Full wwPDB NMR Structure Validation Report (i)

Jun 12, 2024 – 06:31 AM EDT

PDB ID	:	1IRG
Title	:	INTERFERON REGULATORY FACTOR-2 DNA BINDING DOMAIN, NMR, 20 STRUCTURES
Authors	:	Furui, J.; Uegaki, K.; Yamazaki, T.; Shirakawa, M.; Swindells, M.B.; Harada, H.; Taniguchi, T.; Kyogoku, Y.
Deposited on	:	1997-11-25

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/NMRValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

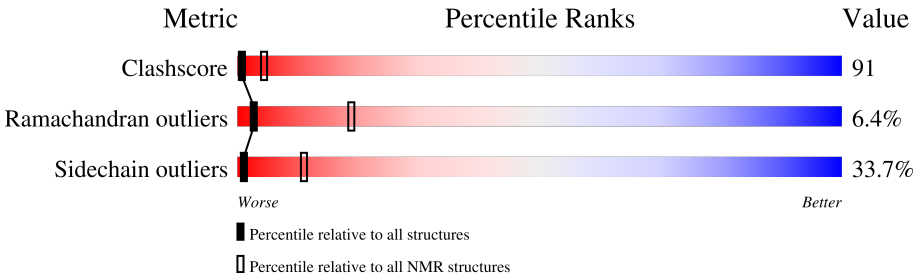
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

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	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	112	13% 51% 9% • 25%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 7 is the overall representative, medoid model (most similar to other models).

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

Well-defined (core) protein residues			
Well-defined core	**Residue range (total)**	**Backbone RMSD (Å)**	**Medoid model**
1	A:7-A:38, A:52-A:95, A:106-A:113 (84)	0.84	7

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. No single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1882 atoms, of which 942 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called INTERFERON REGULATORY FACTOR-2.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	112	1882	601	942	176	157	6	0

4 Residue-property plots (i)

4.1 Average score per residue in the NMR ensemble

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

• Molecule 1: INTERFERON REGULATORY FACTOR-2

Chain A: 13% 51% 9% • 25%

P2 V3 E4 R5 M6 R7 M8 R9 P10 W11 L12 E13 E14 Q15 I16 N17 S18 N19 T20 I21 P22 G23 L24 K25 W26 L27 N28 K29 E30 K31 K32 I33 F34 Q35 I36 P37 W38 M39 H40 A41 A42 R43 H44 G45 W46 D47 V48 E49 K50 D51 A52 P53 L54 F55 R56 N57 W58 A59 I60 H61

T62 G63 K64 H65 Q66 D70 K71 P72 D73 T76 W77 K78 F81 R82 C83 A84 M85 N86 S87 L88 P89 D90 I91 E92 E93 V94 K95 D96 R97 S98 I99 K100 K101 G102 N103 N104 A105 F106 R107 V108 Y109 R110 M111 L112 P113

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: INTERFERON REGULATORY FACTOR-2

Chain A: 15% 40% 18% • 25%

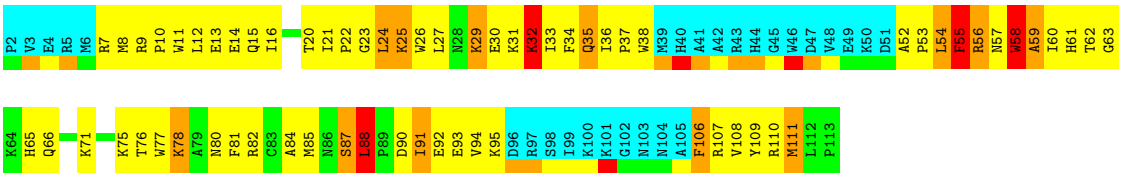
P2 V3 E4 R5 M6 R7 M8 R9 P10 W11 E14 Q15 I16 N17 S18 N19 T20 I21 P22 G23 L24 K25 W26 L27 N28 K29 E30 K31 K32 I33 F34 Q35 I36 P37 W38 M39 H40 A41 A42 R43 H44 G45 W46 D47 V48 E49 K50 D51 A52 P53 L54 F55 R56 N57 W58 A59 I60 H61 T62

G63 K64 H65 Q66 D70 D73 P74 K75 T76 W77 K78 A79 N80 F81 R82 C83 A84 M85 N86 S87 L88 P89 D90 I91 E92 E93 V94 K95 D96 R97 S98 I99 K100 K101 G102 N103 N104 A105 F106 R107 V108 Y109 R110 M111 L112 P113

