



Full wwPDB NMR Structure Validation Report ⓘ

Apr 26, 2016 – 03:09 PM BST

PDB ID : 1HD1
Title : HETEROGENEOUS NUCLEAR RIBONUCLEOPROTEIN D0 (HNRNP D0 RBD1), NMR
Authors : Nagata, T.; Kurihara, Y.; Matsuda, G.; Saeki, J.; Kohno, T.; Yanagida, Y.; Ishikawa, F.; Uesugi, S.; Katahira, M.
Deposited on : 1999-05-18

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/NMRValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

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

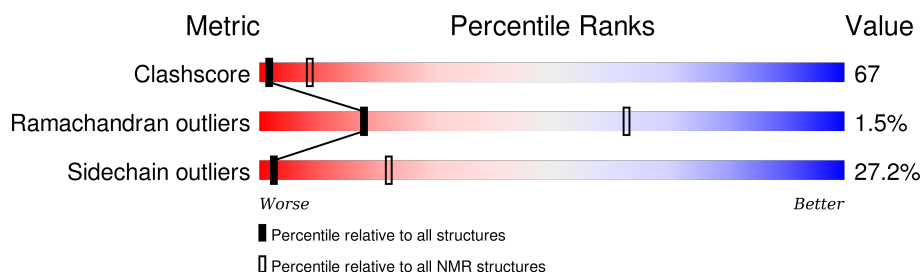
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment 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	114402	11133
Ramachandran outliers	111179	9975
Sidechain outliers	111093	9958

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

Mol	Chain	Length	Quality of chain
1	A	75	

2 Ensemble composition and analysis

This entry contains 20 models. Model 2 is the overall representative, medoid model (most similar to other models).

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:98-A:128, A:140-A:171 (63)	0.25	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. No single-model clusters were found.

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

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 1215 atoms, of which 614 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called PROTEIN (HETEROGENEOUS NUCLEAR RIBONUCLEOPROTEIN D0).

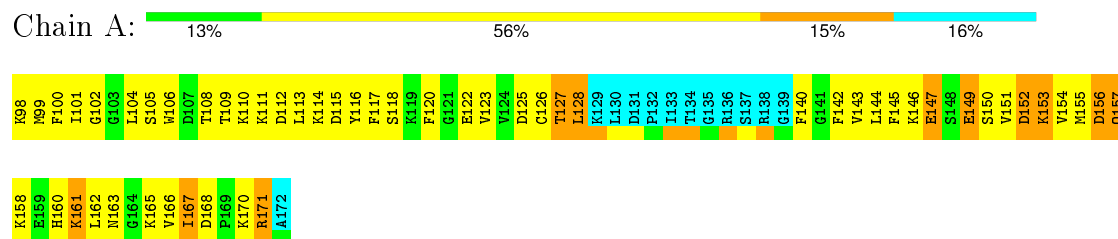
Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	75	1215	386	614	101	111	3	0

4 Residue-property plots [i](#)

4.1 Average score per residue in the NMR ensemble

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

- Molecule 1: PROTEIN (HETEROGENEOUS NUCLEAR RIBONUCLEOPROTEIN D0)

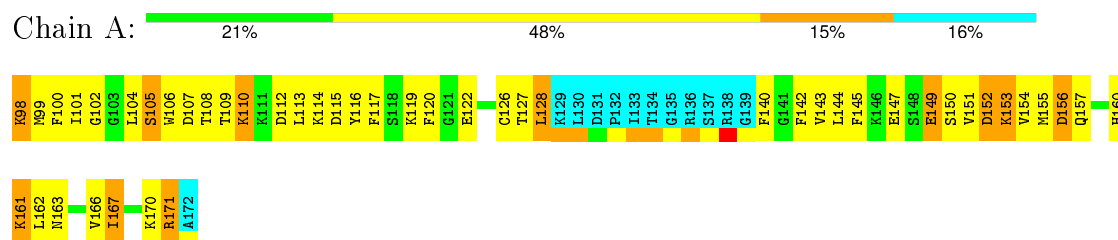


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

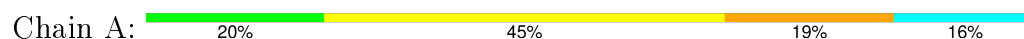
4.2.1 Score per residue for model 1

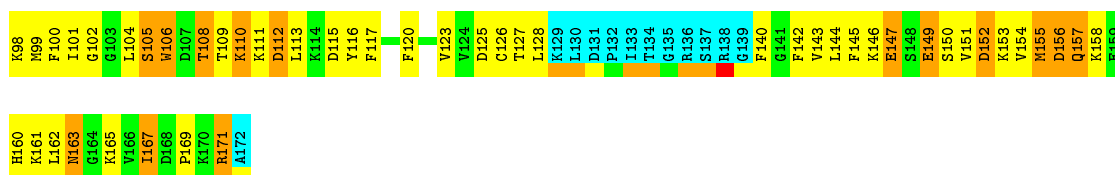
- Molecule 1: PROTEIN (HETEROGENEOUS NUCLEAR RIBONUCLEOPROTEIN D0)



4.2.2 Score per residue for model 2 (medoid)

- Molecule 1: PROTEIN (HETEROGENEOUS NUCLEAR RIBONUCLEOPROTEIN D0)

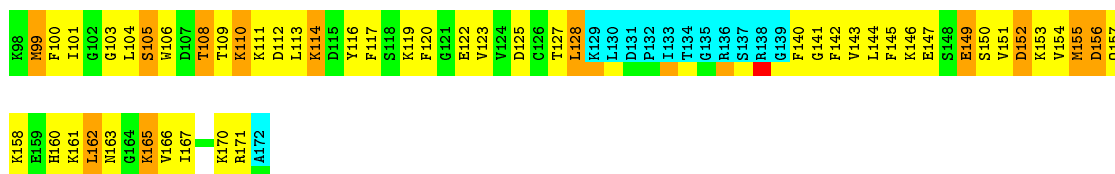




4.2.3 Score per residue for model 3

- Molecule 1: PROTEIN (HETEROGENEOUS NUCLEAR RIBONUCLEOPROTEIN D0)

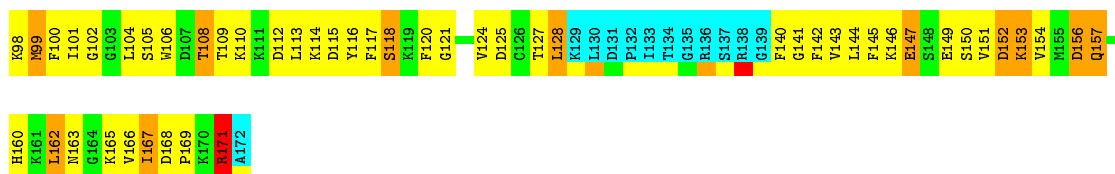
Chain A: 17% 51% 16% 16%



4.2.4 Score per residue for model 4

- Molecule 1: PROTEIN (HETEROGENEOUS NUCLEAR RIBONUCLEOPROTEIN D0)

