



Full wwPDB NMR Structure Validation Report ⓘ

Apr 27, 2016 – 05:10 AM BST

PDB ID : 2RPC
Title : Solution structure of the tandem zf-C2H2 domains from the human zinc finger protein ZIC 3
Authors : Tomizawa, T.; Kigawa, T.; Yokoyama, S.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on : 2008-05-14

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

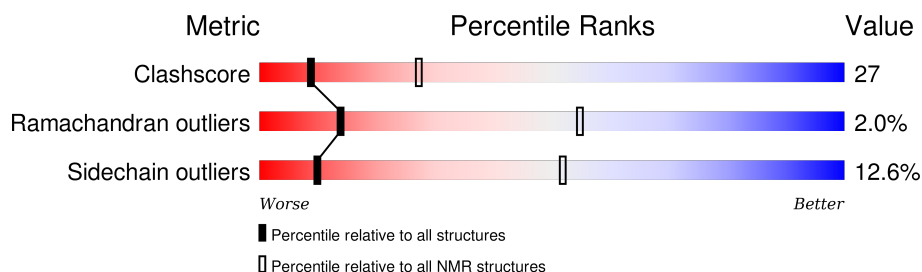
1 Overall quality at a glance

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	155	

2 Ensemble composition and analysis ⓘ

This entry contains 20 models. Model 7 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *fewest violations*.

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:12-A:86 (75)	0.34	7
2	A:91-A:113 (23)	0.17	3
3	A:121-A:145 (25)	0.13	13

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 4 clusters and 2 single-model clusters were found.

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

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2416 atoms, of which 1182 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Zinc finger protein ZIC 3.

Mol	Chain	Residues	Atoms						Trace
1	A	155	Total	C	H	N	O	S	0
			2412	761	1182	232	226	11	

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	EXPRESSION TAG	UNP O60481
A	2	SER	-	EXPRESSION TAG	UNP O60481
A	3	SER	-	EXPRESSION TAG	UNP O60481
A	4	GLY	-	EXPRESSION TAG	UNP O60481
A	5	SER	-	EXPRESSION TAG	UNP O60481
A	6	SER	-	EXPRESSION TAG	UNP O60481
A	7	GLY	-	EXPRESSION TAG	UNP O60481
A	150	SER	-	EXPRESSION TAG	UNP O60481
A	151	GLY	-	EXPRESSION TAG	UNP O60481
A	152	PRO	-	EXPRESSION TAG	UNP O60481
A	153	SER	-	EXPRESSION TAG	UNP O60481
A	154	SER	-	EXPRESSION TAG	UNP O60481
A	155	GLY	-	EXPRESSION TAG	UNP O60481

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

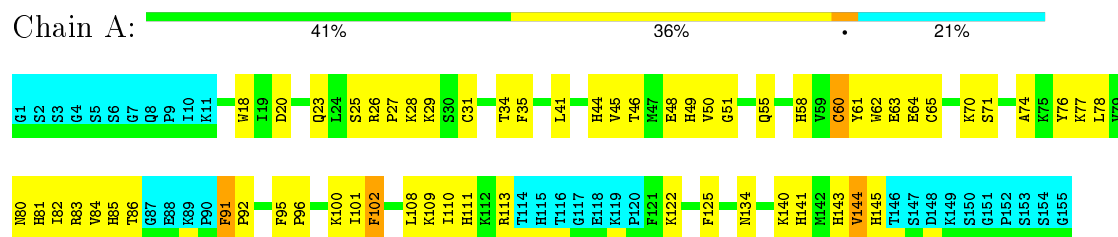
Mol	Chain	Residues	Atoms	
2	A	4	Total	Zn
			4	4