4.2.2 Score per residue for model 2

• Molecule 1: INTERFERON REGULATORY FACTOR-2

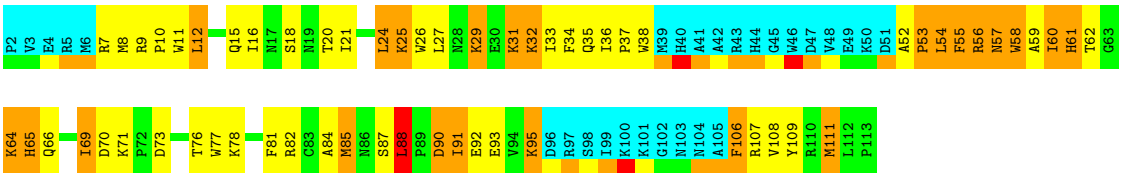
Chain A: 16% 45% 11% • 25%



4.2.3 Score per residue for model 3

- Molecule 1: INTERFERON REGULATORY FACTOR-2

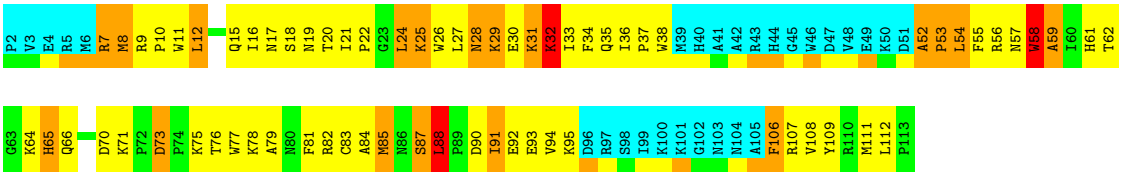
Chain A: 21% 33% 21% • 25%



4.2.4 Score per residue for model 4

- Molecule 1: INTERFERON REGULATORY FACTOR-2

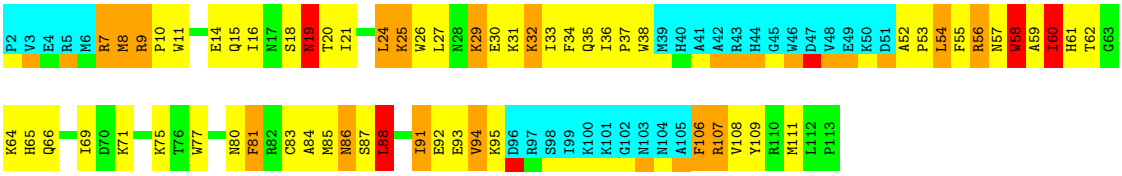
Chain A: 13% 43% 16% • 25%



4.2.5 Score per residue for model 5

- Molecule 1: INTERFERON REGULATORY FACTOR-2

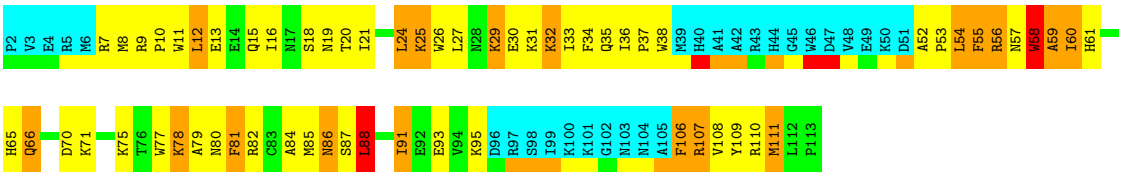
Chain A: 20% 38% 13% • 25%



4.2.6 Score per residue for model 6

- Molecule 1: INTERFERON REGULATORY FACTOR-2

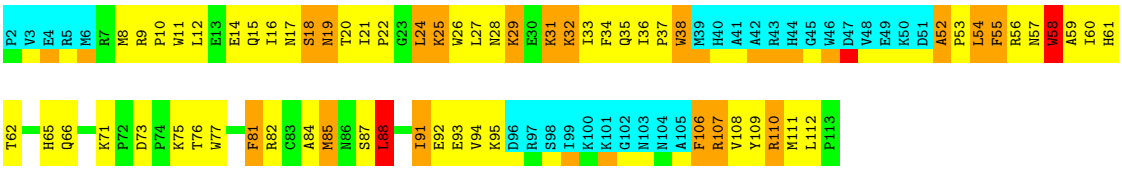
Chain A: 20% 38% 16% • 25%



4.2.7 Score per residue for model 7 (medoid)

- Molecule 1: INTERFERON REGULATORY FACTOR-2

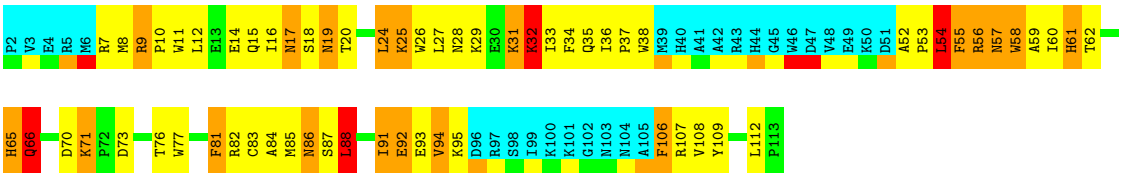
Chain A: 18% 40% 15% • 25%



4.2.8 Score per residue for model 8

- Molecule 1: INTERFERON REGULATORY FACTOR-2

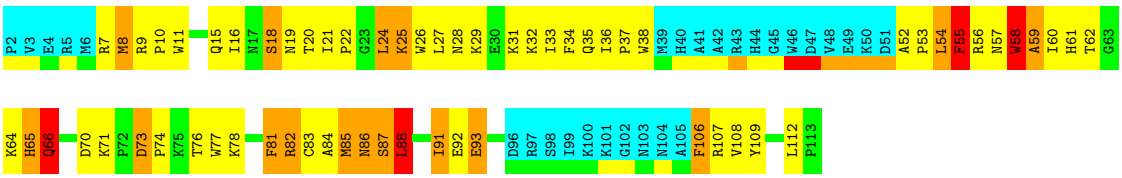
Chain A: 19% 36% 17% • 25%



4.2.9 Score per residue for model 9

- Molecule 1: INTERFERON REGULATORY FACTOR-2

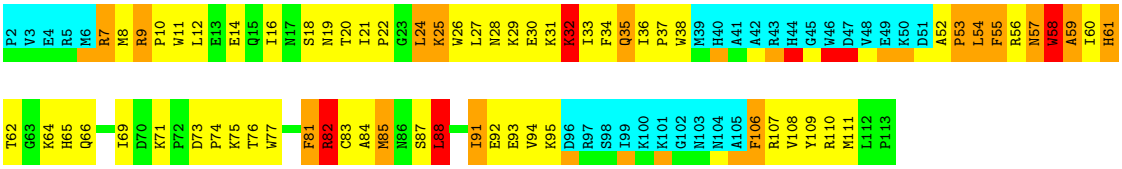
Chain A: 19% 38% 14% • 25%



4.2.10 Score per residue for model 10

- Molecule 1: INTERFERON REGULATORY FACTOR-2

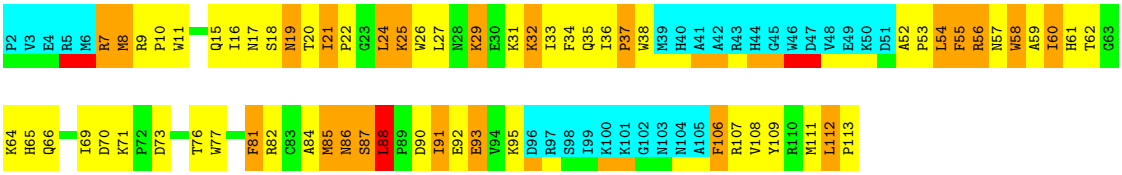
Chain A: 15% 43% 13% • 25%



4.2.11 Score per residue for model 11

- Molecule 1: INTERFERON REGULATORY FACTOR-2

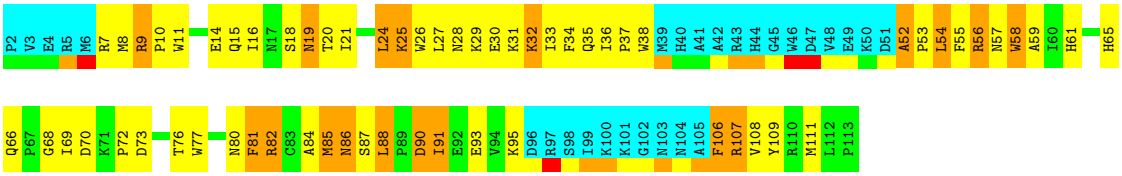
Chain A: 17% 38% 20% • 25%



4.2.12 Score per residue for model 12

- Molecule 1: INTERFERON REGULATORY FACTOR-2

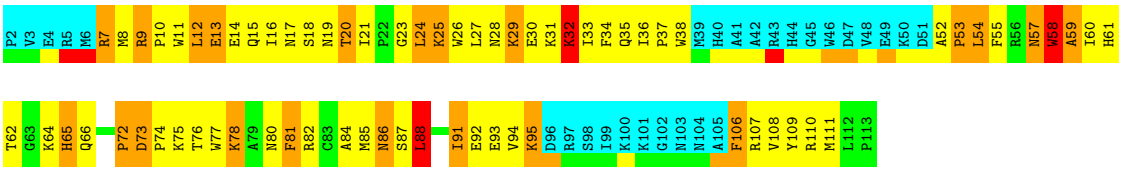
Chain A: 20% 39% 16% 25%



4.2.13 Score per residue for model 13

- Molecule 1: INTERFERON REGULATORY FACTOR-2

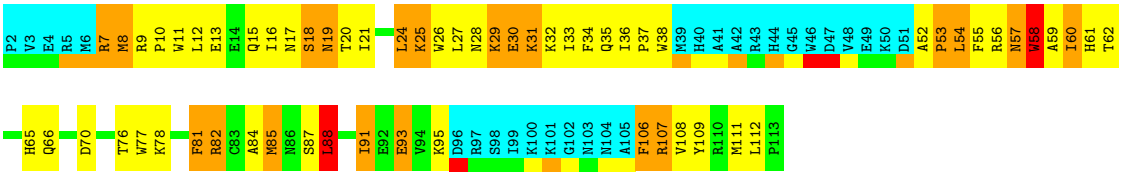
Chain A: 12% 41% 19% • 25%



4.2.14 Score per residue for model 14

- Molecule 1: INTERFERON REGULATORY FACTOR-2

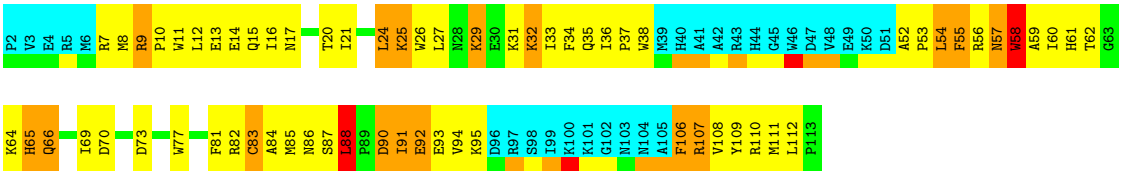
Chain A: 21% 35% 18% • 25%



4.2.15 Score per residue for model 15

- Molecule 1: INTERFERON REGULATORY FACTOR-2

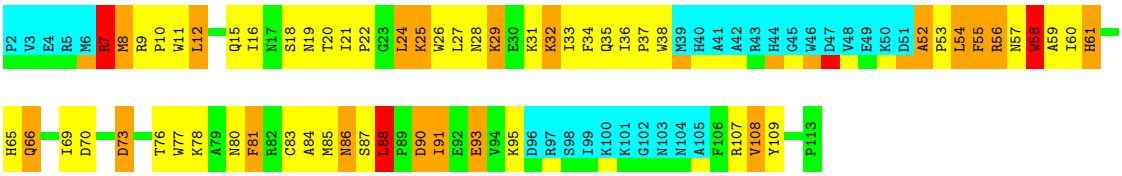
Chain A: 17% 42% 14% • 25%



4.2.16 Score per residue for model 16

- Molecule 1: INTERFERON REGULATORY FACTOR-2

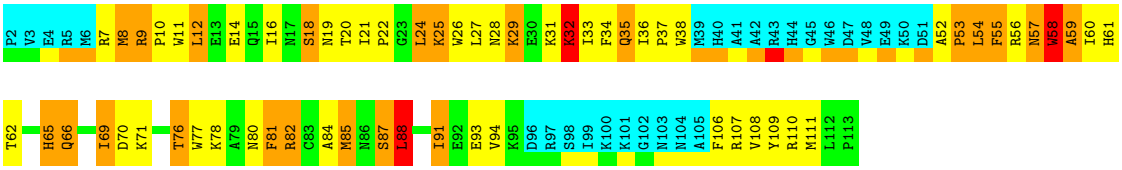
Chain A: 21% 34% 17% • 25%



4.2.17 Score per residue for model 17

- Molecule 1: INTERFERON REGULATORY FACTOR-2

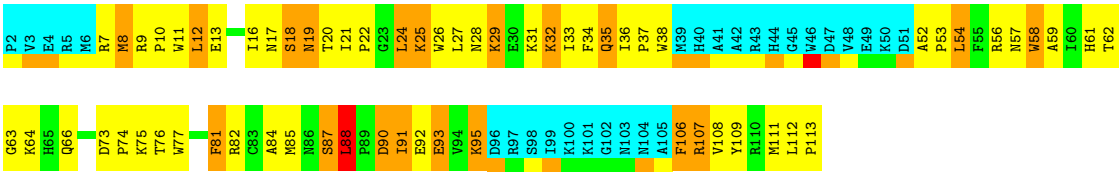
Chain A: 20% 33% 20% • 25%



4.2.18 Score per residue for model 18

- Molecule 1: INTERFERON REGULATORY FACTOR-2

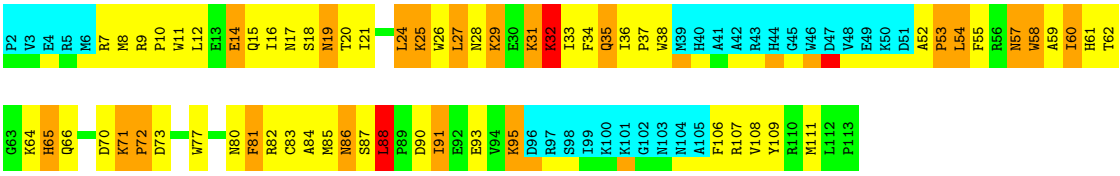
Chain A: 19% 38% 17% • 25%



4.2.19 Score per residue for model 19

- Molecule 1: INTERFERON REGULATORY FACTOR-2

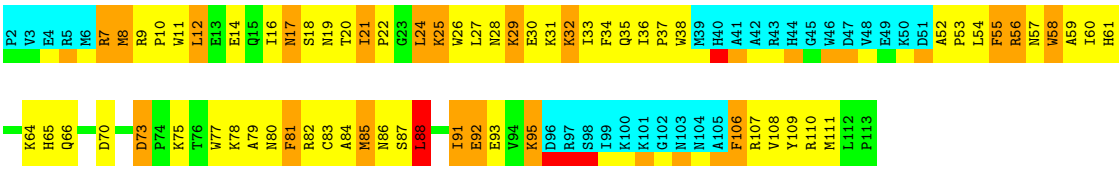
Chain A: 18% 38% 18% • 25%



4.2.20 Score per residue for model 20

- Molecule 1: INTERFERON REGULATORY FACTOR-2

Chain A: 15% 42% 17% • 25%



5 Refinement protocol and experimental data overview (i)

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

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *THE LOWEST TARGET FUNCTIONS*.

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

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

No chemical shift data was provided.