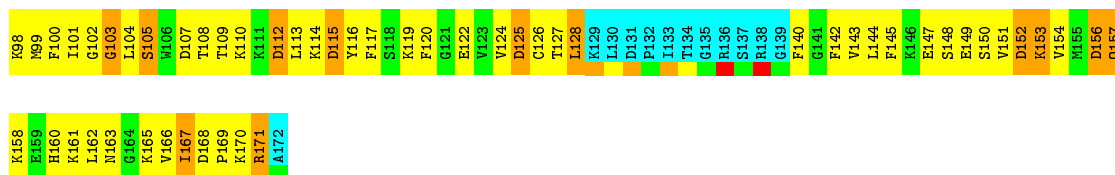
Chain A: 19% 49% 15% 16%



4.2.5 Score per residue for model 5

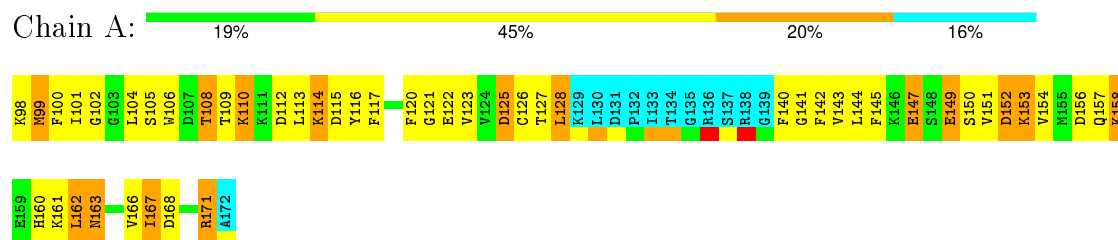
- Molecule 1: PROTEIN (HETEROGENEOUS NUCLEAR RIBONUCLEOPROTEIN D0)

Chain A: 13% 55% 16% 16%



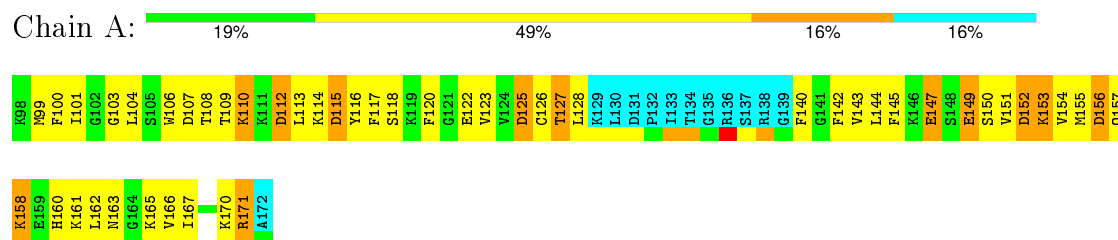
4.2.6 Score per residue for model 6

- Molecule 1: PROTEIN (HETEROGENEOUS NUCLEAR RIBONUCLEOPROTEIN D0)



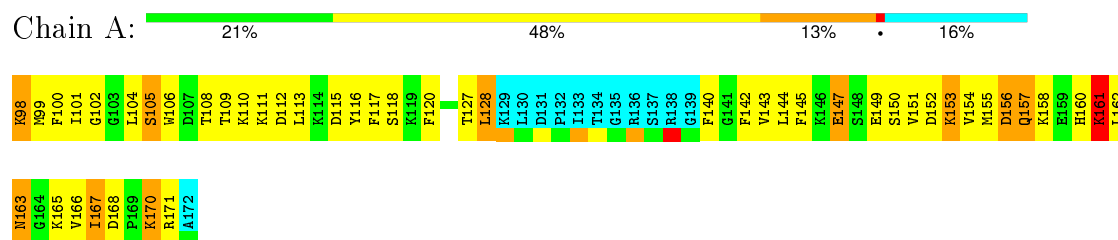
4.2.7 Score per residue for model 7

- Molecule 1: PROTEIN (HETEROGENEOUS NUCLEAR RIBONUCLEOPROTEIN D0)



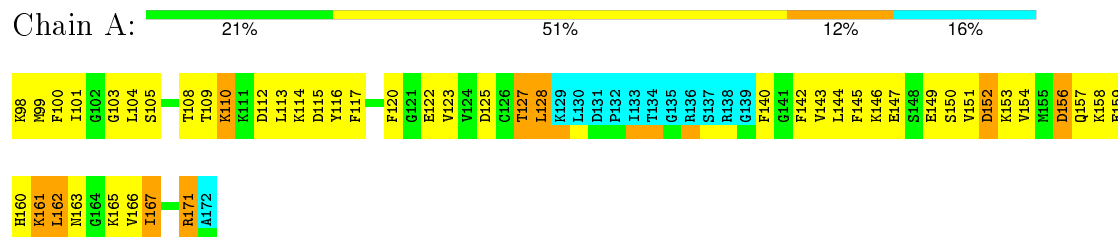
4.2.8 Score per residue for model 8

- Molecule 1: PROTEIN (HETEROGENEOUS NUCLEAR RIBONUCLEOPROTEIN D0)



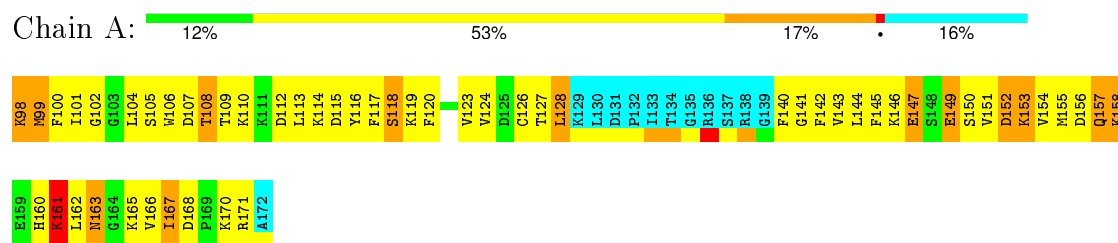
4.2.9 Score per residue for model 9

- Molecule 1: PROTEIN (HETEROGENEOUS NUCLEAR RIBONUCLEOPROTEIN D0)



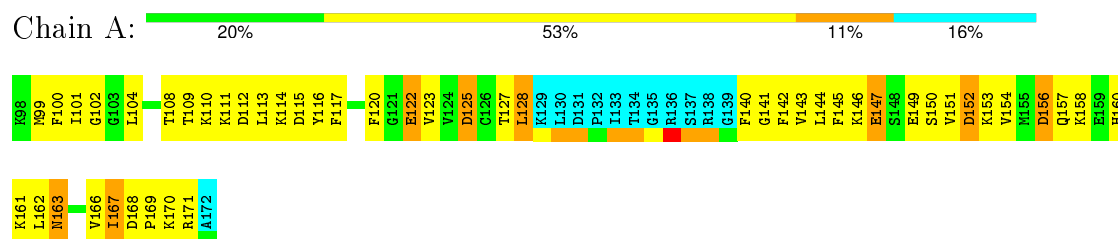
4.2.10 Score per residue for model 10

- Molecule 1: PROTEIN (HETEROGENEOUS NUCLEAR RIBONUCLEOPROTEIN D0)



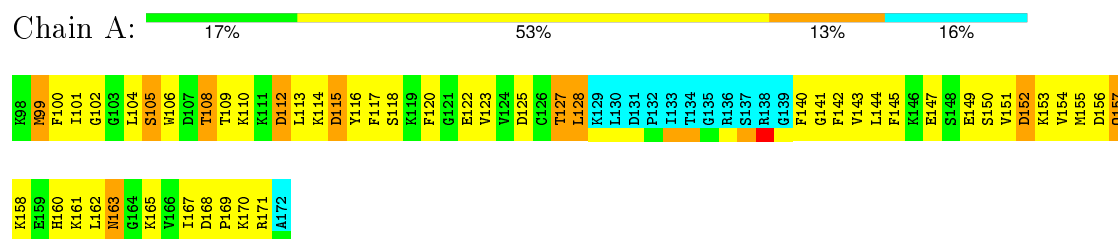
4.2.11 Score per residue for model 11

- Molecule 1: PROTEIN (HETEROGENEOUS NUCLEAR RIBONUCLEOPROTEIN D0)