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: Zinc finger protein ZIC 3

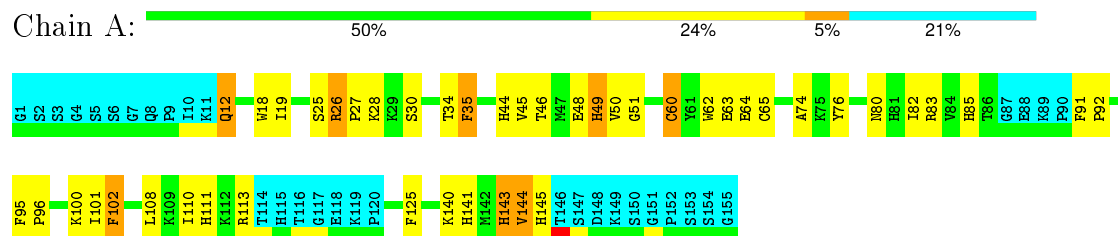


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

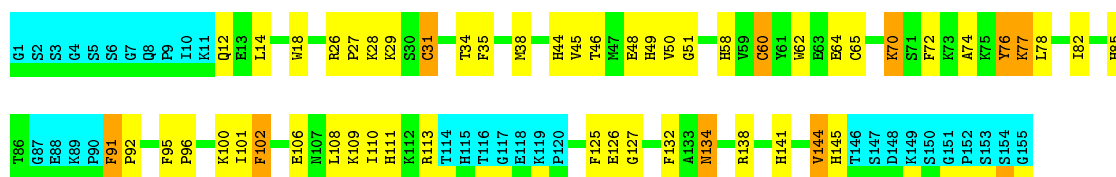
- Molecule 1: Zinc finger protein ZIC 3



4.2.2 Score per residue for model 2

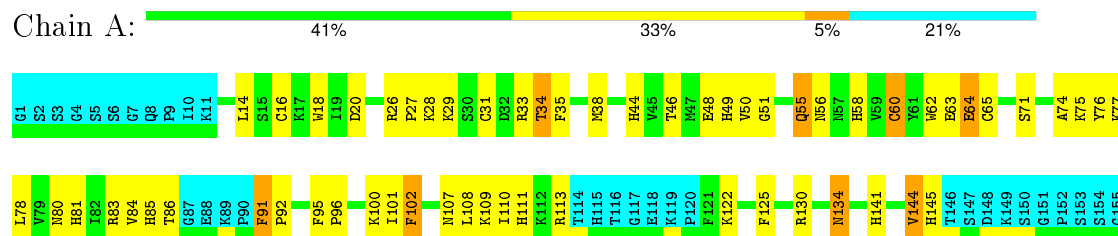
- Molecule 1: Zinc finger protein ZIC 3





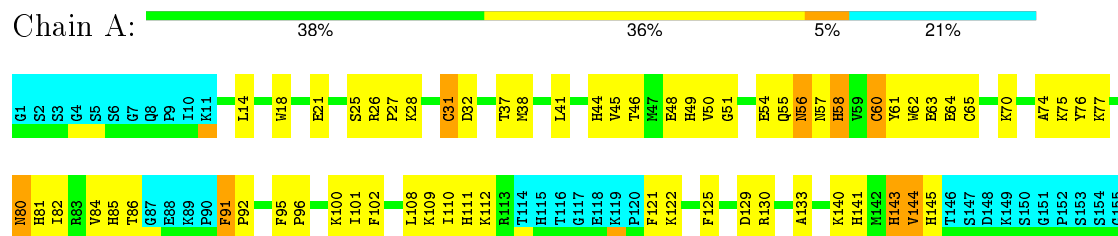
4.2.3 Score per residue for model 3

- Molecule 1: Zinc finger protein ZIC 3



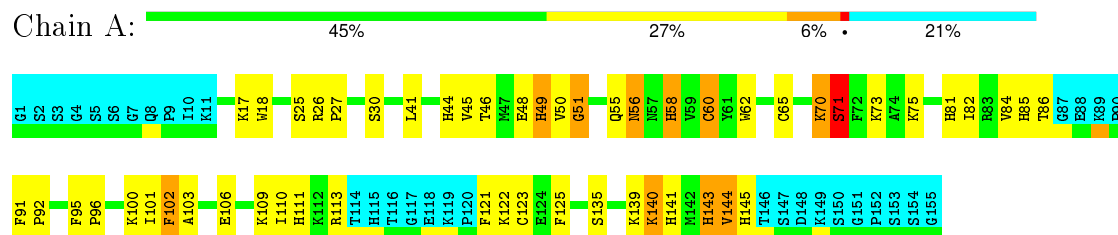
4.2.4 Score per residue for model 4

- Molecule 1: Zinc finger protein ZIC 3



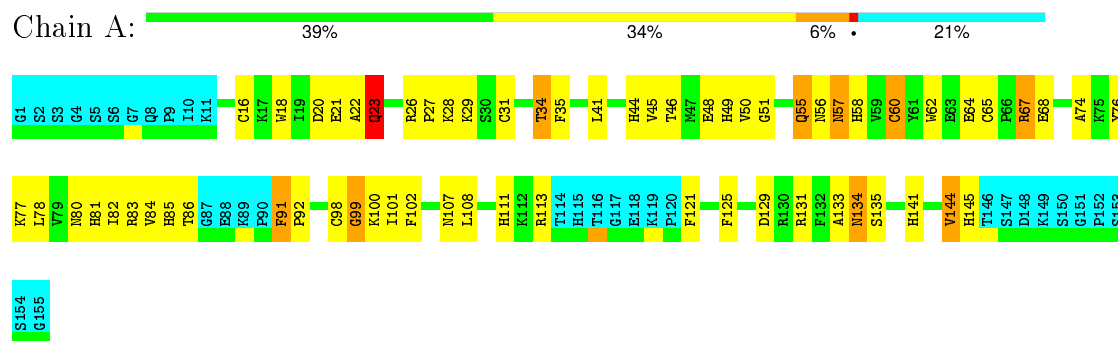
4.2.5 Score per residue for model 5

- Molecule 1: Zinc finger protein ZIC 3



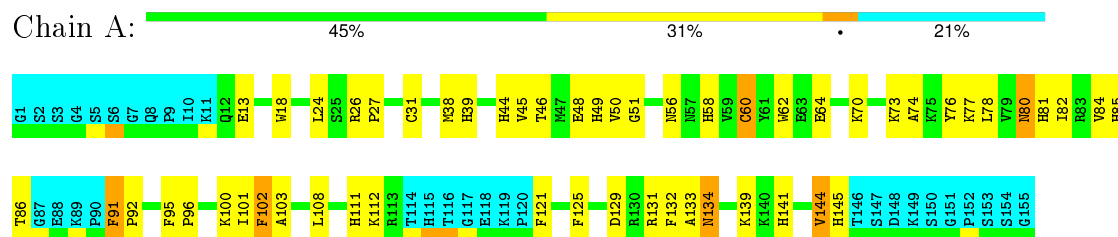
4.2.6 Score per residue for model 6

- Molecule 1: Zinc finger protein ZIC 3



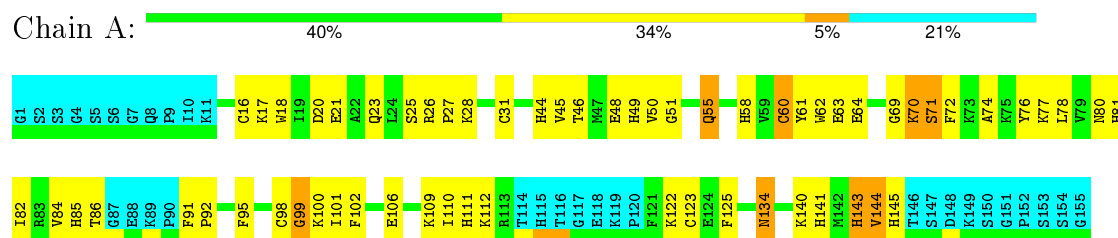
4.2.7 Score per residue for model 7 (medoid)