6 Model quality (i)

6.1 Standard geometry (i)

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 (i)

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	714	722	722	131±10
All	All	14280	14440	14440	2627

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 91.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:88:LEU:HD13	1:A:91:ILE:HG21	1.05	1.27	1	18
1:A:12:LEU:HD23	1:A:16:ILE:HD11	0.97	1.29	13	1
1:A:8:MET:HE1	1:A:84:ALA:HB1	0.96	1.37	4	12
1:A:8:MET:HE2	1:A:84:ALA:HB1	0.96	1.35	10	1
1:A:8:MET:CE	1:A:84:ALA:HB1	0.96	1.90	10	16
1:A:84:ALA:O	1:A:88:LEU:HD11	0.94	1.62	15	12
1:A:27:LEU:HD11	1:A:35:GLN:HB2	0.94	1.40	10	5
1:A:88:LEU:O	1:A:91:ILE:HG23	0.93	1.64	13	20
1:A:59:ALA:HB2	1:A:77:TRP:CE2	0.92	2.00	2	16
1:A:12:LEU:HD12	1:A:16:ILE:HD11	0.90	1.42	17	1
1:A:35:GLN:HB3	1:A:108:VAL:HG13	0.89	1.39	2	6
1:A:27:LEU:HD21	1:A:35:GLN:HB3	0.89	1.44	15	11
1:A:27:LEU:HD11	1:A:35:GLN:CB	0.89	1.97	10	1
1:A:35:GLN:CB	1:A:108:VAL:HG13	0.89	1.98	17	10

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:27:LEU:HD22	1:A:35:GLN:CG	0.88	1.99	19	1
1:A:54:LEU:HD22	1:A:55:PHE:N	0.88	1.84	14	5
1:A:27:LEU:HD22	1:A:35:GLN:HG2	0.88	1.44	19	1
1:A:27:LEU:HD11	1:A:108:VAL:HG13	0.88	1.45	20	15
1:A:20:THR:HG23	1:A:21:ILE:HG12	0.87	1.46	1	8
1:A:16:ILE:HG12	1:A:24:LEU:HD11	0.84	1.49	10	19
1:A:8:MET:HE2	1:A:12:LEU:HD13	0.84	1.49	18	5
1:A:35:GLN:HB2	1:A:108:VAL:HG13	0.84	1.48	7	10
1:A:85:MET:O	1:A:91:ILE:HD11	0.83	1.73	6	13
1:A:87:SER:C	1:A:88:LEU:HD12	0.83	1.94	6	17
1:A:68:GLY:C	1:A:69:ILE:HD12	0.83	1.95	12	1
1:A:54:LEU:C	1:A:54:LEU:HD22	0.82	1.95	8	4
1:A:36:ILE:HG23	1:A:37:PRO:HD2	0.82	1.52	2	20
1:A:59:ALA:O	1:A:60:ILE:HD13	0.81	1.75	19	3
1:A:24:LEU:HD12	1:A:25:LYS:N	0.81	1.90	7	19
1:A:59:ALA:HB1	1:A:65:HIS:CB	0.81	2.06	9	4
1:A:27:LEU:HD21	1:A:35:GLN:CG	0.80	2.05	8	3
1:A:20:THR:O	1:A:21:ILE:HD13	0.80	1.77	9	4
1:A:52:ALA:HB3	1:A:53:PRO:HD3	0.79	1.52	5	2
1:A:16:ILE:HG22	1:A:26:TRP:CD1	0.79	2.13	5	18
1:A:31:LYS:HB3	1:A:33:ILE:HD11	0.79	1.55	8	15
1:A:16:ILE:HG23	1:A:25:LYS:HA	0.78	1.54	8	16
1:A:59:ALA:C	1:A:60:ILE:HD12	0.78	1.98	11	2
1:A:35:GLN:HG3	1:A:108:VAL:HG22	0.78	1.54	10	1
1:A:59:ALA:HB1	1:A:65:HIS:HB3	0.78	1.56	8	14
1:A:16:ILE:CG1	1:A:24:LEU:HD11	0.77	2.09	19	13
1:A:33:ILE:HD12	1:A:33:ILE:N	0.75	1.95	20	14
1:A:52:ALA:N	1:A:53:PRO:CD	0.74	2.51	11	20
1:A:12:LEU:HD12	1:A:16:ILE:CD1	0.73	2.13	17	1
1:A:59:ALA:HB1	1:A:65:HIS:CD2	0.73	2.18	19	3
1:A:60:ILE:HD13	1:A:60:ILE:N	0.73	1.97	5	3
1:A:21:ILE:HD11	1:A:54:LEU:HD11	0.73	1.59	9	8
1:A:81:PHE:CD1	1:A:85:MET:HE1	0.73	2.18	9	1
1:A:27:LEU:HD11	1:A:108:VAL:CG1	0.73	2.14	16	12
1:A:88:LEU:HD13	1:A:91:ILE:CG2	0.72	2.13	6	18
1:A:58:TRP:O	1:A:59:ALA:HB3	0.72	1.85	12	5
1:A:84:ALA:HB3	1:A:85:MET:HE3	0.72	1.60	20	3
1:A:54:LEU:N	1:A:54:LEU:CD1	0.71	2.53	7	19
1:A:31:LYS:CB	1:A:33:ILE:HD11	0.71	2.15	13	13
1:A:36:ILE:HG22	1:A:38:TRP:CD1	0.70	2.20	4	17
1:A:58:TRP:CZ2	1:A:81:PHE:CD2	0.70	2.79	17	19