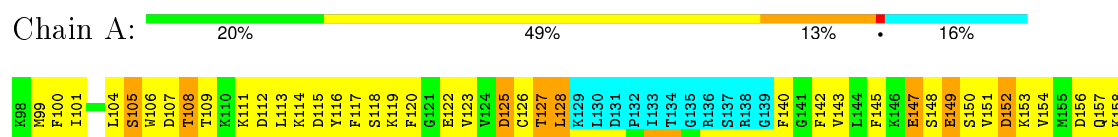
4.2.12 Score per residue for model 12

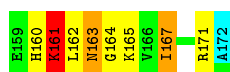
- Molecule 1: PROTEIN (HETEROGENEOUS NUCLEAR RIBONUCLEOPROTEIN D0)



4.2.13 Score per residue for model 13

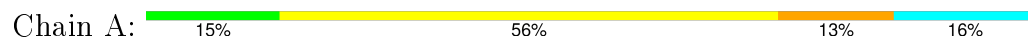
- Molecule 1: PROTEIN (HETEROGENEOUS NUCLEAR RIBONUCLEOPROTEIN D0)





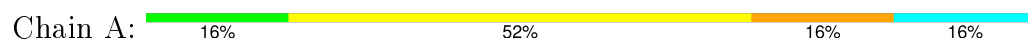
4.2.14 Score per residue for model 14

- Molecule 1: PROTEIN (HETEROGENEOUS NUCLEAR RIBONUCLEOPROTEIN D0)



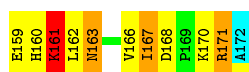
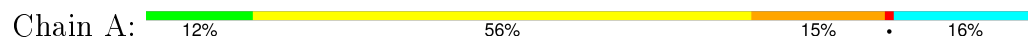
4.2.15 Score per residue for model 15

- Molecule 1: PROTEIN (HETEROGENEOUS NUCLEAR RIBONUCLEOPROTEIN D0)



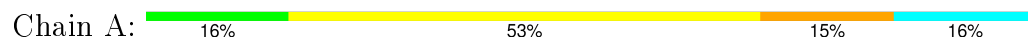
4.2.16 Score per residue for model 16

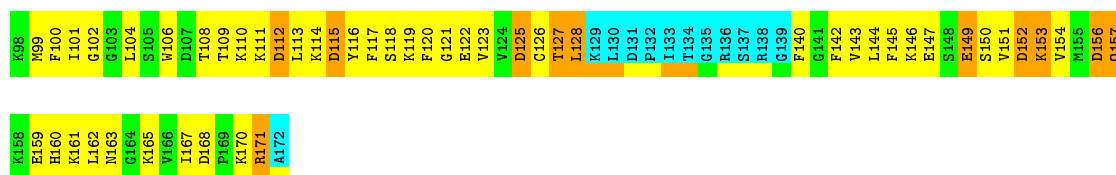
- Molecule 1: PROTEIN (HETEROGENEOUS NUCLEAR RIBONUCLEOPROTEIN D0)



4.2.17 Score per residue for model 17

- Molecule 1: PROTEIN (HETEROGENEOUS NUCLEAR RIBONUCLEOPROTEIN D0)

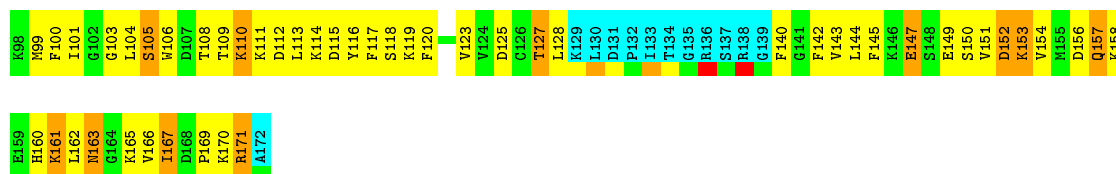




4.2.18 Score per residue for model 18

- Molecule 1: PROTEIN (HETEROGENEOUS NUCLEAR RIBONUCLEOPROTEIN D0)

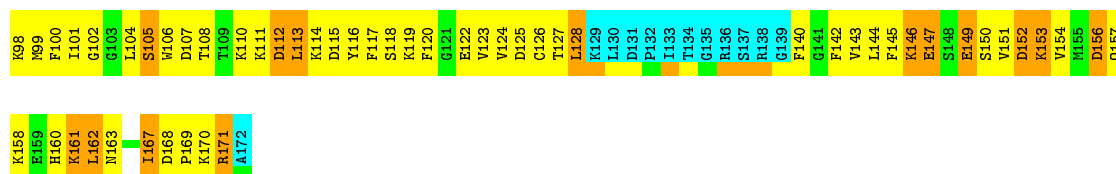
Chain A: 19% 51% 15% 16%



4.2.19 Score per residue for model 19

- Molecule 1: PROTEIN (HETEROGENEOUS NUCLEAR RIBONUCLEOPROTEIN D0)

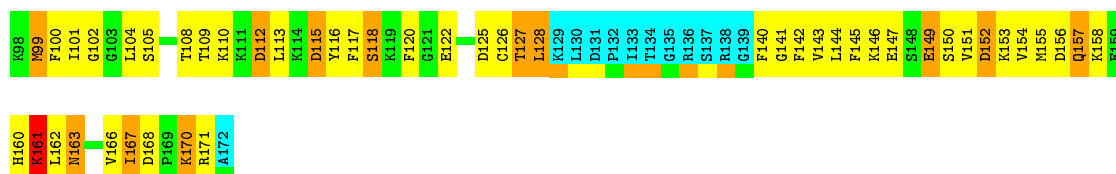
Chain A: 13% 52% 19% 16%



4.2.20 Score per residue for model 20

- Molecule 1: PROTEIN (HETEROGENEOUS NUCLEAR RIBONUCLEOPROTEIN D0)

Chain A: 20% 47% 16% 16%



5 Refinement protocol and experimental data overview

The models were refined using the following method: *SIMULATED ANNEALING*.

Of the 200 calculated structures, 20 were deposited, based on the following criterion: *LOWER ENERGIES*.

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

Software name	Classification	Version
X-PLOR	refinement	3.1
X-PLOR	refinement	3.8
X-PLOR	structure solution	3.1
X-PLOR	structure solution	3.8

No chemical shift data was provided. No validations of the models with respect to experimental NMR restraints is performed at this time.

6 Model quality ⓘ

6.1 Standard geometry ⓘ

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

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	0.9±0.2
All	All	0	19

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	171	ARG	Sidechain	19

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	513	519	518	69±9
All	All	10260	10380	10360	1387

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 67.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:145:PHE:CZ	1:A:154:VAL:HG21	1.06	1.86	8	8
1:A:104:LEU:HD12	1:A:108:THR:HG21	1.05	1.19	20	13

