



Full wwPDB NMR Structure Validation Report ⓘ

Apr 26, 2016 – 10:44 PM BST

PDB ID : 2KEM
Title : Extended structure of citidine deaminase domain of APOBEC3G
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Deposited on : 2009-01-30

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

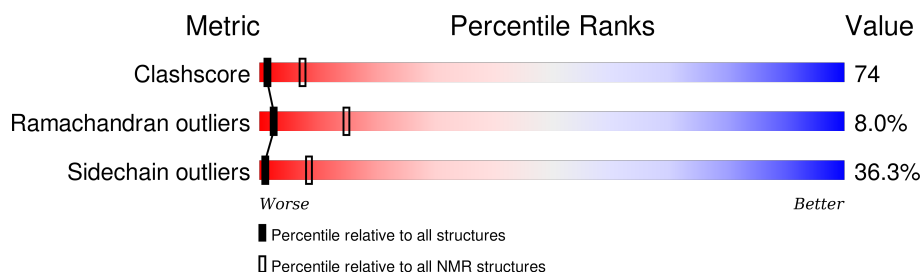
1 Overall quality at a glance

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	202	

2 Ensemble composition and analysis ⓘ

This entry contains 10 models. Model 9 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:28-A:42, A:50-A:56, A:65-A:124, A:131-A:159, A:170-A:190 (132)	0.23	9

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. No single-model clusters were found.

Cluster number	Models
1	1, 2, 4, 5, 6, 8, 9
2	3, 7, 10

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3126 atoms, of which 1521 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called DNA dC->dU-editing enzyme APOBEC-3G.

Mol	Chain	Residues	Atoms						Trace
1	A	194	Total	C	H	N	O	S	0
			3125	1014	1521	288	291	11	

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	GLY	-	EXPRESSION TAG	UNP Q9HC16
A	-6	PRO	-	EXPRESSION TAG	UNP Q9HC16
A	-5	LEU	-	EXPRESSION TAG	UNP Q9HC16
A	-4	GLY	-	EXPRESSION TAG	UNP Q9HC16
A	-3	SER	-	EXPRESSION TAG	UNP Q9HC16
A	-2	PRO	-	EXPRESSION TAG	UNP Q9HC16
A	-1	GLY	-	EXPRESSION TAG	UNP Q9HC16
A	0	PHE	-	EXPRESSION TAG	UNP Q9HC16
A	44	LYS	LEU	ENGINEERED	UNP Q9HC16
A	53	ALA	CYS	ENGINEERED	UNP Q9HC16
A	120	LYS	PHE	ENGINEERED	UNP Q9HC16
A	131	ALA	CYS	ENGINEERED	UNP Q9HC16
A	166	ALA	CYS	ENGINEERED	UNP Q9HC16

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

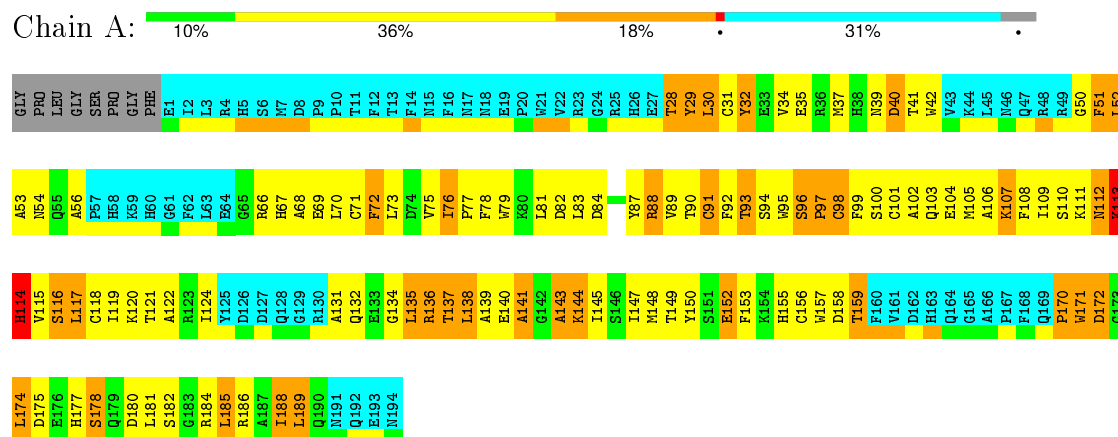
Mol	Chain	Residues	Atoms	
2	A	1	Total	Zn
			1	1

4 Residue-property plots

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: DNA dC->dU-editing enzyme APOBEC-3G

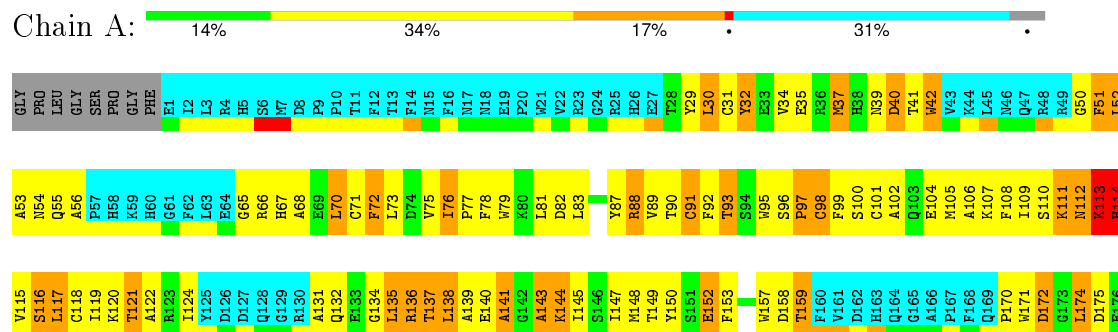


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

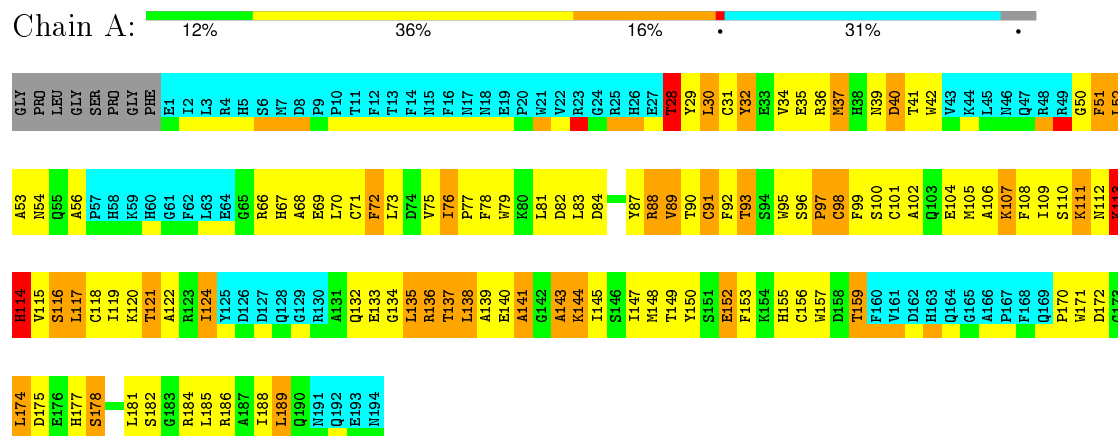
- Molecule 1: DNA dC->dU-editing enzyme APOBEC-3G