- Molecule 1: Zinc finger protein ZIC 3



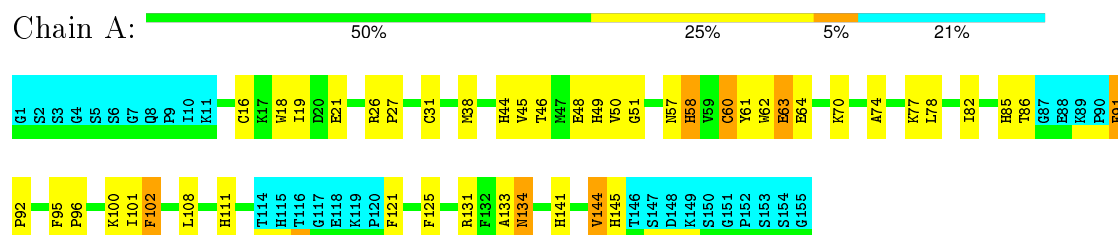
4.2.8 Score per residue for model 8

- Molecule 1: Zinc finger protein ZIC 3



4.2.9 Score per residue for model 9

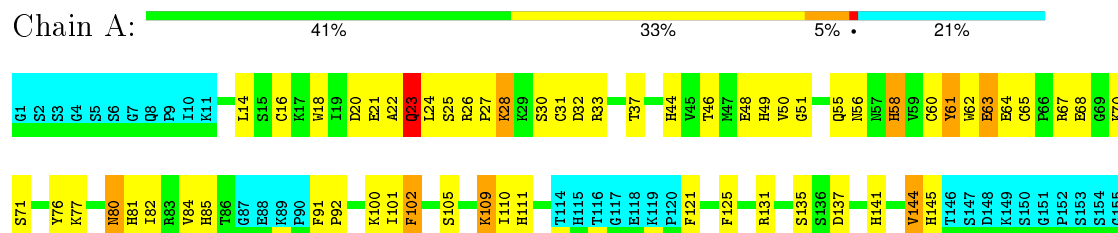
- Molecule 1: Zinc finger protein ZIC 3





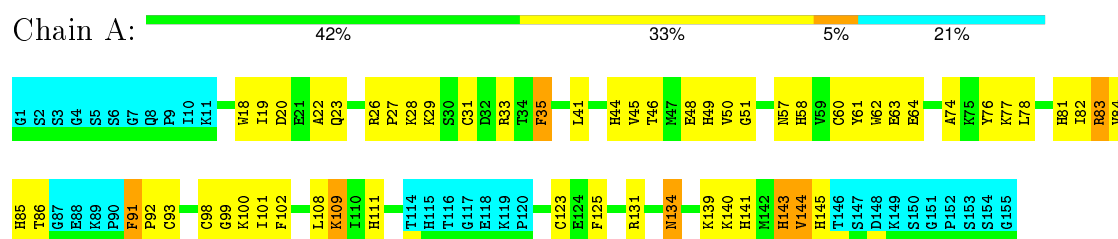
4.2.14 Score per residue for model 14

- Molecule 1: Zinc finger protein ZIC 3



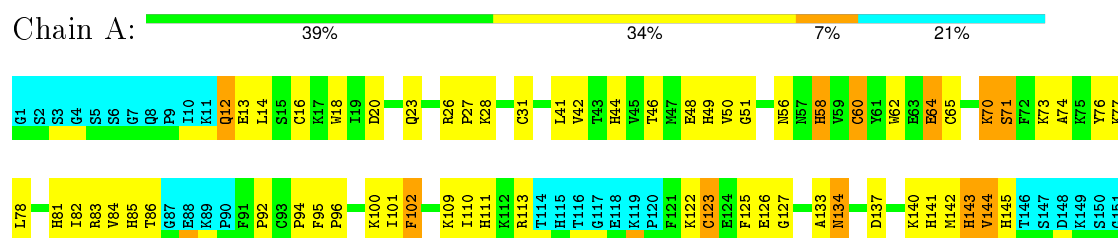
4.2.15 Score per residue for model 15

- Molecule 1: Zinc finger protein ZIC 3



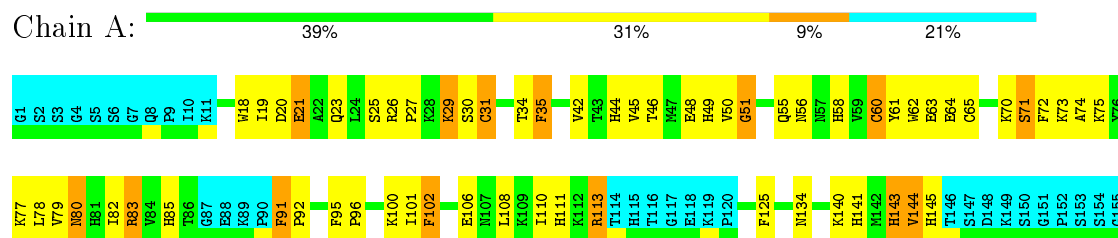
4.2.16 Score per residue for model 16

- Molecule 1: Zinc finger protein ZIC 3



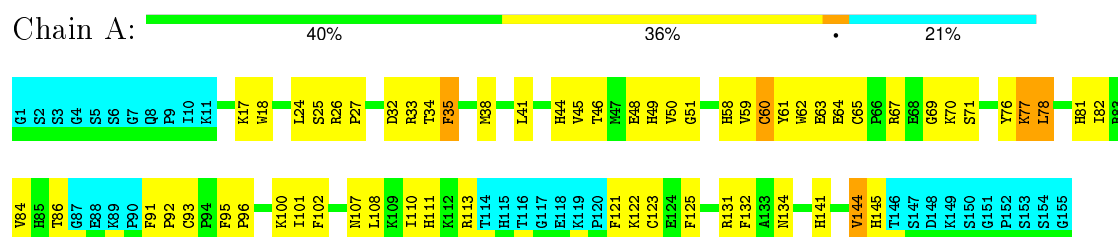
4.2.17 Score per residue for model 17

- Molecule 1: Zinc finger protein ZIC 3



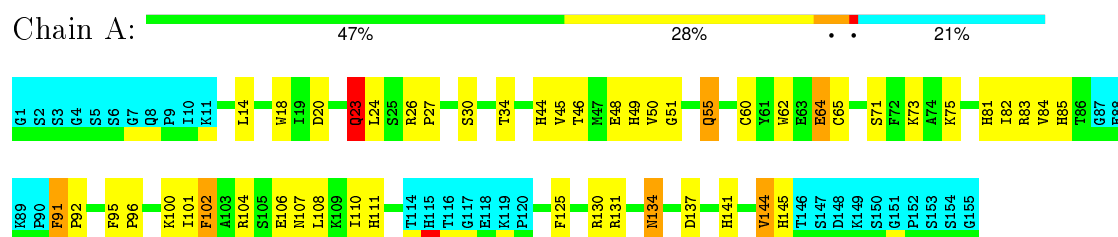
4.2.18 Score per residue for model 18

- Molecule 1: Zinc finger protein ZIC 3



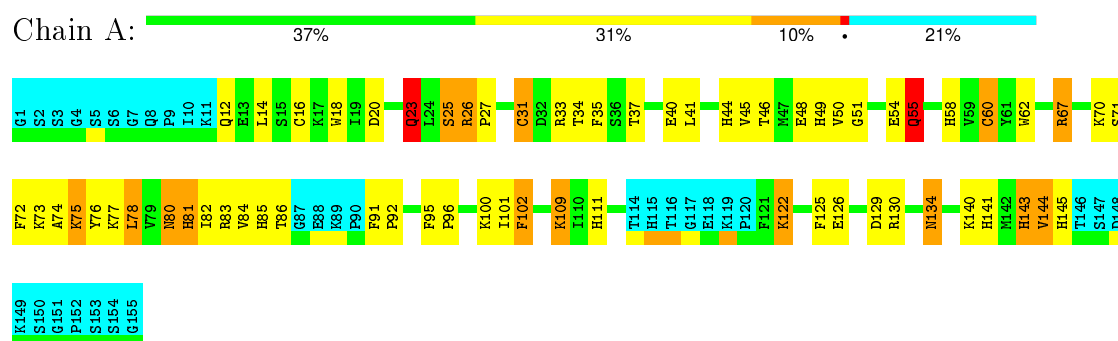
4.2.19 Score per residue for model 19

- Molecule 1: Zinc finger protein ZIC 3



4.2.20 Score per residue for model 20

- Molecule 1: Zinc finger protein ZIC 3



5 Refinement protocol and experimental data overview

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

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

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

Software name	Classification	Version
CYANA	structure solution	
CYANA	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	1016	978	978	55±11
All	All	20400	19560	19560	1095

