



Full wwPDB NMR Structure Validation Report ⓘ

Feb 13, 2017 – 02:05 am GMT

PDB ID : 2RMJ
Title : Solution structure of RIG-I C-terminal domain
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Deposited on : 2007-10-23

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
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : trunk28760
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

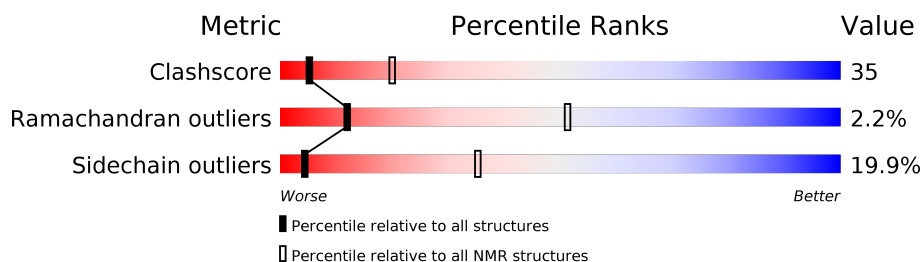
1 Overall quality at a glance

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	125131	11601
Ramachandran outliers	121729	10391
Sidechain outliers	121581	10367

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	134	 30% 50% . . 16%

2 Ensemble composition and analysis

This entry contains 20 models. Model 8 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:805-A:846, A:856-A:925 (112)	0.48	8

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

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

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

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

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 2193 atoms, of which 1094 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Probable ATP-dependent RNA helicase DDX58.

Mol	Chain	Residues	Atoms						Trace
1	A	134	Total	C	H	N	O	S	0
			2193	710	1094	186	195	8	

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: Probable ATP-dependent RNA helicase DDX58

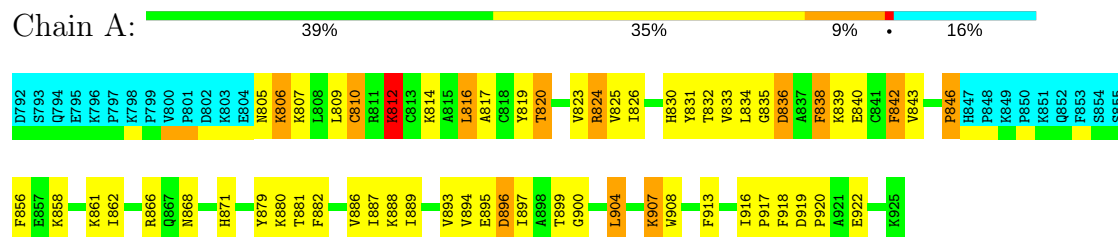


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

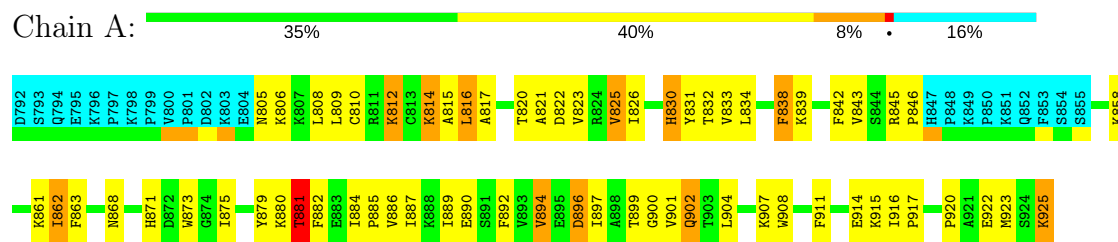
4.2.1 Score per residue for model 1

- Molecule 1: Probable ATP-dependent RNA helicase DDX58



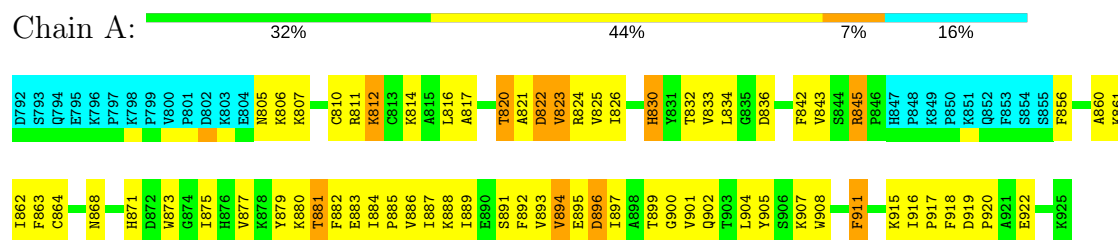
4.2.2 Score per residue for model 2

- Molecule 1: Probable ATP-dependent RNA helicase DDX58



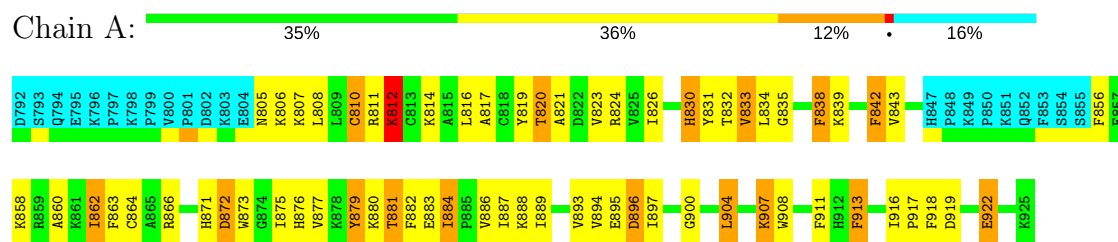
4.2.3 Score per residue for model 3

- Molecule 1: Probable ATP-dependent RNA helicase DDX58



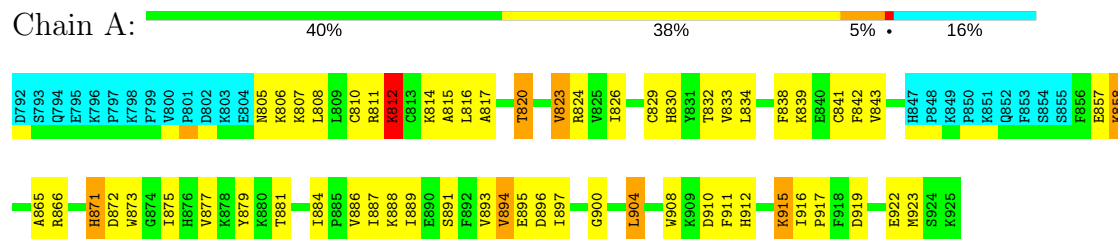
4.2.4 Score per residue for model 4

- Molecule 1: Probable ATP-dependent RNA helicase DDX58



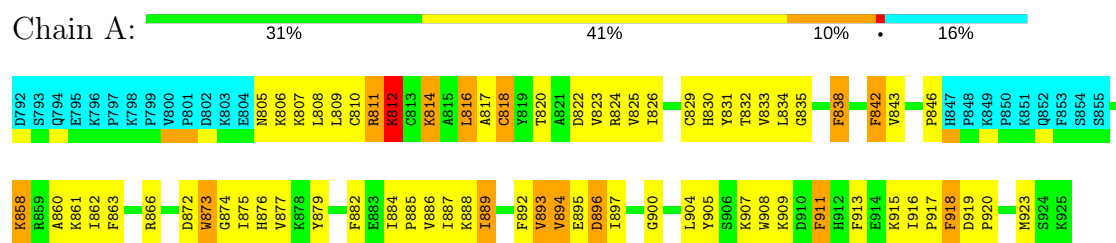
4.2.5 Score per residue for model 5

- Molecule 1: Probable ATP-dependent RNA helicase DDX58



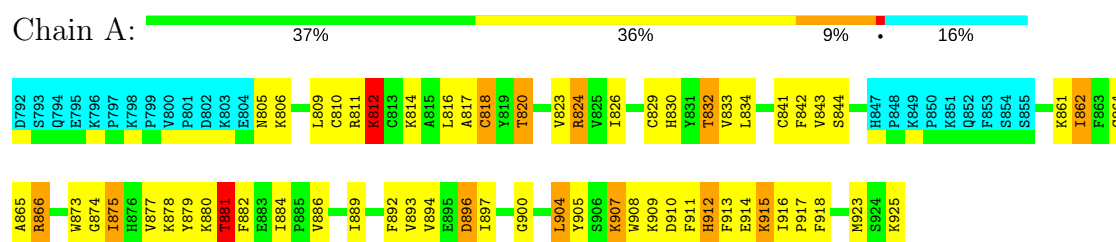
4.2.6 Score per residue for model 6

- Molecule 1: Probable ATP-dependent RNA helicase DDX58



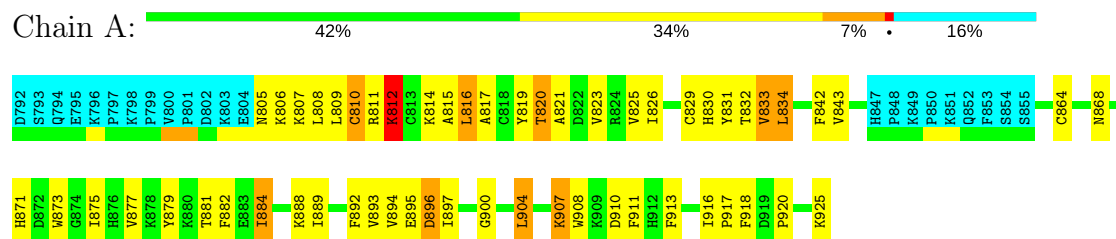
4.2.7 Score per residue for model 7

- Molecule 1: Probable ATP-dependent RNA helicase DDX58



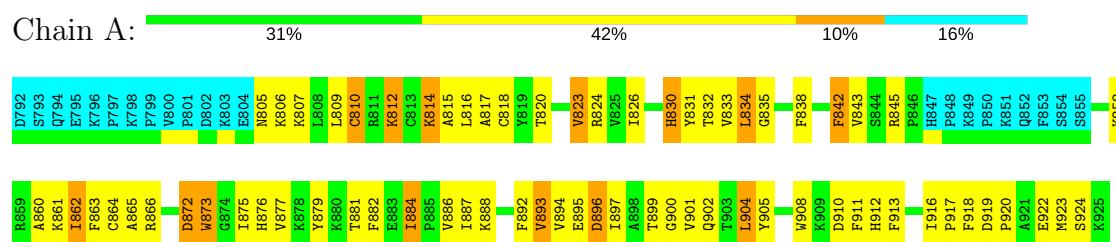
4.2.8 Score per residue for model 8 (medoid)