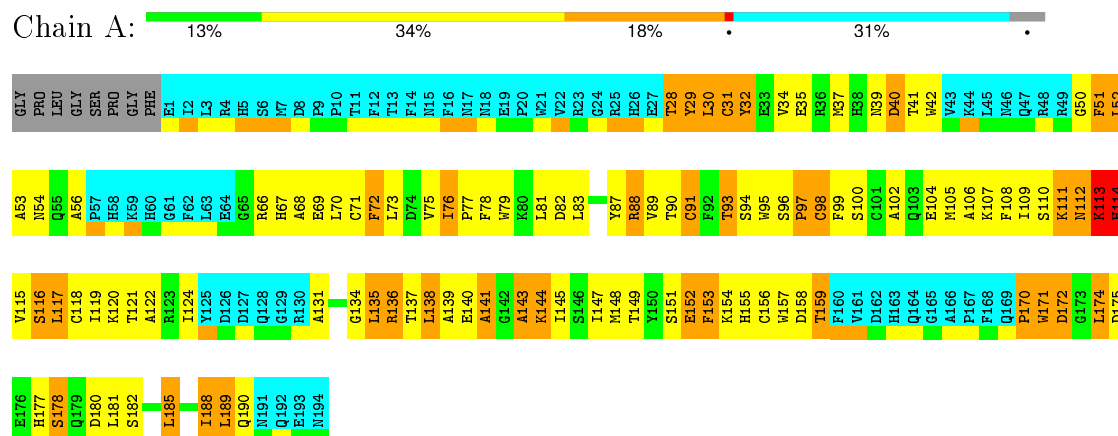
4.2.2 Score per residue for model 2

- Molecule 1: DNA dC->dU-editing enzyme APOBEC-3G



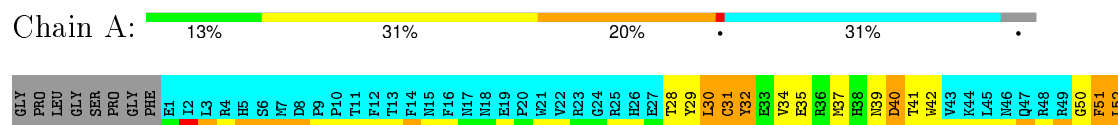
4.2.3 Score per residue for model 3

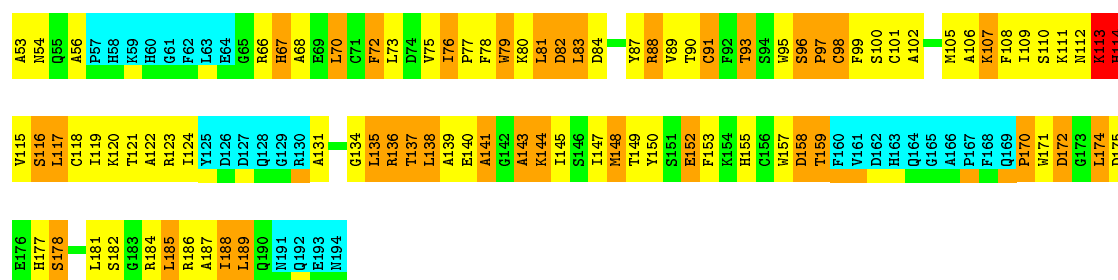
- Molecule 1: DNA dC->dU-editing enzyme APOBEC-3G



4.2.4 Score per residue for model 4

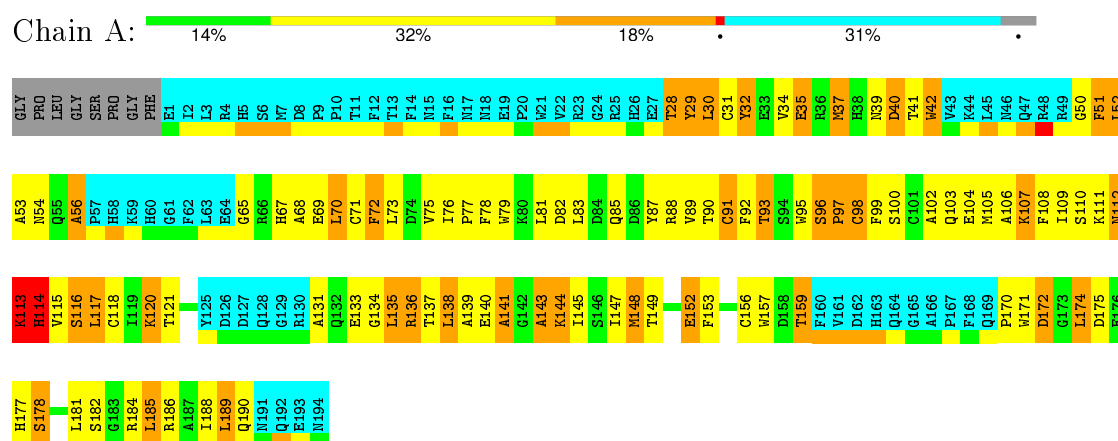
- Molecule 1: DNA dC->dU-editing enzyme APOBEC-3G