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:54:LEU:HD22	1:A:54:LEU:C	0.70	2.05	14	1
1:A:58:TRP:CZ2	1:A:81:PHE:CE2	0.70	2.79	13	8
1:A:112:LEU:N	1:A:112:LEU:HD23	0.70	2.00	11	2
1:A:27:LEU:HD23	1:A:27:LEU:N	0.70	2.02	5	14
1:A:59:ALA:HB2	1:A:77:TRP:NE1	0.70	2.02	20	12
1:A:55:PHE:CE1	1:A:81:PHE:CG	0.70	2.79	2	2
1:A:8:MET:CE	1:A:12:LEU:HD13	0.70	2.16	6	3
1:A:88:LEU:CD1	1:A:91:ILE:HG21	0.69	2.17	19	16
1:A:21:ILE:HD11	1:A:53:PRO:HG2	0.69	1.64	17	3
1:A:33:ILE:HG23	1:A:110:ARG:CG	0.69	2.18	10	2
1:A:54:LEU:HD13	1:A:55:PHE:H	0.69	1.47	8	1
1:A:11:TRP:CH2	1:A:57:ASN:ND2	0.68	2.62	16	11
1:A:12:LEU:O	1:A:16:ILE:HD12	0.68	1.89	18	10
1:A:38:TRP:CE2	1:A:107:ARG:CB	0.68	2.77	16	17
1:A:55:PHE:CE1	1:A:81:PHE:CD2	0.68	2.81	11	6
1:A:88:LEU:HD13	1:A:91:ILE:HD13	0.68	1.64	6	1
1:A:11:TRP:CZ2	1:A:57:ASN:ND2	0.67	2.62	10	13
1:A:11:TRP:CD1	1:A:61:HIS:CE1	0.67	2.82	15	9
1:A:21:ILE:HG13	1:A:54:LEU:HD21	0.67	1.65	2	2
1:A:32:LYS:C	1:A:33:ILE:HD12	0.67	2.09	20	5
1:A:84:ALA:HB3	1:A:85:MET:CE	0.67	2.20	3	6
1:A:54:LEU:N	1:A:54:LEU:HD13	0.67	2.05	14	14
1:A:54:LEU:HD12	1:A:54:LEU:N	0.67	2.04	19	2
1:A:58:TRP:CH2	1:A:81:PHE:CZ	0.67	2.83	16	5
1:A:93:GLU:CB	1:A:109:TYR:CE1	0.67	2.78	9	12
1:A:36:ILE:O	1:A:38:TRP:CD1	0.67	2.48	19	20
1:A:55:PHE:CD1	1:A:81:PHE:CD2	0.67	2.83	2	4
1:A:28:ASN:HB3	1:A:33:ILE:HD13	0.66	1.67	10	2
1:A:27:LEU:HD21	1:A:35:GLN:CB	0.66	2.20	15	3
1:A:27:LEU:HD21	1:A:35:GLN:HG3	0.66	1.66	8	1
1:A:27:LEU:HD23	1:A:27:LEU:H	0.66	1.50	19	1
1:A:58:TRP:CZ2	1:A:81:PHE:CG	0.66	2.84	9	9
1:A:21:ILE:HG22	1:A:23:GLY:H	0.66	1.49	13	1
1:A:8:MET:HE3	1:A:84:ALA:HB1	0.66	1.66	17	7
1:A:85:MET:CG	1:A:109:TYR:CZ	0.66	2.79	2	1
1:A:35:GLN:NE2	1:A:106:PHE:CD2	0.65	2.64	8	1
1:A:58:TRP:CE2	1:A:81:PHE:CD2	0.65	2.84	16	11
1:A:87:SER:O	1:A:88:LEU:O	0.65	2.13	6	20
1:A:88:LEU:CB	1:A:91:ILE:CG2	0.65	2.74	12	1
1:A:87:SER:O	1:A:88:LEU:HD12	0.65	1.92	18	13
1:A:85:MET:CG	1:A:109:TYR:CE2	0.65	2.80	2	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:16:ILE:CG2	1:A:26:TRP:CD1	0.65	2.79	14	15
1:A:84:ALA:HB3	1:A:85:MET:HE1	0.65	1.67	3	3
1:A:21:ILE:HD11	1:A:54:LEU:CD1	0.64	2.21	9	7
1:A:38:TRP:NE1	1:A:107:ARG:CB	0.64	2.60	4	17
1:A:59:ALA:HB2	1:A:77:TRP:CZ2	0.64	2.26	2	3
1:A:81:PHE:CD1	1:A:85:MET:CE	0.64	2.81	6	2
1:A:65:HIS:CG	1:A:66:GLN:N	0.64	2.66	7	19
1:A:55:PHE:CE1	1:A:81:PHE:CB	0.64	2.81	16	2
1:A:27:LEU:HD21	1:A:35:GLN:HG2	0.63	1.69	8	1
1:A:81:PHE:CE1	1:A:85:MET:CE	0.63	2.81	18	3
1:A:16:ILE:HG23	1:A:25:LYS:CA	0.63	2.23	2	9
1:A:55:PHE:CZ	1:A:81:PHE:CG	0.63	2.87	5	3
1:A:91:ILE:HD11	1:A:109:TYR:CE2	0.63	2.28	12	3
1:A:84:ALA:O	1:A:88:LEU:HD12	0.63	1.94	12	2
1:A:91:ILE:HD12	1:A:109:TYR:CD2	0.62	2.29	19	6
1:A:35:GLN:NE2	1:A:106:PHE:CE1	0.62	2.67	20	7
1:A:54:LEU:HD23	1:A:81:PHE:CZ	0.62	2.30	10	5
1:A:106:PHE:N	1:A:106:PHE:CD1	0.62	2.67	15	4
1:A:53:PRO:C	1:A:54:LEU:HD13	0.61	2.14	5	2
1:A:27:LEU:HD11	1:A:33:ILE:CG2	0.61	2.24	19	2
1:A:27:LEU:CD1	1:A:108:VAL:HG13	0.61	2.25	11	9
1:A:112:LEU:N	1:A:113:PRO:CD	0.61	2.64	18	2
1:A:11:TRP:CH2	1:A:54:LEU:HA	0.61	2.30	3	2
1:A:88:LEU:CD1	1:A:91:ILE:HD13	0.61	2.24	6	2
1:A:52:ALA:N	1:A:53:PRO:HD2	0.61	2.11	19	16
1:A:54:LEU:CD2	1:A:81:PHE:CE2	0.61	2.84	8	5
1:A:69:ILE:HG22	1:A:70:ASP:N	0.60	2.10	15	3
1:A:107:ARG:N	1:A:107:ARG:CD	0.60	2.63	9	1
1:A:93:GLU:HB3	1:A:109:TYR:CE1	0.60	2.31	15	8
1:A:38:TRP:CE2	1:A:107:ARG:HB2	0.60	2.31	16	12
1:A:21:ILE:HD12	1:A:21:ILE:N	0.60	2.12	3	2
1:A:8:MET:HE3	1:A:84:ALA:CB	0.60	2.27	2	4
1:A:21:ILE:CG1	1:A:54:LEU:HD21	0.60	2.27	4	1
1:A:12:LEU:CD2	1:A:16:ILE:HD11	0.60	2.19	13	1
1:A:27:LEU:CD1	1:A:108:VAL:CG1	0.60	2.80	11	12
1:A:33:ILE:HG23	1:A:110:ARG:HG3	0.59	1.74	10	2
1:A:21:ILE:HG22	1:A:22:PRO:HD2	0.59	1.74	10	7
1:A:91:ILE:CD1	1:A:109:TYR:CE2	0.59	2.85	12	8
1:A:38:TRP:NE1	1:A:107:ARG:HB2	0.59	2.12	19	19
1:A:34:PHE:CD1	1:A:34:PHE:O	0.59	2.56	9	9
1:A:9:ARG:NH1	1:A:88:LEU:CD2	0.59	2.66	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:20:THR:HG23	1:A:21:ILE:CG1	0.59	2.27	15	5
1:A:24:LEU:HD12	1:A:24:LEU:C	0.59	2.17	2	11
1:A:58:TRP:O	1:A:59:ALA:CB	0.59	2.50	18	3
1:A:9:ARG:HG3	1:A:88:LEU:HD23	0.59	1.75	11	2
1:A:37:PRO:C	1:A:38:TRP:CD1	0.58	2.76	13	20
1:A:38:TRP:CD1	1:A:107:ARG:HB2	0.58	2.33	4	14
1:A:88:LEU:HB2	1:A:91:ILE:CG2	0.58	2.27	12	20
1:A:34:PHE:CZ	1:A:109:TYR:CB	0.58	2.86	13	9
1:A:34:PHE:CE1	1:A:109:TYR:CB	0.58	2.86	16	7
1:A:59:ALA:CB	1:A:77:TRP:CZ2	0.58	2.85	15	5
1:A:91:ILE:CD1	1:A:109:TYR:CE1	0.58	2.86	4	3
1:A:73:ASP:O	1:A:77:TRP:CD1	0.58	2.57	10	3
1:A:53:PRO:O	1:A:54:LEU:HB2	0.58	1.97	20	2
1:A:57:ASN:OD1	1:A:62:THR:HG23	0.58	1.99	19	1
1:A:36:ILE:CG2	1:A:38:TRP:CE2	0.58	2.87	4	14
1:A:38:TRP:CE2	1:A:107:ARG:HB3	0.58	2.34	19	16
1:A:81:PHE:CE1	1:A:85:MET:HE3	0.58	2.34	6	3
1:A:54:LEU:HD13	1:A:55:PHE:N	0.58	2.14	8	1
1:A:54:LEU:CD2	1:A:81:PHE:CZ	0.58	2.87	13	4
1:A:11:TRP:CE3	1:A:12:LEU:HD12	0.58	2.33	16	3
1:A:92:GLU:OE1	1:A:112:LEU:HD11	0.58	1.99	8	1
1:A:88:LEU:HB2	1:A:91:ILE:HG21	0.58	1.75	12	1
1:A:38:TRP:CH2	1:A:85:MET:SD	0.57	2.97	9	1
1:A:18:SER:O	1:A:19:ASN:CB	0.57	2.53	11	15
1:A:36:ILE:HB	1:A:38:TRP:CE2	0.57	2.34	2	17
1:A:93:GLU:HB3	1:A:109:TYR:CZ	0.57	2.34	13	10
1:A:33:ILE:N	1:A:33:ILE:CD1	0.57	2.67	20	6
1:A:80:ASN:O	1:A:81:PHE:CB	0.57	2.51	6	1
1:A:57:ASN:ND2	1:A:58:TRP:CZ3	0.57	2.72	19	7
1:A:11:TRP:CZ3	1:A:12:LEU:HD12	0.57	2.33	8	1
1:A:31:LYS:CB	1:A:33:ILE:CD1	0.57	2.82	16	18
1:A:69:ILE:CG2	1:A:70:ASP:N	0.57	2.67	16	2
1:A:85:MET:O	1:A:109:TYR:CE1	0.57	2.57	15	1
1:A:85:MET:HG2	1:A:109:TYR:CE2	0.57	2.35	9	2
1:A:27:LEU:HD11	1:A:35:GLN:HB3	0.57	1.77	17	9
1:A:52:ALA:HB3	1:A:53:PRO:CD	0.57	2.27	5	1
1:A:93:GLU:CB	1:A:109:TYR:CZ	0.57	2.87	13	4
1:A:21:ILE:CD1	1:A:54:LEU:HD12	0.57	2.29	17	2
1:A:34:PHE:CZ	1:A:109:TYR:HB2	0.57	2.34	16	8
1:A:85:MET:HG3	1:A:109:TYR:CE2	0.57	2.34	2	2
1:A:93:GLU:O	1:A:94:VAL:HG23	0.57	2.00	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:16:ILE:HD13	1:A:34:PHE:CB	0.57	2.30	17	1
1:A:65:HIS:CD2	1:A:66:GLN:N	0.56	2.72	3	4
1:A:54:LEU:C	1:A:54:LEU:CD2	0.56	2.73	10	5
1:A:93:GLU:HB3	1:A:109:TYR:CE2	0.56	2.35	17	5
1:A:60:ILE:HD12	1:A:60:ILE:N	0.56	2.15	11	1
1:A:34:PHE:CE1	1:A:109:TYR:HB3	0.56	2.36	14	6
1:A:16:ILE:CG2	1:A:26:TRP:NE1	0.56	2.69	19	1
1:A:31:LYS:O	1:A:32:LYS:CB	0.56	2.54	19	14
1:A:11:TRP:CH2	1:A:54:LEU:CA	0.56	2.88	3	2
1:A:35:GLN:CD	1:A:106:PHE:CD1	0.56	2.79	13	4
1:A:21:ILE:HB	1:A:24:LEU:HD23	0.56	1.75	3	1
1:A:52:ALA:N	1:A:53:PRO:HD3	0.56	2.15	7	4
1:A:76:THR:CG2	1:A:77:TRP:N	0.56	2.68	4	1
1:A:21:ILE:HG23	1:A:22:PRO:HD2	0.56	1.76	17	2
1:A:54:LEU:O	1:A:57:ASN:N	0.56	2.39	19	5
1:A:9:ARG:CB	1:A:10:PRO:CD	0.56	2.84	15	18
1:A:84:ALA:O	1:A:88:LEU:CD1	0.56	2.54	2	3
1:A:36:ILE:O	1:A:106:PHE:CB	0.56	2.53	20	15
1:A:58:TRP:CH2	1:A:81:PHE:CE2	0.55	2.94	15	10
1:A:54:LEU:O	1:A:57:ASN:ND2	0.55	2.40	6	9
1:A:93:GLU:HA	1:A:109:TYR:CD1	0.55	2.36	14	9
1:A:93:GLU:HB2	1:A:109:TYR:CE1	0.55	2.36	6	7
1:A:25:LYS:CD	1:A:25:LYS:N	0.55	2.69	11	1
1:A:27:LEU:HD11	1:A:108:VAL:HG11	0.55	1.78	16	1
1:A:38:TRP:CZ2	1:A:109:TYR:CE1	0.55	2.94	20	6
1:A:112:LEU:N	1:A:113:PRO:HD2	0.55	2.17	18	2
1:A:88:LEU:O	1:A:91:ILE:CG2	0.55	2.55	2	1
1:A:35:GLN:NE2	1:A:106:PHE:CE2	0.55	2.75	3	2
1:A:69:ILE:HG22	1:A:69:ILE:O	0.55	2.01	5	2
1:A:35:GLN:HG2	1:A:108:VAL:HG13	0.55	1.79	19	1
1:A:35:GLN:CB	1:A:108:VAL:HA	0.55	2.32	1	4
1:A:36:ILE:HB	1:A:38:TRP:NE1	0.55	2.16	4	18
1:A:11:TRP:CH2	1:A:54:LEU:CB	0.55	2.90	3	2
1:A:55:PHE:CZ	1:A:78:LYS:HD3	0.55	2.37	1	1
1:A:55:PHE:CZ	1:A:81:PHE:HB3	0.55	2.37	5	2
1:A:55:PHE:CE2	1:A:81:PHE:CB	0.54	2.90	7	1
1:A:16:ILE:CG2	1:A:26:TRP:N	0.54	2.70	17	8
1:A:11:TRP:CD1	1:A:61:HIS:NE2	0.54	2.75	20	2
1:A:54:LEU:HA	1:A:57:ASN:ND2	0.54	2.17	18	2
1:A:85:MET:SD	1:A:85:MET:N	0.54	2.81	2	5
1:A:21:ILE:HD12	1:A:54:LEU:HD21	0.54	1.79	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:11:TRP:HE3	1:A:12:LEU:HD12	0.54	1.60	16	1
1:A:11:TRP:CZ3	1:A:15:GLN:HG3	0.54	2.38	12	14
1:A:58:TRP:CZ2	1:A:81:PHE:CZ	0.54	2.96	16	4
1:A:33:ILE:HG23	1:A:110:ARG:HA	0.54	1.77	2	1
1:A:55:PHE:CD1	1:A:81:PHE:CE2	0.54	2.95	2	4
1:A:93:GLU:CG	1:A:93:GLU:O	0.54	2.54	13	2
1:A:85:MET:HB2	1:A:109:TYR:CZ	0.54	2.38	10	1
1:A:38:TRP:CZ2	1:A:107:ARG:HB3	0.54	2.38	15	3
1:A:55:PHE:CE1	1:A:81:PHE:HB2	0.54	2.37	16	1
1:A:95:LYS:CB	1:A:106:PHE:O	0.54	2.56	13	1
1:A:57:ASN:O	1:A:61:HIS:CB	0.54	2.56	1	1
1:A:57:ASN:OD1	1:A:61:HIS:CB	0.54	2.55	17	3
1:A:34:PHE:CD1	1:A:34:PHE:C	0.54	2.82	2	7
1:A:35:GLN:CD	1:A:106:PHE:CD2	0.54	2.81	7	3
1:A:55:PHE:CZ	1:A:81:PHE:CB	0.54	2.90	5	2
1:A:94:VAL:O	1:A:94:VAL:HG12	0.54	2.03	15	3
1:A:9:ARG:CB	1:A:10:PRO:HD3	0.54	2.33	15	18
1:A:59:ALA:CB	1:A:77:TRP:CE2	0.54	2.89	15	4
1:A:12:LEU:O	1:A:16:ILE:CD1	0.54	2.56	4	4
1:A:8:MET:CE	1:A:84:ALA:CB	0.53	2.85	3	7
1:A:91:ILE:CD1	1:A:109:TYR:CD2	0.53	2.91	12	9
1:A:73:ASP:O	1:A:77:TRP:CG	0.53	2.61	10	2
1:A:9:ARG:N	1:A:10:PRO:HD2	0.53	2.18	19	20
1:A:26:TRP:CG	1:A:29:LYS:HB3	0.53	2.39	18	6
1:A:36:ILE:O	1:A:106:PHE:HB3	0.53	2.02	15	16
1:A:81:PHE:O	1:A:85:MET:HE1	0.53	2.03	2	1
1:A:54:LEU:N	1:A:54:LEU:HD12	0.53	2.17	20	3
1:A:31:LYS:HB2	1:A:33:ILE:CD1	0.53	2.34	2	7
1:A:11:TRP:CH2	1:A:54:LEU:HB3	0.53	2.38	3	2
1:A:54:LEU:O	1:A:56:ARG:N	0.53	2.42	1	13