- Molecule 1: Probable ATP-dependent RNA helicase DDX58



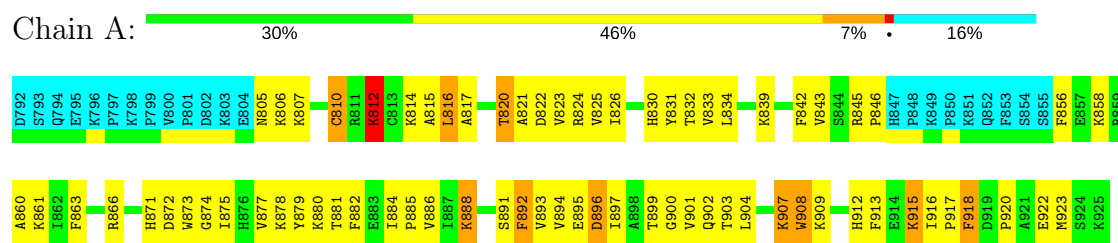
4.2.9 Score per residue for model 9

- Molecule 1: Probable ATP-dependent RNA helicase DDX58



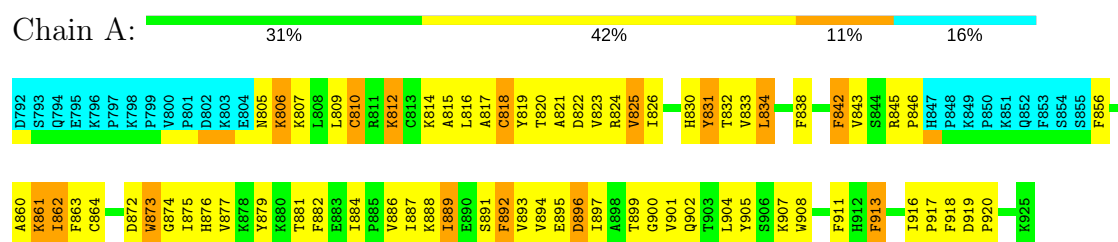
4.2.10 Score per residue for model 10

- Molecule 1: Probable ATP-dependent RNA helicase DDX58



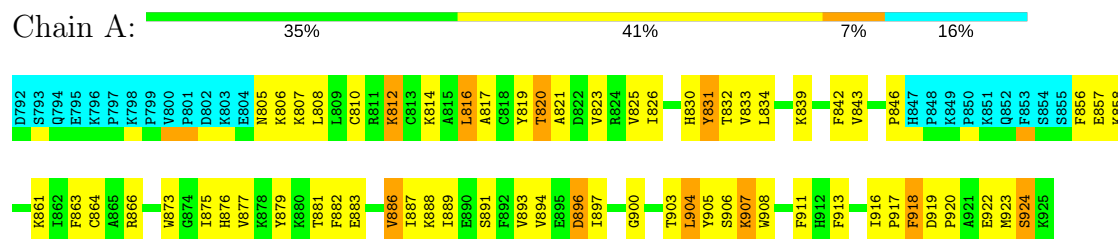
4.2.11 Score per residue for model 11

- Molecule 1: Probable ATP-dependent RNA helicase DDX58



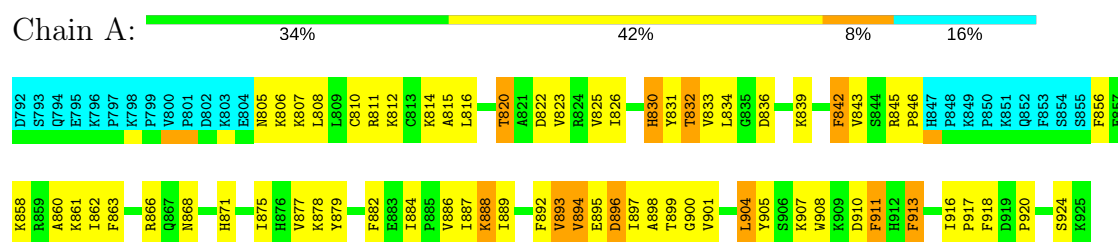
4.2.12 Score per residue for model 12

- Molecule 1: Probable ATP-dependent RNA helicase DDX58



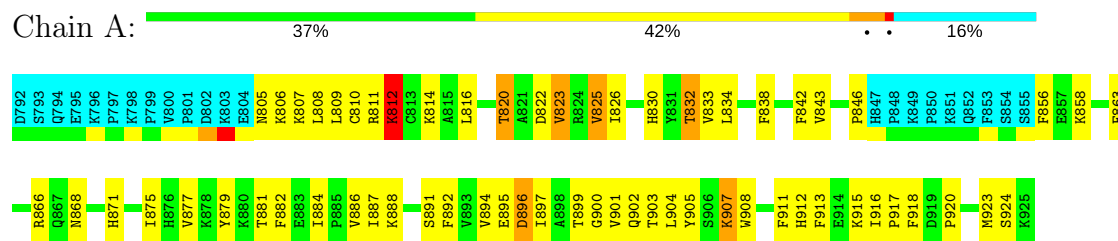
4.2.13 Score per residue for model 13

- Molecule 1: Probable ATP-dependent RNA helicase DDX58



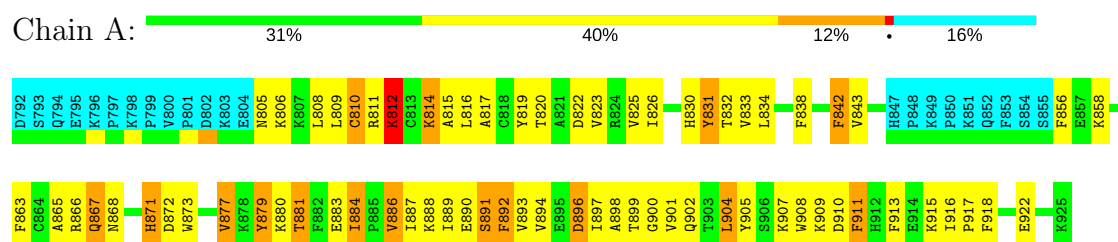
4.2.14 Score per residue for model 14

- Molecule 1: Probable ATP-dependent RNA helicase DDX58



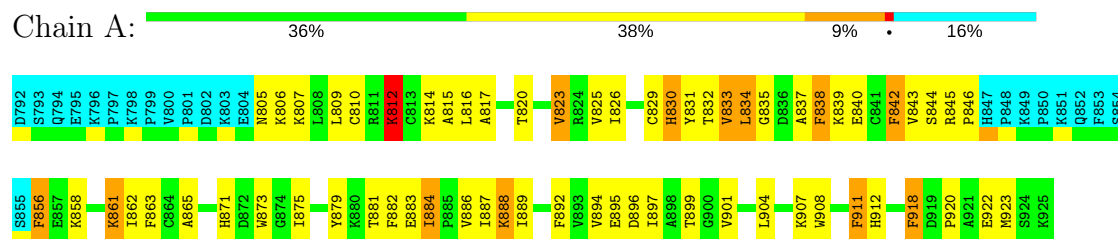
4.2.15 Score per residue for model 15

- Molecule 1: Probable ATP-dependent RNA helicase DDX58



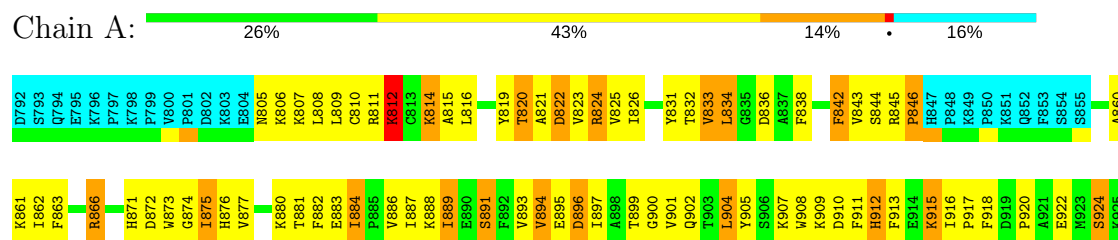
4.2.16 Score per residue for model 16

- Molecule 1: Probable ATP-dependent RNA helicase DDX58



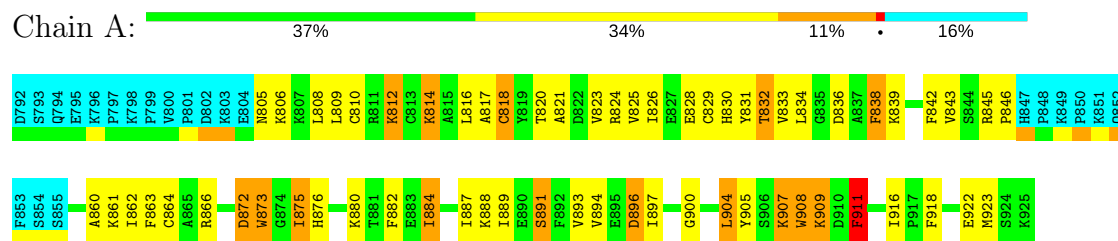
4.2.17 Score per residue for model 17

- Molecule 1: Probable ATP-dependent RNA helicase DDX58



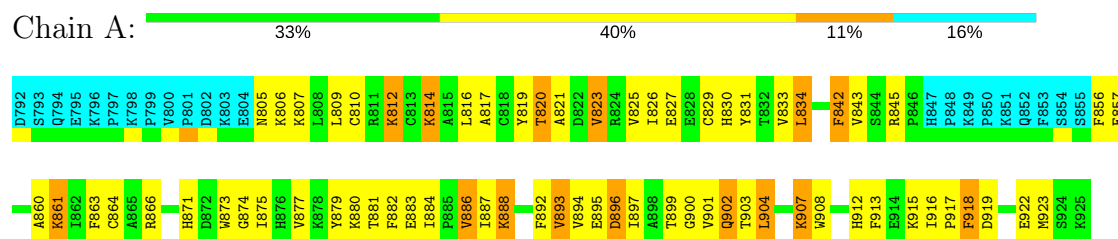
4.2.18 Score per residue for model 18

- Molecule 1: Probable ATP-dependent RNA helicase DDX58



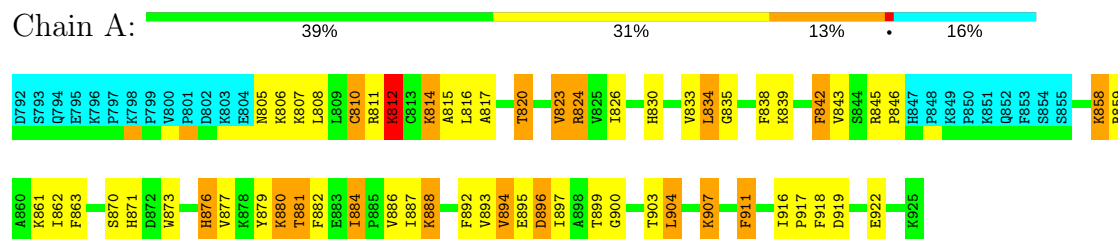
4.2.19 Score per residue for model 19

- Molecule 1: Probable ATP-dependent RNA helicase DDX58



4.2.20 Score per residue for model 20

- Molecule 1: Probable ATP-dependent RNA helicase DDX58



5 Refinement protocol and experimental data overview

The models were refined using the following method: *torsion angle dynamics, distance geometry, simulated annealing*.

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
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

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	921	919	923	65±10
All	All	18420	18380	18460	1306

