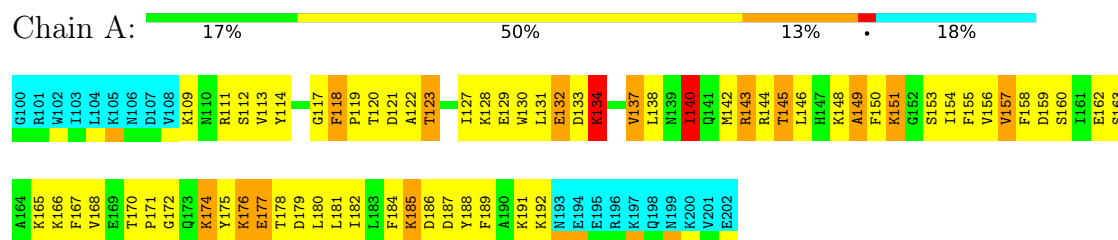
4.2.12 Score per residue for model 12

- Molecule 1: Lupus La protein



4.2.13 Score per residue for model 13

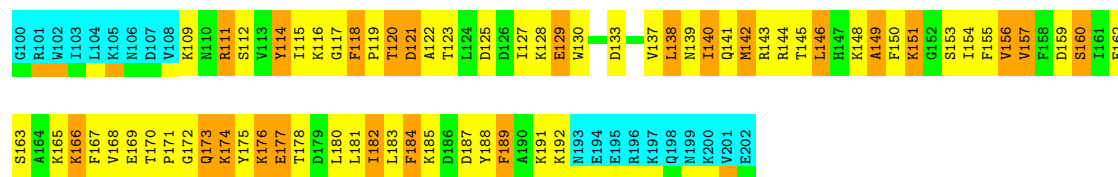
- Molecule 1: Lupus La protein



4.2.14 Score per residue for model 14

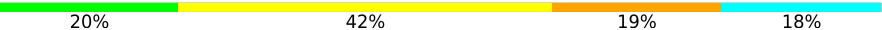
- Molecule 1: Lupus La protein

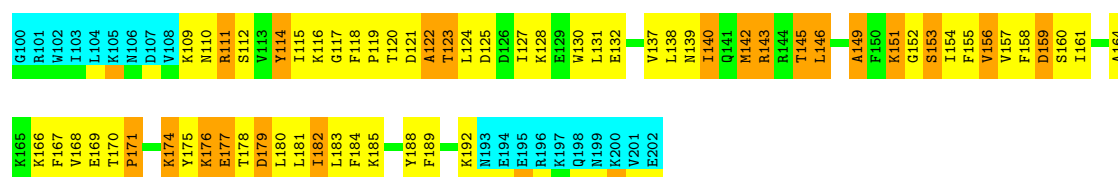
Chain A: 



4.2.15 Score per residue for model 15

- Molecule 1: Lupus La protein

Chain A: 



4.2.16 Score per residue for model 16

- Molecule 1: Lupus La protein

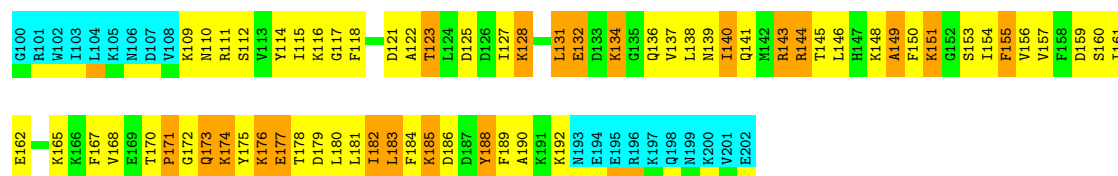
Chain A: 



4.2.17 Score per residue for model 17

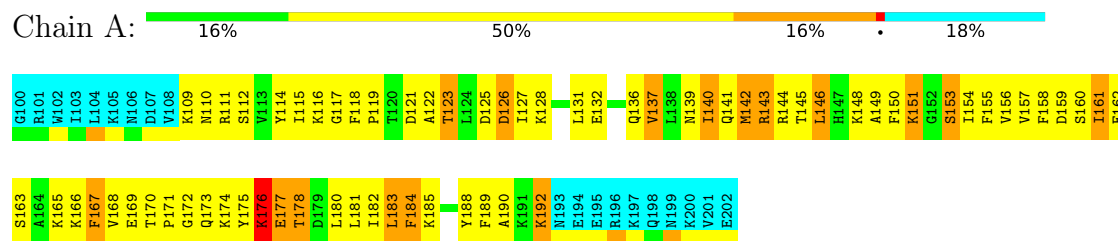
- Molecule 1: Lupus La protein

Chain A: 



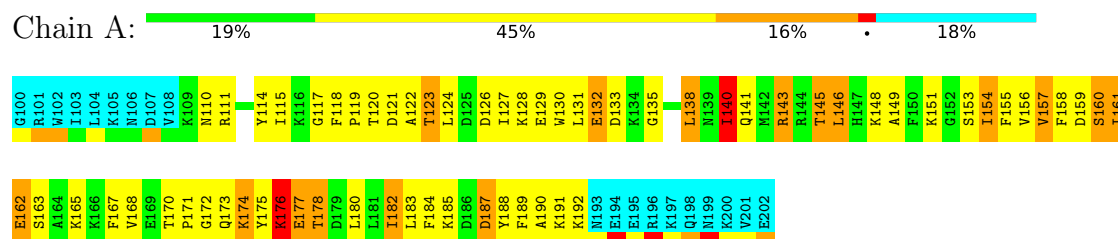
4.2.18 Score per residue for model 18

- Molecule 1: Lupus La protein



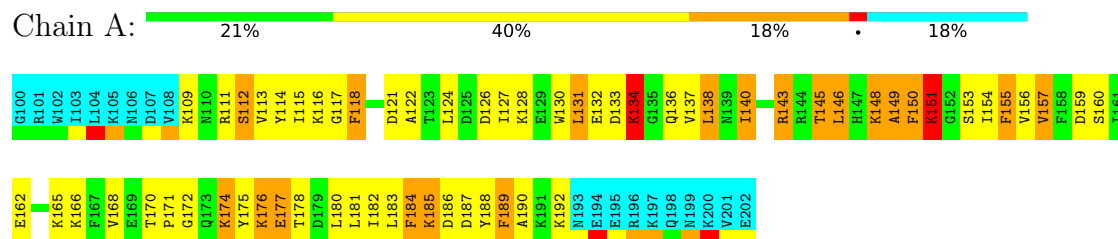
4.2.19 Score per residue for model 19

- Molecule 1: Lupus La protein



4.2.20 Score per residue for model 20

- Molecule 1: Lupus La protein



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: *structures with the lowest energy*.

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

Software name	Classification	Version
X-PLOR	structure solution	3.1
X-PLOR	refinement	3.1

No chemical shift data was provided.

6 Model quality

6.1 Standard geometry

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	1.41±0.01	0±0/710 (0.0± 0.0%)	1.59±0.01	4±1/952 (0.4± 0.1%)
All	All	1.41	0/14200 (0.0%)	1.59	72/19040 (0.4%)

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	140	ILE	N-CA-CB	-5.60	104.94	112.10	15	9
1	A	148	LYS	N-CA-C	-5.46	106.81	112.93	14	4
1	A	182	ILE	N-CA-CB	-5.37	104.92	111.21	2	16
1	A	149	ALA	N-CA-CB	-5.33	102.56	111.20	17	18
1	A	157	VAL	N-CA-CB	-5.32	104.99	111.21	10	16
1	A	137	VAL	N-CA-CB	-5.20	104.91	111.46	4	7
1	A	156	VAL	N-CA-CB	-5.03	104.97	111.82	14	2

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	695	711	711	84±7
All	All	13900	14220	14220	1687