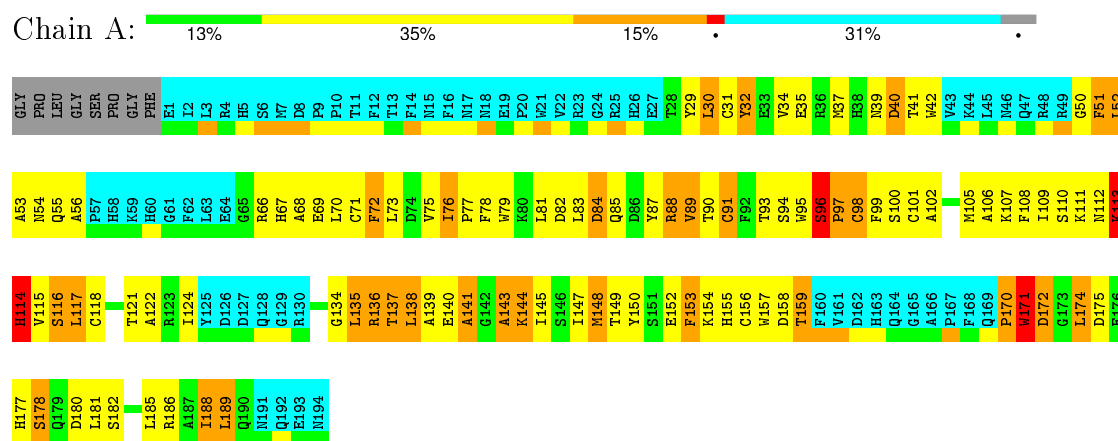
4.2.5 Score per residue for model 5

- Molecule 1: DNA dC->dU-editing enzyme APOBEC-3G



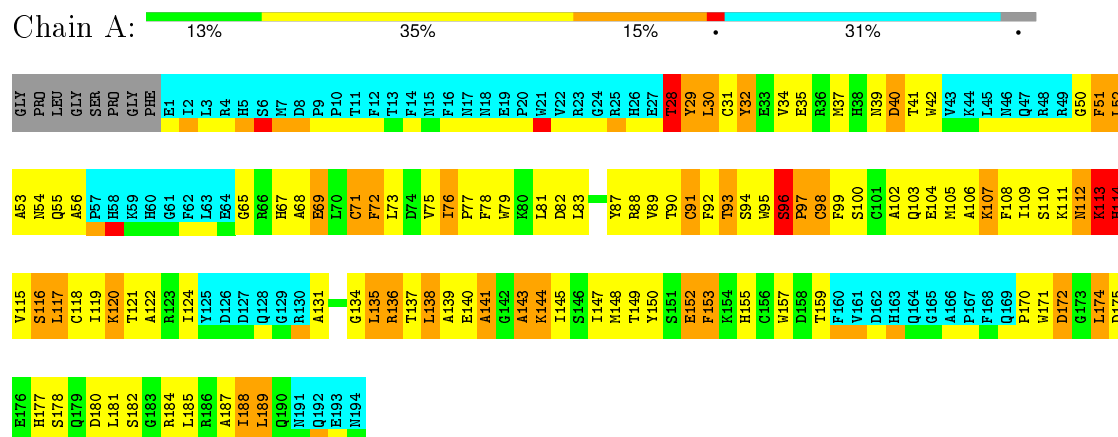
4.2.6 Score per residue for model 6

- Molecule 1: DNA dC->dU-editing enzyme APOBEC-3G



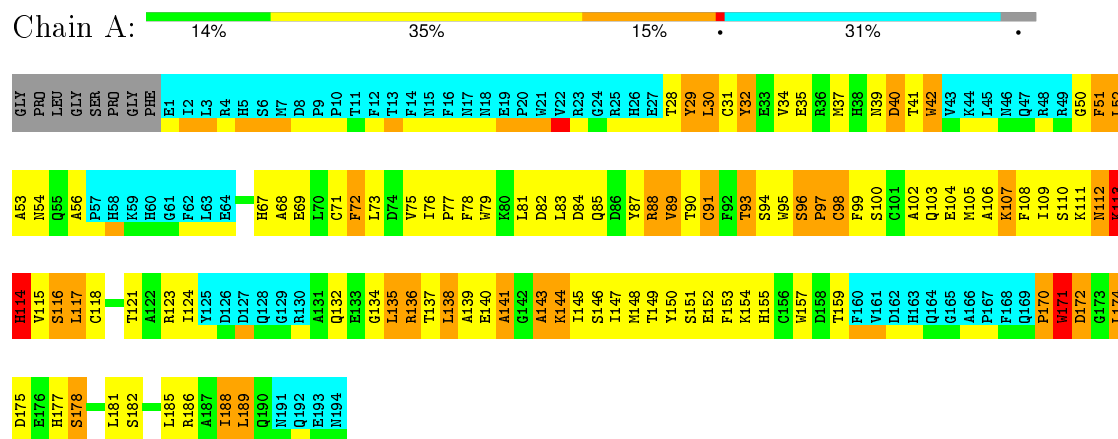
4.2.7 Score per residue for model 7

- Molecule 1: DNA dC->dU-editing enzyme APOBEC-3G



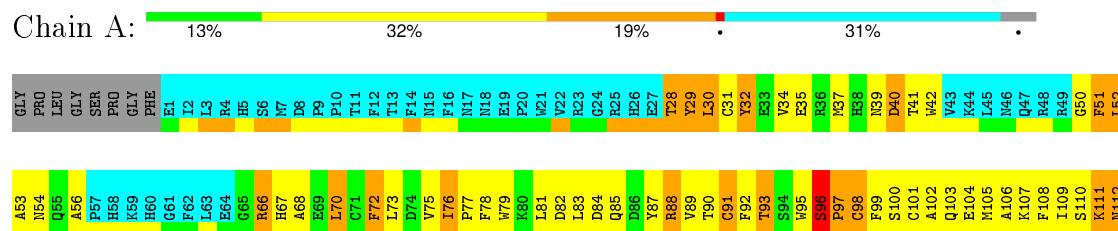
4.2.8 Score per residue for model 8

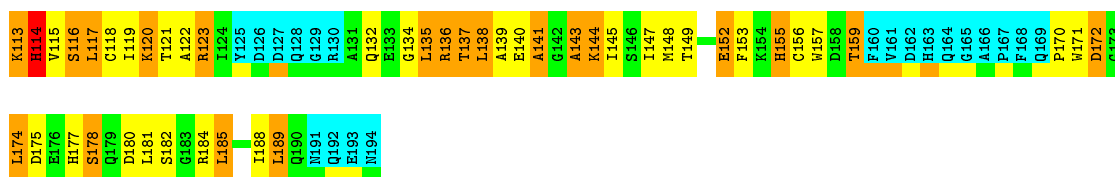
- Molecule 1: DNA dC->dU-editing enzyme APOBEC-3G



4.2.9 Score per residue for model 9 (medoid)

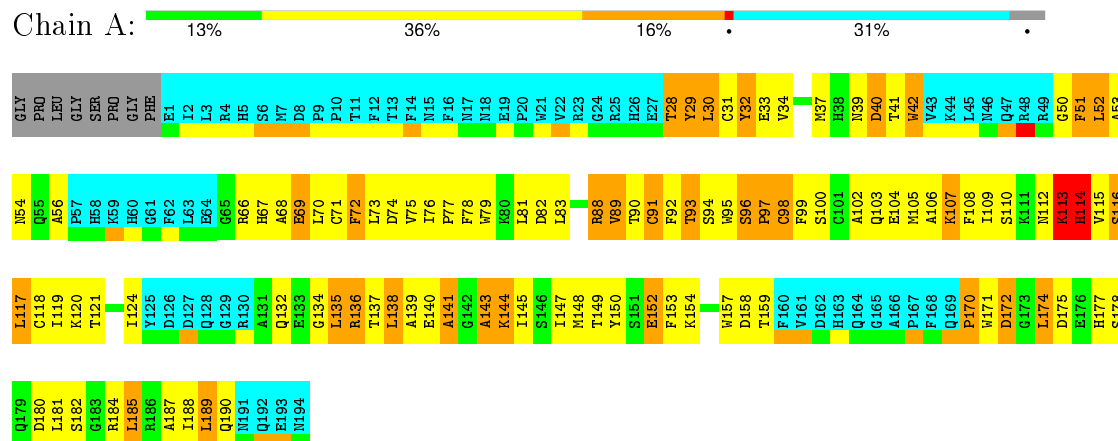
- Molecule 1: DNA dC->dU-editing enzyme APOBEC-3G





4.2.10 Score per residue for model 10

- Molecule 1: DNA dC->dU-editing enzyme APOBEC-3G



5 Refinement protocol and experimental data overview ⓘ

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

Of the 50 calculated structures, 10 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
CNS	refinement	.