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:120:PHE:CE2	1:A:154:VAL:HG23	0.98	1.93	18	6
1:A:104:LEU:HD11	1:A:113:LEU:HD13	0.96	1.35	1	10
1:A:120:PHE:CG	1:A:154:VAL:HG22	0.93	1.98	15	8
1:A:108:THR:HG23	1:A:163:ASN:CG	0.92	1.84	12	1
1:A:120:PHE:CD2	1:A:154:VAL:HG22	0.91	2.00	14	7
1:A:145:PHE:CE2	1:A:154:VAL:HG21	0.90	2.01	14	6
1:A:128:LEU:O	1:A:128:LEU:HD13	0.89	1.68	10	4
1:A:128:LEU:HD13	1:A:128:LEU:O	0.89	1.68	4	10
1:A:99:MET:CE	1:A:101:ILE:HD11	0.88	1.98	16	12
1:A:104:LEU:CD1	1:A:108:THR:HG21	0.88	1.97	2	11
1:A:160:HIS:ND1	1:A:167:ILE:HD11	0.86	1.84	9	4
1:A:151:VAL:O	1:A:154:VAL:HG12	0.86	1.71	3	12
1:A:113:LEU:HD23	1:A:126:CYS:SG	0.85	2.11	5	9
1:A:145:PHE:HB2	1:A:151:VAL:HG22	0.85	1.46	3	20
1:A:108:THR:HG23	1:A:163:ASN:OD1	0.85	1.72	12	6
1:A:104:LEU:HD12	1:A:108:THR:CG2	0.85	2.02	9	10
1:A:116:TYR:CD1	1:A:162:LEU:HD13	0.84	2.06	14	2
1:A:120:PHE:CZ	1:A:154:VAL:HG23	0.83	2.07	7	5
1:A:100:PHE:O	1:A:101:ILE:HD13	0.83	1.74	20	13
1:A:100:PHE:C	1:A:101:ILE:HD13	0.82	1.94	20	18
1:A:99:MET:HE2	1:A:101:ILE:HD11	0.82	1.52	16	11
1:A:104:LEU:HD11	1:A:113:LEU:HD12	0.81	1.51	12	2
1:A:113:LEU:HD12	1:A:162:LEU:CD2	0.79	2.08	17	4
1:A:104:LEU:CD2	1:A:128:LEU:HD23	0.78	2.08	4	3
1:A:160:HIS:O	1:A:166:VAL:HG23	0.77	1.79	9	4
1:A:120:PHE:CD2	1:A:154:VAL:HG23	0.77	2.14	18	3
1:A:128:LEU:HD22	1:A:128:LEU:C	0.77	1.99	16	6
1:A:120:PHE:CE1	1:A:154:VAL:HG23	0.76	2.15	7	5
1:A:147:GLU:O	1:A:151:VAL:HG23	0.76	1.80	1	16
1:A:160:HIS:CB	1:A:167:ILE:HD11	0.75	2.10	15	6
1:A:145:PHE:CB	1:A:151:VAL:HG22	0.74	2.12	3	17
1:A:128:LEU:HD22	1:A:128:LEU:O	0.74	1.82	16	1
1:A:100:PHE:CD2	1:A:142:PHE:CZ	0.74	2.76	17	16
1:A:100:PHE:CE1	1:A:142:PHE:CE1	0.73	2.76	4	4
1:A:160:HIS:CG	1:A:167:ILE:HD11	0.73	2.17	9	5
1:A:162:LEU:HD12	1:A:163:ASN:HB2	0.73	1.59	8	6
1:A:116:TYR:CD2	1:A:162:LEU:HD21	0.73	2.18	5	2
1:A:116:TYR:CG	1:A:162:LEU:HD13	0.72	2.20	13	3
1:A:124:VAL:HG23	1:A:146:LYS:HG2	0.71	1.60	19	1
1:A:113:LEU:HD12	1:A:162:LEU:HD23	0.71	1.63	17	2
1:A:128:LEU:C	1:A:128:LEU:HD12	0.71	2.06	15	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:150:SER:O	1:A:154:VAL:HG23	0.71	1.86	5	6
1:A:143:VAL:O	1:A:144:LEU:HD12	0.70	1.84	18	5
1:A:160:HIS:O	1:A:162:LEU:HD23	0.70	1.86	4	1
1:A:104:LEU:HD21	1:A:113:LEU:HD13	0.70	1.62	17	2
1:A:104:LEU:CD1	1:A:162:LEU:HD11	0.70	2.17	9	2
1:A:100:PHE:CE2	1:A:142:PHE:CZ	0.70	2.79	11	13
1:A:128:LEU:HD13	1:A:128:LEU:C	0.70	2.07	14	10
1:A:104:LEU:HD11	1:A:113:LEU:CD1	0.69	2.17	19	5
1:A:128:LEU:C	1:A:128:LEU:HD13	0.69	2.07	17	2
1:A:120:PHE:CB	1:A:154:VAL:HG22	0.68	2.18	13	6
1:A:108:THR:O	1:A:128:LEU:HD22	0.68	1.89	5	4
1:A:162:LEU:N	1:A:162:LEU:HD23	0.68	2.03	19	1
1:A:128:LEU:C	1:A:128:LEU:HD22	0.68	2.08	13	5
1:A:162:LEU:HD12	1:A:162:LEU:N	0.68	2.03	5	1
1:A:100:PHE:CZ	1:A:140:PHE:CD1	0.67	2.83	14	8
1:A:160:HIS:HB3	1:A:167:ILE:HD11	0.66	1.65	15	6
1:A:145:PHE:CE2	1:A:154:VAL:HG11	0.66	2.25	3	10
1:A:104:LEU:HD23	1:A:128:LEU:HD23	0.65	1.66	4	1
1:A:151:VAL:HG12	1:A:155:MET:SD	0.65	2.31	3	1
1:A:108:THR:O	1:A:128:LEU:HD13	0.64	1.93	12	1
1:A:104:LEU:CD2	1:A:108:THR:HG21	0.64	2.22	11	2
1:A:104:LEU:HD22	1:A:104:LEU:N	0.64	2.08	20	2
1:A:116:TYR:CZ	1:A:162:LEU:CD2	0.63	2.80	19	1
1:A:104:LEU:HD21	1:A:113:LEU:HD22	0.63	1.67	8	2
1:A:123:VAL:HG13	1:A:125:ASP:O	0.63	1.92	15	14
1:A:145:PHE:HE2	1:A:154:VAL:HG11	0.62	1.52	3	2
1:A:104:LEU:HD22	1:A:128:LEU:HD23	0.62	1.71	13	2
1:A:116:TYR:CD2	1:A:162:LEU:CD2	0.61	2.83	5	2
1:A:113:LEU:HD21	1:A:143:VAL:CG2	0.61	2.25	19	2
1:A:162:LEU:HD12	1:A:162:LEU:H	0.61	1.55	5	2
1:A:162:LEU:HD11	1:A:167:ILE:HD13	0.61	1.72	19	1
1:A:100:PHE:CZ	1:A:140:PHE:CD2	0.61	2.88	18	6
1:A:104:LEU:HD23	1:A:108:THR:CG2	0.61	2.26	11	2
1:A:108:THR:C	1:A:128:LEU:HD13	0.60	2.16	12	1
1:A:100:PHE:CD1	1:A:142:PHE:CE1	0.60	2.89	20	4
1:A:162:LEU:H	1:A:162:LEU:HD12	0.60	1.55	3	1
1:A:104:LEU:N	1:A:104:LEU:HD22	0.59	2.12	9	4
1:A:143:VAL:C	1:A:144:LEU:HD12	0.59	2.17	17	12
1:A:120:PHE:HB3	1:A:154:VAL:HG22	0.59	1.74	13	4