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 60.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:168:VAL:HG21	1:A:184:PHE:CD1	1.11	1.81	19	13
1:A:131:LEU:HD13	1:A:137:VAL:HG21	1.10	1.20	20	1
1:A:168:VAL:HG11	1:A:184:PHE:CD2	1.08	1.83	16	9
1:A:131:LEU:HD12	1:A:137:VAL:HG22	1.06	1.27	17	2
1:A:127:ILE:HG21	1:A:140:ILE:HD11	1.05	1.29	14	7
1:A:118:PHE:CD2	1:A:154:ILE:HD13	1.04	1.86	13	3
1:A:131:LEU:HD23	1:A:137:VAL:HG21	1.04	1.29	7	2
1:A:168:VAL:HG21	1:A:184:PHE:CE1	1.02	1.90	10	12
1:A:118:PHE:CD2	1:A:154:ILE:HD12	1.01	1.91	3	8
1:A:118:PHE:CE1	1:A:127:ILE:HG23	1.00	1.89	3	1
1:A:118:PHE:O	1:A:178:THR:HG21	0.98	1.58	3	2
1:A:168:VAL:HG11	1:A:184:PHE:CD1	0.97	1.94	9	5
1:A:131:LEU:HD22	1:A:137:VAL:CG1	0.96	1.91	3	3
1:A:127:ILE:CD1	1:A:154:ILE:HG21	0.94	1.91	1	2
1:A:168:VAL:HG11	1:A:184:PHE:CG	0.93	1.98	11	9
1:A:127:ILE:HD13	1:A:154:ILE:HG21	0.91	1.38	1	3
1:A:118:PHE:CD2	1:A:154:ILE:HD11	0.91	2.00	1	1
1:A:131:LEU:HD21	1:A:156:VAL:CG2	0.90	1.96	7	1
1:A:131:LEU:HD22	1:A:137:VAL:CG2	0.89	1.97	20	1
1:A:111:ARG:O	1:A:157:VAL:HG13	0.86	1.70	3	9
1:A:153:SER:O	1:A:154:ILE:HD13	0.86	1.69	6	1
1:A:110:ASN:O	1:A:161:ILE:HG23	0.85	1.69	17	2
1:A:168:VAL:HG11	1:A:184:PHE:CE2	0.85	2.07	6	4
1:A:122:ALA:HB3	1:A:154:ILE:HD11	0.82	1.50	8	2
1:A:119:PRO:C	1:A:120:THR:HG23	0.82	1.98	15	1
1:A:131:LEU:HD12	1:A:137:VAL:CG2	0.82	2.03	17	2
1:A:167:PHE:O	1:A:170:THR:HG22	0.82	1.73	19	4
1:A:140:ILE:HD13	1:A:156:VAL:HG22	0.82	1.52	17	1
1:A:118:PHE:C	1:A:178:THR:HG21	0.81	2.00	15	10
1:A:115:ILE:CG2	1:A:180:LEU:HD21	0.81	2.04	14	15
1:A:180:LEU:C	1:A:180:LEU:HD13	0.80	2.01	10	20
1:A:145:THR:OG1	1:A:149:ALA:HB1	0.80	1.75	14	3
1:A:142:MET:HA	1:A:154:ILE:HG23	0.79	1.53	14	7
1:A:138:LEU:HD22	1:A:159:ASP:HA	0.79	1.52	15	2
1:A:110:ASN:CB	1:A:161:ILE:HG23	0.79	2.07	12	3
1:A:131:LEU:HD22	1:A:137:VAL:HG23	0.79	1.50	20	1
1:A:127:ILE:CG2	1:A:140:ILE:HD11	0.79	2.07	1	2
1:A:118:PHE:CE2	1:A:154:ILE:HD13	0.79	2.13	14	2
1:A:138:LEU:HD12	1:A:138:LEU:O	0.79	1.77	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:131:LEU:HD21	1:A:156:VAL:HG21	0.78	1.53	7	2
1:A:127:ILE:CD1	1:A:140:ILE:HD11	0.78	2.08	8	1
1:A:137:VAL:CG1	1:A:156:VAL:HG13	0.78	2.09	4	3
1:A:140:ILE:HD13	1:A:141:GLN:N	0.77	1.94	18	2
1:A:127:ILE:HG21	1:A:140:ILE:CD1	0.76	2.08	14	7
1:A:181:LEU:C	1:A:181:LEU:HD13	0.76	2.05	6	5
1:A:145:THR:HG21	1:A:150:PHE:C	0.76	2.05	17	8
1:A:146:LEU:O	1:A:149:ALA:HB3	0.76	1.80	14	19
1:A:122:ALA:O	1:A:127:ILE:HD11	0.75	1.81	20	10
1:A:154:ILE:N	1:A:154:ILE:HD12	0.75	1.97	13	3
1:A:116:LYS:HB3	1:A:181:LEU:HD21	0.75	1.58	11	2
1:A:154:ILE:HD13	1:A:154:ILE:N	0.74	1.97	1	1
1:A:131:LEU:CD1	1:A:137:VAL:HG22	0.74	2.11	17	1
1:A:131:LEU:CD1	1:A:137:VAL:HG21	0.74	2.08	20	1
1:A:112:SER:HA	1:A:157:VAL:HG22	0.74	1.58	13	3
1:A:166:LYS:O	1:A:170:THR:HG23	0.74	1.83	14	3
1:A:119:PRO:N	1:A:178:THR:HG21	0.73	1.98	5	10
1:A:137:VAL:HG21	1:A:156:VAL:HG13	0.73	1.61	1	1
1:A:110:ASN:HB2	1:A:161:ILE:HG23	0.73	1.60	12	1
1:A:131:LEU:CD2	1:A:137:VAL:HG21	0.73	2.12	7	1
1:A:140:ILE:CD1	1:A:156:VAL:HG22	0.72	2.15	17	2
1:A:181:LEU:HD13	1:A:182:ILE:N	0.72	1.98	5	8
1:A:115:ILE:HG21	1:A:180:LEU:HD21	0.71	1.61	10	10
1:A:110:ASN:HB2	1:A:161:ILE:HD12	0.71	1.62	7	2
1:A:118:PHE:CG	1:A:154:ILE:HD12	0.71	2.21	3	4
1:A:181:LEU:HD13	1:A:181:LEU:C	0.70	2.11	14	3
1:A:131:LEU:HB3	1:A:137:VAL:HG11	0.70	1.63	10	1
1:A:153:SER:C	1:A:154:ILE:HD13	0.70	2.12	1	2
1:A:188:TYR:C	1:A:188:TYR:CD1	0.70	2.69	17	19
1:A:161:ILE:C	1:A:161:ILE:HD12	0.70	2.11	19	1
1:A:127:ILE:HD11	1:A:154:ILE:HD13	0.70	1.62	18	4
1:A:146:LEU:N	1:A:149:ALA:HB3	0.69	2.02	19	18
1:A:183:LEU:HD13	1:A:184:PHE:N	0.69	2.03	16	1
1:A:114:TYR:CD1	1:A:155:PHE:CZ	0.69	2.81	3	3
1:A:142:MET:HA	1:A:154:ILE:HG22	0.69	1.63	1	1
1:A:122:ALA:HB1	1:A:154:ILE:HD11	0.69	1.63	3	1
1:A:153:SER:C	1:A:154:ILE:HD12	0.69	2.13	13	3
1:A:131:LEU:HD12	1:A:137:VAL:CG1	0.69	2.17	13	1
1:A:140:ILE:C	1:A:140:ILE:HD13	0.69	2.13	19	1
1:A:114:TYR:CD1	1:A:155:PHE:CE1	0.68	2.82	3	9
1:A:131:LEU:HD13	1:A:137:VAL:HG11	0.68	1.65	2	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:127:ILE:HG21	1:A:140:ILE:HD13	0.68	1.65	11	3
1:A:127:ILE:CG2	1:A:154:ILE:HD13	0.68	2.18	19	3
1:A:138:LEU:HD13	1:A:159:ASP:CG	0.67	2.15	1	3
1:A:158:PHE:CZ	1:A:167:PHE:CD2	0.67	2.82	3	4
1:A:140:ILE:HD13	1:A:140:ILE:C	0.67	2.15	18	1
1:A:111:ARG:HG3	1:A:161:ILE:HD13	0.67	1.66	5	3
1:A:127:ILE:HD11	1:A:154:ILE:HG12	0.66	1.65	12	2
1:A:127:ILE:HG22	1:A:131:LEU:HD12	0.66	1.66	8	3
1:A:124:LEU:HD21	1:A:140:ILE:HG23	0.66	1.67	3	1
1:A:186:ASP:O	1:A:190:ALA:HB2	0.65	1.91	17	5
1:A:137:VAL:HG21	1:A:156:VAL:HB	0.65	1.67	14	2
1:A:138:LEU:HD12	1:A:159:ASP:CB	0.65	2.21	20	1
1:A:127:ILE:HG21	1:A:140:ILE:HD12	0.65	1.66	17	1
1:A:118:PHE:CE2	1:A:154:ILE:HD12	0.65	2.27	8	4
1:A:138:LEU:HD11	1:A:159:ASP:HB3	0.65	1.67	4	1
1:A:188:TYR:CE1	1:A:192:LYS:CD	0.65	2.80	7	1
1:A:137:VAL:HB	1:A:156:VAL:HG22	0.65	1.66	15	1
1:A:145:THR:OG1	1:A:151:LYS:HA	0.64	1.92	12	11
1:A:115:ILE:HG22	1:A:180:LEU:HD21	0.64	1.68	11	3
1:A:122:ALA:CB	1:A:154:ILE:HD11	0.64	2.21	8	2
1:A:146:LEU:HB2	1:A:149:ALA:HB2	0.64	1.70	16	4
1:A:138:LEU:HD12	1:A:159:ASP:HB3	0.64	1.69	20	1
1:A:138:LEU:HD13	1:A:159:ASP:OD2	0.63	1.93	3	1
1:A:118:PHE:CD2	1:A:154:ILE:CD1	0.63	2.82	9	6
1:A:118:PHE:CD2	1:A:154:ILE:CG1	0.63	2.81	6	2
1:A:114:TYR:CB	1:A:155:PHE:CE2	0.63	2.81	15	1
1:A:124:LEU:C	1:A:124:LEU:HD13	0.63	2.18	2	1
1:A:130:TRP:HH2	1:A:182:ILE:HD11	0.63	1.53	20	10
1:A:138:LEU:HD11	1:A:159:ASP:CB	0.63	2.24	4	1
1:A:127:ILE:CG2	1:A:131:LEU:HD22	0.62	2.23	15	2
1:A:119:PRO:O	1:A:120:THR:OG1	0.62	2.17	15	1
1:A:119:PRO:CD	1:A:178:THR:HG21	0.62	2.24	5	4
1:A:145:THR:OG1	1:A:151:LYS:CB	0.62	2.48	19	8
1:A:131:LEU:HD21	1:A:156:VAL:HG22	0.62	1.69	7	1
1:A:127:ILE:HD12	1:A:140:ILE:HD11	0.62	1.71	8	1
1:A:168:VAL:CG1	1:A:184:PHE:CG	0.62	2.80	11	1
1:A:123:THR:N	1:A:126:ASP:OD1	0.62	2.33	19	1
1:A:124:LEU:HD13	1:A:124:LEU:O	0.62	1.94	2	2
1:A:118:PHE:HB3	1:A:122:ALA:HB2	0.62	1.72	1	4
1:A:127:ILE:HG22	1:A:131:LEU:HD22	0.61	1.72	7	2
1:A:121:ASP:O	1:A:123:THR:N	0.61	2.34	1	11