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 ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section:
ZN

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	1071	1031	1027	156±5
All	All	10720	10310	10270	1562

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 74.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:102:ALA:HA	1:A:138:LEU:HD21	1.04	1.29	10	10
1:A:135:LEU:HD23	1:A:145:ILE:HG21	1.03	1.25	6	10
1:A:147:ILE:HG23	1:A:181:LEU:HD13	0.93	1.39	7	10
1:A:56:ALA:HB2	1:A:67:HIS:CE1	0.88	2.04	8	4
1:A:174:LEU:HD23	1:A:175:ASP:N	0.87	1.84	3	10
1:A:72:PHE:O	1:A:75:VAL:HG22	0.86	1.69	2	10
1:A:109:ILE:HG21	1:A:117:LEU:HD21	0.84	1.44	7	10
1:A:34:VAL:HG12	1:A:89:VAL:HA	0.81	1.52	10	10
1:A:117:LEU:HD23	1:A:143:ALA:HA	0.80	1.53	4	10
1:A:90:THR:HG22	1:A:118:CYS:CB	0.79	2.06	2	10
1:A:102:ALA:CA	1:A:138:LEU:HD21	0.78	2.06	10	1
1:A:116:SER:C	1:A:117:LEU:HD13	0.78	1.99	1	10

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:29:TYR:CG	1:A:53:ALA:HB2	0.78	2.13	8	5
1:A:102:ALA:HB2	1:A:134:GLY:HA2	0.77	1.55	4	10
1:A:102:ALA:HA	1:A:138:LEU:CD2	0.77	2.09	10	10
1:A:139:ALA:HB3	1:A:189:LEU:HD21	0.77	1.55	10	10
1:A:139:ALA:CB	1:A:189:LEU:HD11	0.76	2.10	5	10
1:A:54:ASN:O	1:A:67:HIS:HA	0.76	1.80	5	10
1:A:96:SER:OG	1:A:124:ILE:HG23	0.76	1.79	6	2
1:A:76:ILE:HB	1:A:77:PRO:HD3	0.75	1.57	10	10
1:A:96:SER:OG	1:A:135:LEU:HD21	0.75	1.81	9	5
1:A:76:ILE:CG2	1:A:81:LEU:HD12	0.75	2.12	5	10
1:A:34:VAL:HA	1:A:88:ARG:O	0.74	1.82	5	10
1:A:81:LEU:HD22	1:A:82:ASP:N	0.73	1.98	9	10
1:A:76:ILE:HG22	1:A:81:LEU:HB3	0.73	1.59	3	7
1:A:30:LEU:HD13	1:A:91:CYS:SG	0.73	2.24	9	5
1:A:90:THR:HG22	1:A:118:CYS:SG	0.73	2.23	8	8
1:A:32:TYR:HB3	1:A:51:PHE:CG	0.73	2.17	2	10
1:A:149:THR:HG21	1:A:178:SER:OG	0.72	1.84	3	10
1:A:135:LEU:HD23	1:A:145:ILE:CG2	0.71	2.11	6	4
1:A:119:ILE:HB	1:A:145:ILE:HD13	0.71	1.62	4	3
1:A:32:TYR:HB3	1:A:51:PHE:CD1	0.71	2.21	8	10
1:A:72:PHE:CE1	1:A:76:ILE:HD11	0.71	2.20	8	7
1:A:109:ILE:CG2	1:A:117:LEU:HD21	0.70	2.16	4	10
1:A:90:THR:HG22	1:A:118:CYS:HB2	0.70	1.61	1	10
1:A:135:LEU:CD2	1:A:145:ILE:HG21	0.70	2.16	7	6
1:A:70:LEU:HD13	1:A:101:CYS:SG	0.70	2.27	1	5
1:A:124:ILE:HD11	1:A:185:LEU:CD1	0.70	2.17	1	3
1:A:53:ALA:HA	1:A:68:ALA:HB2	0.69	1.64	2	10
1:A:185:LEU:HD13	1:A:188:ILE:HD11	0.69	1.64	10	1
1:A:109:ILE:HG21	1:A:117:LEU:CD2	0.69	2.18	4	10
1:A:31:CYS:O	1:A:91:CYS:HA	0.68	1.88	1	10
1:A:51:PHE:CZ	1:A:75:VAL:HG21	0.68	2.23	3	10
1:A:76:ILE:HG22	1:A:81:LEU:CB	0.68	2.18	3	7
1:A:117:LEU:N	1:A:117:LEU:HD13	0.68	2.03	5	5
1:A:30:LEU:HD23	1:A:93:THR:OG1	0.68	1.87	5	2
1:A:147:ILE:HG22	1:A:149:THR:HG23	0.67	1.66	5	10
1:A:110:SER:OG	1:A:141:ALA:HB3	0.66	1.89	5	10
1:A:37:MET:HA	1:A:41:THR:O	0.65	1.91	5	10
1:A:171:TRP:O	1:A:172:ASP:CB	0.65	2.45	8	10
1:A:30:LEU:HD23	1:A:93:THR:CG2	0.64	2.22	9	1
1:A:30:LEU:HD11	1:A:68:ALA:HB1	0.64	1.68	10	8
1:A:30:LEU:HB3	1:A:93:THR:HG23	0.64	1.68	1	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:39:ASN:O	1:A:40:ASP:CB	0.64	2.46	2	10
1:A:124:ILE:CG2	1:A:135:LEU:HD11	0.64	2.22	2	3
1:A:28:THR:HG22	1:A:54:ASN:O	0.64	1.93	3	1
1:A:149:THR:O	1:A:153:PHE:N	0.63	2.31	8	10
1:A:52:LEU:N	1:A:52:LEU:HD13	0.63	2.09	2	6
1:A:73:LEU:CD1	1:A:105:MET:HE3	0.63	2.22	5	2
1:A:51:PHE:CZ	1:A:75:VAL:HG11	0.63	2.29	6	6
1:A:106:ALA:HA	1:A:110:SER:HB2	0.62	1.70	5	10
1:A:149:THR:HG21	1:A:178:SER:HA	0.62	1.71	4	10
1:A:73:LEU:HD21	1:A:105:MET:HA	0.62	1.70	4	5
1:A:30:LEU:CB	1:A:93:THR:HG23	0.62	2.24	7	6
1:A:117:LEU:HD13	1:A:117:LEU:N	0.62	2.09	9	5
1:A:139:ALA:HA	1:A:144:LYS:HA	0.62	1.70	10	10
1:A:115:VAL:HG13	1:A:117:LEU:HD11	0.61	1.72	9	10
1:A:93:THR:OG1	1:A:119:ILE:HG23	0.61	1.96	3	5
1:A:76:ILE:HG22	1:A:81:LEU:HD12	0.61	1.70	4	7
1:A:52:LEU:HD21	1:A:75:VAL:CG1	0.61	2.26	1	10
1:A:153:PHE:CD2	1:A:174:LEU:CD1	0.61	2.83	3	4
1:A:81:LEU:HD11	1:A:115:VAL:HB	0.61	1.73	4	10
1:A:149:THR:HG21	1:A:178:SER:CB	0.61	2.26	7	10
1:A:174:LEU:HA	1:A:177:HIS:CE1	0.60	2.31	7	1
1:A:51:PHE:HZ	1:A:75:VAL:HG21	0.60	1.54	3	10
1:A:106:ALA:O	1:A:110:SER:N	0.60	2.34	1	10
1:A:32:TYR:CB	1:A:51:PHE:CD1	0.60	2.84	7	10
1:A:29:TYR:CD2	1:A:53:ALA:HB2	0.60	2.31	10	5
1:A:117:LEU:HD22	1:A:117:LEU:H	0.60	1.56	4	6
1:A:117:LEU:H	1:A:117:LEU:HD22	0.60	1.55	10	4
1:A:30:LEU:HD23	1:A:93:THR:HG23	0.59	1.73	9	1
1:A:51:PHE:CD2	1:A:52:LEU:HD22	0.59	2.32	6	8
1:A:153:PHE:CE2	1:A:171:TRP:HB2	0.59	2.32	4	4
