Full wwPDB NMR Structure Validation Report (i)

Feb 7, 2022 – 04:22 PM EST

PDB ID	:	1AJ3
Title	:	SOLUTION STRUCTURE OF THE SPECTRIN REPEAT, NMR, 20 STRUCTURES
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Deposited on	:	1997-05-14

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
https://www.wwpdb.org/validation/2017/NMRValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

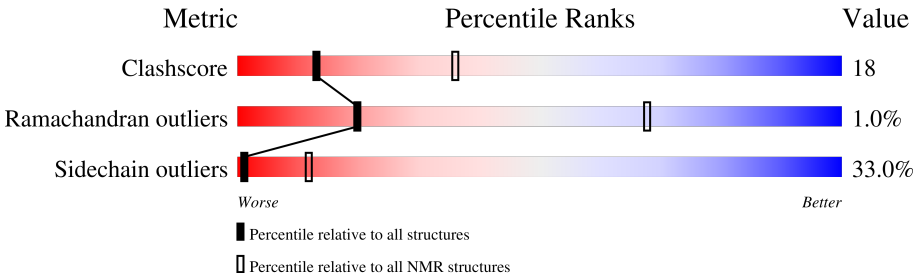
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.26
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.26

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	110	37% 43% • 8% 11%

2 Ensemble composition and analysis (i)

This entry contains 20 models. The atoms present in the NMR models are not consistent. Some calculations may have failed as a result. All residues are included in the validation scores. Model 4 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:10-A:33, A:43-A:107 (89)	1.11	4

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

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

NmrClust was unable to cluster the ensemble.

Error message: Inconsistent models

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1593 atoms, of which 793 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called ALPHA SPECTRIN.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	98	1593	498	793	147	154	1	0

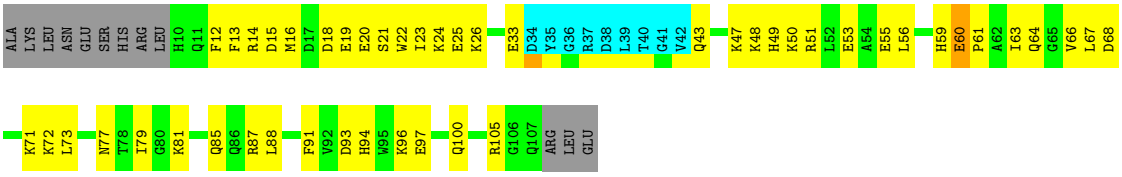
4 Residue-property plots (i)

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: ALPHA SPECTRIN

Chain A: 37% 43% • 8% 11%



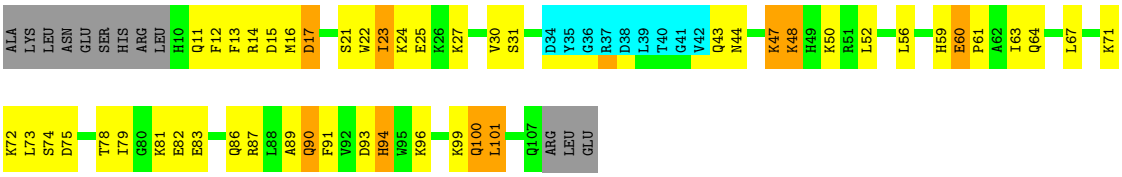
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: ALPHA SPECTRIN