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:111:ARG:HD2	1:A:157:VAL:HG12	0.61	1.71	10	1
1:A:137:VAL:HG13	1:A:156:VAL:HG13	0.60	1.72	7	2
1:A:131:LEU:HD21	1:A:156:VAL:HG11	0.60	1.72	1	1
1:A:175:TYR:CB	1:A:180:LEU:HB3	0.60	2.25	18	20
1:A:180:LEU:C	1:A:180:LEU:CD1	0.60	2.74	10	20
1:A:181:LEU:HD12	1:A:183:LEU:HD12	0.60	1.73	17	1
1:A:150:PHE:O	1:A:150:PHE:CD2	0.60	2.54	14	2
1:A:110:ASN:HB3	1:A:161:ILE:HG23	0.60	1.73	9	3
1:A:185:LYS:O	1:A:189:PHE:CD2	0.60	2.55	11	2
1:A:119:PRO:C	1:A:120:THR:CG2	0.60	2.70	15	1
1:A:122:ALA:CB	1:A:154:ILE:CD1	0.59	2.80	8	1
1:A:168:VAL:HG21	1:A:184:PHE:HD1	0.59	1.53	15	2
1:A:114:TYR:C	1:A:114:TYR:CD1	0.59	2.80	17	5
1:A:156:VAL:O	1:A:156:VAL:HG23	0.59	1.97	14	2
1:A:137:VAL:HG11	1:A:156:VAL:CG1	0.59	2.27	5	1
1:A:127:ILE:CG2	1:A:140:ILE:CD1	0.59	2.81	11	4
1:A:145:THR:HG21	1:A:151:LYS:N	0.59	2.13	7	4
1:A:131:LEU:HD22	1:A:137:VAL:HG11	0.59	1.72	3	2
1:A:168:VAL:CG1	1:A:184:PHE:CD2	0.59	2.78	5	4
1:A:131:LEU:CD1	1:A:140:ILE:HD12	0.59	2.28	5	1
1:A:150:PHE:CG	1:A:150:PHE:O	0.59	2.55	1	1
1:A:137:VAL:HG11	1:A:156:VAL:HB	0.59	1.75	6	1
1:A:167:PHE:O	1:A:170:THR:HG23	0.59	1.98	7	1
1:A:140:ILE:O	1:A:140:ILE:HG23	0.59	1.98	19	6
1:A:175:TYR:CB	1:A:180:LEU:CB	0.58	2.81	16	20
1:A:114:TYR:CD1	1:A:114:TYR:O	0.58	2.56	5	4
1:A:131:LEU:HD22	1:A:137:VAL:HG12	0.58	1.69	3	1
1:A:137:VAL:CG1	1:A:156:VAL:CG1	0.58	2.80	4	2
1:A:127:ILE:HD13	1:A:140:ILE:HD11	0.58	1.73	8	1
1:A:140:ILE:CD1	1:A:156:VAL:HG12	0.58	2.28	12	1
1:A:167:PHE:CE1	1:A:182:ILE:HG21	0.58	2.34	12	1
1:A:184:PHE:CG	1:A:186:ASP:OD1	0.58	2.57	13	1
1:A:167:PHE:HE1	1:A:182:ILE:HD13	0.58	1.59	17	1
1:A:145:THR:OG1	1:A:151:LYS:CA	0.57	2.52	8	8
1:A:167:PHE:CE1	1:A:182:ILE:HD13	0.57	2.34	17	2
1:A:154:ILE:N	1:A:154:ILE:CD1	0.57	2.64	1	4
1:A:134:LYS:CD	1:A:134:LYS:N	0.57	2.67	17	3
1:A:117:GLY:O	1:A:178:THR:CG2	0.57	2.52	5	13
1:A:114:TYR:CE1	1:A:155:PHE:CE1	0.57	2.93	3	2
1:A:110:ASN:CB	1:A:161:ILE:HD12	0.57	2.30	7	1
1:A:184:PHE:CD2	1:A:186:ASP:OD2	0.57	2.57	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:181:LEU:HD21	1:A:183:LEU:HD12	0.57	1.75	18	1
1:A:175:TYR:HB3	1:A:180:LEU:CB	0.57	2.30	13	20
1:A:181:LEU:HD13	1:A:183:LEU:HD13	0.57	1.76	11	1
1:A:137:VAL:CG2	1:A:157:VAL:N	0.57	2.68	8	1
1:A:164:ALA:O	1:A:168:VAL:HG23	0.56	2.00	11	2
1:A:119:PRO:O	1:A:120:THR:C	0.56	2.47	10	5
1:A:137:VAL:O	1:A:137:VAL:HG23	0.56	1.99	4	4
1:A:168:VAL:HG21	1:A:184:PHE:HE1	0.56	1.55	9	1
1:A:118:PHE:CG	1:A:154:ILE:CD1	0.56	2.88	9	1
1:A:127:ILE:HG23	1:A:154:ILE:HD13	0.56	1.78	19	1
1:A:117:GLY:O	1:A:118:PHE:O	0.56	2.24	3	5
1:A:122:ALA:HB3	1:A:154:ILE:CD1	0.56	2.26	8	1
1:A:128:LYS:O	1:A:132:GLU:CG	0.55	2.54	12	2
1:A:138:LEU:HD11	1:A:159:ASP:HB2	0.55	1.78	12	1
1:A:140:ILE:C	1:A:140:ILE:CD1	0.55	2.79	19	2
1:A:118:PHE:CD2	1:A:154:ILE:HG13	0.55	2.35	6	4
1:A:114:TYR:CD1	1:A:115:ILE:N	0.55	2.74	11	1
1:A:131:LEU:HD22	1:A:156:VAL:HG21	0.55	1.75	18	1
1:A:175:TYR:CE1	1:A:176:LYS:HE3	0.55	2.36	2	1
1:A:188:TYR:CE1	1:A:192:LYS:HD2	0.55	2.35	7	3
1:A:119:PRO:HD3	1:A:178:THR:HG21	0.55	1.78	6	1
1:A:127:ILE:HG22	1:A:131:LEU:CD1	0.55	2.31	19	2
1:A:145:THR:HG22	1:A:149:ALA:HB1	0.55	1.76	10	11
1:A:184:PHE:N	1:A:187:ASP:OD2	0.55	2.40	2	1
1:A:145:THR:HG23	1:A:149:ALA:HB3	0.55	1.79	3	5
1:A:181:LEU:C	1:A:181:LEU:HD12	0.55	2.27	11	2
1:A:146:LEU:O	1:A:149:ALA:N	0.55	2.38	20	16
1:A:119:PRO:O	1:A:120:THR:CB	0.55	2.55	15	1
1:A:151:LYS:CG	1:A:152:GLY:N	0.54	2.70	16	9
1:A:181:LEU:HD12	1:A:181:LEU:O	0.54	2.02	11	1
1:A:181:LEU:C	1:A:181:LEU:CD1	0.54	2.80	16	8
1:A:173:GLN:HB3	1:A:182:ILE:HD12	0.54	1.79	14	1
1:A:118:PHE:CD1	1:A:122:ALA:HB1	0.54	2.37	6	1
1:A:154:ILE:HD12	1:A:156:VAL:HG23	0.54	1.78	20	1
1:A:176:LYS:O	1:A:178:THR:N	0.54	2.41	3	18
1:A:138:LEU:CD1	1:A:159:ASP:CB	0.54	2.86	4	1
1:A:114:TYR:HB3	1:A:155:PHE:CE2	0.54	2.38	15	1
1:A:171:PRO:O	1:A:172:GLY:C	0.54	2.50	16	16
1:A:128:LYS:O	1:A:132:GLU:CB	0.54	2.56	7	10
1:A:180:LEU:HD13	1:A:181:LEU:N	0.54	2.17	11	9
1:A:145:THR:HB	1:A:151:LYS:HB2	0.54	1.80	1	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:114:TYR:CD1	1:A:114:TYR:C	0.54	2.85	5	2
1:A:112:SER:O	1:A:185:LYS:CG	0.54	2.56	12	5
1:A:114:TYR:HB2	1:A:155:PHE:CZ	0.54	2.38	15	4
1:A:175:TYR:HB3	1:A:180:LEU:HB2	0.54	1.80	15	20
1:A:113:VAL:CG2	1:A:156:VAL:O	0.54	2.56	5	1
1:A:137:VAL:HG11	1:A:140:ILE:CG1	0.54	2.33	20	1
1:A:116:LYS:HB3	1:A:181:LEU:HD11	0.54	1.79	3	1
1:A:115:ILE:HD11	1:A:156:VAL:HG21	0.54	1.79	16	1
1:A:161:ILE:HG13	1:A:162:GLU:N	0.54	2.17	19	1
1:A:176:LYS:O	1:A:177:GLU:C	0.54	2.51	19	20
1:A:144:ARG:CG	1:A:145:THR:N	0.54	2.70	1	1
1:A:118:PHE:CZ	1:A:127:ILE:HG23	0.54	2.35	3	1
1:A:145:THR:CG2	1:A:149:ALA:C	0.54	2.81	17	6
1:A:112:SER:O	1:A:185:LYS:CE	0.54	2.56	16	2
1:A:130:TRP:O	1:A:134:LYS:CD	0.54	2.55	12	1
1:A:166:LYS:O	1:A:170:THR:CG2	0.54	2.56	14	1
1:A:114:TYR:CB	1:A:155:PHE:CZ	0.54	2.91	15	2
1:A:175:TYR:O	1:A:176:LYS:O	0.53	2.24	12	20
1:A:131:LEU:O	1:A:135:GLY:N	0.53	2.41	3	2
1:A:118:PHE:CE2	1:A:154:ILE:HG12	0.53	2.38	4	4
1:A:153:SER:C	1:A:154:ILE:CD1	0.53	2.81	13	2
1:A:122:ALA:HA	1:A:126:ASP:OD2	0.53	2.03	19	1
1:A:137:VAL:CG2	1:A:156:VAL:HG13	0.53	2.32	1	1
1:A:143:ARG:CB	1:A:153:SER:O	0.53	2.57	1	3