1:A:117:PHE:CD2	1:A:143:VAL:HG21	0.59	2.32	11	9
1:A:154:VAL:HG23	1:A:160:HIS:HE1	0.59	1.57	4	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:157:GLN:O	1:A:160:HIS:CD2	0.59	2.56	8	12
1:A:100:PHE:CD1	1:A:142:PHE:CD1	0.59	2.90	20	2
1:A:99:MET:SD	1:A:143:VAL:HG12	0.59	2.37	4	3
1:A:117:PHE:HA	1:A:120:PHE:CD1	0.59	2.33	8	12
1:A:99:MET:CE	1:A:101:ILE:CD1	0.58	2.81	15	7
1:A:128:LEU:HD12	1:A:128:LEU:C	0.58	2.18	9	1
1:A:116:TYR:CD2	1:A:162:LEU:HD22	0.58	2.33	19	2
1:A:104:LEU:CD2	1:A:104:LEU:N	0.58	2.67	20	2
1:A:104:LEU:CG	1:A:108:THR:HG21	0.58	2.29	9	2
1:A:116:TYR:CE2	1:A:162:LEU:CD2	0.58	2.86	19	1
1:A:99:MET:SD	1:A:101:ILE:HD11	0.57	2.39	18	3
1:A:160:HIS:O	1:A:166:VAL:HG13	0.57	1.99	6	1
1:A:140:PHE:O	1:A:140:PHE:CG	0.57	2.57	14	3
1:A:104:LEU:HD23	1:A:140:PHE:HA	0.57	1.76	7	4
1:A:143:VAL:O	1:A:144:LEU:HD22	0.57	2.00	15	2
1:A:113:LEU:HD12	1:A:162:LEU:HD22	0.56	1.77	5	3
1:A:106:TRP:CD1	1:A:106:TRP:N	0.56	2.72	8	2
1:A:128:LEU:CD1	1:A:128:LEU:O	0.56	2.52	16	4
1:A:159:GLU:CG	1:A:159:GLU:O	0.55	2.55	16	2
1:A:102:GLY:O	1:A:168:ASP:N	0.55	2.39	8	13
1:A:143:VAL:C	1:A:144:LEU:HD22	0.55	2.22	15	2
1:A:161:LYS:C	1:A:162:LEU:HD23	0.55	2.22	19	1
1:A:110:LYS:O	1:A:114:LYS:CB	0.55	2.54	11	11
1:A:99:MET:CE	1:A:170:LYS:O	0.55	2.55	19	2
1:A:117:PHE:HA	1:A:120:PHE:CD2	0.55	2.37	9	7
1:A:120:PHE:CZ	1:A:160:HIS:CE1	0.55	2.95	8	9
1:A:106:TRP:N	1:A:106:TRP:CD1	0.55	2.73	6	1
1:A:117:PHE:CE2	1:A:143:VAL:HG21	0.55	2.37	5	2
1:A:154:VAL:HG22	1:A:160:HIS:HE1	0.54	1.61	1	2
1:A:101:ILE:CG2	1:A:167:ILE:HD13	0.54	2.32	4	1
1:A:101:ILE:O	1:A:104:LEU:CD1	0.54	2.55	13	1
1:A:156:ASP:OD1	1:A:157:GLN:N	0.54	2.41	14	15
1:A:101:ILE:O	1:A:104:LEU:HD23	0.54	2.03	3	3
1:A:120:PHE:CD1	1:A:154:VAL:HG22	0.54	2.37	15	1
1:A:158:LYS:HA	1:A:160:HIS:CD2	0.54	2.37	6	7
1:A:160:HIS:O	1:A:161:LYS:CD	0.54	2.56	6	1
1:A:117:PHE:CD1	1:A:120:PHE:CE2	0.54	2.96	4	7
1:A:160:HIS:HB2	1:A:167:ILE:CG1	0.54	2.32	12	12
1:A:99:MET:CG	1:A:170:LYS:O	0.54	2.56	15	1
1:A:120:PHE:CD2	1:A:154:VAL:CG2	0.53	2.89	18	2
1:A:165:LYS:CE	1:A:166:VAL:O	0.53	2.56	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:113:LEU:HD11	1:A:117:PHE:HE2	0.53	1.64	8	3
1:A:147:GLU:OE1	1:A:149:GLU:CB	0.53	2.56	19	8
1:A:122:GLU:O	1:A:146:LYS:CB	0.53	2.57	3	6
1:A:160:HIS:CB	1:A:167:ILE:CG1	0.53	2.87	16	10
1:A:99:MET:SD	1:A:143:VAL:CG1	0.53	2.97	12	5
1:A:127:THR:CG2	1:A:128:LEU:N	0.53	2.72	12	8
1:A:105:SER:N	1:A:108:THR:OG1	0.53	2.42	8	9
1:A:112:ASP:OD1	1:A:113:LEU:N	0.53	2.42	1	16
1:A:104:LEU:HD23	1:A:108:THR:HG21	0.53	1.78	11	2
1:A:128:LEU:HD23	1:A:128:LEU:O	0.53	2.02	12	1
1:A:101:ILE:O	1:A:104:LEU:CD2	0.53	2.57	14	1
1:A:116:TYR:CE2	1:A:162:LEU:HD22	0.53	2.38	19	1
1:A:160:HIS:O	1:A:166:VAL:HG22	0.53	2.04	3	1
1:A:99:MET:HE2	1:A:101:ILE:CD1	0.53	2.34	18	10
1:A:157:GLN:O	1:A:160:HIS:NE2	0.53	2.41	18	13
1:A:110:LYS:CD	1:A:126:CYS:O	0.53	2.57	7	1
1:A:154:VAL:HG13	1:A:160:HIS:HE1	0.53	1.64	15	3
1:A:152:ASP:OD1	1:A:153:LYS:N	0.52	2.42	2	3
1:A:100:PHE:CE1	1:A:141:GLY:O	0.52	2.62	20	1
1:A:99:MET:HE2	1:A:170:LYS:O	0.52	2.04	8	2
1:A:147:GLU:OE2	1:A:149:GLU:CB	0.52	2.58	15	2
1:A:104:LEU:HD13	1:A:141:GLY:H	0.52	1.65	6	1
1:A:113:LEU:HA	1:A:162:LEU:HD21	0.52	1.79	13	2
1:A:102:GLY:O	1:A:167:ILE:HG22	0.52	2.05	10	1
1:A:154:VAL:HG23	1:A:160:HIS:CE1	0.52	2.40	4	1
1:A:160:HIS:CD2	1:A:160:HIS:N	0.51	2.79	3	2
1:A:101:ILE:CG2	1:A:167:ILE:CD1	0.51	2.88	4	2
1:A:104:LEU:HD13	1:A:162:LEU:HD11	0.51	1.83	7	4
1:A:123:VAL:CG1	1:A:125:ASP:O	0.51	2.59	15	4
1:A:160:HIS:CB	1:A:167:ILE:CD1	0.51	2.86	15	1
1:A:99:MET:CG	1:A:143:VAL:O	0.51	2.59	5	3
1:A:166:VAL:HG12	1:A:167:ILE:N	0.51	2.21	18	6
1:A:108:THR:O	1:A:128:LEU:CD2	0.51	2.59	11	1
1:A:162:LEU:HD21	1:A:167:ILE:CG2	0.51	2.35	9	1
1:A:105:SER:O	1:A:108:THR:OG1	0.51	2.29	19	6
1:A:147:GLU:OE1	1:A:149:GLU:N	0.51	2.44	7	1
1:A:145:PHE:HB2	1:A:151:VAL:CG2	0.51	2.36	2	5
1:A:101:ILE:HG13	1:A:143:VAL:HG23	0.51	1.83	17	6
1:A:99:MET:HE2	1:A:143:VAL:HB	0.51	1.82	16	1
1:A:151:VAL:O	1:A:154:VAL:CG1	0.51	2.58	2	2