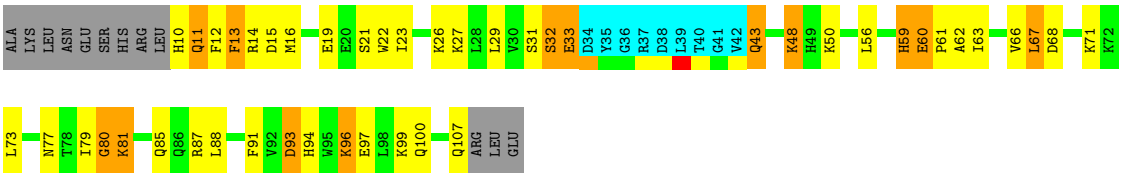
Chain A: 36% 36% 8% 8% 11%



4.2.2 Score per residue for model 2

• Molecule 1: ALPHA SPECTRIN

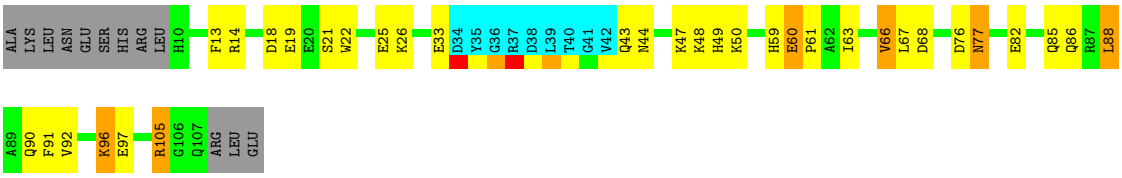
Chain A: 39% 30% 12% 8% 11%



4.2.3 Score per residue for model 3

- Molecule 1: ALPHA SPECTRIN

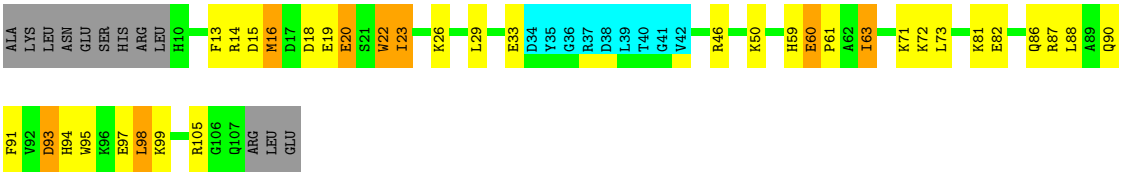
Chain A: 50% 25% 5% 8% 11%



4.2.4 Score per residue for model 4 (medoid)

- Molecule 1: ALPHA SPECTRIN

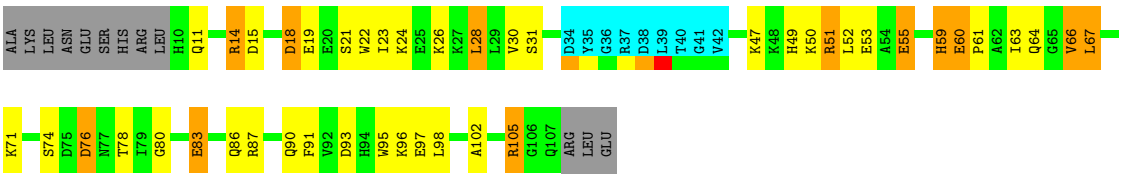
Chain A: 49% 25% 7% 8% 11%



4.2.5 Score per residue for model 5

- Molecule 1: ALPHA SPECTRIN

Chain A: 41% 29% 11% 8% 11%



4.2.6 Score per residue for model 6

- Molecule 1: ALPHA SPECTRIN

Chain A: 44% 32% 5% 8% 11%

ALA LYS LEU ASN GLU SER HIS ARG LEU H10 Q11 F12 F13 D18 E19 E20 S21 W22 E25 K26 K27 L28 L29 V30 S31 S32 E33 D34 Y35 G36 R37 D38 L39 T40 G41 V42 Q43 R46 H49 K50 R51 H59 E60 P61 A62 V66 K71 K72 D75 D76 N77

G80 K81 E82 E83 I84 Q85 Q86 R87 F91 K96 E97 L98 K99 Q100 R105 G106 Q107 ARG LEU GLU

4.2.7 Score per residue for model 7

- Molecule 1: ALPHA SPECTRIN

Chain A: 47% 25% 9% 8% 11%

ALA LYS LEU ASN GLU SER HIS ARG LEU H10 F13 R14 D15 M16 D17 D18 E19 E20 S21 W22 E25 L28 L29 V30 S31 S32 E33 D34 Y35 G36 R37 D38 L39 T40 G41 V42 R46 K47 R51 L52 E53 A54 E55 H59 E60 P61 Q64 G65 V66 L67 K72

D76 N77 T78 E83 F91 V92 D93 H94 W95 K96 E97 Q100 Q107 ARG LEU GLU

4.2.8 Score per residue for model 8

- Molecule 1: ALPHA SPECTRIN

Chain A: 43% 32% 6% 8% 11%

ALA LYS LEU ASN GLU SER HIS ARG LEU H10 Q11 F12 F13 R14 D15 M16 D17 D18 E19 W22 K26 K27 L28 L29 V30 S31 S32 E33 D34 Y35 G36 R37 D38 L39 T40 G41 V42 Q43 N44 L45 R46 H49 K50 E53 A54 E55 L56 A57 A58 H59 E60 P61 V66 K72