1:A:54:LEU:HA	1:A:57:ASN:HB3	0.53	1.79	14	4
1:A:26:TRP:CE3	1:A:34:PHE:HB3	0.53	2.39	8	14
1:A:85:MET:HA	1:A:91:ILE:CD1	0.53	2.34	8	5
1:A:85:MET:HG3	1:A:109:TYR:CZ	0.53	2.39	2	1
1:A:33:ILE:CG2	1:A:110:ARG:CG	0.53	2.87	10	1
1:A:27:LEU:HD22	1:A:35:GLN:HG3	0.53	1.80	19	1
1:A:88:LEU:CB	1:A:91:ILE:HG21	0.53	2.34	12	1
1:A:34:PHE:O	1:A:34:PHE:CG	0.53	2.61	12	13
1:A:57:ASN:C	1:A:57:ASN:OD1	0.53	2.47	3	2
1:A:36:ILE:HG22	1:A:38:TRP:NE1	0.53	2.19	4	9
1:A:35:GLN:OE1	1:A:106:PHE:CD1	0.53	2.62	13	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:12:LEU:O	1:A:16:ILE:CG1	0.53	2.57	14	2
1:A:8:MET:HE2	1:A:12:LEU:HD22	0.53	1.80	16	1
1:A:55:PHE:CE1	1:A:81:PHE:CD1	0.52	2.97	5	2
1:A:54:LEU:O	1:A:58:TRP:CE3	0.52	2.62	18	4
1:A:77:TRP:CD1	1:A:77:TRP:N	0.52	2.76	13	7
1:A:85:MET:CG	1:A:109:TYR:OH	0.52	2.57	14	1
1:A:27:LEU:HD11	1:A:33:ILE:HG21	0.52	1.80	19	1
1:A:34:PHE:O	1:A:34:PHE:CD1	0.52	2.62	12	1
1:A:35:GLN:CG	1:A:108:VAL:HG13	0.52	2.34	19	2
1:A:36:ILE:CB	1:A:38:TRP:NE1	0.52	2.72	4	12
1:A:52:ALA:O	1:A:56:ARG:CB	0.52	2.57	8	2
1:A:58:TRP:O	1:A:60:ILE:N	0.52	2.42	17	6
1:A:59:ALA:HB1	1:A:65:HIS:CG	0.52	2.40	3	2
1:A:21:ILE:CG1	1:A:24:LEU:HD23	0.52	2.35	20	2
1:A:88:LEU:HB3	1:A:91:ILE:CG2	0.52	2.34	12	1
1:A:21:ILE:HD12	1:A:53:PRO:HG2	0.52	1.82	14	1
1:A:26:TRP:CD2	1:A:29:LYS:HG2	0.52	2.40	5	2
1:A:73:ASP:O	1:A:77:TRP:CE2	0.52	2.63	11	3
1:A:65:HIS:CE1	1:A:71:LYS:C	0.52	2.84	8	2
1:A:11:TRP:CD1	1:A:61:HIS:CD2	0.52	2.98	19	2
1:A:65:HIS:O	1:A:66:GLN:CB	0.51	2.58	9	2
1:A:54:LEU:O	1:A:55:PHE:C	0.51	2.48	19	13
1:A:85:MET:O	1:A:91:ILE:CD1	0.51	2.58	1	7
1:A:107:ARG:N	1:A:107:ARG:HD2	0.51	2.20	9	1
1:A:85:MET:N	1:A:85:MET:HE3	0.51	2.21	10	1
1:A:58:TRP:CH2	1:A:81:PHE:CD2	0.51	2.98	15	2
1:A:36:ILE:C	1:A:38:TRP:CD1	0.51	2.84	4	18
1:A:36:ILE:O	1:A:38:TRP:NE1	0.51	2.44	15	19
1:A:8:MET:HE1	1:A:12:LEU:HD13	0.51	1.82	6	1
1:A:81:PHE:O	1:A:83:CYS:N	0.51	2.43	10	1
1:A:27:LEU:HD21	1:A:33:ILE:HG22	0.51	1.82	19	1
1:A:23:GLY:O	1:A:35:GLN:NE2	0.51	2.44	2	1
1:A:86:ASN:N	1:A:86:ASN:OD1	0.51	2.43	9	2
1:A:28:ASN:HB2	1:A:33:ILE:HD13	0.51	1.82	18	3
1:A:31:LYS:HB3	1:A:33:ILE:CD1	0.51	2.36	15	2
1:A:53:PRO:O	1:A:54:LEU:CB	0.51	2.59	5	1
1:A:21:ILE:HG13	1:A:24:LEU:HD23	0.51	1.83	12	2
1:A:38:TRP:CH2	1:A:85:MET:CG	0.51	2.93	9	1
1:A:36:ILE:CG2	1:A:37:PRO:HD2	0.51	2.34	12	18
1:A:37:PRO:O	1:A:38:TRP:HB2	0.51	2.06	13	20
1:A:25:LYS:CE	1:A:27:LEU:CD2	0.51	2.89	4	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:58:TRP:O	1:A:62:THR:OG1	0.50	2.29	19	5
1:A:11:TRP:CE3	1:A:15:GLN:HG3	0.50	2.41	14	2
1:A:87:SER:O	1:A:88:LEU:C	0.50	2.49	13	20
1:A:91:ILE:HG13	1:A:109:TYR:CD2	0.50	2.42	5	6
1:A:57:ASN:OD1	1:A:57:ASN:C	0.50	2.49	19	1
1:A:26:TRP:CE2	1:A:29:LYS:HD2	0.50	2.41	2	5
1:A:82:ARG:O	1:A:86:ASN:HB3	0.50	2.07	12	1
1:A:20:THR:HB	1:A:21:ILE:HD12	0.50	1.83	13	1
1:A:69:ILE:HG23	1:A:70:ASP:N	0.50	2.22	16	1
1:A:33:ILE:HG13	1:A:110:ARG:CG	0.50	2.37	17	1
1:A:27:LEU:HD21	1:A:35:GLN:N	0.50	2.22	1	1
1:A:25:LYS:CD	1:A:25:LYS:C	0.50	2.80	19	3
1:A:58:TRP:HA	1:A:58:TRP:CE3	0.50	2.41	13	6
1:A:55:PHE:CG	1:A:81:PHE:CD2	0.50	2.99	12	1
1:A:72:PRO:O	1:A:73:ASP:CB	0.50	2.60	19	2
1:A:33:ILE:CG2	1:A:110:ARG:HG2	0.50	2.36	10	2
1:A:16:ILE:HG21	1:A:26:TRP:CD1	0.49	2.42	1	2
1:A:81:PHE:O	1:A:85:MET:HE2	0.49	2.07	5	3
1:A:28:ASN:CB	1:A:33:ILE:HD13	0.49	2.37	10	1
1:A:90:ASP:N	1:A:90:ASP:OD1	0.49	2.45	3	2
1:A:21:ILE:CD1	1:A:54:LEU:CD2	0.49	2.90	5	1
1:A:85:MET:HB3	1:A:109:TYR:CZ	0.49	2.42	19	3
1:A:31:LYS:O	1:A:32:LYS:HB2	0.49	2.07	18	15
1:A:35:GLN:HA	1:A:108:VAL:HA	0.49	1.84	19	11
1:A:38:TRP:CD1	1:A:38:TRP:N	0.49	2.80	4	18
1:A:91:ILE:HD12	1:A:109:TYR:CD1	0.49	2.43	4	3
1:A:30:GLU:CG	1:A:31:LYS:N	0.49	2.76	13	2
1:A:57:ASN:O	1:A:58:TRP:O	0.49	2.30	4	5
1:A:57:ASN:ND2	1:A:58:TRP:CE3	0.49	2.81	10	2
1:A:55:PHE:CZ	1:A:78:LYS:HG3	0.49	2.42	13	1
1:A:21:ILE:CD1	1:A:53:PRO:HG2	0.49	2.38	19	7
1:A:35:GLN:OE1	1:A:106:PHE:CB	0.49	2.60	8	2
1:A:21:ILE:HD11	1:A:54:LEU:HD12	0.49	1.84	17	2
1:A:112:LEU:N	1:A:112:LEU:CD2	0.49	2.69	11	1
1:A:11:TRP:CB	1:A:61:HIS:NE2	0.49	2.76	15	1
1:A:34:PHE:CE1	1:A:109:TYR:HB2	0.49	2.43	6	6
1:A:21:ILE:HG13	1:A:54:LEU:CD2	0.49	2.38	4	1
1:A:58:TRP:CZ2	1:A:81:PHE:CD1	0.49	3.00	12	1
1:A:30:GLU:HG3	1:A:31:LYS:N	0.49	2.23	13	2
1:A:36:ILE:CG2	1:A:38:TRP:NE1	0.48	2.76	4	7
1:A:16:ILE:CG2	1:A:25:LYS:HA	0.48	2.35	2	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:35:GLN:OE1	1:A:36:ILE:N	0.48	2.45	2	1
1:A:60:ILE:N	1:A:60:ILE:CD1	0.48	2.72	14	3
1:A:55:PHE:CE2	1:A:81:PHE:HB3	0.48	2.42	12	1
1:A:11:TRP:CZ3	1:A:54:LEU:HB3	0.48	2.43	3	1
1:A:86:ASN:O	1:A:86:ASN:ND2	0.48	2.46	11	2
1:A:8:MET:SD	1:A:84:ALA:HB1	0.48	2.48	14	1
1:A:11:TRP:CH2	1:A:15:GLN:HG3	0.48	2.43	3	2
1:A:37:PRO:O	1:A:38:TRP:CB	0.48	2.60	13	16
1:A:55:PHE:O	1:A:58:TRP:HB2	0.48	2.08	19	9
1:A:36:ILE:HG23	1:A:37:PRO:CD	0.48	2.34	2	5
1:A:59:ALA:C	1:A:60:ILE:CD1	0.48	2.78	11	1
1:A:27:LEU:HD12	1:A:108:VAL:CG1	0.48	2.38	13	1
1:A:16:ILE:CG2	1:A:25:LYS:C	0.48	2.81	13	2
1:A:73:ASP:OD2	1:A:75:LYS:CE	0.48	2.62	4	1
1:A:33:ILE:CG1	1:A:110:ARG:HG3	0.48	2.38	6	1
1:A:9:ARG:N	1:A:10:PRO:CD	0.48	2.77	10	19
1:A:21:ILE:CG2	1:A:22:PRO:HD2	0.48	2.39	16	7
1:A:64:LYS:O	1:A:65:HIS:CB	0.48	2.60	4	5
1:A:86:ASN:O	1:A:86:ASN:CG	0.48	2.52	11	3
1:A:16:ILE:HG21	1:A:26:TRP:NE1	0.48	2.23	19	1
1:A:57:ASN:CB	1:A:61:HIS:HB3	0.48	2.39	3	2
1:A:81:PHE:O	1:A:85:MET:SD	0.48	2.72	10	6
1:A:56:ARG:O	1:A:57:ASN:C	0.48	2.51	18	10
1:A:58:TRP:CE3	1:A:58:TRP:HA	0.48	2.44	10	2
1:A:65:HIS:CE1	1:A:71:LYS:O	0.48	2.67	19	1
1:A:69:ILE:O	1:A:69:ILE:CG2	0.48	2.62	5	1
1:A:31:LYS:HB2	1:A:33:ILE:HD11	0.48	1.85	13	1
1:A:21:ILE:CG1	1:A:53:PRO:HG2	0.47	2.38	3	1
1:A:11:TRP:CD1	1:A:61:HIS:ND1	0.47	2.82	15	1
1:A:55:PHE:CZ	1:A:78:LYS:CD	0.47	2.97	1	1
1:A:26:TRP:CD2	1:A:29:LYS:HD2	0.47	2.45	19	2
1:A:25:LYS:N	1:A:25:LYS:CD	0.47	2.73	7	5
1:A:53:PRO:O	1:A:54:LEU:C	0.47	2.51	19	2
1:A:26:TRP:CZ3	1:A:34:PHE:HB3	0.47	2.44	7	6
1:A:38:TRP:CH2	1:A:85:MET:HG2	0.47	2.45	6	3
1:A:9:ARG:HB2	1:A:10:PRO:HD3	0.47	1.86	18	12
1:A:27:LEU:CD1	1:A:33:ILE:CG2	0.47	2.92	1	1
1:A:27:LEU:HD11	1:A:33:ILE:HG22	0.47	1.86	1	1
1:A:35:GLN:HB2	1:A:108:VAL:HA	0.47	1.86	2	2
1:A:18:SER:O	1:A:19:ASN:HB3	0.47	2.09	20	4
1:A:25:LYS:HE2	1:A:27:LEU:CD2	0.47	2.40	7	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:21:ILE:HG13	1:A:53:PRO:CG	0.47	2.39	3	1
1:A:91:ILE:HD12	1:A:109:TYR:CE2	0.47	2.44	14	3
1:A:29:LYS:O	1:A:29:LYS:CE	0.47	2.61	20	2
1:A:52:ALA:O	1:A:56:ARG:HB2	0.47	2.09	8	1
1:A:54:LEU:HD23	1:A:81:PHE:HZ	0.47	1.68	17	2
1:A:8:MET:HG3	1:A:12:LEU:HD13	0.47	1.85	14	1
1:A:24:LEU:C	1:A:24:LEU:CD1	0.47	2.82	2	4
1:A:20:THR:CG2	1:A:21:ILE:HG12	0.47	2.39	4	2
1:A:11:TRP:CH2	1:A:54:LEU:HB2	0.47	2.43	14	1
1:A:27:LEU:CD1	1:A:33:ILE:HG22	0.47	2.39	1	1
1:A:85:MET:HB3	1:A:109:TYR:CE2	0.47	2.45	19	3
1:A:20:THR:HG23	1:A:21:ILE:CD1	0.47	2.40	17	2
1:A:29:LYS:HE3	1:A:29:LYS:N	0.47	2.25	4	1
1:A:76:THR:HG23	1:A:77:TRP:N	0.47	2.24	4	1
1:A:24:LEU:CB	1:A:37:PRO:HD3	0.47	2.40	7	5
1:A:58:TRP:CD1	1:A:80:ASN:HB2	0.47	2.45	19	2
1:A:38:TRP:CZ2	1:A:109:TYR:CE2	0.47	3.03	15	4
1:A:92:GLU:O	1:A:94:VAL:HG23	0.47	2.09	1	1
1:A:33:ILE:CG1	1:A:110:ARG:HD2	0.47	2.39	7	1
1:A:16:ILE:HG23	1:A:25:LYS:C	0.47	2.30	13	5
1:A:8:MET:HE3	1:A:12:LEU:HD22	0.47	1.86	10	1
1:A:92:GLU:O	1:A:108:VAL:O	0.47	2.33	20	1
1:A:35:GLN:NE2	1:A:106:PHE:CD1	0.46	2.83	1	3
1:A:56:ARG:O	1:A:58:TRP:N	0.46	2.48	2	8
1:A:54:LEU:HD13	1:A:54:LEU:N	0.46	2.24	5	1
1:A:33:ILE:HG23	1:A:110:ARG:HG2	0.46	1.86	20	2
1:A:25:LYS:HE3	1:A:27:LEU:CD2	0.46	2.40	8	5
1:A:54:LEU:CB	1:A:58:TRP:CZ3	0.46	2.98	3	1
1:A:83:CYS:O	1:A:86:ASN:OD1	0.46	2.33	20	2
1:A:27:LEU:CD2	1:A:35:GLN:N	0.46	2.78	1	1
1:A:58:TRP:O	1:A:61:HIS:O	0.46	2.34	2	1
1:A:88:LEU:HB2	1:A:91:ILE:HG22	0.46	1.86	2	1
1:A:60:ILE:O	1:A:61:HIS:C	0.46	2.54	16	5
1:A:55:PHE:CD1	1:A:56:ARG:N	0.46	2.83	8	1
1:A:24:LEU:CA	1:A:37:PRO:HD3	0.46	2.41	9	5
1:A:81:PHE:O	1:A:82:ARG:C	0.46	2.53	10	4
1:A:106:PHE:CD1	1:A:106:PHE:N	0.46	2.83	14	2
1:A:90:ASP:OD1	1:A:90:ASP:N	0.46	2.48	16	1
1:A:35:GLN:OE1	1:A:106:PHE:HB2	0.46	2.11	2	3
1:A:90:ASP:HB3	1:A:113:PRO:CD	0.46	2.40	11	1
1:A:32:LYS:HE2	1:A:111:MET:CB	0.46	2.40	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:20:THR:C	1:A:21:ILE:HD13	0.46	2.31	1	1
1:A:58:TRP:CD1	1:A:77:TRP:O	0.46	2.69	12	7
1:A:57:ASN:O	1:A:61:HIS:HB3	0.46	2.11	13	3
1:A:58:TRP:O	1:A:59:ALA:C	0.46	2.53	2	7
1:A:91:ILE:HD11	1:A:109:TYR:CD1	0.46	2.46	2	2
1:A:29:LYS:O	1:A:29:LYS:HE2	0.46	2.11	20	2
1:A:95:LYS:HB3	1:A:107:ARG:CD	0.46	2.41	3	1
1:A:11:TRP:CZ3	1:A:12:LEU:CD1	0.46	2.99	8	1
1:A:73:ASP:O	1:A:77:TRP:CD2	0.46	2.68	9	2
1:A:12:LEU:HD21	1:A:34:PHE:CE2	0.46	2.46	10	1
1:A:34:PHE:CD2	1:A:111:MET:CE	0.46	2.99	11	1
1:A:16:ILE:HG13	1:A:24:LEU:HD11	0.46	1.85	19	1
1:A:12:LEU:O	1:A:13:GLU:C	0.46	2.53	2	3
1:A:25:LYS:HE3	1:A:27:LEU:HD22	0.46	1.87	2	2
1:A:35:GLN:HB3	1:A:108:VAL:CG1	0.46	2.39	19	1
1:A:35:GLN:OE1	1:A:36:ILE:O	0.45	2.33	2	1
1:A:7:ARG:HB3	1:A:10:PRO:CD	0.45	2.41	10	5
1:A:38:TRP:CH2	1:A:85:MET:HE3	0.45	2.46	12	1
1:A:8:MET:SD	1:A:84:ALA:CB	0.45	3.04	14	1
1:A:27:LEU:CD1	1:A:108:VAL:HG11	0.45	2.40	16	1
1:A:55:PHE:CD1	1:A:78:LYS:HG2	0.45	2.45	16	1
1:A:8:MET:O	1:A:8:MET:SD	0.45	2.73	17	1