1:A:136:ARG:CG	1:A:137:THR:N	0.59	2.66	10	10
1:A:52:LEU:HD13	1:A:52:LEU:N	0.59	2.12	4	4
1:A:140:GLU:HG2	1:A:189:LEU:HD13	0.58	1.74	6	10
1:A:122:ALA:HB2	1:A:148:MET:CE	0.58	2.28	9	4
1:A:34:VAL:HG11	1:A:79:TRP:CH2	0.58	2.34	5	9
1:A:177:HIS:O	1:A:181:LEU:N	0.58	2.37	7	10
1:A:117:LEU:HD22	1:A:117:LEU:N	0.58	2.13	4	7
1:A:99:PHE:O	1:A:102:ALA:HB3	0.57	2.00	1	10
1:A:52:LEU:HD21	1:A:75:VAL:HG11	0.57	1.77	7	7
1:A:97:PRO:O	1:A:98:CYS:HB3	0.57	1.99	1	9
1:A:145:ILE:O	1:A:185:LEU:HD11	0.57	1.99	3	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:81:LEU:HD13	1:A:81:LEU:O	0.56	2.01	4	3
1:A:56:ALA:HB3	1:A:67:HIS:CE1	0.56	2.35	4	3
1:A:72:PHE:HZ	1:A:117:LEU:HD12	0.56	1.58	5	3
1:A:150:TYR:HA	1:A:174:LEU:HD11	0.56	1.78	7	5
1:A:90:THR:HG22	1:A:118:CYS:HB3	0.56	1.75	2	2
1:A:32:TYR:CE2	1:A:34:VAL:CG1	0.56	2.89	4	2
1:A:32:TYR:CD2	1:A:51:PHE:CE1	0.56	2.93	4	10
1:A:76:ILE:HG22	1:A:81:LEU:CG	0.56	2.31	3	6
1:A:79:TRP:CH2	1:A:89:VAL:HG22	0.56	2.36	1	9
1:A:30:LEU:CD1	1:A:68:ALA:HB1	0.55	2.31	5	7
1:A:149:THR:HG21	1:A:178:SER:CA	0.55	2.32	3	10
1:A:147:ILE:CG1	1:A:181:LEU:HD22	0.55	2.32	5	3
1:A:117:LEU:N	1:A:117:LEU:HD22	0.55	2.16	10	3
1:A:122:ALA:HB2	1:A:148:MET:HE3	0.55	1.77	6	2
1:A:32:TYR:CD2	1:A:34:VAL:HG13	0.55	2.36	5	10
1:A:32:TYR:O	1:A:32:TYR:CD1	0.55	2.60	6	7
1:A:75:VAL:O	1:A:79:TRP:N	0.55	2.39	3	9
1:A:122:ALA:HB2	1:A:148:MET:HE2	0.55	1.77	9	1
1:A:28:THR:HG21	1:A:67:HIS:HB3	0.55	1.79	3	1
1:A:139:ALA:HB3	1:A:189:LEU:CD2	0.54	2.31	6	8
1:A:30:LEU:CG	1:A:93:THR:HG23	0.54	2.33	9	3
1:A:181:LEU:CD2	1:A:185:LEU:HD23	0.54	2.32	7	1
1:A:138:LEU:HD13	1:A:143:ALA:HB3	0.53	1.79	5	9
1:A:95:TRP:CE3	1:A:96:SER:O	0.53	2.61	2	7
1:A:171:TRP:HD1	1:A:174:LEU:HB3	0.53	1.62	7	1
1:A:72:PHE:CD1	1:A:76:ILE:HD11	0.53	2.38	10	3
1:A:147:ILE:HG13	1:A:185:LEU:HD22	0.53	1.81	2	4
1:A:174:LEU:C	1:A:174:LEU:HD23	0.53	2.22	8	2
1:A:32:TYR:CD1	1:A:32:TYR:O	0.53	2.62	9	3
1:A:147:ILE:HG13	1:A:181:LEU:HD22	0.53	1.80	5	1
1:A:135:LEU:O	1:A:139:ALA:N	0.53	2.42	6	10
1:A:76:ILE:HG23	1:A:81:LEU:CG	0.53	2.33	10	3
1:A:106:ALA:HA	1:A:110:SER:CB	0.53	2.34	7	10
1:A:34:VAL:HG12	1:A:89:VAL:CA	0.53	2.31	10	7
1:A:97:PRO:O	1:A:98:CYS:CB	0.53	2.54	3	10
1:A:73:LEU:O	1:A:77:PRO:CD	0.52	2.57	4	9
1:A:139:ALA:HB1	1:A:189:LEU:HD11	0.52	1.78	5	8
1:A:28:THR:HG22	1:A:93:THR:HG22	0.51	1.82	4	1
1:A:76:ILE:HB	1:A:77:PRO:CD	0.51	2.35	5	10
1:A:174:LEU:HD23	1:A:175:ASP:H	0.51	1.64	3	5
1:A:84:ASP:O	1:A:85:GLN:CG	0.51	2.59	6	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:30:LEU:CD2	1:A:93:THR:HG23	0.51	2.35	9	1
1:A:139:ALA:CB	1:A:189:LEU:HD21	0.51	2.34	6	7
1:A:56:ALA:CB	1:A:67:HIS:CE1	0.51	2.94	10	7
1:A:124:ILE:HG23	1:A:181:LEU:HD21	0.51	1.81	4	1
1:A:81:LEU:C	1:A:81:LEU:HD13	0.51	2.27	10	2
1:A:32:TYR:CD1	1:A:50:GLY:O	0.51	2.64	9	10
1:A:121:THR:O	1:A:181:LEU:HD11	0.51	2.07	2	2
1:A:66:ARG:HB3	1:A:70:LEU:HD23	0.51	1.83	2	3
1:A:102:ALA:O	1:A:106:ALA:HB2	0.50	2.06	7	9
1:A:72:PHE:CE1	1:A:76:ILE:CD1	0.50	2.94	3	6
1:A:32:TYR:CG	1:A:51:PHE:CD1	0.50	3.00	4	10
1:A:156:CYS:O	1:A:159:THR:HG22	0.50	2.06	6	5
1:A:81:LEU:HD13	1:A:81:LEU:C	0.50	2.27	4	6
1:A:72:PHE:CZ	1:A:117:LEU:HD12	0.50	2.42	6	2
1:A:147:ILE:CG2	1:A:149:THR:HG23	0.50	2.36	2	8
1:A:96:SER:OG	1:A:124:ILE:HA	0.50	2.06	7	1
1:A:29:TYR:CD2	1:A:53:ALA:CB	0.50	2.95	10	5
1:A:79:TRP:CZ3	1:A:89:VAL:HG22	0.49	2.42	1	9
1:A:73:LEU:HD21	1:A:105:MET:CA	0.49	2.37	4	2
1:A:148:MET:HA	1:A:152:GLU:HB3	0.49	1.84	3	10
1:A:122:ALA:O	1:A:177:HIS:CE1	0.49	2.65	7	1
1:A:145:ILE:O	1:A:185:LEU:HD21	0.49	2.08	1	3
1:A:124:ILE:HD11	1:A:181:LEU:CD2	0.49	2.37	6	2
1:A:157:TRP:CZ3	1:A:158:ASP:HB2	0.49	2.43	10	1
1:A:124:ILE:HG23	1:A:135:LEU:HD11	0.49	1.83	1	2
1:A:149:THR:CG2	1:A:178:SER:HA	0.49	2.38	7	10
1:A:147:ILE:HG23	1:A:181:LEU:CD1	0.49	2.35	4	3
1:A:30:LEU:HD23	1:A:93:THR:HG1	0.49	1.65	5	1
1:A:133:GLU:HA	1:A:136:ARG:HB3	0.49	1.84	5	2
1:A:35:GLU:O	1:A:87:TYR:CD2	0.48	2.66	8	9
1:A:28:THR:CG2	1:A:54:ASN:O	0.48	2.60	3	1
1:A:108:PHE:O	1:A:112:ASN:CB	0.48	2.61	5	10
1:A:96:SER:CB	1:A:97:PRO:CD	0.48	2.92	2	7
1:A:117:LEU:CD1	1:A:117:LEU:N	0.48	2.74	3	2
1:A:32:TYR:CB	1:A:51:PHE:CG	0.48	2.96	2	9
1:A:105:MET:O	1:A:109:ILE:HD12	0.48	2.07	1	2
1:A:171:TRP:CE3	1:A:171:TRP:C	0.48	2.87	8	2
1:A:149:THR:O	1:A:153:PHE:HB2	0.48	2.09	7	2
1:A:76:ILE:CB	1:A:77:PRO:HD3	0.48	2.39	6	7
1:A:30:LEU:O	1:A:51:PHE:CB	0.48	2.61	10	8
1:A:106:ALA:O	1:A:111:LYS:N	0.48	2.44	4	7