1:A:120:PHE:CG	1:A:154:VAL:HB	0.50	2.41	7	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:162:LEU:CD2	1:A:162:LEU:N	0.50	2.67	19	1
1:A:99:MET:HE3	1:A:101:ILE:HD11	0.50	1.79	16	1
1:A:124:VAL:HG23	1:A:146:LYS:CE	0.50	2.36	10	1
1:A:147:GLU:O	1:A:150:SER:OG	0.50	2.29	7	19
1:A:140:PHE:CD1	1:A:140:PHE:O	0.50	2.65	3	2
1:A:99:MET:SD	1:A:145:PHE:CD2	0.50	3.05	10	2
1:A:104:LEU:HD23	1:A:108:THR:CB	0.50	2.36	11	1
1:A:104:LEU:HD23	1:A:141:GLY:H	0.50	1.67	12	2
1:A:162:LEU:H	1:A:162:LEU:HD23	0.50	1.65	6	2
1:A:128:LEU:CD1	1:A:128:LEU:C	0.50	2.77	17	5
1:A:112:ASP:N	1:A:112:ASP:OD1	0.50	2.45	3	1
1:A:107:ASP:OD1	1:A:107:ASP:N	0.50	2.45	7	2
1:A:125:ASP:CB	1:A:144:LEU:HB2	0.49	2.37	17	9
1:A:145:PHE:CD1	1:A:150:SER:HB2	0.49	2.42	6	2
1:A:128:LEU:CD2	1:A:128:LEU:O	0.49	2.57	16	1
1:A:128:LEU:C	1:A:128:LEU:CD1	0.49	2.77	15	4
1:A:162:LEU:HD21	1:A:167:ILE:HG21	0.49	1.84	9	3
1:A:120:PHE:CD2	1:A:154:VAL:HA	0.49	2.42	3	7
1:A:101:ILE:HG13	1:A:143:VAL:CG2	0.49	2.38	6	14
1:A:128:LEU:O	1:A:128:LEU:CD1	0.49	2.56	7	1
1:A:162:LEU:HD23	1:A:167:ILE:HD13	0.49	1.84	16	1
1:A:113:LEU:CD2	1:A:126:CYS:SG	0.49	3.01	19	1
1:A:101:ILE:HG23	1:A:167:ILE:CD1	0.49	2.38	4	1
1:A:101:ILE:HD13	1:A:101:ILE:N	0.49	2.22	2	3
1:A:110:LYS:CE	1:A:126:CYS:O	0.49	2.61	2	1
1:A:109:THR:O	1:A:112:ASP:OD1	0.49	2.31	7	14
1:A:153:LYS:O	1:A:156:ASP:OD1	0.49	2.31	14	13
1:A:160:HIS:HB2	1:A:167:ILE:HG13	0.48	1.84	16	16
1:A:123:VAL:HG23	1:A:145:PHE:CD1	0.48	2.42	14	4
1:A:100:PHE:C	1:A:100:PHE:CD1	0.48	2.86	17	5
1:A:153:LYS:O	1:A:156:ASP:OD2	0.48	2.32	7	7
1:A:103:GLY:O	1:A:165:LYS:CD	0.48	2.61	3	1
1:A:161:LYS:CE	1:A:164:GLY:C	0.48	2.81	13	1
1:A:162:LEU:N	1:A:162:LEU:CD1	0.48	2.72	5	1
1:A:101:ILE:HG21	1:A:117:PHE:CE2	0.48	2.43	10	1
1:A:128:LEU:C	1:A:128:LEU:CD2	0.48	2.80	3	1
1:A:120:PHE:CE1	1:A:154:VAL:HA	0.48	2.43	9	5
1:A:98:LYS:HE3	1:A:144:LEU:HD11	0.48	1.83	15	1
1:A:162:LEU:N	1:A:162:LEU:HD12	0.48	2.22	3	1
1:A:149:GLU:HA	1:A:152:ASP:OD2	0.48	2.08	12	16
1:A:144:LEU:N	1:A:144:LEU:CD2	0.48	2.76	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:103:GLY:O	1:A:165:LYS:CE	0.48	2.62	3	1
1:A:149:GLU:O	1:A:152:ASP:OD1	0.48	2.32	7	3
1:A:162:LEU:C	1:A:162:LEU:HD12	0.48	2.29	1	2
1:A:125:ASP:CB	1:A:144:LEU:HD22	0.48	2.39	14	2
1:A:100:PHE:CD1	1:A:101:ILE:N	0.48	2.81	16	3
1:A:125:ASP:HB2	1:A:144:LEU:CB	0.48	2.39	6	7
1:A:115:ASP:O	1:A:118:SER:N	0.48	2.45	12	11
1:A:120:PHE:CD1	1:A:154:VAL:HA	0.48	2.43	4	3
1:A:116:TYR:CE2	1:A:162:LEU:HD21	0.48	2.43	15	1
1:A:162:LEU:HD12	1:A:163:ASN:CB	0.48	2.37	1	1
1:A:124:VAL:O	1:A:125:ASP:OD1	0.48	2.31	5	4
1:A:120:PHE:CE2	1:A:154:VAL:HA	0.48	2.44	17	3
1:A:108:THR:HB	1:A:128:LEU:HD12	0.48	1.86	12	1
1:A:104:LEU:HG	1:A:128:LEU:HD23	0.47	1.85	19	3
1:A:149:GLU:O	1:A:152:ASP:OD2	0.47	2.32	20	15
1:A:110:LYS:CG	1:A:126:CYS:O	0.47	2.61	1	1
1:A:114:LYS:HG3	1:A:123:VAL:HG11	0.47	1.86	18	1
1:A:160:HIS:O	1:A:161:LYS:CG	0.47	2.62	6	2
1:A:120:PHE:CD1	1:A:154:VAL:CB	0.47	2.97	7	2
1:A:116:TYR:CG	1:A:162:LEU:HD23	0.47	2.44	15	2
1:A:105:SER:HB3	1:A:163:ASN:CB	0.47	2.39	19	1
1:A:116:TYR:CE1	1:A:162:LEU:HG	0.47	2.44	5	2
1:A:98:LYS:CG	1:A:144:LEU:HG	0.47	2.40	10	4
1:A:143:VAL:C	1:A:144:LEU:CD2	0.47	2.83	15	1
1:A:120:PHE:CE2	1:A:154:VAL:HG13	0.47	2.45	14	3
1:A:99:MET:SD	1:A:145:PHE:CE2	0.47	3.07	16	2
1:A:100:PHE:CD1	1:A:100:PHE:C	0.47	2.88	3	4
1:A:160:HIS:N	1:A:160:HIS:CD2	0.47	2.81	7	1
1:A:108:THR:HB	1:A:128:LEU:CD1	0.47	2.39	12	1
1:A:113:LEU:HD21	1:A:143:VAL:HG22	0.47	1.87	19	1
1:A:108:THR:HG22	1:A:109:THR:N	0.47	2.24	16	2
1:A:162:LEU:O	1:A:163:ASN:CB	0.47	2.62	6	4
1:A:103:GLY:O	1:A:165:LYS:HD2	0.47	2.10	3	1
1:A:98:LYS:HG2	1:A:144:LEU:CD1	0.47	2.40	2	3
1:A:145:PHE:CZ	1:A:154:VAL:CG2	0.47	2.91	15	1
1:A:99:MET:HG3	1:A:170:LYS:O	0.47	2.10	15	1
1:A:99:MET:SD	1:A:170:LYS:O	0.46	2.73	20	2
1:A:110:LYS:CG	1:A:127:THR:HA	0.46	2.40	7	2
1:A:161:LYS:HG3	1:A:166:VAL:HG22	0.46	1.86	8	1
1:A:115:ASP:O	1:A:116:TYR:C	0.46	2.53	8	19
1:A:108:THR:C	1:A:109:THR:HG23	0.46	2.31	6	8