1:A:62:THR:O	1:A:63:GLY:C	0.45	2.52	2	2
1:A:13:GLU:O	1:A:17:ASN:HB2	0.45	2.10	13	1
1:A:61:HIS:CG	1:A:62:THR:N	0.45	2.81	1	1
1:A:93:GLU:O	1:A:94:VAL:CG2	0.45	2.64	5	1
1:A:25:LYS:N	1:A:25:LYS:HD2	0.45	2.24	11	3
1:A:81:PHE:CE1	1:A:85:MET:HE1	0.45	2.46	9	1
1:A:86:ASN:ND2	1:A:86:ASN:C	0.45	2.69	13	2
1:A:55:PHE:CD1	1:A:55:PHE:C	0.45	2.89	17	1
1:A:9:ARG:CZ	1:A:9:ARG:HA	0.45	2.41	18	1
1:A:35:GLN:OE1	1:A:35:GLN:C	0.45	2.55	1	3
1:A:37:PRO:HA	1:A:106:PHE:HB3	0.45	1.88	11	7
1:A:85:MET:HB3	1:A:109:TYR:OH	0.45	2.11	16	4
1:A:11:TRP:HB2	1:A:61:HIS:CE1	0.45	2.47	15	1
1:A:86:ASN:OD1	1:A:109:TYR:OH	0.45	2.33	15	1
1:A:72:PRO:HB2	1:A:77:TRP:CH2	0.45	2.47	19	1
1:A:111:MET:O	1:A:112:LEU:C	0.45	2.55	15	1
1:A:95:LYS:HA	1:A:106:PHE:O	0.45	2.12	5	3
1:A:65:HIS:CE1	1:A:70:ASP:O	0.45	2.70	8	2
1:A:72:PRO:O	1:A:73:ASP:OD1	0.45	2.34	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:31:LYS:HB2	1:A:33:ILE:HD13	0.45	1.87	20	1
1:A:16:ILE:CG2	1:A:26:TRP:CG	0.45	2.99	7	2
1:A:17:ASN:O	1:A:18:SER:C	0.45	2.54	13	2
1:A:95:LYS:HB2	1:A:106:PHE:O	0.45	2.12	13	1
1:A:54:LEU:C	1:A:56:ARG:N	0.45	2.70	20	9
1:A:56:ARG:CD	1:A:56:ARG:C	0.45	2.85	5	1
1:A:57:ASN:O	1:A:58:TRP:C	0.45	2.55	5	6
1:A:82:ARG:HD2	1:A:83:CYS:N	0.45	2.27	9	1
1:A:83:CYS:O	1:A:84:ALA:C	0.45	2.55	9	1
1:A:83:CYS:O	1:A:87:SER:N	0.45	2.50	9	1
1:A:61:HIS:O	1:A:62:THR:C	0.45	2.55	11	13
1:A:83:CYS:HA	1:A:86:ASN:OD1	0.45	2.11	8	5
1:A:21:ILE:N	1:A:21:ILE:CD1	0.45	2.80	3	1
1:A:11:TRP:CD1	1:A:61:HIS:CG	0.45	3.05	15	1
1:A:14:GLU:O	1:A:15:GLN:C	0.44	2.54	8	4
1:A:55:PHE:C	1:A:55:PHE:CD1	0.44	2.89	13	1
1:A:32:LYS:CE	1:A:111:MET:HB3	0.44	2.42	14	1
1:A:11:TRP:HB2	1:A:61:HIS:NE2	0.44	2.27	19	2
1:A:78:LYS:O	1:A:79:ALA:C	0.44	2.56	6	1
1:A:94:VAL:O	1:A:108:VAL:HG23	0.44	2.13	7	1
1:A:57:ASN:OD1	1:A:61:HIS:HB2	0.44	2.12	10	3
1:A:24:LEU:C	1:A:25:LYS:CD	0.44	2.86	10	1
1:A:31:LYS:O	1:A:32:LYS:HB3	0.44	2.12	19	1
1:A:95:LYS:HD3	1:A:107:ARG:NH1	0.44	2.28	5	1
1:A:38:TRP:NE1	1:A:107:ARG:HB3	0.44	2.27	4	2
1:A:95:LYS:HB3	1:A:107:ARG:NE	0.44	2.28	6	1
1:A:71:LYS:N	1:A:71:LYS:HD3	0.44	2.27	17	1
1:A:31:LYS:C	1:A:32:LYS:CG	0.44	2.84	17	1
1:A:11:TRP:CZ2	1:A:57:ASN:CG	0.44	2.91	2	1
1:A:92:GLU:O	1:A:109:TYR:HA	0.44	2.12	10	3
1:A:91:ILE:HD12	1:A:109:TYR:CE1	0.44	2.47	4	1
1:A:95:LYS:CB	1:A:107:ARG:HD2	0.44	2.43	6	1
1:A:65:HIS:ND1	1:A:71:LYS:O	0.44	2.51	8	2
1:A:18:SER:O	1:A:19:ASN:HB2	0.44	2.12	18	2
1:A:66:GLN:NE2	1:A:69:ILE:HD13	0.44	2.28	11	1
1:A:16:ILE:HG12	1:A:24:LEU:CD1	0.44	2.43	19	3
1:A:59:ALA:O	1:A:60:ILE:C	0.44	2.55	2	2
1:A:54:LEU:HB2	1:A:58:TRP:CZ3	0.44	2.48	3	1
1:A:59:ALA:CB	1:A:65:HIS:HB3	0.44	2.42	3	1
1:A:27:LEU:HD11	1:A:35:GLN:OE1	0.44	2.12	5	2
1:A:36:ILE:HB	1:A:38:TRP:CZ2	0.44	2.47	2	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:55:PHE:CE2	1:A:78:LYS:HA	0.44	2.47	2	1
1:A:56:ARG:C	1:A:58:TRP:N	0.44	2.71	12	6
1:A:59:ALA:O	1:A:60:ILE:CD1	0.44	2.60	19	1
1:A:34:PHE:CD1	1:A:109:TYR:O	0.44	2.71	20	1
1:A:91:ILE:CG1	1:A:109:TYR:CD1	0.44	3.01	15	2
1:A:7:ARG:HB3	1:A:10:PRO:CG	0.44	2.43	13	1
1:A:11:TRP:CE3	1:A:11:TRP:C	0.44	2.91	14	1
1:A:35:GLN:OE1	1:A:108:VAL:HG22	0.44	2.13	14	1
1:A:27:LEU:N	1:A:27:LEU:CD2	0.44	2.73	19	1
1:A:74:PRO:HA	1:A:77:TRP:CD2	0.43	2.48	13	2
1:A:16:ILE:CG1	1:A:24:LEU:CD1	0.43	2.92	19	1
1:A:90:ASP:O	1:A:111:MET:HA	0.43	2.14	12	4
1:A:24:LEU:HD13	1:A:36:ILE:CG1	0.43	2.43	2	1
1:A:54:LEU:HD13	1:A:54:LEU:H	0.43	1.73	2	1
1:A:65:HIS:O	1:A:66:GLN:HB2	0.43	2.12	8	2
1:A:21:ILE:CG1	1:A:53:PRO:CG	0.43	2.97	3	1
1:A:24:LEU:HA	1:A:35:GLN:O	0.43	2.14	14	6
1:A:32:LYS:O	1:A:111:MET:HB2	0.43	2.12	6	1
1:A:69:ILE:HD12	1:A:69:ILE:N	0.43	2.27	12	1
1:A:11:TRP:CG	1:A:61:HIS:NE2	0.43	2.86	18	2
1:A:12:LEU:O	1:A:16:ILE:HG13	0.43	2.13	14	2
1:A:16:ILE:O	1:A:17:ASN:C	0.43	2.56	19	3
1:A:73:ASP:O	1:A:77:TRP:NE1	0.43	2.52	16	1
1:A:54:LEU:HD22	1:A:81:PHE:CE2	0.43	2.49	19	1
1:A:9:ARG:HG3	1:A:88:LEU:CD2	0.43	2.43	2	1
1:A:29:LYS:CE	1:A:32:LYS:HD3	0.43	2.44	16	1
1:A:25:LYS:HE2	1:A:35:GLN:NE2	0.43	2.29	17	1
1:A:85:MET:HG2	1:A:109:TYR:OH	0.43	2.12	3	1
1:A:83:CYS:O	1:A:87:SER:HB2	0.43	2.13	15	2
1:A:54:LEU:CD1	1:A:54:LEU:H	0.43	2.27	10	5
1:A:54:LEU:O	1:A:57:ASN:HB3	0.43	2.13	14	2
1:A:32:LYS:HB3	1:A:111:MET:O	0.43	2.14	14	1
1:A:26:TRP:CB	1:A:29:LYS:HB3	0.43	2.44	1	1
1:A:34:PHE:CD1	1:A:111:MET:SD	0.43	3.11	5	2
1:A:15:GLN:OE1	1:A:20:THR:HG21	0.43	2.12	7	1
1:A:53:PRO:C	1:A:54:LEU:HD12	0.43	2.34	9	1
1:A:57:ASN:O	1:A:57:ASN:CG	0.43	2.56	13	1
1:A:21:ILE:CD1	1:A:54:LEU:HD21	0.43	2.44	5	1
1:A:65:HIS:C	1:A:66:GLN:OE1	0.43	2.57	7	1
1:A:8:MET:SD	1:A:8:MET:C	0.43	2.97	9	1
1:A:68:GLY:O	1:A:69:ILE:HD12	0.43	2.11	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:34:PHE:HE1	1:A:36:ILE:HD12	0.43	1.74	15	1
1:A:55:PHE:CE1	1:A:78:LYS:HD3	0.43	2.49	1	1
1:A:21:ILE:HD12	1:A:54:LEU:CD2	0.43	2.42	5	1
1:A:35:GLN:HB2	1:A:108:VAL:CG1	0.43	2.35	17	1
1:A:29:LYS:O	1:A:29:LYS:HD3	0.42	2.14	5	1
1:A:35:GLN:HB2	1:A:108:VAL:HG22	0.42	1.90	2	1
1:A:60:ILE:N	1:A:60:ILE:HD13	0.42	2.28	8	1
1:A:33:ILE:CG1	1:A:110:ARG:HG2	0.42	2.44	15	2
1:A:35:GLN:C	1:A:35:GLN:CD	0.42	2.78	2	1
1:A:57:ASN:OD1	1:A:61:HIS:HB3	0.42	2.15	3	1
1:A:32:LYS:HE2	1:A:111:MET:HB3	0.42	1.91	14	1
1:A:82:ARG:O	1:A:85:MET:HG2	0.42	2.15	12	1
1:A:35:GLN:CG	1:A:106:PHE:HB2	0.42	2.44	13	1
1:A:95:LYS:HD3	1:A:107:ARG:CZ	0.42	2.43	5	1
1:A:29:LYS:NZ	1:A:32:LYS:HE3	0.42	2.29	15	1
1:A:38:TRP:CH2	1:A:85:MET:HG3	0.42	2.49	18	2
1:A:11:TRP:O	1:A:15:GLN:HG2	0.42	2.13	16	3
1:A:38:TRP:CZ3	1:A:85:MET:HG3	0.42	2.50	18	1
1:A:27:LEU:HD13	1:A:108:VAL:HG11	0.42	1.90	1	1
1:A:36:ILE:CB	1:A:38:TRP:CE2	0.42	3.02	2	4
1:A:80:ASN:C	1:A:83:CYS:SG	0.42	2.98	5	1
1:A:94:VAL:HB	1:A:108:VAL:O	0.42	2.14	2	2
1:A:91:ILE:O	1:A:91:ILE:HG12	0.42	2.15	3	1
1:A:7:ARG:HG2	1:A:10:PRO:CG	0.42	2.45	4	1
1:A:76:THR:O	1:A:78:LYS:N	0.42	2.53	4	1
1:A:7:ARG:C	1:A:10:PRO:HD2	0.42	2.35	16	1
1:A:19:ASN:N	1:A:19:ASN:OD1	0.42	2.50	1	1
1:A:64:LYS:O	1:A:65:HIS:HB2	0.42	2.15	15	2
1:A:59:ALA:C	1:A:60:ILE:HD13	0.42	2.35	20	1
1:A:74:PRO:HA	1:A:77:TRP:CE3	0.41	2.50	10	3
1:A:85:MET:CB	1:A:109:TYR:CZ	0.41	3.03	2	1
1:A:32:LYS:CE	1:A:111:MET:CB	0.41	2.98	14	1
1:A:75:LYS:HG3	1:A:76:THR:N	0.41	2.30	4	1
1:A:27:LEU:CG	1:A:35:GLN:HB3	0.41	2.45	12	1
1:A:55:PHE:CD1	1:A:55:PHE:O	0.41	2.73	13	1
1:A:20:THR:HG23	1:A:21:ILE:HG13	0.41	1.92	16	1
1:A:21:ILE:HD11	1:A:54:LEU:CD2	0.41	2.45	11	1
1:A:87:SER:OG	1:A:88:LEU:CD1	0.41	2.69	13	1
1:A:79:ALA:O	1:A:80:ASN:C	0.41	2.57	20	1
1:A:76:THR:O	1:A:77:TRP:C	0.41	2.56	4	2
1:A:24:LEU:HD13	1:A:36:ILE:HG12	0.41	1.93	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:8:MET:HE2	1:A:84:ALA:CB	0.41	2.46	11	1
1:A:33:ILE:HG13	1:A:110:ARG:HG3	0.41	1.91	17	1
1:A:58:TRP:CE3	1:A:58:TRP:CA	0.41	3.03	13	3
1:A:7:ARG:O	1:A:10:PRO:HD2	0.41	2.16	16	1
1:A:35:GLN:NE2	1:A:106:PHE:CG	0.41	2.89	8	1
1:A:11:TRP:CD2	1:A:15:GLN:HG3	0.41	2.51	14	1
1:A:15:GLN:OE1	1:A:15:GLN:HA	0.41	2.15	15	1
1:A:84:ALA:HB3	1:A:85:MET:HE2	0.41	1.92	16	1
1:A:35:GLN:HB3	1:A:108:VAL:HA	0.41	1.91	19	1
1:A:36:ILE:HG22	1:A:38:TRP:CE2	0.41	2.50	2	2
1:A:57:ASN:C	1:A:58:TRP:O	0.41	2.59	6	1
1:A:65:HIS:O	1:A:66:GLN:OE1	0.41	2.39	7	1
1:A:25:LYS:C	1:A:25:LYS:HD3	0.41	2.36	9	3
1:A:55:PHE:CE1	1:A:81:PHE:CE2	0.41	3.08	11	1
1:A:16:ILE:HG22	1:A:26:TRP:N	0.41	2.31	13	1
1:A:11:TRP:CE3	1:A:11:TRP:O	0.41	2.74	14	1
1:A:25:LYS:C	1:A:25:LYS:CD	0.41	2.89	8	3
1:A:27:LEU:HD13	1:A:108:VAL:CG1	0.41	2.45	1	1
1:A:87:SER:OG	1:A:88:LEU:HG	0.41	2.15	13	1
1:A:87:SER:C	1:A:88:LEU:CD1	0.41	2.81	18	2
1:A:57:ASN:O	1:A:61:HIS:N	0.41	2.54	3	1
1:A:36:ILE:HG22	1:A:38:TRP:CG	0.41	2.50	4	1
1:A:38:TRP:CE3	1:A:107:ARG:NH1	0.41	2.89	4	1
1:A:34:PHE:CD2	1:A:111:MET:HE3	0.41	2.51	11	1
1:A:35:GLN:CD	1:A:106:PHE:CG	0.41	2.94	13	1
1:A:26:TRP:O	1:A:27:LEU:C	0.41	2.58	16	1
1:A:27:LEU:HD21	1:A:35:GLN:HB2	0.41	1.91	16	1
1:A:29:LYS:O	1:A:29:LYS:HG3	0.41	2.15	19	1
1:A:95:LYS:HB3	1:A:107:ARG:HG2	0.41	1.92	20	1
1:A:35:GLN:CA	1:A:108:VAL:HA	0.41	2.46	1	1
1:A:83:CYS:O	1:A:86:ASN:N	0.41	2.55	9	1
1:A:72:PRO:O	1:A:73:ASP:HB2	0.41	2.16	19	1
1:A:29:LYS:HG2	1:A:30:GLU:N	0.40	2.30	4	2
1:A:79:ALA:O	1:A:83:CYS:SG	0.40	2.79	4	1
1:A:55:PHE:CE1	1:A:78:LYS:HE3	0.40	2.51	16	1
1:A:11:TRP:CZ3	1:A:12:LEU:HD22	0.40	2.51	17	1
1:A:54:LEU:HD12	1:A:54:LEU:H	0.40	1.74	19	1
1:A:93:GLU:O	1:A:93:GLU:HG3	0.40	2.17	4	1
1:A:58:TRP:NE1	1:A:80:ASN:HB2	0.40	2.31	6	1
1:A:59:ALA:O	1:A:60:ILE:HG13	0.40	2.16	11	1
1:A:93:GLU:CB	1:A:109:TYR:CE2	0.40	3.04	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:32:LYS:HB2	1:A:111:MET:O	0.40	2.17	18	1
1:A:26:TRP:CD1	1:A:29:LYS:CG	0.40	3.05	20	1
1:A:29:LYS:HE3	1:A:32:LYS:CD	0.40	2.46	7	1
1:A:8:MET:C	1:A:8:MET:SD	0.40	3.00	8	1
1:A:53:PRO:O	1:A:54:LEU:HB3	0.40	2.16	8	1
1:A:52:ALA:H	1:A:53:PRO:CD	0.40	2.29	10	1
1:A:27:LEU:CD2	1:A:35:GLN:HB3	0.40	2.46	1	1
1:A:26:TRP:CE2	1:A:29:LYS:HE3	0.40	2.51	3	1
1:A:91:ILE:CD1	1:A:109:TYR:CD1	0.40	3.05	4	1
1:A:65:HIS:O	1:A:66:GLN:HG3	0.40	2.16	7	1
1:A:112:LEU:HB2	1:A:113:PRO:HD3	0.40	1.92	18	1
1:A:90:ASP:HB3	1:A:113:PRO:HD3	0.40	1.93	18	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	83/112 (74%)	61±3 (73±3%)	17±3 (20±4%)	5±2 (6±2%)	3 19
All	All	1660/2240 (74%)	1216 (73%)	338 (20%)	106 (6%)	3 19