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:32:TYR:H	1:A:50:GLY:C	0.48	2.12	4	5
1:A:147:ILE:HG23	1:A:181:LEU:HD22	0.48	1.85	8	3
1:A:76:ILE:CG2	1:A:81:LEU:CG	0.48	2.92	3	7
1:A:103:GLN:O	1:A:107:LYS:CG	0.48	2.62	7	4
1:A:138:LEU:CD1	1:A:143:ALA:HB3	0.47	2.39	3	10
1:A:32:TYR:HB3	1:A:51:PHE:CB	0.47	2.38	2	10
1:A:124:ILE:HG23	1:A:135:LEU:HD21	0.47	1.85	10	1
1:A:32:TYR:CE2	1:A:34:VAL:HG11	0.47	2.44	4	1
1:A:75:VAL:O	1:A:79:TRP:CB	0.47	2.63	8	4
1:A:157:TRP:CZ3	1:A:158:ASP:HB3	0.47	2.43	6	1
1:A:174:LEU:HB2	1:A:177:HIS:CE1	0.47	2.45	7	1
1:A:81:LEU:CD1	1:A:114:HIS:CE1	0.47	2.97	10	9
1:A:95:TRP:CE3	1:A:96:SER:N	0.47	2.82	6	3
1:A:81:LEU:HD12	1:A:114:HIS:NE2	0.47	2.24	4	10
1:A:39:ASN:O	1:A:40:ASP:HB3	0.47	2.09	8	1
1:A:136:ARG:O	1:A:140:GLU:CG	0.47	2.62	3	10
1:A:28:THR:O	1:A:53:ALA:HB1	0.47	2.09	10	2
1:A:81:LEU:CD1	1:A:114:HIS:NE2	0.47	2.77	8	10
1:A:170:PRO:O	1:A:171:TRP:HB3	0.47	2.09	6	2
1:A:174:LEU:HD23	1:A:174:LEU:C	0.47	2.30	3	4
1:A:177:HIS:O	1:A:181:LEU:CB	0.46	2.64	7	10
1:A:157:TRP:CE3	1:A:158:ASP:HB2	0.46	2.46	4	2
1:A:188:ILE:CD1	1:A:189:LEU:HD23	0.46	2.40	5	2
1:A:76:ILE:HG22	1:A:81:LEU:CD1	0.46	2.40	3	7
1:A:139:ALA:HB3	1:A:189:LEU:HD11	0.46	1.86	5	1
1:A:92:PHE:CE2	1:A:120:LYS:HD2	0.46	2.45	5	2
1:A:109:ILE:O	1:A:113:LYS:CG	0.46	2.63	5	9
1:A:32:TYR:CD1	1:A:32:TYR:C	0.46	2.87	5	4
1:A:29:TYR:HB3	1:A:53:ALA:CB	0.46	2.41	6	5
1:A:42:TRP:CD1	1:A:42:TRP:N	0.46	2.84	5	3
1:A:144:LYS:O	1:A:144:LYS:CG	0.46	2.63	6	7
1:A:135:LEU:HD13	1:A:188:ILE:HD13	0.46	1.87	10	3
1:A:76:ILE:CG2	1:A:81:LEU:CD1	0.46	2.92	4	7
1:A:178:SER:O	1:A:182:SER:CB	0.46	2.64	2	10
1:A:34:VAL:HG11	1:A:79:TRP:HH2	0.46	1.69	7	7
1:A:122:ALA:HB2	1:A:148:MET:HE1	0.46	1.87	1	1
1:A:92:PHE:CD1	1:A:92:PHE:N	0.46	2.84	10	1
1:A:102:ALA:O	1:A:106:ALA:CB	0.46	2.64	6	8
1:A:80:LYS:O	1:A:83:LEU:HG	0.46	2.11	4	1
1:A:185:LEU:O	1:A:189:LEU:HD23	0.45	2.11	8	4
1:A:42:TRP:N	1:A:42:TRP:CD1	0.45	2.84	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:67:HIS:N	1:A:67:HIS:ND1	0.45	2.65	4	3
1:A:28:THR:O	1:A:53:ALA:HA	0.45	2.11	2	2
1:A:76:ILE:CB	1:A:77:PRO:CD	0.45	2.95	3	6
1:A:105:MET:CG	1:A:138:LEU:HD11	0.45	2.42	4	6
1:A:139:ALA:N	1:A:143:ALA:O	0.45	2.49	5	10
1:A:28:THR:CG2	1:A:93:THR:HG22	0.45	2.42	4	1
1:A:75:VAL:HG23	1:A:76:ILE:HD13	0.45	1.87	5	3
1:A:92:PHE:CE2	1:A:120:LYS:CD	0.45	3.00	5	1
1:A:81:LEU:O	1:A:82:ASP:HB3	0.45	2.12	4	7
1:A:188:ILE:HD12	1:A:189:LEU:CD2	0.45	2.41	5	1
1:A:153:PHE:CG	1:A:174:LEU:CD1	0.45	3.00	7	2
1:A:92:PHE:CE2	1:A:120:LYS:CE	0.45	2.99	7	1
1:A:52:LEU:H	1:A:52:LEU:HD22	0.45	1.72	7	6
1:A:29:TYR:HB3	1:A:53:ALA:HB1	0.45	1.87	2	1
1:A:185:LEU:O	1:A:189:LEU:CG	0.45	2.65	1	8
1:A:138:LEU:N	1:A:138:LEU:HD23	0.45	2.26	10	1
1:A:32:TYR:C	1:A:32:TYR:CD1	0.45	2.89	7	4
1:A:75:VAL:O	1:A:79:TRP:HB2	0.44	2.12	8	4
1:A:56:ALA:HB1	1:A:65:GLY:HA2	0.44	1.89	1	1
1:A:75:VAL:O	1:A:79:TRP:CG	0.44	2.71	5	7
1:A:95:TRP:CD2	1:A:96:SER:O	0.44	2.70	8	2
1:A:150:TYR:N	1:A:174:LEU:HD11	0.44	2.27	2	1
1:A:29:TYR:CG	1:A:53:ALA:CB	0.44	2.93	8	3
1:A:72:PHE:HA	1:A:75:VAL:HG13	0.44	1.89	9	3
1:A:52:LEU:HD22	1:A:52:LEU:H	0.44	1.72	8	3
1:A:69:GLU:O	1:A:72:PHE:HB3	0.44	2.13	7	6
1:A:29:TYR:CB	1:A:53:ALA:HB2	0.44	2.42	6	1
1:A:138:LEU:HD13	1:A:143:ALA:CB	0.44	2.42	5	3
1:A:144:LYS:CG	1:A:144:LYS:O	0.44	2.66	1	2
1:A:92:PHE:N	1:A:92:PHE:CD1	0.44	2.86	5	1
1:A:96:SER:CB	1:A:135:LEU:HD21	0.44	2.43	8	1
1:A:171:TRP:CG	1:A:172:ASP:N	0.44	2.85	6	1
1:A:171:TRP:CD1	1:A:174:LEU:N	0.44	2.86	7	1
1:A:122:ALA:O	1:A:181:LEU:HD12	0.44	2.13	7	2
1:A:67:HIS:ND1	1:A:67:HIS:N	0.44	2.66	10	2
1:A:32:TYR:CE2	1:A:34:VAL:HG13	0.43	2.48	4	1
1:A:184:ARG:O	1:A:188:ILE:N	0.43	2.47	5	3
1:A:34:VAL:CG1	1:A:89:VAL:HG13	0.43	2.43	4	3
1:A:136:ARG:HB2	1:A:188:ILE:O	0.43	2.13	2	3
1:A:67:HIS:O	1:A:70:LEU:N	0.43	2.51	6	2
1:A:29:TYR:CD1	1:A:53:ALA:HB2	0.43	2.48	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:171:TRP:O	1:A:171:TRP:CE3	0.43	2.72	3	1
1:A:31:CYS:SG	1:A:159:THR:HG23	0.43	2.54	4	1
1:A:81:LEU:O	1:A:82:ASP:CB	0.43	2.66	4	1
1:A:96:SER:OG	1:A:97:PRO:CD	0.43	2.66	4	1
1:A:107:LYS:HE3	1:A:108:PHE:HB2	0.43	1.90	2	2
1:A:94:SER:O	1:A:95:TRP:CD2	0.43	2.72	3	3