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 35.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:830:HIS:CE1	1:A:886:VAL:HG22	1.08	1.84	2	1
1:A:830:HIS:CD2	1:A:886:VAL:HG13	1.05	1.87	11	2
1:A:823:VAL:HG23	1:A:833:VAL:HG22	0.98	1.31	9	4
1:A:823:VAL:HG22	1:A:833:VAL:CG1	0.97	1.90	4	2
1:A:823:VAL:HG23	1:A:833:VAL:HG12	0.97	1.34	16	2
1:A:823:VAL:HG22	1:A:833:VAL:HG12	0.91	1.43	4	2
1:A:834:LEU:HD22	1:A:918:PHE:CZ	0.90	2.01	17	4
1:A:845:ARG:O	1:A:860:ALA:HB1	0.89	1.67	13	7
1:A:899:THR:OG1	1:A:901:VAL:HG12	0.89	1.68	11	7
1:A:830:HIS:NE2	1:A:886:VAL:HG22	0.88	1.83	2	1
1:A:886:VAL:O	1:A:887:ILE:HD13	0.87	1.68	14	5
1:A:819:TYR:O	1:A:823:VAL:HG23	0.87	1.70	15	7
1:A:824:ARG:NH1	1:A:834:LEU:HD13	0.85	1.87	3	2
1:A:823:VAL:HG11	1:A:831:TYR:CE2	0.84	2.06	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:834:LEU:HD22	1:A:918:PHE:CE1	0.83	2.09	19	4
1:A:823:VAL:HG23	1:A:833:VAL:CG2	0.83	2.04	3	3
1:A:823:VAL:HG21	1:A:831:TYR:CE2	0.82	2.09	13	1
1:A:820:THR:O	1:A:823:VAL:HG12	0.82	1.75	13	3
1:A:823:VAL:HG12	1:A:831:TYR:CE1	0.81	2.09	15	2
1:A:826:ILE:HG21	1:A:879:TYR:CE1	0.79	2.13	3	1
1:A:856:PHE:CZ	1:A:879:TYR:CE1	0.79	2.70	13	1
1:A:834:LEU:N	1:A:834:LEU:HD23	0.76	1.95	17	1
1:A:884:ILE:HD13	1:A:884:ILE:N	0.75	1.95	17	1
1:A:893:VAL:HG12	1:A:904:LEU:HD23	0.75	1.57	1	11
1:A:858:LYS:NZ	1:A:875:ILE:HG21	0.75	1.96	16	1
1:A:884:ILE:HG21	1:A:918:PHE:CZ	0.75	2.17	17	9
1:A:858:LYS:HZ1	1:A:875:ILE:HG21	0.74	1.41	16	1
1:A:856:PHE:CZ	1:A:879:TYR:CG	0.74	2.76	15	1
1:A:874:GLY:O	1:A:875:ILE:HG23	0.74	1.82	17	4
1:A:806:LYS:HD2	1:A:894:VAL:HG22	0.74	1.60	10	7
1:A:823:VAL:HG23	1:A:833:VAL:CG1	0.73	2.13	20	2
1:A:832:THR:HG23	1:A:885:PRO:O	0.73	1.82	3	3
1:A:818:CYS:SG	1:A:833:VAL:HG11	0.73	2.23	18	3
1:A:861:LYS:HG3	1:A:875:ILE:HG22	0.73	1.58	16	4
1:A:806:LYS:HD2	1:A:894:VAL:HG12	0.72	1.62	5	8
1:A:856:PHE:CE2	1:A:879:TYR:CE1	0.70	2.80	13	3
1:A:805:ASN:ND2	1:A:821:ALA:HB2	0.70	2.01	4	6
1:A:881:THR:HG22	1:A:882:PHE:CE1	0.70	2.22	17	1
1:A:834:LEU:CD2	1:A:918:PHE:CZ	0.69	2.75	14	11
1:A:823:VAL:HG22	1:A:833:VAL:HG22	0.69	1.64	2	5
1:A:824:ARG:CZ	1:A:834:LEU:HD13	0.69	2.17	3	1
1:A:808:LEU:HG	1:A:894:VAL:HG13	0.69	1.64	12	5
1:A:843:VAL:HG22	1:A:863:PHE:O	0.68	1.88	11	8
1:A:887:ILE:HG21	1:A:892:PHE:CE2	0.68	2.23	11	3
1:A:893:VAL:CG1	1:A:904:LEU:HD23	0.68	2.18	1	10
1:A:834:LEU:CD2	1:A:918:PHE:CE2	0.68	2.76	4	1
1:A:817:ALA:HB1	1:A:873:TRP:CH2	0.68	2.24	19	2
1:A:886:VAL:C	1:A:887:ILE:HD13	0.68	2.09	6	3
1:A:888:LYS:HZ2	1:A:908:TRP:HE1	0.68	1.32	19	1
1:A:856:PHE:CZ	1:A:879:TYR:CE2	0.67	2.82	16	2
1:A:874:GLY:HA3	1:A:887:ILE:HD12	0.67	1.64	6	1
1:A:856:PHE:CD2	1:A:879:TYR:CE1	0.67	2.82	14	2
1:A:805:ASN:HB2	1:A:821:ALA:HB2	0.67	1.64	19	2
1:A:858:LYS:HD3	1:A:875:ILE:HG21	0.67	1.65	13	1
1:A:871:HIS:CE1	1:A:873:TRP:CD1	0.67	2.83	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:823:VAL:CG1	1:A:831:TYR:CE2	0.66	2.79	11	1
1:A:834:LEU:HD21	1:A:918:PHE:CZ	0.66	2.26	18	4
1:A:881:THR:HG22	1:A:882:PHE:CD1	0.66	2.26	17	1
1:A:816:LEU:HD22	1:A:817:ALA:N	0.66	2.06	2	14
1:A:856:PHE:CE2	1:A:879:TYR:CD1	0.66	2.84	15	1
1:A:823:VAL:HG22	1:A:833:VAL:CG2	0.66	2.21	15	4
1:A:834:LEU:HD22	1:A:922:GLU:HB2	0.66	1.68	20	7
1:A:834:LEU:HD21	1:A:918:PHE:CE2	0.66	2.26	4	1
1:A:806:LYS:CD	1:A:894:VAL:HG22	0.65	2.21	8	7
1:A:868:ASN:CB	1:A:871:HIS:CD2	0.65	2.79	13	4
1:A:816:LEU:HD13	1:A:816:LEU:C	0.65	2.12	6	12
1:A:808:LEU:HG	1:A:894:VAL:HG23	0.65	1.69	8	4
1:A:825:VAL:CG1	1:A:831:TYR:CD1	0.65	2.80	11	6
1:A:912:HIS:NE2	1:A:913:PHE:CE1	0.65	2.65	17	1
1:A:830:HIS:CG	1:A:886:VAL:CG1	0.64	2.80	20	2
1:A:860:ALA:HB3	1:A:876:HIS:HB3	0.64	1.70	9	4
1:A:816:LEU:C	1:A:816:LEU:HD13	0.64	2.12	8	8
1:A:825:VAL:HG12	1:A:830:HIS:O	0.64	1.93	12	8
1:A:826:ILE:O	1:A:826:ILE:HG22	0.64	1.93	20	6
1:A:823:VAL:CG2	1:A:833:VAL:HG12	0.64	2.21	20	3
1:A:834:LEU:CD2	1:A:918:PHE:CE1	0.64	2.80	7	7
1:A:857:GLU:C	1:A:877:VAL:HG22	0.63	2.13	19	1
1:A:884:ILE:HG23	1:A:923:MET:HE2	0.63	1.69	5	1
1:A:826:ILE:HG22	1:A:826:ILE:O	0.63	1.94	4	13
1:A:806:LYS:CD	1:A:894:VAL:HG12	0.63	2.23	5	8
1:A:879:TYR:CB	1:A:884:ILE:HD11	0.63	2.23	20	1
1:A:875:ILE:HD13	1:A:877:VAL:HG13	0.62	1.70	4	6
1:A:809:LEU:HD23	1:A:814:LYS:O	0.62	1.93	8	4
1:A:805:ASN:CB	1:A:821:ALA:HB2	0.62	2.24	8	2
1:A:807:LYS:HG3	1:A:816:LEU:HD23	0.62	1.70	13	6
1:A:830:HIS:CD2	1:A:886:VAL:CG2	0.62	2.83	19	1
1:A:830:HIS:HB3	1:A:886:VAL:HG13	0.62	1.70	4	5
1:A:858:LYS:HA	1:A:877:VAL:HG12	0.62	1.69	9	1
1:A:875:ILE:HD13	1:A:877:VAL:HG23	0.62	1.70	19	1
1:A:856:PHE:CE2	1:A:879:TYR:CZ	0.62	2.88	13	1
1:A:823:VAL:HG22	1:A:833:VAL:HG11	0.61	1.71	4	1
1:A:862:ILE:C	1:A:863:PHE:CD1	0.61	2.74	18	7
1:A:884:ILE:N	1:A:884:ILE:HD12	0.61	2.10	4	2
1:A:879:TYR:N	1:A:879:TYR:CD1	0.61	2.67	4	3
1:A:834:LEU:HD21	1:A:918:PHE:CE1	0.61	2.31	7	5
1:A:822:ASP:CG	1:A:838:PHE:CZ	0.61	2.75	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:918:PHE:CE1	1:A:923:MET:CG	0.61	2.84	19	2
1:A:818:CYS:HB2	1:A:833:VAL:HG11	0.61	1.73	9	1
1:A:882:PHE:CD1	1:A:923:MET:CE	0.60	2.84	16	1
1:A:911:PHE:N	1:A:911:PHE:CD1	0.60	2.66	18	1
1:A:875:ILE:O	1:A:875:ILE:HD12	0.60	1.97	10	2
1:A:830:HIS:CD2	1:A:830:HIS:N	0.60	2.69	16	2
1:A:881:THR:HG23	1:A:881:THR:O	0.60	1.97	3	1
1:A:835:GLY:O	1:A:838:PHE:CD2	0.60	2.55	20	6
1:A:823:VAL:HA	1:A:833:VAL:HG12	0.60	1.73	20	2
1:A:825:VAL:HG23	1:A:915:LYS:HA	0.60	1.73	17	3
1:A:908:TRP:O	1:A:911:PHE:CD1	0.60	2.55	16	5
1:A:838:PHE:CD1	1:A:838:PHE:C	0.60	2.75	6	4
1:A:882:PHE:CD1	1:A:923:MET:HE3	0.60	2.32	16	1
1:A:838:PHE:C	1:A:838:PHE:CD1	0.59	2.75	4	4