All 21 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	88	LEU	20
1	A	58	TRP	13
1	A	32	LYS	10
1	A	55	PHE	9
1	A	59	ALA	8
1	A	53	PRO	7
1	A	65	HIS	7
1	A	60	ILE	5
1	A	61	HIS	4
1	A	52	ALA	4

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Mol	Chain	Res	Type	Models (Total)
1	A	19	ASN	3
1	A	94	VAL	3
1	A	69	ILE	2
1	A	17	ASN	2
1	A	66	GLN	2
1	A	72	PRO	2
1	A	38	TRP	1
1	A	54	LEU	1
1	A	82	ARG	1
1	A	37	PRO	1
1	A	7	ARG	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	77/100 (77%)	51±2 (66±2%)	26±2 (34±2%)	1 11
All	All	1540/2000 (77%)	1021 (66%)	519 (34%)	1 11

All 54 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	24	LEU	20
1	A	25	LYS	20
1	A	29	LYS	20
1	A	58	TRP	20
1	A	91	ILE	20
1	A	54	LEU	19
1	A	88	LEU	19
1	A	7	ARG	18
1	A	106	PHE	18
1	A	82	ARG	17
1	A	81	PHE	16
1	A	32	LYS	14
1	A	76	THR	13
1	A	92	GLU	12