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 27.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:91:PHE:CE2	1:A:108:LEU:HD23	0.95	1.97	18	1
1:A:78:LEU:O	1:A:78:LEU:HD12	0.88	1.69	18	1
1:A:91:PHE:CD2	1:A:108:LEU:HD23	0.84	2.06	18	1
1:A:81:HIS:O	1:A:84:VAL:HG22	0.84	1.72	10	16
1:A:20:ASP:OD2	1:A:22:ALA:HB3	0.82	1.73	15	1
1:A:14:LEU:O	1:A:34:THR:HG22	0.81	1.75	20	3
1:A:74:ALA:HB3	1:A:77:LYS:HG2	0.80	1.54	16	12
1:A:24:LEU:HD13	1:A:24:LEU:O	0.80	1.76	14	1
1:A:62:TRP:CE3	1:A:85:HIS:CD2	0.79	2.69	20	16
1:A:125:PHE:CD2	1:A:145:HIS:CE1	0.79	2.71	20	18
1:A:92:PRO:O	1:A:108:LEU:HD21	0.78	1.77	9	6
1:A:92:PRO:HA	1:A:101:ILE:HG23	0.76	1.57	7	20

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:78:LEU:HD12	1:A:78:LEU:O	0.76	1.79	20	5
1:A:18:TRP:CG	1:A:49:HIS:CE1	0.75	2.75	8	10
1:A:24:LEU:O	1:A:24:LEU:HD23	0.74	1.82	7	2
1:A:50:VAL:HG21	1:A:82:ILE:HD11	0.74	1.59	18	13
1:A:24:LEU:HD23	1:A:24:LEU:O	0.74	1.82	18	2
1:A:38:MET:CE	1:A:41:LEU:HD23	0.74	2.11	18	2
1:A:125:PHE:CG	1:A:145:HIS:CE1	0.74	2.76	20	15
1:A:18:TRP:CE3	1:A:49:HIS:CD2	0.73	2.76	10	13
1:A:75:LYS:O	1:A:79:VAL:HG23	0.71	1.85	17	1
1:A:45:VAL:CG1	1:A:82:ILE:HG21	0.70	2.17	5	16
1:A:91:PHE:CE2	1:A:108:LEU:CD2	0.69	2.75	18	1
1:A:106:GLU:OE2	1:A:110:ILE:HD12	0.69	1.86	11	1
1:A:74:ALA:HB3	1:A:77:LYS:CG	0.69	2.18	17	9
1:A:35:PHE:CE1	1:A:41:LEU:HD13	0.68	2.24	18	2
1:A:12:GLN:NE2	1:A:14:LEU:HD21	0.68	2.03	20	1
1:A:42:VAL:HG11	1:A:83:ARG:NH1	0.68	2.03	16	1
1:A:45:VAL:HG11	1:A:82:ILE:CG2	0.66	2.20	6	16
1:A:76:TYR:CE1	1:A:77:LYS:CD	0.65	2.79	16	4
1:A:76:TYR:CE2	1:A:77:LYS:CD	0.65	2.79	8	5
1:A:78:LEU:C	1:A:78:LEU:HD12	0.64	2.13	18	1
1:A:58:HIS:HB3	1:A:78:LEU:HD23	0.64	1.70	3	6
1:A:59:VAL:CG1	1:A:61:TYR:CZ	0.64	2.80	18	3
1:A:34:THR:C	1:A:35:PHE:CD1	0.64	2.71	17	5
1:A:83:ARG:N	1:A:83:ARG:NE	0.64	2.46	17	1
1:A:38:MET:SD	1:A:86:THR:HG21	0.64	2.33	12	5
1:A:55:GLN:HE21	1:A:55:GLN:N	0.62	1.92	19	1
1:A:19:ILE:HG23	1:A:23:GLN:HE22	0.62	1.54	10	2
1:A:125:PHE:CD1	1:A:145:HIS:CG	0.62	2.87	20	4
1:A:102:PHE:CZ	1:A:111:HIS:CG	0.62	2.88	18	18
1:A:130:ARG:NH1	1:A:141:HIS:CE1	0.61	2.68	19	1
1:A:106:GLU:O	1:A:110:ILE:HD12	0.61	1.96	5	1
1:A:91:PHE:CD1	1:A:91:PHE:N	0.61	2.67	17	2
1:A:67:ARG:NH2	1:A:72:PHE:CE2	0.60	2.69	20	1
1:A:140:LYS:O	1:A:143:HIS:CD2	0.60	2.55	5	10
1:A:91:PHE:N	1:A:91:PHE:CD1	0.60	2.69	19	3
1:A:33:ARG:CG	1:A:35:PHE:CZ	0.60	2.85	18	1
1:A:67:ARG:NH2	1:A:72:PHE:CD2	0.60	2.69	20	1
1:A:58:HIS:HB2	1:A:78:LEU:HD23	0.59	1.73	16	2
1:A:102:PHE:CD1	1:A:102:PHE:N	0.59	2.69	3	8
1:A:18:TRP:CD2	1:A:49:HIS:CE1	0.59	2.89	19	6
1:A:102:PHE:N	1:A:102:PHE:CD1	0.59	2.71	13	11