1:A:113:VAL:HG22	1:A:156:VAL:O	0.53	2.03	5	1
1:A:133:ASP:O	1:A:134:LYS:CD	0.53	2.57	1	1
1:A:120:THR:HG22	1:A:120:THR:O	0.53	2.03	6	2
1:A:131:LEU:CD2	1:A:156:VAL:HG11	0.53	2.33	1	1
1:A:181:LEU:CD1	1:A:183:LEU:HD13	0.53	2.33	11	1
1:A:117:GLY:O	1:A:178:THR:HG22	0.53	2.03	10	4
1:A:121:ASP:O	1:A:122:ALA:C	0.53	2.52	16	9
1:A:114:TYR:HB2	1:A:155:PHE:CE2	0.53	2.38	15	5
1:A:109:LYS:O	1:A:185:LYS:CE	0.53	2.56	8	2
1:A:120:THR:HG23	1:A:121:ASP:N	0.53	2.18	14	4
1:A:145:THR:OG1	1:A:149:ALA:CB	0.53	2.53	14	2
1:A:167:PHE:O	1:A:170:THR:CG2	0.53	2.55	3	5
1:A:111:ARG:CD	1:A:158:PHE:O	0.53	2.57	10	1
1:A:142:MET:CG	1:A:142:MET:O	0.53	2.57	12	1
1:A:115:ILE:CG2	1:A:180:LEU:CD2	0.53	2.87	10	6
1:A:186:ASP:OD1	1:A:186:ASP:N	0.53	2.42	10	1
1:A:137:VAL:HG23	1:A:157:VAL:O	0.53	2.04	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:137:VAL:O	1:A:137:VAL:CG2	0.53	2.57	4	4
1:A:138:LEU:HD12	1:A:159:ASP:CG	0.53	2.29	14	1
1:A:110:ASN:OD1	1:A:111:ARG:N	0.53	2.41	18	1
1:A:125:ASP:N	1:A:125:ASP:OD1	0.52	2.39	18	1
1:A:122:ALA:O	1:A:127:ILE:CD1	0.52	2.57	1	7
1:A:168:VAL:HG21	1:A:184:PHE:CE2	0.52	2.38	3	1
1:A:158:PHE:CE2	1:A:167:PHE:CD2	0.52	2.97	6	1
1:A:110:ASN:O	1:A:164:ALA:CB	0.52	2.57	12	3
1:A:138:LEU:CB	1:A:157:VAL:O	0.52	2.57	17	1
1:A:146:LEU:O	1:A:149:ALA:CB	0.52	2.56	14	2
1:A:137:VAL:HG22	1:A:156:VAL:CG1	0.52	2.34	20	1
1:A:117:GLY:O	1:A:118:PHE:C	0.52	2.53	5	4
1:A:173:GLN:HB2	1:A:182:ILE:HD12	0.52	1.82	10	1
1:A:145:THR:HG21	1:A:149:ALA:C	0.52	2.29	6	4
1:A:119:PRO:O	1:A:120:THR:HG23	0.52	2.03	15	1
1:A:150:PHE:O	1:A:151:LYS:O	0.52	2.26	17	1
1:A:168:VAL:HG21	1:A:184:PHE:CZ	0.52	2.39	3	2
1:A:130:TRP:CH2	1:A:182:ILE:HD11	0.52	2.38	13	5
1:A:119:PRO:HG2	1:A:122:ALA:HB2	0.52	1.82	10	1
1:A:111:ARG:CG	1:A:161:ILE:HD13	0.52	2.34	5	1
1:A:111:ARG:O	1:A:158:PHE:N	0.52	2.43	19	2
1:A:154:ILE:C	1:A:155:PHE:CD1	0.52	2.88	7	3
1:A:140:ILE:O	1:A:140:ILE:CG2	0.52	2.58	19	2
1:A:137:VAL:HG22	1:A:156:VAL:HG13	0.52	1.82	20	1
1:A:153:SER:C	1:A:154:ILE:CG1	0.51	2.83	2	14
1:A:158:PHE:HB2	1:A:164:ALA:HB2	0.51	1.82	15	1
1:A:121:ASP:N	1:A:121:ASP:OD1	0.51	2.43	7	3
1:A:188:TYR:O	1:A:192:LYS:CB	0.51	2.58	5	4
1:A:125:ASP:OD1	1:A:126:ASP:N	0.51	2.42	18	1
1:A:110:ASN:ND2	1:A:111:ARG:HG3	0.51	2.21	19	1
1:A:131:LEU:HD13	1:A:137:VAL:CG2	0.51	2.14	20	1
1:A:119:PRO:HD2	1:A:122:ALA:HB2	0.51	1.83	7	4
1:A:145:THR:CG2	1:A:149:ALA:HB1	0.51	2.36	10	11
1:A:115:ILE:CG2	1:A:118:PHE:CE2	0.51	2.92	17	2
1:A:175:TYR:HB2	1:A:180:LEU:HB3	0.51	1.83	10	19
1:A:184:PHE:CB	1:A:187:ASP:OD2	0.51	2.59	2	2
1:A:121:ASP:OD1	1:A:122:ALA:N	0.51	2.43	10	1
1:A:145:THR:CG2	1:A:150:PHE:C	0.51	2.82	17	1
1:A:110:ASN:ND2	1:A:111:ARG:CG	0.51	2.73	19	1
1:A:175:TYR:CE1	1:A:176:LYS:CE	0.51	2.94	2	1
1:A:131:LEU:HD11	1:A:156:VAL:HG21	0.51	1.81	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:142:MET:SD	1:A:142:MET:O	0.51	2.69	9	2
1:A:109:LYS:O	1:A:185:LYS:NZ	0.51	2.44	20	2
1:A:155:PHE:CZ	1:A:185:LYS:HD3	0.51	2.41	17	1
1:A:160:SER:OG	1:A:163:SER:CB	0.51	2.59	14	4
1:A:192:LYS:CD	1:A:192:LYS:C	0.51	2.84	2	1
1:A:143:ARG:HB3	1:A:153:SER:CB	0.51	2.36	6	9
1:A:136:GLN:NE2	1:A:160:SER:OG	0.51	2.43	16	1
1:A:174:LYS:HA	1:A:180:LEU:O	0.50	2.06	15	20
1:A:119:PRO:O	1:A:122:ALA:N	0.50	2.43	3	1
1:A:130:TRP:CZ2	1:A:134:LYS:HE2	0.50	2.41	4	1
1:A:118:PHE:CD1	1:A:122:ALA:CB	0.50	2.94	6	1
1:A:121:ASP:OD1	1:A:121:ASP:N	0.50	2.43	10	3
1:A:138:LEU:HD21	1:A:157:VAL:HG12	0.50	1.83	15	1
1:A:118:PHE:CD1	1:A:127:ILE:HG12	0.50	2.41	3	1
1:A:161:ILE:CG1	1:A:162:GLU:N	0.50	2.72	6	2
1:A:177:GLU:N	1:A:177:GLU:CD	0.50	2.69	17	1
1:A:133:ASP:O	1:A:134:LYS:CG	0.50	2.60	1	1
1:A:118:PHE:CZ	1:A:154:ILE:HD12	0.50	2.42	8	2
1:A:134:LYS:N	1:A:134:LYS:HD2	0.50	2.22	10	1
1:A:145:THR:CG2	1:A:151:LYS:N	0.50	2.75	6	5
1:A:124:LEU:CD1	1:A:140:ILE:HD13	0.50	2.37	15	1
1:A:110:ASN:N	1:A:110:ASN:OD1	0.50	2.43	1	1
1:A:130:TRP:CE2	1:A:134:LYS:HE2	0.50	2.42	4	1
1:A:138:LEU:HD12	1:A:159:ASP:HA	0.50	1.83	5	1
1:A:111:ARG:NH2	1:A:159:ASP:O	0.50	2.43	1	1
1:A:127:ILE:HG21	1:A:154:ILE:HD13	0.50	1.82	20	3
1:A:138:LEU:H	1:A:138:LEU:HD23	0.50	1.66	15	1
1:A:140:ILE:HG12	1:A:156:VAL:HG12	0.50	1.84	19	1
1:A:168:VAL:CG2	1:A:184:PHE:CD1	0.50	2.79	18	4
1:A:131:LEU:CD1	1:A:137:VAL:HG11	0.50	2.37	13	2
1:A:168:VAL:HG11	1:A:184:PHE:HB2	0.49	1.82	15	2
1:A:123:THR:N	1:A:126:ASP:CG	0.49	2.70	19	1
1:A:131:LEU:CD2	1:A:156:VAL:HG21	0.49	2.36	15	1
1:A:187:ASP:OD1	1:A:188:TYR:N	0.49	2.45	2	1
1:A:131:LEU:CD1	1:A:140:ILE:CD1	0.49	2.90	5	1
1:A:118:PHE:CD2	1:A:154:ILE:HG12	0.49	2.43	6	4
1:A:111:ARG:O	1:A:157:VAL:CG1	0.49	2.57	20	4
1:A:118:PHE:CE1	1:A:127:ILE:HG12	0.49	2.43	13	1
1:A:179:ASP:N	1:A:179:ASP:OD1	0.49	2.43	11	3
1:A:137:VAL:HG21	1:A:156:VAL:CG1	0.49	2.34	1	1
1:A:144:ARG:HG2	1:A:145:THR:N	0.49	2.22	1	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:168:VAL:CG1	1:A:184:PHE:CE2	0.49	2.91	6	2
1:A:131:LEU:HD11	1:A:140:ILE:HD12	0.49	1.84	5	1
1:A:168:VAL:HG11	1:A:184:PHE:CE1	0.49	2.42	9	1
1:A:114:TYR:CD1	1:A:155:PHE:CD1	0.49	3.01	12	1
1:A:138:LEU:N	1:A:157:VAL:O	0.49	2.46	19	2
1:A:181:LEU:HD21	1:A:183:LEU:HG	0.49	1.83	7	1
1:A:134:LYS:HB3	1:A:167:PHE:CZ	0.49	2.42	11	1