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Mol	Chain	Res	Type	Models (Total)
1	A	95	LYS	11
1	A	56	ARG	11
1	A	71	LYS	11
1	A	8	MET	11
1	A	73	ASP	10
1	A	86	ASN	10
1	A	111	MET	10
1	A	20	THR	10
1	A	85	MET	10
1	A	14	GLU	9
1	A	57	ASN	9
1	A	75	LYS	9
1	A	78	LYS	9
1	A	12	LEU	9
1	A	28	ASN	9
1	A	64	LYS	8
1	A	66	GLN	8
1	A	70	ASP	8
1	A	107	ARG	8
1	A	19	ASN	7
1	A	30	GLU	7
1	A	90	ASP	7
1	A	9	ARG	7
1	A	55	PHE	6
1	A	87	SER	6
1	A	18	SER	6
1	A	31	LYS	6
1	A	80	ASN	5
1	A	35	GLN	5
1	A	17	ASN	5
1	A	112	LEU	5
1	A	93	GLU	5
1	A	13	GLU	4
1	A	21	ILE	3
1	A	27	LEU	2
1	A	60	ILE	2
1	A	110	ARG	2
1	A	83	CYS	1
1	A	108	VAL	1
1	A	65	HIS	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 monosaccharides 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 (i)

No chemical shift data were provided