1:A:117:LEU:N	1:A:117:LEU:CD1	0.43	2.78	9	5
1:A:76:ILE:HG23	1:A:81:LEU:HD12	0.43	1.90	5	2
1:A:109:ILE:O	1:A:113:LYS:HG2	0.43	2.13	4	2
1:A:147:ILE:CD1	1:A:182:SER:CB	0.43	2.96	1	5
1:A:153:PHE:O	1:A:156:CYS:N	0.43	2.52	5	2
1:A:97:PRO:CB	1:A:105:MET:CE	0.43	2.97	10	2
1:A:139:ALA:C	1:A:189:LEU:HD11	0.43	2.35	10	2
1:A:138:LEU:CD2	1:A:138:LEU:N	0.43	2.81	10	1
1:A:135:LEU:CD1	1:A:188:ILE:HD13	0.42	2.44	4	1
1:A:134:GLY:O	1:A:138:LEU:HG	0.42	2.13	10	3
1:A:91:CYS:O	1:A:119:ILE:HA	0.42	2.14	10	1
1:A:147:ILE:HD12	1:A:147:ILE:H	0.42	1.74	5	1
1:A:132:GLN:O	1:A:136:ARG:HB3	0.42	2.15	9	1
1:A:30:LEU:HA	1:A:92:PHE:O	0.42	2.14	9	1
1:A:52:LEU:N	1:A:52:LEU:CD1	0.42	2.80	9	2
1:A:75:VAL:CG2	1:A:76:ILE:HD13	0.42	2.44	4	1
1:A:119:ILE:O	1:A:119:ILE:HG22	0.42	2.15	9	1
1:A:105:MET:HE3	1:A:138:LEU:HD11	0.42	1.91	1	1
1:A:88:ARG:HA	1:A:116:SER:CB	0.42	2.44	8	3
1:A:89:VAL:CB	1:A:116:SER:O	0.42	2.67	5	3
1:A:92:PHE:CD2	1:A:120:LYS:HG3	0.42	2.50	2	2
1:A:184:ARG:O	1:A:187:ALA:N	0.42	2.53	10	1
1:A:147:ILE:H	1:A:147:ILE:HD12	0.42	1.74	10	1
1:A:136:ARG:HA	1:A:189:LEU:HD22	0.42	1.92	5	2
1:A:28:THR:HG22	1:A:93:THR:CG2	0.42	2.45	7	2
1:A:96:SER:HG	1:A:135:LEU:HD21	0.42	1.74	9	1
1:A:138:LEU:O	1:A:141:ALA:N	0.42	2.52	7	4
1:A:151:SER:O	1:A:154:LYS:CG	0.42	2.68	8	2
1:A:68:ALA:HA	1:A:71:CYS:HB2	0.42	1.91	7	1
1:A:96:SER:OG	1:A:135:LEU:CD2	0.42	2.67	3	2
1:A:105:MET:CE	1:A:138:LEU:CD1	0.42	2.98	1	1
1:A:79:TRP:CZ3	1:A:89:VAL:CG2	0.42	3.03	7	2
1:A:123:ARG:HA	1:A:181:LEU:HD12	0.42	1.92	9	2
1:A:76:ILE:HG23	1:A:81:LEU:CD1	0.42	2.45	10	1
1:A:96:SER:HB3	1:A:97:PRO:CD	0.42	2.45	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:153:PHE:CD2	1:A:174:LEU:HD13	0.41	2.49	3	2
1:A:138:LEU:C	1:A:143:ALA:O	0.41	2.57	10	1
1:A:76:ILE:HG23	1:A:81:LEU:HG	0.41	1.91	10	1
1:A:79:TRP:CH2	1:A:89:VAL:CG2	0.41	3.03	7	1
1:A:185:LEU:O	1:A:189:LEU:HB2	0.41	2.14	5	2
1:A:147:ILE:CG1	1:A:185:LEU:HD22	0.41	2.44	2	2
1:A:124:ILE:HG21	1:A:135:LEU:HD11	0.41	1.90	8	1
1:A:171:TRP:O	1:A:172:ASP:HB2	0.41	2.11	8	1
1:A:110:SER:O	1:A:113:LYS:CG	0.41	2.69	2	1
1:A:81:LEU:O	1:A:81:LEU:HD13	0.41	2.15	5	1
1:A:124:ILE:HG13	1:A:181:LEU:HG	0.41	1.93	8	1
1:A:28:THR:O	1:A:53:ALA:CA	0.41	2.68	8	2
1:A:136:ARG:HG3	1:A:137:THR:N	0.41	2.30	9	5
1:A:30:LEU:HD11	1:A:68:ALA:CB	0.41	2.43	5	1
1:A:52:LEU:CD1	1:A:52:LEU:N	0.41	2.82	5	1
1:A:177:HIS:C	1:A:177:HIS:CD2	0.41	2.93	7	1
1:A:32:TYR:CD2	1:A:34:VAL:CG1	0.41	3.03	5	2
1:A:150:TYR:N	1:A:174:LEU:HG	0.41	2.31	7	2
1:A:155:HIS:O	1:A:159:THR:HB	0.41	2.16	9	2
1:A:172:ASP:O	1:A:175:ASP:HB3	0.41	2.15	6	1
1:A:95:TRP:HB2	1:A:123:ARG:O	0.41	2.16	4	1
1:A:75:VAL:O	1:A:79:TRP:CD1	0.41	2.74	4	1
1:A:66:ARG:CB	1:A:70:LEU:HD23	0.41	2.45	10	1
1:A:115:VAL:CG2	1:A:116:SER:N	0.41	2.84	7	5
1:A:39:ASN:O	1:A:40:ASP:HB2	0.41	2.16	3	3
1:A:170:PRO:O	1:A:171:TRP:CB	0.41	2.69	4	2
1:A:122:ALA:HA	1:A:148:MET:HB3	0.41	1.92	4	1
1:A:117:LEU:N	1:A:117:LEU:CD2	0.41	2.81	8	2
1:A:171:TRP:CE3	1:A:171:TRP:CA	0.41	3.04	8	1
1:A:131:ALA:O	1:A:134:GLY:N	0.41	2.54	4	1
1:A:135:LEU:HB2	1:A:188:ILE:CD1	0.41	2.46	6	1
1:A:153:PHE:CZ	1:A:171:TRP:HE3	0.40	2.34	5	1
1:A:181:LEU:O	1:A:181:LEU:HD23	0.40	2.16	7	1
1:A:101:CYS:O	1:A:105:MET:HG3	0.40	2.17	2	1
1:A:73:LEU:CD1	1:A:105:MET:CE	0.40	2.99	3	1
1:A:105:MET:HB2	1:A:138:LEU:CD1	0.40	2.46	5	1
1:A:109:ILE:HG21	1:A:117:LEU:CG	0.40	2.46	6	1
1:A:171:TRP:CA	1:A:171:TRP:CE3	0.40	3.04	6	1
1:A:94:SER:O	1:A:95:TRP:CE3	0.40	2.75	3	1
1:A:184:ARG:O	1:A:188:ILE:CG1	0.40	2.70	4	1
1:A:32:TYR:HB3	1:A:51:PHE:HB2	0.40	1.93	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:74:ASP:O	1:A:77:PRO:HD2	0.40	2.16	10	1
1:A:81:LEU:HD22	1:A:81:LEU:C	0.40	2.36	1	1
1:A:124:ILE:HD11	1:A:181:LEU:HD23	0.40	1.94	7	1
1:A:109:ILE:O	1:A:113:LYS:CA	0.40	2.70	2	1
1:A:185:LEU:O	1:A:189:LEU:HG	0.40	2.17	3	1
1:A:170:PRO:O	1:A:172:ASP:N	0.40	2.55	3	1
1:A:96:SER:HB2	1:A:135:LEU:HD21	0.40	1.94	1	1
1:A:73:LEU:O	1:A:77:PRO:HD3	0.40	2.17	10	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	132/202 (65%)	100±1 (76±1%)	21±1 (16±1%)	11±1 (8±1%)	2	15
All	All	1320/2020 (65%)	1001 (76%)	214 (16%)	105 (8%)	2	15