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:160:HIS:C	1:A:161:LYS:CG	0.46	2.84	3	2
1:A:116:TYR:CG	1:A:162:LEU:CD2	0.46	2.97	5	2
1:A:114:LYS:CG	1:A:126:CYS:CB	0.46	2.93	6	1
1:A:141:GLY:C	1:A:142:PHE:CD1	0.46	2.89	15	2
1:A:120:PHE:CD1	1:A:154:VAL:HB	0.46	2.46	9	3
1:A:117:PHE:HA	1:A:120:PHE:CE2	0.46	2.46	4	4
1:A:154:VAL:HG13	1:A:160:HIS:CE1	0.46	2.45	11	2
1:A:120:PHE:CD2	1:A:154:VAL:CB	0.46	2.99	18	2
1:A:100:PHE:CE2	1:A:142:PHE:CE1	0.46	3.04	17	1
1:A:104:LEU:HD23	1:A:108:THR:HB	0.46	1.87	11	1
1:A:99:MET:CB	1:A:170:LYS:O	0.46	2.64	12	3
1:A:105:SER:CB	1:A:108:THR:HG1	0.46	2.23	15	1
1:A:152:ASP:C	1:A:152:ASP:OD1	0.46	2.55	20	5
1:A:99:MET:HG2	1:A:143:VAL:O	0.46	2.10	5	6
1:A:166:VAL:CG1	1:A:167:ILE:N	0.46	2.78	20	2
1:A:100:PHE:CE1	1:A:142:PHE:CD1	0.46	3.04	6	2
1:A:161:LYS:O	1:A:161:LYS:CG	0.46	2.64	20	1
1:A:99:MET:CG	1:A:143:VAL:HB	0.46	2.41	18	1
1:A:147:GLU:OE2	1:A:150:SER:OG	0.46	2.33	14	1
1:A:110:LYS:HG3	1:A:126:CYS:O	0.45	2.11	1	1
1:A:113:LEU:CD2	1:A:143:VAL:CG2	0.45	2.94	12	1
1:A:116:TYR:HH	1:A:160:HIS:CG	0.45	2.29	9	1
1:A:102:GLY:O	1:A:167:ILE:HA	0.45	2.11	6	7
1:A:101:ILE:HG23	1:A:167:ILE:HD12	0.45	1.87	4	2
1:A:151:VAL:O	1:A:155:MET:SD	0.45	2.74	3	1
1:A:117:PHE:HZ	1:A:167:ILE:HD12	0.45	1.71	13	1
1:A:99:MET:CE	1:A:143:VAL:HB	0.45	2.41	10	2
1:A:112:ASP:OD1	1:A:112:ASP:C	0.45	2.55	19	3
1:A:158:LYS:HB2	1:A:169:PRO:CG	0.45	2.42	2	3
1:A:158:LYS:HG2	1:A:158:LYS:O	0.45	2.12	9	1
1:A:110:LYS:O	1:A:114:LYS:HB2	0.45	2.12	12	8
1:A:99:MET:SD	1:A:143:VAL:O	0.45	2.75	4	2
1:A:122:GLU:O	1:A:146:LYS:HB2	0.45	2.11	11	2
1:A:128:LEU:CD2	1:A:128:LEU:C	0.45	2.78	17	3
1:A:128:LEU:O	1:A:128:LEU:HG	0.45	2.11	11	1
1:A:99:MET:HG3	1:A:143:VAL:O	0.45	2.11	16	2
1:A:162:LEU:CD2	1:A:167:ILE:HD13	0.45	2.42	10	3
1:A:159:GLU:O	1:A:159:GLU:HG2	0.45	2.12	16	1
1:A:122:GLU:O	1:A:146:LYS:HB3	0.45	2.11	9	2
1:A:116:TYR:CG	1:A:162:LEU:HD22	0.45	2.47	19	1
1:A:101:ILE:HD11	1:A:143:VAL:HB	0.45	1.89	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:101:ILE:HG22	1:A:167:ILE:CG2	0.45	2.42	16	5
1:A:156:ASP:OD1	1:A:156:ASP:C	0.45	2.55	9	9
1:A:99:MET:HG2	1:A:151:VAL:HG13	0.45	1.89	12	2
1:A:161:LYS:HA	1:A:165:LYS:O	0.45	2.12	10	2
1:A:157:GLN:O	1:A:157:GLN:HG3	0.45	2.12	11	1
1:A:117:PHE:HZ	1:A:167:ILE:HD13	0.45	1.71	9	1
1:A:120:PHE:CD1	1:A:154:VAL:HG23	0.44	2.46	10	1
1:A:109:THR:OG1	1:A:112:ASP:OD2	0.44	2.33	15	2
1:A:112:ASP:OD1	1:A:112:ASP:N	0.44	2.51	8	1
1:A:147:GLU:OE1	1:A:149:GLU:HB3	0.44	2.12	5	2
1:A:104:LEU:HG	1:A:108:THR:HG21	0.44	1.89	8	1
1:A:128:LEU:HA	1:A:141:GLY:CA	0.44	2.41	15	2
1:A:101:ILE:N	1:A:101:ILE:HD13	0.44	2.27	5	6
1:A:160:HIS:O	1:A:161:LYS:HG2	0.44	2.13	3	2
1:A:105:SER:HB3	1:A:163:ASN:ND2	0.44	2.28	6	1
1:A:103:GLY:O	1:A:166:VAL:O	0.44	2.35	16	2
1:A:113:LEU:HD22	1:A:127:THR:O	0.44	2.12	17	1
1:A:110:LYS:O	1:A:114:LYS:HB3	0.44	2.12	10	3
1:A:162:LEU:O	1:A:163:ASN:HB2	0.44	2.13	10	7
1:A:100:PHE:CD1	1:A:142:PHE:CZ	0.44	3.06	4	1
1:A:162:LEU:HD11	1:A:167:ILE:HG12	0.44	1.89	15	1
1:A:145:PHE:CD2	1:A:151:VAL:HG22	0.43	2.48	2	1
1:A:125:ASP:HB2	1:A:144:LEU:HB2	0.43	1.89	6	5
1:A:117:PHE:HA	1:A:120:PHE:CE1	0.43	2.48	6	3
1:A:116:TYR:OH	1:A:160:HIS:HA	0.43	2.12	15	1
1:A:166:VAL:HG22	1:A:167:ILE:H	0.43	1.73	11	1
1:A:147:GLU:OE2	1:A:149:GLU:HB2	0.43	2.14	15	1
1:A:100:PHE:CZ	1:A:140:PHE:CE1	0.43	3.06	5	1
1:A:140:PHE:O	1:A:140:PHE:CD1	0.43	2.71	14	1
1:A:104:LEU:HD13	1:A:140:PHE:HA	0.43	1.91	5	1
1:A:100:PHE:O	1:A:169:PRO:HA	0.43	2.13	5	4
1:A:110:LYS:HD3	1:A:126:CYS:O	0.43	2.13	10	1
1:A:98:LYS:HG2	1:A:144:LEU:CD2	0.43	2.44	5	2
1:A:162:LEU:HD23	1:A:167:ILE:CD1	0.43	2.44	11	1
1:A:116:TYR:CZ	1:A:162:LEU:HD21	0.43	2.48	19	1
1:A:162:LEU:HD11	1:A:167:ILE:CD1	0.43	2.43	3	1
1:A:101:ILE:O	1:A:104:LEU:HD13	0.43	2.13	13	1
1:A:166:VAL:HG12	1:A:167:ILE:H	0.43	1.74	7	3
1:A:108:THR:HB	1:A:128:LEU:CD2	0.43	2.44	2	1
1:A:114:LYS:HB2	1:A:126:CYS:CB	0.43	2.44	13	1
1:A:112:ASP:CG	1:A:113:LEU:N	0.43	2.72	18	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:113:LEU:O	1:A:114:LYS:C	0.43	2.56	12	1
1:A:121:GLY:HA3	1:A:150:SER:CB	0.43	2.44	17	3
1:A:160:HIS:O	1:A:161:LYS:HB2	0.42	2.14	1	4
1:A:102:GLY:HA2	1:A:140:PHE:CB	0.42	2.44	15	4
1:A:98:LYS:HA	1:A:144:LEU:HD13	0.42	1.91	15	1
1:A:108:THR:C	1:A:109:THR:CG2	0.42	2.88	12	3
1:A:147:GLU:OE1	1:A:149:GLU:HB2	0.42	2.14	20	3
1:A:160:HIS:HB3	1:A:167:ILE:CD1	0.42	2.40	15	1
1:A:116:TYR:CD1	1:A:162:LEU:CD1	0.42	2.92	14	1
1:A:103:GLY:O	1:A:165:LYS:HE3	0.42	2.14	3	1
1:A:147:GLU:OE2	1:A:149:GLU:HB3	0.42	2.14	6	2
1:A:165:LYS:HG2	1:A:166:VAL:N	0.42	2.29	3	1
1:A:124:VAL:HG23	1:A:146:LYS:HE2	0.42	1.90	10	1
1:A:105:SER:CB	1:A:108:THR:OG1	0.42	2.67	3	2
1:A:156:ASP:OD1	1:A:157:GLN:HG2	0.42	2.14	2	1
1:A:152:ASP:OD1	1:A:152:ASP:C	0.42	2.57	11	1
1:A:113:LEU:CD1	1:A:162:LEU:HD23	0.42	2.44	14	1
1:A:149:GLU:O	1:A:150:SER:C	0.42	2.58	20	3
1:A:158:LYS:O	1:A:158:LYS:CG	0.42	2.67	8	1
1:A:144:LEU:CD1	1:A:144:LEU:N	0.42	2.83	4	1
1:A:120:PHE:N	1:A:120:PHE:CD1	0.42	2.87	18	2
1:A:100:PHE:CD2	1:A:142:PHE:CE2	0.42	3.07	11	2
1:A:104:LEU:HD13	1:A:141:GLY:N	0.42	2.30	4	1
1:A:105:SER:O	1:A:107:ASP:N	0.42	2.53	19	2
1:A:155:MET:O	1:A:156:ASP:C	0.42	2.57	14	3
1:A:140:PHE:CD1	1:A:140:PHE:C	0.42	2.93	3	2
1:A:156:ASP:OD2	1:A:157:GLN:OE1	0.42	2.37	20	1
1:A:108:THR:O	1:A:128:LEU:CD1	0.42	2.67	12	1
1:A:160:HIS:O	1:A:161:LYS:HD3	0.42	2.13	6	1
1:A:120:PHE:CE2	1:A:160:HIS:CE1	0.42	3.07	8	1
1:A:99:MET:HB3	1:A:155:MET:HE1	0.42	1.92	3	1
1:A:128:LEU:HA	1:A:141:GLY:HA3	0.41	1.90	10	1
1:A:105:SER:OG	1:A:106:TRP:N	0.41	2.53	18	1
1:A:119:LYS:O	1:A:119:LYS:HG2	0.41	2.15	10	1
1:A:142:PHE:N	1:A:142:PHE:CD1	0.41	2.88	7	1
1:A:148:SER:O	1:A:149:GLU:C	0.41	2.57	14	1
1:A:104:LEU:N	1:A:104:LEU:CD2	0.41	2.83	14	1
1:A:152:ASP:CG	1:A:153:LYS:N	0.41	2.73	13	1
1:A:100:PHE:C	1:A:101:ILE:CD1	0.41	2.81	20	1
1:A:110:LYS:O	1:A:114:LYS:HG3	0.41	2.16	6	1
1:A:102:GLY:HA2	1:A:140:PHE:HB2	0.41	1.92	12	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:113:LEU:HD11	1:A:117:PHE:CE2	0.41	2.47	8	1
1:A:153:LYS:HA	1:A:156:ASP:OD2	0.41	2.15	5	1
1:A:160:HIS:O	1:A:166:VAL:HA	0.41	2.16	15	1
1:A:101:ILE:HG22	1:A:167:ILE:HG21	0.41	1.93	4	1
1:A:120:PHE:CD2	1:A:154:VAL:CA	0.41	3.03	3	1
1:A:158:LYS:CB	1:A:169:PRO:CG	0.41	2.99	2	1
1:A:99:MET:SD	1:A:143:VAL:HB	0.41	2.55	6	1
1:A:102:GLY:O	1:A:167:ILE:CA	0.41	2.68	10	1
1:A:99:MET:HE3	1:A:101:ILE:CD1	0.41	2.46	15	1
1:A:110:LYS:HG2	1:A:110:LYS:O	0.41	2.16	8	1
1:A:98:LYS:HD3	1:A:144:LEU:HD21	0.41	1.92	9	1
1:A:102:GLY:O	1:A:168:ASP:CB	0.41	2.69	5	1
1:A:143:VAL:C	1:A:144:LEU:CD1	0.41	2.89	4	1
1:A:158:LYS:HB2	1:A:169:PRO:HG2	0.41	1.92	19	1
1:A:98:LYS:CG	1:A:144:LEU:CD1	0.41	2.99	6	1
1:A:98:LYS:HG2	1:A:144:LEU:HG	0.40	1.91	10	1
1:A:125:ASP:CB	1:A:144:LEU:CB	0.40	2.99	16	1
1:A:157:GLN:O	1:A:157:GLN:CG	0.40	2.69	11	1
1:A:113:LEU:CD1	1:A:162:LEU:HD22	0.40	2.47	3	1
1:A:117:PHE:CZ	1:A:167:ILE:HD12	0.40	2.51	13	1
1:A:101:ILE:N	1:A:101:ILE:CD1	0.40	2.82	2	1
1:A:120:PHE:CD1	1:A:120:PHE:N	0.40	2.89	5	1
1:A:162:LEU:HD13	1:A:167:ILE:CG2	0.40	2.47	5	1
1:A:104:LEU:HD22	1:A:167:ILE:HG22	0.40	1.94	12	1
1:A:102:GLY:O	1:A:167:ILE:C	0.40	2.60	16	1
1:A:124:VAL:CG2	1:A:146:LYS:HE2	0.40	2.47	10	1
1:A:161:LYS:O	1:A:161:LYS:HG3	0.40	2.16	20	1
1:A:120:PHE:CD1	1:A:154:VAL:CA	0.40	3.04	7	1
1:A:124:VAL:CG2	1:A:146:LYS:HG2	0.40	2.42	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	62/75 (83%)	56±1 (90±2%)	5±2 (8±3%)	1±1 (1±1%)	18 63