1:A:184:PHE:CD2	1:A:186:ASP:OD1	0.49	2.66	13	1
1:A:114:TYR:HB2	1:A:155:PHE:CD2	0.49	2.42	15	2
1:A:161:ILE:HD12	1:A:161:ILE:O	0.49	2.07	19	1
1:A:145:THR:CG2	1:A:151:LYS:HB2	0.49	2.38	19	4
1:A:145:THR:OG1	1:A:151:LYS:HB3	0.49	2.08	11	9
1:A:156:VAL:O	1:A:156:VAL:CG2	0.49	2.60	14	2
1:A:114:TYR:HB2	1:A:155:PHE:CE1	0.49	2.42	15	3
1:A:127:ILE:O	1:A:131:LEU:HD12	0.49	2.07	1	1
1:A:137:VAL:CG2	1:A:156:VAL:CG1	0.49	2.91	1	1
1:A:114:TYR:OH	1:A:153:SER:OG	0.49	2.31	4	2
1:A:142:MET:HG3	1:A:154:ILE:HD12	0.49	1.83	6	1
1:A:186:ASP:O	1:A:190:ALA:CB	0.49	2.61	10	2
1:A:138:LEU:O	1:A:139:ASN:CG	0.49	2.56	11	1
1:A:111:ARG:HD2	1:A:157:VAL:CG1	0.49	2.38	3	1
1:A:118:PHE:CE2	1:A:154:ILE:HB	0.49	2.43	3	1
1:A:138:LEU:CD1	1:A:159:ASP:HB3	0.49	2.36	4	1
1:A:130:TRP:CD2	1:A:134:LYS:NZ	0.49	2.81	10	1
1:A:118:PHE:CE2	1:A:154:ILE:HG13	0.49	2.42	6	1
1:A:155:PHE:CE2	1:A:185:LYS:HD3	0.49	2.43	6	1
1:A:117:GLY:HA3	1:A:179:ASP:O	0.48	2.08	2	6
1:A:131:LEU:CD1	1:A:137:VAL:CG1	0.48	2.90	13	1
1:A:161:ILE:C	1:A:161:ILE:CD1	0.48	2.77	19	1
1:A:137:VAL:HB	1:A:156:VAL:CG1	0.48	2.38	1	1
1:A:188:TYR:CZ	1:A:192:LYS:HD2	0.48	2.43	5	2
1:A:114:TYR:OH	1:A:153:SER:CB	0.48	2.61	12	1
1:A:131:LEU:HD12	1:A:137:VAL:HG13	0.48	1.84	13	1
1:A:184:PHE:CD1	1:A:185:LYS:HD3	0.48	2.44	20	1
1:A:111:ARG:HD2	1:A:157:VAL:HG13	0.48	1.85	4	1
1:A:168:VAL:HG21	1:A:184:PHE:CG	0.48	2.39	4	1
1:A:119:PRO:CD	1:A:122:ALA:HB2	0.48	2.37	10	1
1:A:134:LYS:HG3	1:A:167:PHE:CE1	0.48	2.42	11	1
1:A:173:GLN:O	1:A:173:GLN:CG	0.48	2.61	8	1
1:A:120:THR:CG2	1:A:121:ASP:N	0.48	2.77	14	1
1:A:142:MET:SD	1:A:142:MET:C	0.48	2.96	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:131:LEU:HB3	1:A:137:VAL:CG2	0.48	2.38	18	1
1:A:170:THR:O	1:A:171:PRO:O	0.48	2.32	2	4
1:A:161:ILE:HG23	1:A:162:GLU:N	0.48	2.23	18	2
1:A:137:VAL:CG1	1:A:139:ASN:O	0.48	2.61	9	1
1:A:137:VAL:HG11	1:A:140:ILE:HD11	0.48	1.84	12	1
1:A:153:SER:C	1:A:154:ILE:CG2	0.48	2.87	16	3
1:A:143:ARG:HD3	1:A:155:PHE:CE1	0.48	2.43	18	1
1:A:131:LEU:O	1:A:135:GLY:O	0.48	2.32	3	4
1:A:187:ASP:O	1:A:190:ALA:HB3	0.48	2.08	6	5
1:A:110:ASN:HB3	1:A:161:ILE:CG2	0.48	2.38	9	2
1:A:110:ASN:OD1	1:A:110:ASN:C	0.48	2.56	18	1
1:A:137:VAL:HG11	1:A:156:VAL:HG11	0.48	1.85	5	1
1:A:143:ARG:CB	1:A:153:SER:HB3	0.48	2.39	8	2
1:A:131:LEU:CD2	1:A:137:VAL:CG2	0.48	2.82	20	1
1:A:183:LEU:CD2	1:A:187:ASP:HB2	0.48	2.38	10	1
1:A:123:THR:O	1:A:126:ASP:CG	0.48	2.56	19	1
1:A:184:PHE:CE1	1:A:185:LYS:HD3	0.48	2.43	20	1
1:A:137:VAL:CG1	1:A:156:VAL:CG2	0.47	2.92	2	1
1:A:115:ILE:HG23	1:A:181:LEU:O	0.47	2.09	15	2
1:A:138:LEU:HD23	1:A:159:ASP:N	0.47	2.24	16	1
1:A:183:LEU:HD11	1:A:187:ASP:HB3	0.47	1.86	16	1
1:A:123:THR:O	1:A:126:ASP:OD1	0.47	2.32	19	1
1:A:129:GLU:OE1	1:A:129:GLU:CA	0.47	2.59	1	1
1:A:133:ASP:O	1:A:134:LYS:CB	0.47	2.59	13	4
1:A:132:GLU:OE1	1:A:132:GLU:C	0.47	2.57	2	1
1:A:170:THR:HG23	1:A:171:PRO:HD2	0.47	1.86	5	9
1:A:111:ARG:HD2	1:A:158:PHE:O	0.47	2.10	10	1
1:A:124:LEU:C	1:A:124:LEU:CD1	0.47	2.87	2	1
1:A:159:ASP:CG	1:A:160:SER:N	0.47	2.73	5	1
1:A:114:TYR:CD1	1:A:154:ILE:O	0.47	2.68	12	1
1:A:114:TYR:O	1:A:183:LEU:O	0.47	2.32	7	3
1:A:124:LEU:HD21	1:A:140:ILE:CG2	0.47	2.40	7	2
1:A:133:ASP:O	1:A:133:ASP:CG	0.47	2.57	13	2
1:A:137:VAL:HG13	1:A:157:VAL:O	0.47	2.09	14	1
1:A:112:SER:CA	1:A:157:VAL:HG22	0.47	2.37	13	1
1:A:145:THR:HG23	1:A:149:ALA:CB	0.47	2.40	17	1
1:A:145:THR:HB	1:A:151:LYS:HB3	0.47	1.87	7	3
1:A:114:TYR:CE2	1:A:188:TYR:CD2	0.47	3.03	6	1
1:A:109:LYS:O	1:A:185:LYS:HE3	0.47	2.10	16	2
1:A:168:VAL:HG11	1:A:184:PHE:CB	0.47	2.40	15	3
1:A:173:GLN:O	1:A:173:GLN:HG3	0.47	2.10	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:115:ILE:HD12	1:A:156:VAL:HG11	0.47	1.87	12	1
1:A:150:PHE:CD1	1:A:150:PHE:N	0.46	2.79	3	1
1:A:180:LEU:HD11	1:A:182:ILE:HG13	0.46	1.86	11	1
1:A:111:ARG:CD	1:A:161:ILE:HG22	0.46	2.40	19	1
1:A:184:PHE:O	1:A:187:ASP:OD1	0.46	2.34	2	1
1:A:168:VAL:CG1	1:A:184:PHE:CD1	0.46	2.84	9	2
1:A:143:ARG:CB	1:A:153:SER:HB2	0.46	2.40	16	1
1:A:127:ILE:HD11	1:A:154:ILE:HG21	0.46	1.79	1	1
1:A:117:GLY:O	1:A:179:ASP:O	0.46	2.34	15	3
1:A:189:PHE:HA	1:A:192:LYS:CG	0.46	2.40	2	1
1:A:137:VAL:HG11	1:A:156:VAL:HG13	0.46	1.82	4	1
1:A:170:THR:OG1	1:A:173:GLN:OE1	0.46	2.34	10	1
1:A:128:LYS:O	1:A:132:GLU:HB3	0.46	2.10	8	6
1:A:140:ILE:HA	1:A:155:PHE:O	0.46	2.11	2	9
1:A:119:PRO:HG2	1:A:122:ALA:CB	0.46	2.40	10	1
1:A:177:GLU:HG3	1:A:178:THR:N	0.46	2.25	10	1
1:A:159:ASP:O	1:A:159:ASP:OD1	0.46	2.34	11	1
1:A:173:GLN:HB3	1:A:182:ILE:CD1	0.46	2.39	12	2
1:A:145:THR:HG21	1:A:150:PHE:N	0.46	2.25	17	1
1:A:111:ARG:CG	1:A:161:ILE:HG22	0.46	2.40	6	1
1:A:134:LYS:N	1:A:134:LYS:HD3	0.46	2.26	17	1
1:A:184:PHE:HB3	1:A:187:ASP:OD2	0.46	2.10	2	1
1:A:177:GLU:HG2	1:A:178:THR:N	0.46	2.26	5	2
1:A:185:LYS:HB3	1:A:189:PHE:CE2	0.46	2.45	10	1
1:A:114:TYR:CD2	1:A:188:TYR:CD2	0.46	3.03	11	1
1:A:145:THR:OG1	1:A:151:LYS:HB2	0.46	2.09	19	1
1:A:143:ARG:N	1:A:153:SER:O	0.46	2.48	18	7
1:A:173:GLN:OE1	1:A:173:GLN:CA	0.46	2.64	1	1
1:A:123:THR:O	1:A:127:ILE:HD12	0.46	2.11	19	3
1:A:181:LEU:O	1:A:181:LEU:CD1	0.46	2.64	11	1
1:A:154:ILE:CD1	1:A:156:VAL:HG23	0.46	2.41	20	1
1:A:188:TYR:O	1:A:192:LYS:HB2	0.46	2.11	20	1