1:A:887:ILE:CG2	1:A:891:SER:CB	0.59	2.80	12	1
1:A:831:TYR:OH	1:A:913:PHE:CD1	0.59	2.55	12	1
1:A:877:VAL:CG2	1:A:886:VAL:HG23	0.59	2.27	13	4
1:A:911:PHE:O	1:A:911:PHE:CD1	0.59	2.55	4	6
1:A:829:CYS:O	1:A:830:HIS:CD2	0.59	2.55	6	2
1:A:811:ARG:CD	1:A:904:LEU:CD2	0.59	2.80	13	1
1:A:862:ILE:O	1:A:863:PHE:CD1	0.59	2.55	13	1
1:A:809:LEU:HD22	1:A:902:GLN:NE2	0.59	2.13	11	1
1:A:905:TYR:CD2	1:A:910:ASP:O	0.59	2.56	17	1
1:A:838:PHE:CD1	1:A:838:PHE:O	0.59	2.55	18	2
1:A:822:ASP:OD2	1:A:838:PHE:CE1	0.59	2.55	17	1
1:A:880:LYS:O	1:A:882:PHE:CD2	0.59	2.55	20	2
1:A:826:ILE:CG2	1:A:879:TYR:CE1	0.59	2.85	3	1
1:A:830:HIS:CE1	1:A:832:THR:OG1	0.59	2.56	2	2
1:A:806:LYS:HZ1	1:A:912:HIS:CD2	0.59	2.15	17	1
1:A:820:THR:OG1	1:A:913:PHE:CE2	0.59	2.55	12	1
1:A:882:PHE:CD2	1:A:923:MET:SD	0.59	2.96	18	1
1:A:881:THR:C	1:A:882:PHE:CD1	0.59	2.77	17	1
1:A:858:LYS:HB3	1:A:877:VAL:HG12	0.59	1.73	14	2
1:A:834:LEU:HD13	1:A:922:GLU:OE2	0.59	1.98	16	1
1:A:833:VAL:O	1:A:838:PHE:CE2	0.59	2.55	1	1
1:A:809:LEU:HD23	1:A:814:LYS:C	0.58	2.18	8	12
1:A:818:CYS:SG	1:A:838:PHE:CD1	0.58	2.96	18	2
1:A:830:HIS:NE2	1:A:856:PHE:CE2	0.58	2.72	3	1
1:A:881:THR:O	1:A:881:THR:HG23	0.58	1.99	20	1
1:A:881:THR:O	1:A:882:PHE:CD1	0.58	2.55	14	3
1:A:823:VAL:CG1	1:A:913:PHE:CZ	0.58	2.86	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:834:LEU:N	1:A:834:LEU:CD2	0.58	2.67	17	1
1:A:889:ILE:HD13	1:A:889:ILE:O	0.58	1.98	17	2
1:A:856:PHE:CE1	1:A:879:TYR:OH	0.58	2.55	19	1
1:A:830:HIS:NE2	1:A:886:VAL:HG13	0.58	2.13	11	1
1:A:873:TRP:O	1:A:887:ILE:HG23	0.58	1.99	17	2
1:A:875:ILE:HD13	1:A:877:VAL:CG1	0.58	2.29	4	6
1:A:820:THR:OG1	1:A:913:PHE:CE1	0.57	2.57	8	4
1:A:858:LYS:HB2	1:A:877:VAL:HG12	0.57	1.75	9	1
1:A:831:TYR:OH	1:A:913:PHE:CD2	0.57	2.55	15	2
1:A:879:TYR:CE2	1:A:881:THR:OG1	0.57	2.55	10	1
1:A:831:TYR:OH	1:A:913:PHE:CE1	0.57	2.56	12	1
1:A:826:ILE:HG21	1:A:879:TYR:CD1	0.57	2.34	3	1
1:A:858:LYS:CA	1:A:877:VAL:HG12	0.57	2.29	9	1
1:A:808:LEU:HD23	1:A:892:PHE:CD1	0.57	2.34	15	1
1:A:805:ASN:OD1	1:A:821:ALA:HB2	0.57	1.99	11	2
1:A:825:VAL:HG12	1:A:831:TYR:HA	0.57	1.77	11	2
1:A:842:PHE:CD2	1:A:843:VAL:N	0.57	2.73	2	7
1:A:916:ILE:HG23	1:A:917:PRO:HD2	0.57	1.77	9	16
1:A:808:LEU:O	1:A:809:LEU:HD12	0.57	1.99	14	1
1:A:873:TRP:CD1	1:A:873:TRP:N	0.56	2.73	6	3
1:A:809:LEU:HD13	1:A:895:GLU:CB	0.56	2.30	11	1
1:A:899:THR:OG1	1:A:901:VAL:HG23	0.56	1.99	17	4
1:A:873:TRP:N	1:A:873:TRP:CD1	0.56	2.73	9	1
1:A:908:TRP:O	1:A:911:PHE:CG	0.56	2.59	3	5
1:A:834:LEU:HD12	1:A:834:LEU:N	0.56	2.16	8	2
1:A:834:LEU:HD13	1:A:922:GLU:HB2	0.56	1.76	4	2
1:A:884:ILE:HG21	1:A:918:PHE:HZ	0.56	1.61	20	5
1:A:874:GLY:HA3	1:A:887:ILE:HD13	0.56	1.76	11	1
1:A:856:PHE:CZ	1:A:879:TYR:CD2	0.56	2.94	15	2
1:A:875:ILE:HD12	1:A:875:ILE:O	0.56	2.01	4	5
1:A:845:ARG:CG	1:A:863:PHE:CE1	0.56	2.88	2	1
1:A:882:PHE:CG	1:A:923:MET:SD	0.55	3.00	19	2
1:A:911:PHE:CD1	1:A:911:PHE:O	0.55	2.60	20	4
1:A:868:ASN:CG	1:A:871:HIS:CD2	0.55	2.80	13	3
1:A:831:TYR:OH	1:A:913:PHE:CG	0.55	2.60	12	1
1:A:830:HIS:ND1	1:A:886:VAL:CG1	0.55	2.70	4	1
1:A:823:VAL:CG1	1:A:831:TYR:CE1	0.55	2.86	15	1
1:A:880:LYS:O	1:A:882:PHE:CG	0.55	2.60	3	2
1:A:830:HIS:CD2	1:A:831:TYR:O	0.55	2.60	2	2
1:A:826:ILE:O	1:A:827:GLU:CG	0.55	2.55	19	1
1:A:899:THR:HG1	1:A:901:VAL:HG12	0.54	1.61	11	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:829:CYS:O	1:A:830:HIS:CG	0.54	2.60	5	4
1:A:806:LYS:CE	1:A:912:HIS:NE2	0.54	2.71	17	1
1:A:864:CYS:SG	1:A:873:TRP:CZ2	0.54	2.96	3	4
1:A:918:PHE:CE1	1:A:923:MET:HG2	0.54	2.38	19	2
1:A:809:LEU:HD13	1:A:895:GLU:HB3	0.54	1.79	11	1
1:A:830:HIS:NE2	1:A:856:PHE:CZ	0.54	2.76	10	2
1:A:806:LYS:H	1:A:820:THR:HG22	0.54	1.63	5	10
1:A:912:HIS:O	1:A:913:PHE:CD1	0.54	2.61	9	1
1:A:830:HIS:CD2	1:A:886:VAL:HG21	0.54	2.38	19	3
1:A:879:TYR:OH	1:A:884:ILE:HD11	0.53	2.03	4	2
1:A:830:HIS:CB	1:A:886:VAL:HG13	0.53	2.33	20	2
1:A:814:LYS:NZ	1:A:902:GLN:HE22	0.53	2.02	19	2
1:A:894:VAL:O	1:A:894:VAL:CG1	0.53	2.56	11	4
1:A:822:ASP:O	1:A:833:VAL:HG13	0.53	2.03	3	2
1:A:834:LEU:HD13	1:A:918:PHE:CE2	0.53	2.38	17	1
1:A:861:LYS:CD	1:A:861:LYS:N	0.53	2.70	19	3
1:A:834:LEU:HD23	1:A:918:PHE:CE1	0.53	2.38	8	1
1:A:816:LEU:HD22	1:A:817:ALA:H	0.53	1.62	2	6
1:A:868:ASN:HB3	1:A:871:HIS:CD2	0.53	2.39	13	4
1:A:889:ILE:HG21	1:A:907:LYS:O	0.53	2.03	8	2
1:A:830:HIS:CE1	1:A:856:PHE:CE2	0.53	2.97	1	3
1:A:863:PHE:CD1	1:A:863:PHE:N	0.53	2.76	16	4
1:A:889:ILE:CD1	1:A:905:TYR:CB	0.53	2.87	11	2
1:A:810:CYS:SG	1:A:873:TRP:CG	0.53	3.02	9	1
1:A:830:HIS:CE1	1:A:856:PHE:CD2	0.53	2.97	15	2
1:A:894:VAL:CG1	1:A:894:VAL:O	0.53	2.56	10	3
1:A:905:TYR:CD1	1:A:910:ASP:CG	0.53	2.83	9	1
1:A:831:TYR:OH	1:A:913:PHE:CZ	0.52	2.62	12	1
1:A:835:GLY:O	1:A:838:PHE:CE2	0.52	2.62	20	1
1:A:858:LYS:CB	1:A:877:VAL:HG12	0.52	2.35	9	3
1:A:879:TYR:OH	1:A:886:VAL:HG21	0.52	2.05	13	1
1:A:805:ASN:ND2	1:A:806:LYS:H	0.52	2.02	7	2
1:A:826:ILE:CD1	1:A:832:THR:HG21	0.52	2.35	9	1
1:A:894:VAL:O	1:A:894:VAL:HG13	0.52	2.05	11	6
1:A:830:HIS:CD2	1:A:886:VAL:CG1	0.52	2.87	2	4
1:A:893:VAL:HG12	1:A:904:LEU:HB3	0.52	1.82	15	3
1:A:839:LYS:O	1:A:842:PHE:CD1	0.52	2.63	5	3
1:A:831:TYR:OH	1:A:911:PHE:CD2	0.52	2.62	16	1
1:A:887:ILE:HG22	1:A:888:LYS:H	0.52	1.65	9	12
1:A:812:LYS:N	1:A:812:LYS:CE	0.51	2.73	11	1
1:A:833:VAL:HG21	1:A:838:PHE:CD2	0.51	2.40	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:831:TYR:CD2	1:A:908:TRP:CZ2	0.51	2.97	9	1
1:A:805:ASN:ND2	1:A:806:LYS:N	0.51	2.58	7	16
1:A:839:LYS:HA	1:A:842:PHE:CE1	0.51	2.41	1	4
1:A:877:VAL:CG1	1:A:886:VAL:CG1	0.51	2.88	15	1
1:A:830:HIS:CE1	1:A:856:PHE:CZ	0.51	2.98	10	3