L73 D76 E83 Q86 R87 L88 D93 H94 W95 K96 E97 L98 K99 Q100 L101 Q107 ARG LEU GLU

4.2.9 Score per residue for model 9

- Molecule 1: ALPHA SPECTRIN

Chain A: 42% 32% 7% 8% 11%

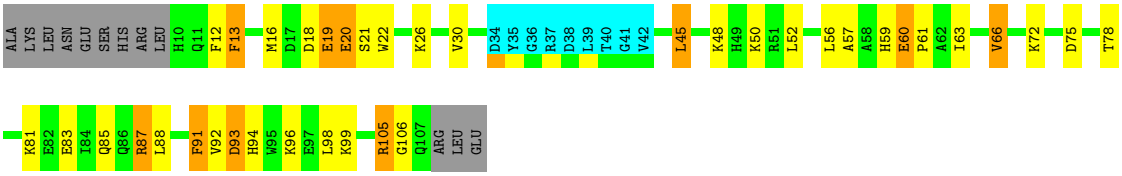
ALA LYS LEU ASN GLU SER HIS ARG LEU H10 Q11 F12 F13 R14 D17 D18 E19 E20 S21 W22 T23 K24 E25 K26 K27 L28 L29 V30 S31 S32 E33 D34 Y35 G36 R37 D38 L39 T40 G41 V42 Q43 K47 K48 H49 K50 R51 E55 L56 H59 E60 P61 Q64 D68