1:A:116:LYS:HG3	1:A:117:GLY:N	0.46	2.25	12	3
1:A:138:LEU:HD23	1:A:158:PHE:C	0.46	2.36	16	1
1:A:143:ARG:O	1:A:151:LYS:CG	0.46	2.64	18	1
1:A:118:PHE:HD2	1:A:154:ILE:HD11	0.46	1.63	1	1
1:A:138:LEU:HD13	1:A:159:ASP:OD1	0.46	2.11	1	1
1:A:166:LYS:HG3	1:A:167:PHE:N	0.46	2.26	2	2
1:A:185:LYS:O	1:A:189:PHE:HB2	0.46	2.11	8	2
1:A:160:SER:HG	1:A:163:SER:HB2	0.46	1.70	16	1
1:A:115:ILE:HB	1:A:118:PHE:CE2	0.45	2.46	10	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:111:ARG:HB2	1:A:161:ILE:CD1	0.45	2.41	5	1
1:A:116:LYS:CG	1:A:117:GLY:N	0.45	2.79	15	2
1:A:123:THR:HG22	1:A:124:LEU:H	0.45	1.71	11	2
1:A:138:LEU:HB3	1:A:157:VAL:O	0.45	2.11	17	1
1:A:118:PHE:CE2	1:A:154:ILE:CG1	0.45	2.99	6	2
1:A:133:ASP:C	1:A:134:LYS:HD2	0.45	2.36	10	1
1:A:113:VAL:N	1:A:156:VAL:O	0.45	2.50	20	2
1:A:138:LEU:CD2	1:A:158:PHE:C	0.45	2.89	15	1
1:A:188:TYR:CD1	1:A:192:LYS:HG2	0.45	2.46	18	1
1:A:115:ILE:CD1	1:A:156:VAL:HG21	0.45	2.42	1	1
1:A:124:LEU:HD13	1:A:124:LEU:C	0.45	2.37	1	1
1:A:137:VAL:HG11	1:A:156:VAL:HG21	0.45	1.88	2	1
1:A:133:ASP:O	1:A:134:LYS:HB3	0.45	2.11	9	2
1:A:112:SER:O	1:A:185:LYS:HG2	0.45	2.11	8	2
1:A:118:PHE:HB3	1:A:122:ALA:CB	0.45	2.42	4	4
1:A:111:ARG:O	1:A:157:VAL:HA	0.45	2.11	18	8
1:A:142:MET:CA	1:A:154:ILE:HG23	0.45	2.33	14	1
1:A:192:LYS:C	1:A:192:LYS:HD2	0.45	2.36	2	1
1:A:145:THR:N	1:A:151:LYS:HB3	0.45	2.25	3	5
1:A:158:PHE:CE1	1:A:167:PHE:CD2	0.45	3.03	13	2
1:A:143:ARG:HB3	1:A:153:SER:OG	0.45	2.11	13	1
1:A:171:PRO:O	1:A:173:GLN:OE1	0.45	2.35	14	1
1:A:120:THR:HG23	1:A:121:ASP:H	0.45	1.72	10	2
1:A:114:TYR:HB2	1:A:155:PHE:CG	0.45	2.47	15	2
1:A:138:LEU:HD22	1:A:159:ASP:CA	0.45	2.32	15	1
1:A:115:ILE:HG22	1:A:118:PHE:CE2	0.45	2.46	9	1
1:A:153:SER:C	1:A:154:ILE:HG23	0.45	2.37	16	4
1:A:145:THR:O	1:A:146:LEU:C	0.45	2.60	6	20
1:A:143:ARG:HB3	1:A:153:SER:O	0.45	2.12	3	2
1:A:138:LEU:CD2	1:A:159:ASP:HB2	0.45	2.42	11	1
1:A:125:ASP:O	1:A:129:GLU:OE1	0.45	2.34	14	1
1:A:141:GLN:O	1:A:155:PHE:N	0.45	2.50	10	9
1:A:111:ARG:HG3	1:A:161:ILE:CD1	0.45	2.42	11	2
1:A:139:ASN:O	1:A:157:VAL:N	0.45	2.49	5	1
1:A:145:THR:CB	1:A:151:LYS:HB3	0.45	2.42	7	3
1:A:166:LYS:HA	1:A:169:GLU:HG2	0.45	1.88	8	1
1:A:181:LEU:O	1:A:181:LEU:HG	0.45	2.11	12	2
1:A:127:ILE:O	1:A:131:LEU:HD23	0.44	2.13	13	1
1:A:133:ASP:O	1:A:133:ASP:OD1	0.44	2.34	19	1
1:A:142:MET:HG3	1:A:154:ILE:CD1	0.44	2.42	6	1
1:A:183:LEU:CD2	1:A:187:ASP:CB	0.44	2.96	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:153:SER:O	1:A:154:ILE:HG13	0.44	2.13	13	2
1:A:114:TYR:HB2	1:A:155:PHE:CD1	0.44	2.47	15	1
1:A:119:PRO:O	1:A:120:THR:CG2	0.44	2.65	15	1
1:A:180:LEU:CD1	1:A:182:ILE:HG13	0.44	2.42	11	1
1:A:185:LYS:HD3	1:A:189:PHE:CE2	0.44	2.48	5	1
1:A:110:ASN:O	1:A:161:ILE:CB	0.44	2.65	7	1
1:A:137:VAL:HG21	1:A:156:VAL:CA	0.44	2.41	8	1
1:A:123:THR:HG22	1:A:124:LEU:N	0.44	2.26	11	2
1:A:181:LEU:HD13	1:A:183:LEU:CD1	0.44	2.41	11	1
1:A:120:THR:O	1:A:121:ASP:OD1	0.44	2.34	6	1
1:A:181:LEU:O	1:A:181:LEU:CG	0.44	2.65	11	2
1:A:119:PRO:HG2	1:A:122:ALA:CA	0.44	2.43	10	1
1:A:160:SER:OG	1:A:163:SER:HB3	0.44	2.13	14	2
1:A:111:ARG:HD3	1:A:161:ILE:HG22	0.44	1.88	19	1
1:A:112:SER:HA	1:A:156:VAL:O	0.44	2.13	4	1
1:A:137:VAL:HG12	1:A:156:VAL:CG1	0.44	2.42	4	1
1:A:141:GLN:CB	1:A:155:PHE:HB2	0.44	2.43	4	3
1:A:114:TYR:CZ	1:A:116:LYS:HB2	0.44	2.48	5	1
1:A:130:TRP:CZ3	1:A:134:LYS:HD3	0.44	2.47	5	1
1:A:127:ILE:CD1	1:A:154:ILE:HG12	0.44	2.41	12	1
1:A:183:LEU:HD11	1:A:187:ASP:CB	0.44	2.43	16	1
1:A:130:TRP:O	1:A:134:LYS:HD3	0.44	2.12	12	1
1:A:110:ASN:HB2	1:A:161:ILE:CD1	0.44	2.43	18	1
1:A:166:LYS:O	1:A:170:THR:OG1	0.44	2.36	1	1
1:A:175:TYR:CE1	1:A:176:LYS:HE2	0.44	2.48	5	1
1:A:188:TYR:O	1:A:192:LYS:HB3	0.44	2.11	5	2
1:A:113:VAL:O	1:A:155:PHE:HA	0.44	2.13	8	1
1:A:112:SER:O	1:A:185:LYS:HG3	0.44	2.12	9	3
1:A:159:ASP:OD1	1:A:159:ASP:C	0.44	2.60	19	2
1:A:119:PRO:CG	1:A:122:ALA:HB2	0.44	2.43	10	1
1:A:183:LEU:HD21	1:A:187:ASP:HB3	0.44	1.88	10	1
1:A:145:THR:CB	1:A:151:LYS:HB2	0.43	2.43	18	3
1:A:112:SER:CB	1:A:185:LYS:HE2	0.43	2.43	4	2
1:A:111:ARG:CD	1:A:157:VAL:CG1	0.43	2.95	9	1
1:A:116:LYS:HG2	1:A:117:GLY:N	0.43	2.28	15	1
1:A:173:GLN:OE1	1:A:173:GLN:HA	0.43	2.12	1	1
1:A:155:PHE:CD2	1:A:185:LYS:HE2	0.43	2.47	5	1
1:A:111:ARG:O	1:A:157:VAL:HG22	0.43	2.13	8	2
1:A:175:TYR:HB2	1:A:180:LEU:CB	0.43	2.41	20	4
1:A:138:LEU:CD1	1:A:159:ASP:HB2	0.43	2.43	12	1
1:A:137:VAL:CG1	1:A:156:VAL:HG21	0.43	2.43	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:131:LEU:CD1	1:A:131:LEU:N	0.43	2.81	4	1
1:A:112:SER:HB2	1:A:185:LYS:CG	0.43	2.43	5	1
1:A:115:ILE:HD12	1:A:156:VAL:CG2	0.43	2.43	1	1
1:A:115:ILE:HD11	1:A:156:VAL:HG11	0.43	1.90	18	1
1:A:117:GLY:O	1:A:178:THR:HG23	0.43	2.14	5	1
1:A:127:ILE:CG2	1:A:131:LEU:HD11	0.43	2.44	18	1
1:A:119:PRO:HG3	1:A:178:THR:CB	0.43	2.44	5	1
1:A:188:TYR:CD1	1:A:188:TYR:O	0.43	2.72	17	2
1:A:139:ASN:CB	1:A:157:VAL:HB	0.43	2.44	16	2
1:A:115:ILE:HG22	1:A:180:LEU:CD2	0.43	2.42	11	1
1:A:179:ASP:OD1	1:A:179:ASP:O	0.43	2.36	11	1
1:A:137:VAL:O	1:A:137:VAL:HG13	0.43	2.13	12	1
1:A:124:LEU:O	1:A:128:LYS:HB2	0.43	2.14	9	2
1:A:128:LYS:O	1:A:132:GLU:HG3	0.43	2.13	10	1
1:A:110:ASN:O	1:A:164:ALA:HB3	0.43	2.14	11	1
1:A:130:TRP:CZ2	1:A:180:LEU:HG	0.43	2.48	6	1