1:A:882:PHE:CB	1:A:923:MET:HE2	0.51	2.35	19	1
1:A:861:LYS:HB3	1:A:863:PHE:CZ	0.51	2.41	11	4
1:A:888:LYS:NZ	1:A:908:TRP:HE1	0.51	2.01	19	1
1:A:842:PHE:CG	1:A:843:VAL:N	0.51	2.78	1	20
1:A:825:VAL:HG23	1:A:830:HIS:C	0.51	2.26	19	2
1:A:832:THR:HG22	1:A:886:VAL:HA	0.51	1.82	16	1
1:A:832:THR:CG2	1:A:918:PHE:CE1	0.51	2.94	15	1
1:A:883:GLU:CG	1:A:883:GLU:O	0.51	2.59	15	1
1:A:826:ILE:HG21	1:A:879:TYR:CE2	0.51	2.40	6	3
1:A:856:PHE:CE2	1:A:879:TYR:OH	0.51	2.61	13	1
1:A:877:VAL:CG2	1:A:886:VAL:CG2	0.51	2.89	4	5
1:A:805:ASN:CG	1:A:821:ALA:HB2	0.51	2.26	17	1
1:A:820:THR:HG21	1:A:913:PHE:CE1	0.51	2.41	17	1
1:A:823:VAL:HG12	1:A:831:TYR:HE1	0.51	1.63	15	1
1:A:856:PHE:CZ	1:A:879:TYR:CD1	0.51	2.98	14	2
1:A:883:GLU:O	1:A:883:GLU:CG	0.51	2.59	4	4
1:A:829:CYS:SG	1:A:830:HIS:CE1	0.51	3.03	18	1
1:A:858:LYS:HZ3	1:A:858:LYS:H	0.51	1.49	5	1
1:A:823:VAL:CG2	1:A:831:TYR:CE2	0.51	2.91	13	1
1:A:860:ALA:O	1:A:876:HIS:CB	0.50	2.59	17	2
1:A:806:LYS:NZ	1:A:912:HIS:NE2	0.50	2.59	17	1
1:A:915:LYS:O	1:A:915:LYS:CD	0.50	2.59	7	4
1:A:832:THR:HG22	1:A:833:VAL:H	0.50	1.67	10	2
1:A:856:PHE:CE1	1:A:879:TYR:CE1	0.50	3.00	13	1
1:A:817:ALA:HA	1:A:873:TRP:CH2	0.50	2.41	2	2
1:A:823:VAL:HG23	1:A:833:VAL:HG23	0.50	1.82	5	1
1:A:862:ILE:HD11	1:A:873:TRP:HB2	0.50	1.83	7	1
1:A:856:PHE:CE1	1:A:879:TYR:HB3	0.50	2.41	15	1
1:A:843:VAL:HG13	1:A:865:ALA:HB2	0.50	1.84	9	3
1:A:824:ARG:HD2	1:A:834:LEU:HD11	0.50	1.83	10	1
1:A:909:LYS:O	1:A:911:PHE:CE1	0.50	2.64	18	1
1:A:805:ASN:OD1	1:A:821:ALA:CB	0.50	2.60	11	1
1:A:887:ILE:CG2	1:A:892:PHE:CE2	0.50	2.94	13	3
1:A:807:LYS:HD3	1:A:816:LEU:HD23	0.50	1.84	6	1
1:A:823:VAL:O	1:A:824:ARG:CD	0.50	2.60	6	2
1:A:831:TYR:O	1:A:832:THR:CG2	0.50	2.60	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:823:VAL:O	1:A:823:VAL:CG1	0.50	2.60	18	1
1:A:812:LYS:HD2	1:A:871:HIS:CD2	0.49	2.41	20	1
1:A:908:TRP:HA	1:A:911:PHE:CE1	0.49	2.42	12	1
1:A:811:ARG:HD2	1:A:904:LEU:HD22	0.49	1.84	17	1
1:A:871:HIS:NE2	1:A:873:TRP:CD1	0.49	2.80	10	3
1:A:844:SER:O	1:A:845:ARG:CZ	0.49	2.60	17	1
1:A:888:LYS:CG	1:A:891:SER:OG	0.49	2.61	17	3
1:A:894:VAL:HG13	1:A:894:VAL:O	0.49	2.06	8	1
1:A:845:ARG:HG3	1:A:863:PHE:CE1	0.49	2.42	2	5
1:A:830:HIS:HB2	1:A:886:VAL:HG13	0.49	1.84	9	1
1:A:814:LYS:NZ	1:A:902:GLN:NE2	0.49	2.60	19	1
1:A:882:PHE:CE2	1:A:920:PRO:HB3	0.49	2.43	9	5
1:A:805:ASN:OD1	1:A:821:ALA:N	0.49	2.46	11	2
1:A:884:ILE:CD1	1:A:884:ILE:N	0.49	2.67	17	2
1:A:842:PHE:CD1	1:A:842:PHE:C	0.49	2.83	6	1
1:A:832:THR:HG21	1:A:918:PHE:HE2	0.49	1.68	12	1
1:A:830:HIS:CD2	1:A:886:VAL:HG11	0.49	2.43	1	2
1:A:826:ILE:O	1:A:829:CYS:CB	0.49	2.60	8	2
1:A:838:PHE:CD1	1:A:838:PHE:N	0.49	2.78	5	1
1:A:887:ILE:HG22	1:A:891:SER:CB	0.49	2.38	15	3
1:A:832:THR:HG21	1:A:884:ILE:HD13	0.49	1.84	5	2
1:A:830:HIS:NE2	1:A:886:VAL:CG2	0.49	2.70	2	1
1:A:863:PHE:CE2	1:A:872:ASP:HB3	0.49	2.43	18	1
1:A:812:LYS:CD	1:A:871:HIS:CD2	0.49	2.96	14	3
1:A:812:LYS:CG	1:A:871:HIS:CG	0.49	2.96	19	1
1:A:824:ARG:CZ	1:A:922:GLU:OE1	0.48	2.60	10	1
1:A:912:HIS:CG	1:A:912:HIS:O	0.48	2.66	16	1
1:A:887:ILE:HG21	1:A:892:PHE:CD2	0.48	2.43	13	2
1:A:889:ILE:HD11	1:A:905:TYR:CD2	0.48	2.43	18	1
1:A:884:ILE:HG12	1:A:918:PHE:CZ	0.48	2.43	4	2
1:A:887:ILE:CG2	1:A:891:SER:OG	0.48	2.61	11	1
1:A:863:PHE:CD2	1:A:872:ASP:CB	0.48	2.97	17	1
1:A:826:ILE:HD13	1:A:879:TYR:OH	0.48	2.08	15	1
1:A:814:LYS:NZ	1:A:893:VAL:HG11	0.48	2.24	15	1
1:A:807:LYS:HG3	1:A:819:TYR:CE1	0.48	2.43	19	1
1:A:918:PHE:CE1	1:A:923:MET:HG3	0.48	2.43	19	1
1:A:861:LYS:CB	1:A:863:PHE:CZ	0.48	2.96	11	1
1:A:834:LEU:HG	1:A:918:PHE:CZ	0.48	2.44	8	2
1:A:912:HIS:N	1:A:912:HIS:ND1	0.48	2.61	7	1
1:A:839:LYS:HA	1:A:842:PHE:CD1	0.48	2.43	16	3
1:A:812:LYS:HD3	1:A:871:HIS:CD2	0.48	2.43	19	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:807:LYS:CG	1:A:816:LEU:HD23	0.48	2.38	6	2
1:A:845:ARG:O	1:A:860:ALA:CB	0.48	2.61	11	2
1:A:858:LYS:HZ1	1:A:861:LYS:HE3	0.48	1.68	20	1
1:A:842:PHE:CD2	1:A:843:VAL:O	0.48	2.66	18	5
1:A:879:TYR:OH	1:A:886:VAL:CG2	0.48	2.60	13	1
1:A:905:TYR:CD1	1:A:910:ASP:HB3	0.48	2.44	15	1
1:A:823:VAL:O	1:A:823:VAL:HG13	0.48	2.09	18	1
1:A:805:ASN:CG	1:A:806:LYS:N	0.48	2.67	11	4
1:A:896:ASP:O	1:A:900:GLY:N	0.48	2.47	17	19
1:A:889:ILE:CD1	1:A:907:LYS:O	0.48	2.62	12	1
1:A:829:CYS:HB3	1:A:830:HIS:CD2	0.48	2.44	16	1
1:A:884:ILE:H	1:A:884:ILE:HD12	0.48	1.68	4	1
1:A:830:HIS:ND1	1:A:856:PHE:CZ	0.48	2.82	19	1
1:A:881:THR:HG23	1:A:882:PHE:CD2	0.48	2.44	19	1
1:A:824:ARG:O	1:A:832:THR:HG23	0.47	2.09	18	2
1:A:884:ILE:HG23	1:A:923:MET:CE	0.47	2.36	5	2
1:A:881:THR:CG2	1:A:881:THR:O	0.47	2.63	3	1
1:A:863:PHE:CD1	1:A:872:ASP:HB3	0.47	2.45	11	1
1:A:833:VAL:CG1	1:A:834:LEU:N	0.47	2.76	10	1
1:A:862:ILE:O	1:A:872:ASP:CB	0.47	2.62	18	1
1:A:831:TYR:O	1:A:832:THR:HG23	0.47	2.10	17	1
1:A:877:VAL:HG21	1:A:886:VAL:CG2	0.47	2.39	7	4
1:A:887:ILE:HG22	1:A:888:LYS:N	0.47	2.25	12	2
1:A:861:LYS:HB3	1:A:863:PHE:CE1	0.47	2.44	18	1
1:A:807:LYS:CG	1:A:808:LEU:N	0.47	2.78	17	3
1:A:918:PHE:CZ	1:A:923:MET:HE2	0.47	2.45	12	1
1:A:805:ASN:ND2	1:A:821:ALA:CB	0.47	2.76	4	2
1:A:879:TYR:CD1	1:A:880:LYS:HG2	0.47	2.44	3	1
1:A:882:PHE:CZ	1:A:920:PRO:HB3	0.47	2.45	17	7
1:A:908:TRP:O	1:A:911:PHE:N	0.47	2.48	17	7
1:A:843:VAL:CG1	1:A:865:ALA:HB2	0.47	2.40	9	1
1:A:895:GLU:OE1	1:A:902:GLN:CG	0.47	2.63	9	1
1:A:823:VAL:HA	1:A:833:VAL:HG22	0.47	1.85	3	1
1:A:884:ILE:HG12	1:A:918:PHE:CE2	0.47	2.45	15	6
1:A:834:LEU:HD13	1:A:922:GLU:CD	0.47	2.29	1	1
1:A:807:LYS:O	1:A:895:GLU:N	0.47	2.48	11	15
1:A:828:GLU:HB3	1:A:911:PHE:CD2	0.47	2.45	18	1
1:A:814:LYS:HZ1	1:A:893:VAL:HG11	0.47	1.70	6	1