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:67:ARG:HH22	1:A:78:LEU:HD13	0.58	1.57	20	1
1:A:102:PHE:CZ	1:A:111:HIS:CD2	0.58	2.92	14	16
1:A:83:ARG:N	1:A:83:ARG:HE	0.58	1.96	17	1
1:A:50:VAL:HG12	1:A:50:VAL:O	0.57	1.99	17	12
1:A:50:VAL:O	1:A:50:VAL:HG12	0.57	1.99	14	6
1:A:45:VAL:HG11	1:A:82:ILE:HG21	0.57	1.76	5	7
1:A:134:ASN:ND2	1:A:134:ASN:N	0.57	2.53	6	7
1:A:35:PHE:N	1:A:35:PHE:CD1	0.57	2.72	17	4
1:A:125:PHE:CD1	1:A:145:HIS:CE1	0.57	2.93	18	2
1:A:83:ARG:CA	1:A:83:ARG:NE	0.56	2.68	17	1
1:A:76:TYR:CE2	1:A:77:LYS:HD3	0.56	2.36	8	1
1:A:91:PHE:CD2	1:A:108:LEU:CD2	0.56	2.85	18	1
1:A:76:TYR:CE2	1:A:77:LYS:HD2	0.56	2.36	8	4
1:A:58:HIS:CB	1:A:78:LEU:HD23	0.56	2.30	20	2
1:A:41:LEU:CD2	1:A:86:THR:HG22	0.56	2.30	10	4
1:A:35:PHE:CE1	1:A:41:LEU:CD1	0.56	2.89	18	1
1:A:108:LEU:HD11	1:A:112:LYS:HD2	0.56	1.77	4	1
1:A:59:VAL:HG11	1:A:61:TYR:CZ	0.56	2.36	10	3
1:A:134:ASN:N	1:A:134:ASN:ND2	0.55	2.54	19	5
1:A:76:TYR:CE1	1:A:77:LYS:HD2	0.55	2.36	16	2
1:A:64:GLU:CG	1:A:64:GLU:O	0.55	2.54	12	2
1:A:45:VAL:HG12	1:A:82:ILE:HD13	0.55	1.77	17	8
1:A:41:LEU:HD23	1:A:86:THR:HG22	0.55	1.79	16	1
1:A:141:HIS:CG	1:A:141:HIS:O	0.54	2.60	19	13
1:A:41:LEU:HD21	1:A:86:THR:HG22	0.54	1.78	20	2
1:A:109:LYS:CG	1:A:110:ILE:N	0.54	2.71	3	8
1:A:55:GLN:N	1:A:55:GLN:CD	0.54	2.61	3	3
1:A:100:LYS:HG3	1:A:102:PHE:CE1	0.54	2.38	18	20
1:A:62:TRP:O	1:A:64:GLU:N	0.54	2.41	11	13
1:A:141:HIS:O	1:A:141:HIS:CG	0.54	2.60	18	7
1:A:18:TRP:CE3	1:A:49:HIS:CG	0.54	2.96	11	12
1:A:33:ARG:HG3	1:A:35:PHE:CZ	0.54	2.37	18	2
1:A:101:ILE:C	1:A:102:PHE:CD1	0.54	2.81	13	3
1:A:100:LYS:HG2	1:A:102:PHE:CZ	0.54	2.38	4	17
1:A:83:ARG:CD	1:A:83:ARG:N	0.53	2.72	11	1
1:A:34:THR:O	1:A:35:PHE:CD1	0.53	2.61	6	2
1:A:100:LYS:HG3	1:A:102:PHE:CZ	0.53	2.39	8	2
1:A:44:HIS:O	1:A:48:GLU:N	0.53	2.42	18	20
1:A:45:VAL:CG1	1:A:82:ILE:CG2	0.53	2.87	10	11
1:A:18:TRP:CD2	1:A:49:HIS:ND1	0.53	2.76	13	6
1:A:67:ARG:HG2	1:A:81:HIS:CE1	0.53	2.39	10	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:55:GLN:CD	1:A:55:GLN:N	0.53	2.61	8	1
1:A:91:PHE:HD1	1:A:108:LEU:HD23	0.53	1.63	9	2
1:A:74:ALA:HB3	1:A:77:LYS:HG3	0.53	1.81	2	1
1:A:18:TRP:CB	1:A:49:HIS:NE2	0.53	2.72	10	6
1:A:12:GLN:HE21	1:A:14:LEU:HD21	0.53	1.63	20	1
1:A:18:TRP:CB	1:A:49:HIS:CE1	0.52	2.92	2	8
1:A:61:TYR:CE2	1:A:69:GLY:HA2	0.52	2.40	10	3
1:A:58:HIS:CE1	1:A:75:LYS:HG2	0.52	2.39	3	2
1:A:143:HIS:ND1	1:A:144:VAL:N	0.52	2.58	16	9
1:A:19:ILE:HD12	1:A:63:GLU:CD	0.52	2.25	9	1
1:A:134:ASN:HD22	1:A:134:ASN:N	0.51	2.03	20	4
1:A:100:LYS:CG	1:A:102:PHE:CE1	0.51	2.93	14	5
1:A:16:CYS:SG	1:A:45:VAL:HG22	0.51	2.46	20	1
1:A:64:GLU:N	1:A:64:GLU:OE1	0.51	2.44	19	1
1:A:13:GLU:CD	1:A:14:LEU:N	0.51	2.64	12	1
1:A:46:THR:O	1:A:51:GLY:N	0.51	2.44	16	20
1:A:67:ARG:CG	1:A:81:HIS:CE1	0.51	2.94	10	2
1:A:91:PHE:CD1	1:A:108:LEU:HD23	0.51	2.41	3	5
1:A:74:ALA:CB	1:A:76:TYR:CE1	0.51	2.93	2	3
1:A:76:TYR:CE1	1:A:77:LYS:HD3	0.51	2.40	16	3
1:A:50:VAL:CG1	1:A:50:VAL:O	0.50	2.59	3	12
1:A:58:HIS:CE1	1:A:75:LYS:HE3	0.50	2.41	20	1
1:A:121:PHE:CD2	1:A:133:ALA:O	0.50	2.64	7	2
1:A:94:PRO:O	1:A:133:ALA:HB1	0.50	2.06	16	1
1:A:50:VAL:O	1:A:50:VAL:CG1	0.50	2.59	1	8
1:A:76:TYR:CD2	1:A:77:LYS:HD2	0.50	2.42	8	1
1:A:100:LYS:CG	1:A:102:PHE:CZ	0.50	2.95	8	14
1:A:67:ARG:O	1:A:69:GLY:N	0.50	2.45	11	1
1:A:13:GLU:OE1	1:A:14:LEU:N	0.50	2.45	12	1
1:A:44:HIS:ND1	1:A:48:GLU:CB	0.50	2.75	20	20
1:A:23:GLN:OE1	1:A:28:LYS:CD	0.50	2.60	10	1
1:A:98:CYS:O	1:A:100:LYS:N	0.50	2.45	15	4
1:A:144:VAL:O	1:A:144:VAL:CG2	0.49	2.60	9	13
1:A:18:TRP:CH2	1:A:60:CYS:HA	0.49	2.42	20	17
1:A:110:ILE:O	1:A:113:ARG:CG	0.49	2.60	3	10
1:A:102:PHE:CD1	1:A:108:LEU:HD13	0.49	2.41	13	5
1:A:45:VAL:HG12	1:A:82:ILE:HG21	0.49	1.84	5	3
1:A:143:HIS:C	1:A:143:HIS:ND1	0.49	2.65	17	6
1:A:28:LYS:CB	1:A:28:LYS:NZ	0.49	2.76	14	1
1:A:143:HIS:ND1	1:A:143:HIS:C	0.49	2.66	15	4
1:A:94:PRO:O	1:A:133:ALA:CB	0.49	2.61	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:20:ASP:O	1:A:23:GLN:N	0.49	2.45	20	5