1:A:184:PHE:HB2	1:A:187:ASP:OD2	0.43	2.14	6	1
1:A:165:LYS:O	1:A:169:GLU:CG	0.43	2.66	8	1
1:A:188:TYR:CE1	1:A:192:LYS:HB2	0.43	2.49	11	1
1:A:175:TYR:HB3	1:A:180:LEU:HB3	0.43	1.90	12	1
1:A:123:THR:C	1:A:126:ASP:OD1	0.43	2.61	19	1
1:A:137:VAL:CB	1:A:156:VAL:CG1	0.43	2.96	1	1
1:A:185:LYS:O	1:A:189:PHE:CD1	0.43	2.72	7	1
1:A:128:LYS:O	1:A:132:GLU:HB2	0.43	2.14	12	5
1:A:171:PRO:O	1:A:173:GLN:HG3	0.43	2.13	10	1
1:A:143:ARG:O	1:A:151:LYS:HG2	0.42	2.13	14	2
1:A:127:ILE:CD1	1:A:154:ILE:HD13	0.42	2.41	18	2
1:A:143:ARG:CB	1:A:153:SER:OG	0.42	2.67	13	1
1:A:170:THR:O	1:A:171:PRO:C	0.42	2.62	15	1
1:A:141:GLN:HB2	1:A:155:PHE:CB	0.42	2.44	16	1
1:A:154:ILE:HD12	1:A:154:ILE:C	0.42	2.39	16	1
1:A:184:PHE:HB3	1:A:186:ASP:OD1	0.42	2.14	10	1
1:A:130:TRP:O	1:A:134:LYS:HD2	0.42	2.14	12	1
1:A:137:VAL:CG1	1:A:140:ILE:HG13	0.42	2.45	20	1
1:A:170:THR:HG22	1:A:173:GLN:OE1	0.42	2.14	4	1
1:A:114:TYR:OH	1:A:116:LYS:HB2	0.42	2.14	16	3
1:A:165:LYS:O	1:A:169:GLU:CB	0.42	2.68	11	1
1:A:113:VAL:O	1:A:156:VAL:N	0.42	2.53	13	1
1:A:153:SER:C	1:A:154:ILE:HG13	0.42	2.38	17	4
1:A:155:PHE:CD1	1:A:155:PHE:N	0.42	2.86	7	1
1:A:134:LYS:O	1:A:134:LYS:CG	0.42	2.67	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:145:THR:OG1	1:A:150:PHE:O	0.42	2.33	20	3
1:A:123:THR:N	1:A:126:ASP:OD2	0.42	2.53	19	1
1:A:109:LYS:O	1:A:185:LYS:HE2	0.42	2.14	10	1
1:A:183:LEU:HD21	1:A:187:ASP:CB	0.42	2.44	10	1
1:A:138:LEU:CD2	1:A:159:ASP:CA	0.42	2.98	16	1
1:A:112:SER:O	1:A:185:LYS:CD	0.42	2.68	8	1
1:A:174:LYS:CD	1:A:174:LYS:C	0.42	2.92	9	1
1:A:140:ILE:HG13	1:A:155:PHE:O	0.42	2.15	11	1
1:A:137:VAL:HG13	1:A:157:VAL:N	0.42	2.29	14	1
1:A:112:SER:C	1:A:113:VAL:HG23	0.42	2.40	16	1
1:A:123:THR:CA	1:A:126:ASP:OD1	0.42	2.68	19	1
1:A:174:LYS:CD	1:A:174:LYS:N	0.42	2.82	4	1
1:A:130:TRP:CE3	1:A:131:LEU:HD22	0.42	2.49	6	1
1:A:110:ASN:O	1:A:161:ILE:HG13	0.42	2.15	18	2
1:A:160:SER:O	1:A:163:SER:OG	0.42	2.33	7	1
1:A:131:LEU:HD13	1:A:137:VAL:CG1	0.42	2.45	8	1
1:A:174:LYS:C	1:A:174:LYS:HD3	0.42	2.40	9	1
1:A:143:ARG:HB2	1:A:153:SER:O	0.42	2.14	2	2
1:A:155:PHE:CE2	1:A:185:LYS:HE2	0.42	2.50	5	1
1:A:165:LYS:O	1:A:169:GLU:HB2	0.42	2.15	10	2
1:A:143:ARG:HB3	1:A:153:SER:HB3	0.42	1.92	17	1
1:A:136:GLN:OE1	1:A:159:ASP:CG	0.42	2.62	20	1
1:A:170:THR:HG22	1:A:171:PRO:HD2	0.41	1.90	1	1
1:A:150:PHE:CD1	1:A:151:LYS:O	0.41	2.73	12	1
1:A:138:LEU:HG	1:A:139:ASN:N	0.41	2.29	15	1
1:A:163:SER:O	1:A:166:LYS:HG2	0.41	2.15	2	1
1:A:111:ARG:CD	1:A:157:VAL:HG13	0.41	2.45	9	1
1:A:117:GLY:C	1:A:118:PHE:O	0.41	2.63	13	2
1:A:138:LEU:CD1	1:A:159:ASP:HA	0.41	2.44	5	1
1:A:188:TYR:CD1	1:A:188:TYR:C	0.41	2.98	8	1
1:A:112:SER:O	1:A:185:LYS:HE2	0.41	2.15	11	1
1:A:167:PHE:C	1:A:167:PHE:CD1	0.41	2.98	12	1
1:A:142:MET:CG	1:A:154:ILE:HG23	0.41	2.45	18	1
1:A:144:ARG:C	1:A:151:LYS:HG2	0.41	2.40	18	1
1:A:141:GLN:HB2	1:A:155:PHE:HB2	0.41	1.93	10	1
1:A:117:GLY:CA	1:A:179:ASP:O	0.41	2.67	2	1
1:A:145:THR:HG21	1:A:150:PHE:CA	0.41	2.46	6	1
1:A:165:LYS:O	1:A:169:GLU:HB3	0.41	2.16	8	1
1:A:110:ASN:OD1	1:A:111:ARG:HG3	0.41	2.15	18	1
1:A:165:LYS:O	1:A:169:GLU:HG2	0.41	2.15	8	1
1:A:188:TYR:CE1	1:A:192:LYS:CB	0.41	3.04	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:118:PHE:CE1	1:A:127:ILE:HA	0.41	2.50	19	1
1:A:130:TRP:O	1:A:134:LYS:HG2	0.41	2.15	4	1
1:A:174:LYS:O	1:A:174:LYS:HG3	0.41	2.15	10	1
1:A:142:MET:O	1:A:142:MET:HG3	0.41	2.15	12	1
1:A:127:ILE:HG22	1:A:140:ILE:CD1	0.41	2.46	1	1
1:A:133:ASP:O	1:A:134:LYS:HD3	0.41	2.14	1	1
1:A:131:LEU:HD21	1:A:156:VAL:CG1	0.41	2.45	9	1
1:A:115:ILE:HD12	1:A:156:VAL:HG21	0.41	1.91	1	1
1:A:168:VAL:CG1	1:A:184:PHE:HB2	0.41	2.45	2	1
1:A:158:PHE:CZ	1:A:167:PHE:CE2	0.41	3.09	3	1
1:A:112:SER:CB	1:A:185:LYS:HE3	0.41	2.45	10	1
1:A:141:GLN:O	1:A:154:ILE:HA	0.41	2.16	16	1
1:A:171:PRO:O	1:A:173:GLN:HG2	0.41	2.16	17	1
1:A:111:ARG:HD3	1:A:159:ASP:O	0.41	2.15	18	1
1:A:145:THR:HG23	1:A:151:LYS:HB2	0.41	1.93	19	1
1:A:116:LYS:CD	1:A:116:LYS:C	0.41	2.94	20	1
1:A:183:LEU:HD13	1:A:184:PHE:H	0.41	1.74	16	1
1:A:122:ALA:C	1:A:126:ASP:OD2	0.41	2.64	19	1
1:A:156:VAL:O	1:A:156:VAL:HG13	0.40	2.17	3	1
1:A:125:ASP:OD1	1:A:125:ASP:N	0.40	2.54	12	1
1:A:137:VAL:CB	1:A:156:VAL:HG22	0.40	2.43	15	1
1:A:127:ILE:O	1:A:131:LEU:HB2	0.40	2.17	17	1
1:A:163:SER:HA	1:A:166:LYS:HG2	0.40	1.94	2	1
1:A:142:MET:HE3	1:A:142:MET:HB2	0.40	1.81	13	1
1:A:136:GLN:O	1:A:136:GLN:HG3	0.40	2.15	9	1
1:A:114:TYR:OH	1:A:153:SER:HB3	0.40	2.16	12	1
1:A:116:LYS:O	1:A:181:LEU:HG	0.40	2.16	12	1
1:A:141:GLN:N	1:A:155:PHE:O	0.40	2.49	2	1
1:A:189:PHE:HA	1:A:192:LYS:HG2	0.40	1.93	7	1
1:A:177:GLU:CG	1:A:178:THR:N	0.40	2.84	14	1
1:A:132:GLU:CD	1:A:132:GLU:C	0.40	2.90	16	1
1:A:133:ASP:O	1:A:134:LYS:HB2	0.40	2.16	20	1
1:A:124:LEU:O	1:A:128:LYS:CD	0.40	2.69	6	1
1:A:145:THR:CG2	1:A:149:ALA:O	0.40	2.70	6	1
1:A:139:ASN:HB3	1:A:157:VAL:HB	0.40	1.93	8	1
1:A:137:VAL:HG23	1:A:157:VAL:N	0.40	2.31	12	1
1:A:141:GLN:O	1:A:154:ILE:HG23	0.40	2.16	12	1
1:A:140:ILE:HG23	1:A:140:ILE:O	0.40	2.16	14	1
1:A:129:GLU:O	1:A:132:GLU:HG3	0.40	2.16	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	84/103 (82%)	74±2 (88±2%)	6±2 (7±2%)	4±1 (5±1%)	3	23
All	All	1680/2060 (82%)	1479 (88%)	114 (7%)	87 (5%)	3	23