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1240/1500 (83%)	1121 (90%)	101 (8%)	18 (1%)	18	63

All 2 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	161	LYS	14
1	A	103	GLY	4

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	58/67 (87%)	42±2 (73±3%)	16±2 (27±3%)	2	22
All	All	1160/1340 (87%)	844 (73%)	316 (27%)	2	22

All 38 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	127	THR	20
1	A	152	ASP	19
1	A	167	ILE	16
1	A	128	LEU	15
1	A	156	ASP	14
1	A	165	LYS	13
1	A	163	ASN	12
1	A	105	SER	12
1	A	149	GLU	12
1	A	111	LYS	11
1	A	158	LYS	11
1	A	153	LYS	11
1	A	147	GLU	11
1	A	122	GLU	10
1	A	157	GLN	10
1	A	171	ARG	9
1	A	112	ASP	8

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Mol	Chain	Res	Type	Models (Total)
1	A	108	THR	8
1	A	110	LYS	8
1	A	119	LYS	8
1	A	170	LYS	8
1	A	162	LEU	7
1	A	155	MET	7
1	A	161	LYS	6
1	A	125	ASP	6
1	A	99	MET	6
1	A	98	LYS	6
1	A	115	ASP	5
1	A	118	SER	5
1	A	146	LYS	5
1	A	114	LYS	4
1	A	107	ASP	4
1	A	148	SER	3
1	A	106	TRP	2
1	A	104	LEU	1
1	A	159	GLU	1
1	A	113	LEU	1
1	A	150	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

No chemical shift data were provided