1:A:58:HIS:CB	1:A:78:LEU:CD2	0.49	2.91	6	1
1:A:76:TYR:CD1	1:A:77:LYS:N	0.49	2.81	18	2
1:A:78:LEU:HD12	1:A:78:LEU:C	0.49	2.28	20	1
1:A:64:GLU:OE1	1:A:64:GLU:N	0.49	2.45	16	1
1:A:74:ALA:HB3	1:A:76:TYR:CE1	0.49	2.42	15	1
1:A:95:PHE:CD1	1:A:96:PRO:HD2	0.49	2.43	9	15
1:A:121:PHE:O	1:A:132:PHE:N	0.49	2.46	18	3
1:A:58:HIS:CE1	1:A:75:LYS:CG	0.49	2.95	3	1
1:A:144:VAL:CG2	1:A:144:VAL:O	0.49	2.60	5	5
1:A:59:VAL:HB	1:A:61:TYR:CE1	0.49	2.43	10	3
1:A:18:TRP:CZ3	1:A:49:HIS:HB3	0.49	2.43	20	8
1:A:74:ALA:HB1	1:A:76:TYR:CE1	0.49	2.42	6	2
1:A:92:PRO:CA	1:A:101:ILE:HG23	0.49	2.38	18	3
1:A:21:GLU:HG3	1:A:61:TYR:CD2	0.49	2.42	8	3
1:A:67:ARG:O	1:A:70:LYS:N	0.48	2.46	11	2
1:A:91:PHE:O	1:A:108:LEU:CD2	0.48	2.60	18	4
1:A:93:CYS:N	1:A:100:LYS:O	0.48	2.45	15	2
1:A:21:GLU:HG2	1:A:61:TYR:CD2	0.48	2.42	17	2
1:A:19:ILE:CD1	1:A:63:GLU:CD	0.48	2.82	9	1
1:A:76:TYR:CE1	1:A:77:LYS:HG2	0.48	2.44	20	1
1:A:74:ALA:HB3	1:A:77:LYS:CB	0.48	2.38	17	1
1:A:27:PRO:O	1:A:29:LYS:CD	0.48	2.61	11	1
1:A:33:ARG:HG2	1:A:35:PHE:CZ	0.48	2.44	18	2
1:A:109:LYS:NZ	1:A:109:LYS:CB	0.47	2.76	14	1
1:A:38:MET:SD	1:A:86:THR:CG2	0.47	3.02	9	3
1:A:26:ARG:HA	1:A:27:PRO:C	0.47	2.30	7	20
1:A:83:ARG:HD2	1:A:83:ARG:N	0.47	2.23	11	1
1:A:69:GLY:O	1:A:71:SER:N	0.47	2.47	8	1
1:A:72:PHE:CE1	1:A:78:LEU:HD13	0.47	2.44	13	1
1:A:62:TRP:CH2	1:A:85:HIS:HB3	0.47	2.45	6	3
1:A:58:HIS:O	1:A:78:LEU:HD22	0.47	2.10	8	2
1:A:18:TRP:CZ2	1:A:60:CYS:HA	0.47	2.45	20	6
1:A:130:ARG:NE	1:A:141:HIS:CE1	0.47	2.83	3	1
1:A:129:ASP:O	1:A:130:ARG:CD	0.47	2.63	20	2
1:A:74:ALA:HB3	1:A:77:LYS:HB2	0.47	1.86	17	1
1:A:74:ALA:HB1	1:A:76:TYR:CE2	0.47	2.45	20	2
1:A:76:TYR:CD1	1:A:76:TYR:C	0.46	2.88	20	1
1:A:126:GLU:CD	1:A:127:GLY:N	0.46	2.68	16	2
1:A:70:LYS:O	1:A:72:PHE:CE1	0.46	2.68	17	1
1:A:70:LYS:CG	1:A:70:LYS:O	0.46	2.61	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:27:PRO:O	1:A:28:LYS:C	0.46	2.53	1	5
1:A:54:GLU:O	1:A:54:GLU:CG	0.46	2.63	4	1
1:A:38:MET:HE3	1:A:41:LEU:HD23	0.46	1.87	18	1
1:A:72:PHE:CD1	1:A:72:PHE:N	0.46	2.84	8	2
1:A:62:TRP:CB	1:A:65:CYS:HB2	0.46	2.41	11	14
1:A:58:HIS:H	1:A:58:HIS:CD2	0.46	2.28	4	1
1:A:62:TRP:CZ2	1:A:85:HIS:HB3	0.46	2.46	16	2
1:A:31:CYS:SG	1:A:33:ARG:CB	0.46	3.04	20	1
1:A:67:ARG:NE	1:A:67:ARG:N	0.46	2.63	6	1
1:A:77:LYS:O	1:A:80:ASN:ND2	0.46	2.48	4	2
1:A:108:LEU:CD1	1:A:112:LYS:CD	0.46	2.94	4	1
1:A:21:GLU:HG3	1:A:61:TYR:CD1	0.46	2.46	12	1
1:A:41:LEU:O	1:A:45:VAL:HG23	0.45	2.12	5	2
1:A:20:ASP:O	1:A:23:GLN:NE2	0.45	2.50	16	1
1:A:44:HIS:CG	1:A:48:GLU:HB2	0.45	2.46	20	18
1:A:20:ASP:O	1:A:23:GLN:CD	0.45	2.55	6	6
1:A:80:ASN:OD1	1:A:80:ASN:C	0.45	2.55	14	2
1:A:67:ARG:O	1:A:68:GLU:C	0.45	2.55	11	1
1:A:63:GLU:CD	1:A:64:GLU:OE1	0.45	2.55	4	1
1:A:70:LYS:O	1:A:71:SER:C	0.45	2.55	20	4
1:A:65:CYS:SG	1:A:67:ARG:CG	0.45	3.04	18	1
1:A:132:PHE:CD2	1:A:138:ARG:HA	0.45	2.46	2	1
1:A:134:ASN:OD1	1:A:137:ASP:CG	0.45	2.55	10	3
1:A:80:ASN:C	1:A:80:ASN:OD1	0.45	2.55	13	5
1:A:125:PHE:CE1	1:A:145:HIS:HB3	0.45	2.46	4	2
1:A:59:VAL:CG1	1:A:69:GLY:O	0.45	2.65	18	1
1:A:13:GLU:CD	1:A:13:GLU:C	0.45	2.75	12	1
1:A:58:HIS:ND1	1:A:75:LYS:CD	0.45	2.79	4	1
1:A:20:ASP:O	1:A:23:GLN:CG	0.45	2.65	15	1
1:A:62:TRP:C	1:A:64:GLU:N	0.45	2.69	18	15
1:A:74:ALA:HB1	1:A:76:TYR:CD2	0.45	2.47	20	1
1:A:106:GLU:HG2	1:A:110:ILE:HD12	0.45	1.87	8	1
1:A:35:PHE:CD1	1:A:40:GLU:HB3	0.45	2.46	20	1
1:A:121:PHE:CE2	1:A:135:SER:HB3	0.44	2.46	14	1
1:A:72:PHE:CD1	1:A:78:LEU:HB2	0.44	2.46	10	2
1:A:109:LYS:HG3	1:A:110:ILE:N	0.44	2.27	4	2
1:A:54:GLU:O	1:A:54:GLU:CD	0.44	2.55	4	1
1:A:50:VAL:HG21	1:A:82:ILE:CD1	0.44	2.38	18	1
1:A:121:PHE:CE1	1:A:135:SER:HB2	0.44	2.46	6	1
1:A:67:ARG:O	1:A:68:GLU:CB	0.44	2.65	14	2
1:A:20:ASP:O	1:A:22:ALA:N	0.44	2.51	6	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:121:PHE:CD2	1:A:133:ALA:C	0.44	2.91	7	2
1:A:12:GLN:NE2	1:A:13:GLU:O	0.44	2.50	16	1
1:A:122:LYS:O	1:A:123:CYS:C	0.44	2.56	8	6
1:A:62:TRP:CZ3	1:A:85:HIS:CD2	0.44	3.05	20	1
1:A:20:ASP:O	1:A:21:GLU:C	0.43	2.56	14	2