K71 K72 L73 S74 D75 D76 I79 E83 I84 Q85 A89 Q90 F91 V92 D93 H94 W95 L98 K99 Q100 R105 G106 Q107 ARG LEU GLU

4.2.10 Score per residue for model 10

- Molecule 1: ALPHA SPECTRIN

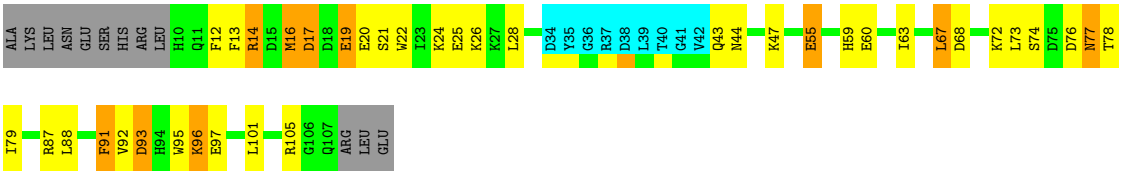
Chain A: 46% 25% 9% 8% 11%



4.2.11 Score per residue for model 11

- Molecule 1: ALPHA SPECTRIN

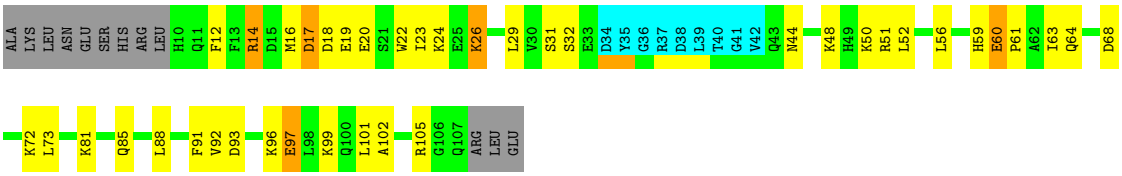
Chain A: 45% 26% 9% 8% 11%



4.2.12 Score per residue for model 12

- Molecule 1: ALPHA SPECTRIN

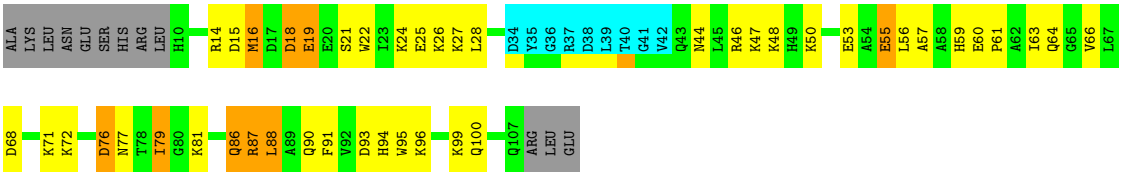
Chain A: 45% 32% 5% 8% 11%



4.2.13 Score per residue for model 13

- Molecule 1: ALPHA SPECTRIN

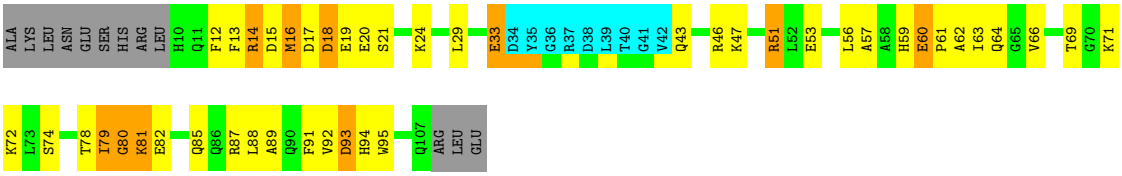
Chain A: 40% 33% 8% 8% 11%



4.2.14 Score per residue for model 14

- Molecule 1: ALPHA SPECTRIN

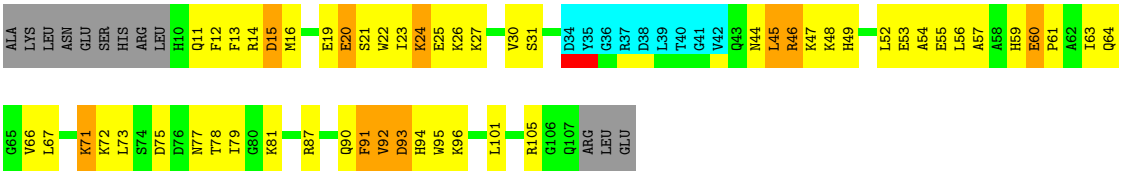
Chain A: 40% 32% 9% 8% 11%



4.2.15 Score per residue for model 15

- Molecule 1: ALPHA SPECTRIN

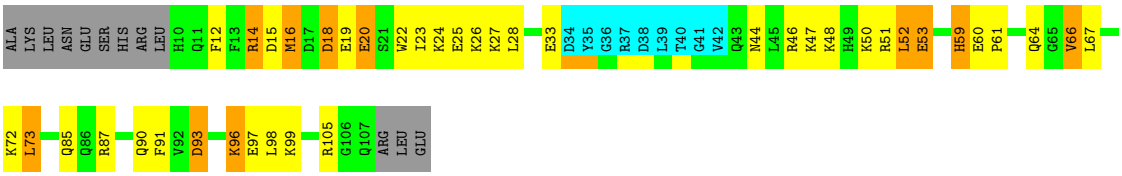
Chain A: 32% 40% 9% 8% 11%



4.2.16 Score per residue for model 16

- Molecule 1: ALPHA SPECTRIN

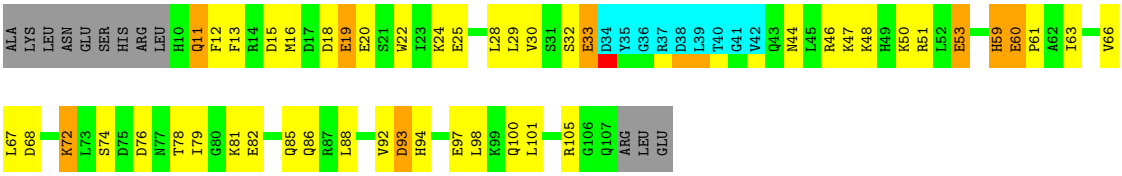
Chain A: 44% 27% 10% 8% 11%



4.2.17 Score per residue for model 17

- Molecule 1: ALPHA SPECTRIN

Chain A: 37% 36% 7% 8% 11%



4.2.18 Score per residue for model 18

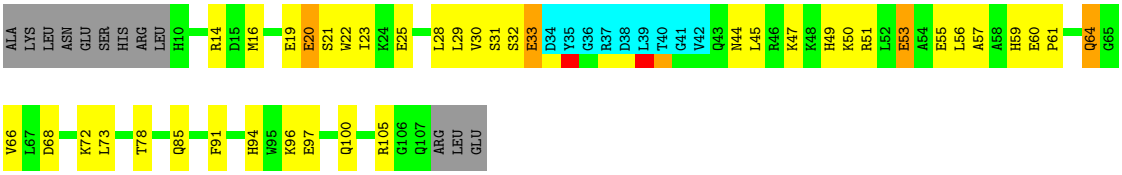
- Molecule 1: ALPHA SPECTRIN

Chain A: 55% 22% • • 8% 11%

4.2.19 Score per residue for model 19

- Molecule 1: ALPHA SPECTRIN

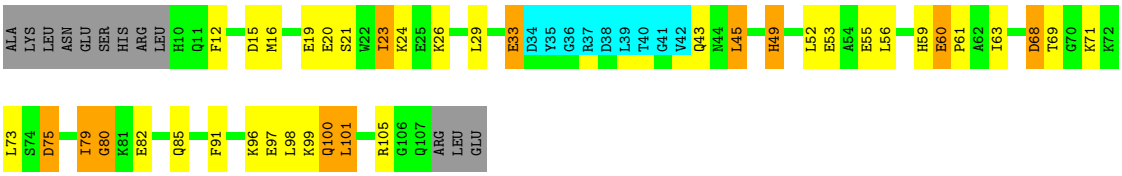
Chain A: 45% 33% • 8% 11%



4.2.20 Score per residue for model 20

- Molecule 1: ALPHA SPECTRIN

Chain A: 45% 25% 10% 8% 11%



5 Refinement protocol and experimental data overview (i)

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