1:A:823:VAL:CG1	1:A:823:VAL:O	0.46	2.62	14	1
1:A:877:VAL:HG22	1:A:886:VAL:CG2	0.46	2.40	14	1
1:A:879:TYR:CD2	1:A:881:THR:HG22	0.46	2.45	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:881:THR:CG2	1:A:882:PHE:N	0.46	2.78	19	1
1:A:888:LYS:NZ	1:A:908:TRP:NE1	0.46	2.61	19	1
1:A:816:LEU:HD13	1:A:817:ALA:N	0.46	2.25	5	3
1:A:882:PHE:CG	1:A:923:MET:CE	0.46	2.98	16	1
1:A:889:ILE:HB	1:A:908:TRP:CD1	0.46	2.46	2	5
1:A:810:CYS:O	1:A:814:LYS:N	0.46	2.48	8	20
1:A:833:VAL:CG2	1:A:838:PHE:CD2	0.46	2.98	4	2
1:A:831:TYR:C	1:A:832:THR:CG2	0.46	2.83	4	1
1:A:884:ILE:O	1:A:884:ILE:HD12	0.46	2.09	19	1
1:A:823:VAL:CG2	1:A:833:VAL:HG22	0.46	2.33	3	1
1:A:863:PHE:CE1	1:A:872:ASP:HB3	0.46	2.45	11	2
1:A:877:VAL:CG2	1:A:879:TYR:CE1	0.46	2.98	14	1
1:A:882:PHE:CE2	1:A:920:PRO:HG3	0.46	2.46	9	1
1:A:905:TYR:CD2	1:A:910:ASP:HB3	0.46	2.45	13	1
1:A:862:ILE:HG23	1:A:875:ILE:C	0.46	2.30	6	2
1:A:879:TYR:CE2	1:A:884:ILE:HD11	0.46	2.46	11	1
1:A:810:CYS:SG	1:A:873:TRP:CZ2	0.46	3.09	19	2
1:A:834:LEU:HD13	1:A:922:GLU:CB	0.46	2.40	19	2
1:A:891:SER:OG	1:A:892:PHE:CD2	0.46	2.69	11	1
1:A:905:TYR:N	1:A:905:TYR:CD1	0.46	2.78	6	2
1:A:832:THR:HG21	1:A:918:PHE:CE2	0.46	2.46	12	1
1:A:832:THR:OG1	1:A:833:VAL:N	0.46	2.49	7	3
1:A:830:HIS:CG	1:A:886:VAL:HG21	0.46	2.45	19	1
1:A:912:HIS:O	1:A:912:HIS:CG	0.46	2.69	5	1
1:A:874:GLY:O	1:A:875:ILE:CG2	0.45	2.60	17	1
1:A:856:PHE:CE1	1:A:879:TYR:CB	0.45	2.99	15	1
1:A:824:ARG:NH1	1:A:834:LEU:HD12	0.45	2.26	1	1
1:A:882:PHE:CZ	1:A:920:PRO:HG3	0.45	2.46	9	1
1:A:812:LYS:HD3	1:A:871:HIS:CG	0.45	2.46	19	1
1:A:882:PHE:CE1	1:A:920:PRO:HB3	0.45	2.46	11	4
1:A:832:THR:HG21	1:A:884:ILE:HB	0.45	1.87	3	1
1:A:830:HIS:CD2	1:A:831:TYR:N	0.45	2.85	2	2
1:A:842:PHE:C	1:A:842:PHE:CD1	0.45	2.89	16	1
1:A:824:ARG:O	1:A:832:THR:CG2	0.45	2.64	7	2
1:A:880:LYS:O	1:A:881:THR:C	0.45	2.55	20	3
1:A:826:ILE:O	1:A:826:ILE:CG2	0.45	2.63	20	3
1:A:896:ASP:CB	1:A:899:THR:OG1	0.45	2.65	19	4
1:A:812:LYS:HG3	1:A:871:HIS:CD2	0.45	2.47	2	1
1:A:810:CYS:O	1:A:812:LYS:N	0.45	2.50	6	7
1:A:826:ILE:HD12	1:A:832:THR:CG2	0.45	2.41	9	1
1:A:843:VAL:N	1:A:863:PHE:O	0.45	2.49	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:830:HIS:NE2	1:A:832:THR:OG1	0.45	2.50	2	2
1:A:911:PHE:CD1	1:A:911:PHE:C	0.45	2.89	13	3
1:A:889:ILE:HG21	1:A:907:LYS:C	0.45	2.32	4	3
1:A:833:VAL:HB	1:A:838:PHE:CE2	0.45	2.46	15	1
1:A:860:ALA:O	1:A:876:HIS:N	0.45	2.50	6	1
1:A:833:VAL:HB	1:A:838:PHE:CD2	0.45	2.47	14	2
1:A:911:PHE:C	1:A:911:PHE:CD1	0.45	2.89	3	2
1:A:879:TYR:C	1:A:881:THR:N	0.45	2.70	9	4
1:A:880:LYS:N	1:A:880:LYS:CD	0.45	2.79	19	1
1:A:877:VAL:HG22	1:A:886:VAL:HG23	0.45	1.87	13	1
1:A:825:VAL:HG13	1:A:831:TYR:CD1	0.45	2.47	17	1
1:A:836:ASP:O	1:A:840:GLU:N	0.45	2.50	1	1
1:A:881:THR:OG1	1:A:882:PHE:N	0.44	2.50	7	4
1:A:879:TYR:HB2	1:A:884:ILE:HD11	0.44	1.88	20	1
1:A:833:VAL:HG23	1:A:838:PHE:CD2	0.44	2.47	16	1
1:A:845:ARG:HG2	1:A:863:PHE:CE1	0.44	2.47	2	1
1:A:883:GLU:O	1:A:884:ILE:HG23	0.44	2.12	3	4
1:A:907:LYS:CD	1:A:908:TRP:CZ3	0.44	3.01	10	1
1:A:824:ARG:NH1	1:A:922:GLU:OE2	0.44	2.50	17	1
1:A:810:CYS:SG	1:A:873:TRP:NE1	0.44	2.90	15	1
1:A:907:LYS:HZ3	1:A:907:LYS:HA	0.44	1.72	18	4
1:A:839:LYS:NZ	1:A:923:MET:O	0.44	2.50	10	1
1:A:889:ILE:CD1	1:A:905:TYR:HB2	0.44	2.42	11	1
1:A:864:CYS:N	1:A:873:TRP:HE1	0.44	2.11	9	3
1:A:861:LYS:O	1:A:862:ILE:CG2	0.44	2.66	17	1
1:A:820:THR:HG1	1:A:913:PHE:HE1	0.44	1.54	14	1
1:A:810:CYS:C	1:A:812:LYS:N	0.44	2.71	1	13
1:A:822:ASP:O	1:A:834:LEU:HD12	0.44	2.12	15	1
1:A:882:PHE:CD1	1:A:923:MET:SD	0.44	3.11	6	1
1:A:824:ARG:NH2	1:A:922:GLU:OE1	0.44	2.50	17	1
1:A:812:LYS:HE2	1:A:871:HIS:CD2	0.44	2.47	3	1
1:A:864:CYS:SG	1:A:866:ARG:CG	0.44	3.05	19	2
1:A:836:ASP:O	1:A:839:LYS:N	0.44	2.51	18	1
1:A:816:LEU:CD1	1:A:816:LEU:C	0.44	2.85	6	1
1:A:879:TYR:O	1:A:880:LYS:C	0.44	2.55	7	4
1:A:881:THR:HG23	1:A:882:PHE:H	0.44	1.72	7	1
1:A:811:ARG:HD2	1:A:904:LEU:CD2	0.44	2.42	13	1
1:A:912:HIS:CD2	1:A:913:PHE:CE1	0.44	3.05	17	1
1:A:841:CYS:O	1:A:865:ALA:HB3	0.44	2.13	5	2
1:A:879:TYR:CE1	1:A:880:LYS:HE2	0.44	2.47	20	1
1:A:829:CYS:O	1:A:830:HIS:ND1	0.44	2.51	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:882:PHE:CB	1:A:923:MET:CE	0.44	2.96	19	1
1:A:884:ILE:HD12	1:A:884:ILE:H	0.43	1.72	15	1
1:A:879:TYR:CE2	1:A:881:THR:HG23	0.43	2.48	8	1
1:A:842:PHE:CZ	1:A:885:PRO:HG3	0.43	2.48	6	1
1:A:831:TYR:C	1:A:832:THR:HG23	0.43	2.33	17	1
1:A:920:PRO:O	1:A:924:SER:N	0.43	2.51	17	1
1:A:826:ILE:HG12	1:A:879:TYR:CZ	0.43	2.48	20	1
1:A:818:CYS:CB	1:A:833:VAL:HG11	0.43	2.41	9	1
1:A:889:ILE:CD1	1:A:905:TYR:CD2	0.43	3.01	18	1
1:A:875:ILE:C	1:A:875:ILE:CD1	0.43	2.86	17	1
1:A:811:ARG:O	1:A:814:LYS:CD	0.43	2.66	7	3
1:A:913:PHE:N	1:A:913:PHE:CD1	0.43	2.83	1	2
1:A:820:THR:O	1:A:913:PHE:CZ	0.43	2.72	6	1
1:A:825:VAL:HG13	1:A:831:TYR:CE1	0.43	2.49	17	1
1:A:908:TRP:C	1:A:910:ASP:N	0.43	2.71	17	4
1:A:878:LYS:NZ	1:A:879:TYR:O	0.43	2.52	7	1
1:A:923:MET:CG	1:A:924:SER:N	0.43	2.81	14	2
1:A:884:ILE:N	1:A:884:ILE:CD1	0.43	2.76	4	1
1:A:832:THR:HB	1:A:918:PHE:CE1	0.43	2.48	9	1
1:A:824:ARG:HD2	1:A:916:ILE:HG21	0.43	1.91	18	1
1:A:812:LYS:HG3	1:A:871:HIS:CE1	0.43	2.48	5	1
1:A:816:LEU:C	1:A:816:LEU:CD1	0.43	2.86	8	4
1:A:845:ARG:O	1:A:860:ALA:CA	0.43	2.67	11	1
1:A:820:THR:HG23	1:A:913:PHE:CE1	0.43	2.49	7	1
1:A:889:ILE:HD11	1:A:905:TYR:HD2	0.43	1.73	7	1
1:A:839:LYS:NZ	1:A:924:SER:O	0.43	2.51	12	1
1:A:822:ASP:HA	1:A:824:ARG:HH21	0.43	1.73	3	1
1:A:845:ARG:HG2	1:A:863:PHE:CD1	0.43	2.49	16	2
1:A:817:ALA:CB	1:A:873:TRP:CH2	0.43	3.01	19	1
1:A:830:HIS:CE1	1:A:879:TYR:OH	0.42	2.72	11	1