1:A:106:GLU:HG3	1:A:110:ILE:CD1	0.43	2.43	17	1
1:A:80:ASN:O	1:A:83:ARG:CG	0.43	2.66	20	4
1:A:58:HIS:HB3	1:A:78:LEU:CD2	0.43	2.43	6	1
1:A:56:ASN:OD1	1:A:57:ASN:N	0.43	2.51	6	1
1:A:106:GLU:O	1:A:110:ILE:CD1	0.43	2.66	5	1
1:A:35:PHE:CE2	1:A:41:LEU:HA	0.43	2.48	12	1
1:A:83:ARG:CZ	1:A:83:ARG:HB3	0.43	2.42	15	1
1:A:14:LEU:HD11	1:A:37:THR:O	0.43	2.13	13	5
1:A:38:MET:SD	1:A:41:LEU:HD23	0.43	2.54	4	1
1:A:20:ASP:OD1	1:A:20:ASP:C	0.43	2.56	17	1
1:A:55:GLN:O	1:A:56:ASN:C	0.43	2.57	5	2
1:A:58:HIS:CE1	1:A:75:LYS:HD3	0.43	2.49	17	1
1:A:123:CYS:SG	1:A:125:PHE:CB	0.43	3.07	8	3
1:A:70:LYS:O	1:A:72:PHE:CD1	0.43	2.72	17	1
1:A:50:VAL:CG2	1:A:82:ILE:HD11	0.43	2.44	1	1
1:A:30:SER:O	1:A:31:CYS:C	0.43	2.56	17	1
1:A:14:LEU:CD1	1:A:37:THR:O	0.43	2.66	14	2
1:A:54:GLU:O	1:A:55:GLN:C	0.43	2.57	11	2
1:A:19:ILE:CG2	1:A:23:GLN:OE1	0.43	2.67	15	1
1:A:98:CYS:O	1:A:99:GLY:C	0.42	2.58	6	3
1:A:50:VAL:O	1:A:55:GLN:NE2	0.42	2.52	17	1
1:A:25:SER:CB	1:A:29:LYS:HD3	0.42	2.44	17	1
1:A:76:TYR:CZ	1:A:77:LYS:HG2	0.42	2.49	20	1
1:A:108:LEU:CD1	1:A:112:LYS:HD2	0.42	2.44	4	1
1:A:35:PHE:CD2	1:A:41:LEU:HA	0.42	2.49	12	1
1:A:12:GLN:O	1:A:12:GLN:NE2	0.42	2.52	1	1
1:A:73:LYS:CG	1:A:73:LYS:O	0.42	2.67	11	1
1:A:93:CYS:CB	1:A:100:LYS:O	0.42	2.67	18	1
1:A:125:PHE:CD2	1:A:145:HIS:CG	0.42	3.07	18	1
1:A:59:VAL:HG11	1:A:61:TYR:OH	0.42	2.14	18	1
1:A:121:PHE:CE2	1:A:133:ALA:O	0.42	2.72	7	1
1:A:83:ARG:HA	1:A:83:ARG:NE	0.42	2.29	15	1
1:A:58:HIS:CD2	1:A:58:HIS:H	0.42	2.31	14	1
1:A:41:LEU:HD12	1:A:45:VAL:HG23	0.42	1.90	20	1
1:A:100:LYS:HE2	1:A:102:PHE:CE2	0.42	2.49	11	1
1:A:67:ARG:CZ	1:A:72:PHE:CE2	0.42	3.02	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:80:ASN:OD1	1:A:81:HIS:N	0.42	2.52	13	1
1:A:33:ARG:HD3	1:A:44:HIS:CE1	0.42	2.49	11	1
1:A:76:TYR:O	1:A:80:ASN:ND2	0.42	2.52	11	1
1:A:14:LEU:HD11	1:A:38:MET:HA	0.42	1.92	2	1
1:A:35:PHE:CD1	1:A:35:PHE:N	0.42	2.87	15	2
1:A:25:SER:O	1:A:26:ARG:NH1	0.42	2.52	20	1
1:A:59:VAL:HB	1:A:61:TYR:CZ	0.42	2.50	10	2
1:A:134:ASN:N	1:A:134:ASN:HD22	0.42	2.11	19	1
1:A:83:ARG:N	1:A:83:ARG:CD	0.42	2.83	17	1
1:A:106:GLU:CG	1:A:110:ILE:CD1	0.42	2.97	17	1
1:A:14:LEU:O	1:A:34:THR:CG2	0.41	2.61	20	1
1:A:61:TYR:N	1:A:61:TYR:CD1	0.41	2.89	14	2
1:A:98:CYS:C	1:A:100:LYS:N	0.41	2.73	8	3
1:A:23:GLN:NE2	1:A:28:LYS:HD3	0.41	2.30	8	1
1:A:45:VAL:HG11	1:A:82:ILE:HG23	0.41	1.92	20	1
1:A:125:PHE:CE2	1:A:145:HIS:ND1	0.41	2.88	4	1
1:A:42:VAL:CG1	1:A:83:ARG:NH1	0.41	2.80	16	1
1:A:67:ARG:C	1:A:69:GLY:N	0.41	2.74	11	1
1:A:102:PHE:CE1	1:A:108:LEU:HD13	0.41	2.50	6	1
1:A:91:PHE:CE2	1:A:108:LEU:CG	0.41	3.03	18	1
1:A:20:ASP:OD1	1:A:21:GLU:N	0.41	2.54	13	1
1:A:61:TYR:CE2	1:A:69:GLY:CA	0.41	3.03	11	1
1:A:62:TRP:O	1:A:63:GLU:C	0.41	2.58	11	2
1:A:106:GLU:HG2	1:A:110:ILE:CD1	0.41	2.46	19	1
1:A:125:PHE:CD2	1:A:145:HIS:ND1	0.41	2.88	4	1
1:A:19:ILE:O	1:A:61:TYR:CB	0.41	2.68	15	1
1:A:132:PHE:CD2	1:A:138:ARG:HB2	0.41	2.51	13	1
1:A:126:GLU:CG	1:A:127:GLY:N	0.41	2.84	2	1
1:A:42:VAL:HG22	1:A:83:ARG:HH22	0.41	1.75	17	1
1:A:58:HIS:C	1:A:78:LEU:CD2	0.41	2.88	20	1
1:A:71:SER:OG	1:A:72:PHE:N	0.41	2.54	8	1
1:A:109:LYS:HD2	1:A:109:LYS:N	0.41	2.31	15	1
1:A:31:CYS:SG	1:A:32:ASP:N	0.40	2.94	13	1
1:A:55:GLN:NE2	1:A:55:GLN:CA	0.40	2.84	6	1
1:A:67:ARG:CD	1:A:67:ARG:N	0.40	2.84	6	1
1:A:69:GLY:O	1:A:70:LYS:C	0.40	2.60	8	1
1:A:63:GLU:OE1	1:A:63:GLU:O	0.40	2.38	9	1
1:A:19:ILE:CG2	1:A:28:LYS:HE2	0.40	2.46	1	1
1:A:14:LEU:CD1	1:A:41:LEU:HB2	0.40	2.47	13	1
1:A:109:LYS:N	1:A:109:LYS:HD2	0.40	2.30	20	1
1:A:14:LEU:HD12	1:A:41:LEU:HB2	0.40	1.92	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:44:HIS:ND1	1:A:48:GLU:HB2	0.40	2.32	5	2
1:A:121:PHE:CE1	1:A:135:SER:OG	0.40	2.63	5	1
1:A:29:LYS:CD	1:A:29:LYS:H	0.40	2.30	10	1
1:A:20:ASP:OD2	1:A:23:GLN:N	0.40	2.54	8	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	123/155 (79%)	109±2 (88±2%)	12±2 (10±2%)	3±1 (2±1%)	14	55
All	All	2460/3100 (79%)	2175 (88%)	235 (10%)	50 (2%)	14	55