All 16 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	141	ALA	10
1	A	40	ASP	10
1	A	143	ALA	10
1	A	98	CYS	10
1	A	97	PRO	10
1	A	113	LYS	10
1	A	114	HIS	10
1	A	170	PRO	10
1	A	172	ASP	7
1	A	28	THR	6
1	A	96	SER	6
1	A	171	TRP	2
1	A	82	ASP	1
1	A	65	GLY	1

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Mol	Chain	Res	Type	Models (Total)
1	A	56	ALA	1
1	A	131	ALA	1

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	115/177 (65%)	73±2 (64±2%)	42±2 (36±2%)	1	8
All	All	1150/1770 (65%)	732 (64%)	418 (36%)	1	8

All 71 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	174	LEU	10
1	A	138	LEU	10
1	A	91	CYS	10
1	A	93	THR	10
1	A	114	HIS	10
1	A	100	SER	10
1	A	136	ARG	10
1	A	32	TYR	10
1	A	83	LEU	10
1	A	135	LEU	10
1	A	42	TRP	10
1	A	78	PHE	10
1	A	72	PHE	10
1	A	144	LYS	10
1	A	30	LEU	10
1	A	159	THR	10
1	A	121	THR	10
1	A	189	LEU	10
1	A	117	LEU	10
1	A	107	LYS	10
1	A	51	PHE	10
1	A	116	SER	10
1	A	52	LEU	10

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Mol	Chain	Res	Type	Models (Total)
1	A	113	LYS	9
1	A	71	CYS	8
1	A	104	GLU	8
1	A	88	ARG	8
1	A	152	GLU	8
1	A	178	SER	8
1	A	188	ILE	7
1	A	76	ILE	7
1	A	155	HIS	6
1	A	111	LYS	6
1	A	29	TYR	6
1	A	112	ASN	6
1	A	120	LYS	6
1	A	180	ASP	6
1	A	66	ARG	5
1	A	185	LEU	5
1	A	186	ARG	5
1	A	137	THR	5
1	A	70	LEU	5
1	A	132	GLN	4
1	A	89	VAL	4
1	A	96	SER	4
1	A	84	ASP	4
1	A	171	TRP	3
1	A	69	GLU	3
1	A	158	ASP	3
1	A	37	MET	3
1	A	55	GLN	3
1	A	190	GLN	3
1	A	148	MET	3
1	A	153	PHE	3
1	A	31	CYS	2
1	A	172	ASP	2
1	A	85	GLN	2
1	A	94	SER	2
1	A	28	THR	2
1	A	184	ARG	2
1	A	154	LYS	2
1	A	103	GLN	1
1	A	81	LEU	1
1	A	36	ARG	1
1	A	67	HIS	1

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Mol	Chain	Res	Type	Models (Total)
1	A	35	GLU	1
1	A	79	TRP	1
1	A	146	SER	1
1	A	123	ARG	1
1	A	124	ILE	1
1	A	33	GLU	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](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

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