1:A:856:PHE:CE1	1:A:879:TYR:CD1	0.42	3.07	14	1
1:A:912:HIS:ND1	1:A:912:HIS:O	0.42	2.52	14	1
1:A:842:PHE:C	1:A:843:VAL:CG1	0.42	2.86	8	1
1:A:905:TYR:CD1	1:A:910:ASP:OD2	0.42	2.71	13	2
1:A:889:ILE:O	1:A:889:ILE:CD1	0.42	2.67	6	1
1:A:818:CYS:SG	1:A:838:PHE:CG	0.42	3.12	11	1
1:A:820:THR:HA	1:A:823:VAL:HG12	0.42	1.89	20	2
1:A:810:CYS:SG	1:A:873:TRP:CE2	0.42	3.07	16	2
1:A:879:TYR:O	1:A:881:THR:N	0.42	2.53	9	1
1:A:807:LYS:CD	1:A:816:LEU:HD23	0.42	2.43	6	1
1:A:807:LYS:HE2	1:A:819:TYR:CE2	0.42	2.49	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:837:ALA:O	1:A:840:GLU:CG	0.42	2.67	16	1
1:A:862:ILE:C	1:A:863:PHE:CG	0.42	2.92	9	1
1:A:826:ILE:CG2	1:A:826:ILE:O	0.42	2.68	18	3
1:A:905:TYR:OH	1:A:912:HIS:CB	0.42	2.67	14	1
1:A:879:TYR:CD2	1:A:881:THR:HG23	0.42	2.50	8	1
1:A:823:VAL:HG11	1:A:831:TYR:HE2	0.42	1.66	11	1
1:A:862:ILE:O	1:A:863:PHE:CG	0.42	2.72	20	2
1:A:880:LYS:N	1:A:880:LYS:CE	0.42	2.83	18	1
1:A:823:VAL:HG13	1:A:913:PHE:CZ	0.42	2.49	13	1
1:A:806:LYS:CG	1:A:894:VAL:HG12	0.42	2.45	6	3
1:A:856:PHE:CE2	1:A:879:TYR:CE2	0.42	3.08	16	1
1:A:826:ILE:HD12	1:A:832:THR:HG21	0.42	1.91	9	1
1:A:879:TYR:CD2	1:A:884:ILE:HD11	0.42	2.50	20	1
1:A:907:LYS:HD3	1:A:908:TRP:CZ3	0.42	2.49	8	3
1:A:831:TYR:OH	1:A:911:PHE:CB	0.42	2.68	8	2
1:A:871:HIS:CD2	1:A:873:TRP:CD1	0.42	3.08	16	1
1:A:812:LYS:HZ2	1:A:871:HIS:CD2	0.42	2.31	4	1
1:A:811:ARG:HD3	1:A:904:LEU:HD22	0.42	1.91	13	1
1:A:824:ARG:NH1	1:A:922:GLU:OE1	0.42	2.52	20	1
1:A:888:LYS:O	1:A:892:PHE:CZ	0.42	2.73	10	1
1:A:856:PHE:CD2	1:A:877:VAL:HG11	0.42	2.50	19	1
1:A:912:HIS:CD2	1:A:913:PHE:CZ	0.42	3.08	17	1
1:A:879:TYR:CE1	1:A:880:LYS:HG2	0.42	2.49	3	1
1:A:862:ILE:CG1	1:A:874:GLY:C	0.41	2.89	11	1
1:A:838:PHE:CZ	1:A:839:LYS:HG2	0.41	2.50	1	1
1:A:825:VAL:HB	1:A:831:TYR:CD1	0.41	2.49	19	1
1:A:912:HIS:C	1:A:913:PHE:CD1	0.41	2.94	19	1
1:A:871:HIS:ND1	1:A:871:HIS:C	0.41	2.74	5	1
1:A:877:VAL:HG23	1:A:879:TYR:CE1	0.41	2.50	14	1
1:A:871:HIS:NE2	1:A:873:TRP:NE1	0.41	2.67	10	1
1:A:811:ARG:HD3	1:A:904:LEU:CD2	0.41	2.43	13	1
1:A:811:ARG:HA	1:A:814:LYS:HZ3	0.41	1.75	6	1
1:A:903:THR:CG2	1:A:905:TYR:CE1	0.41	3.03	12	1
1:A:871:HIS:C	1:A:871:HIS:CD2	0.41	2.92	20	1
1:A:826:ILE:HG23	1:A:879:TYR:OH	0.41	2.14	20	1
1:A:879:TYR:HB2	1:A:884:ILE:CD1	0.41	2.46	20	1
1:A:825:VAL:CG2	1:A:914:GLU:O	0.41	2.68	2	1
1:A:872:ASP:N	1:A:872:ASP:OD2	0.41	2.53	4	1
1:A:808:LEU:C	1:A:809:LEU:HD12	0.41	2.34	14	1
1:A:830:HIS:CG	1:A:886:VAL:HB	0.41	2.50	12	1
1:A:838:PHE:CE1	1:A:839:LYS:HG2	0.41	2.50	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:830:HIS:ND1	1:A:886:VAL:HG12	0.41	2.30	4	1
1:A:876:HIS:C	1:A:877:VAL:CG1	0.41	2.89	12	1
1:A:881:THR:O	1:A:881:THR:CG2	0.41	2.68	20	1
1:A:863:PHE:N	1:A:863:PHE:CD1	0.41	2.89	4	1
1:A:871:HIS:CE1	1:A:873:TRP:NE1	0.41	2.89	5	1
1:A:808:LEU:CD2	1:A:892:PHE:CE1	0.41	3.04	15	1
1:A:834:LEU:N	1:A:834:LEU:HD12	0.41	2.31	20	1
1:A:812:LYS:HD2	1:A:871:HIS:CG	0.41	2.50	16	1
1:A:820:THR:HA	1:A:823:VAL:CG1	0.41	2.46	3	1
1:A:916:ILE:CG2	1:A:917:PRO:HD2	0.41	2.46	13	8
1:A:815:ALA:O	1:A:816:LEU:C	0.41	2.60	15	11
1:A:877:VAL:CG2	1:A:886:VAL:HG12	0.41	2.46	15	1
1:A:868:ASN:HB2	1:A:871:HIS:CD2	0.41	2.48	8	1
1:A:861:LYS:N	1:A:861:LYS:CD	0.41	2.83	17	1
1:A:889:ILE:HD12	1:A:905:TYR:HB2	0.41	1.93	17	1
1:A:823:VAL:HG12	1:A:831:TYR:CD1	0.41	2.51	15	1
1:A:842:PHE:C	1:A:843:VAL:HG13	0.41	2.36	15	1
1:A:812:LYS:HG2	1:A:871:HIS:CG	0.41	2.50	15	1
1:A:877:VAL:HG22	1:A:886:VAL:HG12	0.41	1.92	15	1
1:A:911:PHE:HB2	1:A:913:PHE:CD2	0.41	2.51	15	1
1:A:830:HIS:CG	1:A:886:VAL:HG11	0.41	2.51	20	2
1:A:887:ILE:HG22	1:A:891:SER:OG	0.41	2.16	14	1
1:A:902:GLN:C	1:A:903:THR:OG1	0.41	2.60	14	2
1:A:875:ILE:HD12	1:A:875:ILE:C	0.41	2.37	8	1
1:A:875:ILE:CD1	1:A:877:VAL:HG13	0.41	2.41	4	1
1:A:826:ILE:HB	1:A:830:HIS:CD2	0.41	2.51	9	1
1:A:824:ARG:HD2	1:A:916:ILE:CD1	0.41	2.46	18	1
1:A:825:VAL:O	1:A:916:ILE:O	0.41	2.39	19	2
1:A:884:ILE:HG21	1:A:918:PHE:CE2	0.41	2.50	17	1
1:A:820:THR:HG21	1:A:913:PHE:HE1	0.41	1.73	17	1
1:A:842:PHE:O	1:A:843:VAL:CG1	0.41	2.69	15	1
1:A:866:ARG:O	1:A:867:GLN:C	0.41	2.59	15	1
1:A:862:ILE:HG23	1:A:876:HIS:HB2	0.41	1.93	20	1
1:A:925:LYS:CE	1:A:925:LYS:HA	0.41	2.46	2	1
1:A:812:LYS:HG2	1:A:871:HIS:CE1	0.41	2.51	19	1
1:A:861:LYS:C	1:A:862:ILE:HG23	0.40	2.36	17	1
1:A:873:TRP:C	1:A:887:ILE:HG23	0.40	2.37	17	1
1:A:858:LYS:HZ1	1:A:861:LYS:CE	0.40	2.29	20	1
1:A:834:LEU:CD1	1:A:834:LEU:N	0.40	2.84	8	1
1:A:872:ASP:OD2	1:A:874:GLY:N	0.40	2.54	10	1
1:A:830:HIS:ND1	1:A:856:PHE:CE2	0.40	2.90	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:915:LYS:O	1:A:915:LYS:CG	0.40	2.69	7	3
1:A:908:TRP:HA	1:A:911:PHE:CD1	0.40	2.50	12	1
1:A:858:LYS:HD2	1:A:875:ILE:HG21	0.40	1.92	2	1
1:A:879:TYR:CD2	1:A:881:THR:HB	0.40	2.52	4	1
1:A:822:ASP:CG	1:A:838:PHE:CE1	0.40	2.94	17	1
1:A:893:VAL:HG11	1:A:904:LEU:HD23	0.40	1.93	12	1
1:A:862:ILE:HG23	1:A:876:HIS:N	0.40	2.32	4	1
1:A:918:PHE:CD1	1:A:923:MET:HG3	0.40	2.52	19	1
1:A:838:PHE:CZ	1:A:839:LYS:CG	0.40	3.05	1	1
1:A:875:ILE:O	1:A:885:PRO:CB	0.40	2.70	2	1
1:A:882:PHE:HB3	1:A:923:MET:CE	0.40	2.47	18	1
1:A:812:LYS:HG3	1:A:871:HIS:CG	0.40	2.51	17	1
1:A:907:LYS:CE	1:A:907:LYS:HA	0.40	2.47	12	1
1:A:879:TYR:CG	1:A:884:ILE:HD11	0.40	2.50	20	1
1:A:808:LEU:CG	1:A:894:VAL:HG23	0.40	2.44	8	1
1:A:884:ILE:CG2	1:A:923:MET:SD	0.40	3.09	10	1
1:A:806:LYS:CG	1:A:894:VAL:HG22	0.40	2.46	2	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	111/134 (83%)	92±3 (83±2%)	16±2 (15±2%)	2±1 (2±1%)	12	51
All	All	2220/2680 (83%)	1846 (83%)	325 (15%)	49 (2%)	12	51