All 9 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	176	LYS	20
1	A	177	GLU	20
1	A	122	ALA	12
1	A	134	LYS	11
1	A	171	PRO	8
1	A	151	LYS	6
1	A	118	PHE	5
1	A	119	PRO	3
1	A	120	THR	2

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	76/94 (81%)	53±3 (70±4%)	23±3 (30±4%)	1	16
All	All	1520/1880 (81%)	1059 (70%)	461 (30%)	1	16

All 62 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	160	SER	17

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Mol	Chain	Res	Type	Models (Total)
1	A	123	THR	16
1	A	151	LYS	16
1	A	185	LYS	16
1	A	183	LEU	15
1	A	192	LYS	15
1	A	134	LYS	14
1	A	174	LYS	13
1	A	109	LYS	12
1	A	162	GLU	12
1	A	143	ARG	12
1	A	145	THR	12
1	A	146	LEU	12
1	A	153	SER	11
1	A	166	LYS	11
1	A	144	ARG	11
1	A	176	LYS	11
1	A	140	ILE	10
1	A	148	LYS	10
1	A	184	PHE	10
1	A	165	LYS	10
1	A	124	LEU	9
1	A	138	LEU	9
1	A	191	LYS	9
1	A	131	LEU	8
1	A	142	MET	8
1	A	111	ARG	8
1	A	129	GLU	7
1	A	126	ASP	7
1	A	116	LYS	7
1	A	128	LYS	7
1	A	173	GLN	7
1	A	178	THR	6
1	A	139	ASN	6
1	A	169	GLU	6
1	A	167	PHE	6
1	A	136	GLN	6
1	A	187	ASP	6
1	A	163	SER	5
1	A	189	PHE	5
1	A	132	GLU	5
1	A	133	ASP	5
1	A	141	GLN	5

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Mol	Chain	Res	Type	Models (Total)
1	A	112	SER	5
1	A	121	ASP	4
1	A	154	ILE	4
1	A	125	ASP	4
1	A	114	TYR	4
1	A	186	ASP	3
1	A	150	PHE	3
1	A	161	ILE	3
1	A	155	PHE	3
1	A	181	LEU	2
1	A	159	ASP	2
1	A	188	TYR	2
1	A	179	ASP	2
1	A	120	THR	2
1	A	170	THR	1
1	A	177	GLU	1
1	A	110	ASN	1
1	A	147	HIS	1
1	A	156	VAL	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