All 13 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	63	GLU	12
1	A	71	SER	8
1	A	56	ASN	6
1	A	99	GLY	4
1	A	23	GLN	4
1	A	70	LYS	3
1	A	31	CYS	3
1	A	51	GLY	3
1	A	28	LYS	2
1	A	55	GLN	2
1	A	21	GLU	1
1	A	68	GLU	1
1	A	123	CYS	1

6.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR

entries. The Analysed column shows the number of residues for which the sidechain conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	113/138 (82%)	99±3 (87±2%)	14±3 (13±2%)	10	52
All	All	2260/2760 (82%)	1975 (87%)	285 (13%)	10	52

All 61 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	60	CYS	20
1	A	144	VAL	20
1	A	91	PHE	18
1	A	134	ASN	16
1	A	31	CYS	14
1	A	102	PHE	14
1	A	25	SER	11
1	A	143	HIS	10
1	A	58	HIS	9
1	A	70	LYS	9
1	A	55	GLN	9
1	A	80	ASN	8
1	A	16	CYS	8
1	A	29	LYS	7
1	A	131	ARG	6
1	A	73	LYS	6
1	A	109	LYS	5
1	A	35	PHE	5
1	A	30	SER	5
1	A	28	LYS	4
1	A	122	LYS	4
1	A	23	GLN	4
1	A	57	ASN	4
1	A	107	ASN	4
1	A	75	LYS	4
1	A	64	GLU	3
1	A	26	ARG	3
1	A	12	GLN	3
1	A	126	GLU	3
1	A	83	ARG	3
1	A	17	LYS	3
1	A	32	ASP	3
1	A	139	LYS	3

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Mol	Chain	Res	Type	Models (Total)
1	A	106	GLU	2
1	A	33	ARG	2
1	A	78	LEU	2
1	A	34	THR	2
1	A	49	HIS	2
1	A	129	ASP	2
1	A	77	LYS	2
1	A	71	SER	2
1	A	67	ARG	2
1	A	21	GLU	1
1	A	68	GLU	1
1	A	137	ASP	1
1	A	14	LEU	1
1	A	37	THR	1
1	A	56	ASN	1
1	A	105	SER	1
1	A	39	HIS	1
1	A	140	LYS	1
1	A	76	TYR	1
1	A	113	ARG	1
1	A	104	ARG	1
1	A	63	GLU	1
1	A	13	GLU	1
1	A	142	MET	1
1	A	47	MET	1
1	A	20	ASP	1
1	A	61	TYR	1
1	A	81	HIS	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 carbohydrates in this entry.

6.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 are 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