All 9 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	812	LYS	20
1	A	866	ARG	12
1	A	881	THR	5
1	A	846	PRO	4
1	A	918	PHE	3

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Mol	Chain	Res	Type	Models (Total)
1	A	924	SER	2
1	A	811	ARG	1
1	A	911	PHE	1
1	A	913	PHE	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	101/123 (82%)	81±4 (80±4%)	20±4 (20±4%)	4	35
All	All	2020/2460 (82%)	1618 (80%)	402 (20%)	4	35

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	904	LEU	20
1	A	897	ILE	20
1	A	896	ASP	19
1	A	820	THR	18
1	A	907	LYS	18
1	A	812	LYS	15
1	A	894	VAL	12
1	A	892	PHE	12
1	A	842	PHE	11
1	A	919	ASP	10
1	A	884	ILE	10
1	A	915	LYS	9
1	A	861	LYS	9
1	A	911	PHE	8
1	A	814	LYS	8
1	A	810	CYS	8
1	A	823	VAL	7
1	A	893	VAL	7
1	A	834	LEU	7
1	A	858	LYS	7
1	A	888	LYS	7

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Mol	Chain	Res	Type	Models (Total)
1	A	822	ASP	7
1	A	909	LYS	6
1	A	862	ILE	6
1	A	824	ARG	6
1	A	872	ASP	6
1	A	811	ARG	6
1	A	838	PHE	6
1	A	830	HIS	6
1	A	816	LEU	6
1	A	832	THR	5
1	A	891	SER	5
1	A	889	ILE	5
1	A	902	GLN	5
1	A	886	VAL	4
1	A	833	VAL	4
1	A	818	CYS	4
1	A	873	TRP	4
1	A	836	ASP	4
1	A	875	ILE	4
1	A	881	THR	4
1	A	880	LYS	4
1	A	831	TYR	4
1	A	825	VAL	3
1	A	925	LYS	3
1	A	908	TRP	3
1	A	913	PHE	3
1	A	922	GLU	3
1	A	871	HIS	2
1	A	890	GLU	2
1	A	879	TYR	2
1	A	806	LYS	2
1	A	912	HIS	2
1	A	878	LYS	2
1	A	918	PHE	2
1	A	856	PHE	2
1	A	903	THR	2
1	A	844	SER	2
1	A	857	GLU	2
1	A	877	VAL	1
1	A	870	SER	1
1	A	924	SER	1
1	A	867	GLN	1

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Mol	Chain	Res	Type	Models (Total)
1	A	866	ARG	1
1	A	859	ARG	1
1	A	876	HIS	1
1	A	845	ARG	1
1	A	914	GLU	1
1	A	906	SER	1
1	A	839	LYS	1
1	A	868	ASN	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