Of the 40 calculated structures, 20 were deposited, based on the following criterion: *ENERGY, GEOMETRY, VIOLATIONS*.

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

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

No chemical shift data was provided.

6 Model quality (i)

6.1 Standard geometry (i)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the (average) root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.26±0.06	0±0/742 (0.0± 0.1%)	0.33±0.01	0±0/991 (0.0± 0.0%)
All	All	0.27	3/14840 (0.0%)	0.33	0/19820 (0.0%)

All unique bond outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	91	PHE	CE1-CZ	8.24	1.53	1.37	18	2
1	A	91	PHE	CE2-CZ	-7.29	1.23	1.37	18	1

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	731	730	729	27±7
All	All	14620	14600	14580	537

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 18.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:20:GLU:OE1	1:A:91:PHE:CD2	1.50	1.64	20	1
1:A:16:MET:CA	1:A:19:GLU:OE1	1.46	1.64	10	2
1:A:26:LYS:CE	1:A:55:GLU:OE2	1.39	1.71	8	1
1:A:20:GLU:OE1	1:A:91:PHE:HB2	1.32	1.24	6	2
1:A:15:ASP:HA	1:A:18:ASP:OD2	1.26	1.17	16	5
1:A:50:LYS:CA	1:A:53:GLU:OE1	1.24	1.85	17	1
1:A:15:ASP:CA	1:A:18:ASP:OD2	1.23	1.86	16	4
1:A:97:GLU:OE1	1:A:101:LEU:CD1	1.23	1.87	12	2
1:A:19:GLU:OE1	1:A:66:VAL:HG11	1.21	1.34	17	1
1:A:20:GLU:OE1	1:A:91:PHE:HD2	1.21	0.81	20	1
1:A:19:GLU:N	1:A:19:GLU:OE2	1.21	1.72	8	1
1:A:20:GLU:OE2	1:A:91:PHE:HA	1.20	1.30	6	1
1:A:20:GLU:OE1	1:A:91:PHE:CB	1.19	1.90	6	2
1:A:50:LYS:HA	1:A:53:GLU:OE1	1.17	0.97	17	1
1:A:13:PHE:O	1:A:17:ASP:OD1	1.17	1.60	11	3
1:A:33:GLU:OE2	1:A:51:ARG:NH1	1.16	1.78	19	1
1:A:71:LYS:O	1:A:75:ASP:OD1	1.11	1.69	15	1
1:A:60:GLU:OE1	1:A:64:GLN:NE2	1.10	1.84	13	1
1:A:97:GLU:OE1	1:A:101:LEU:HD12	1.10	1.41	12	2
1:A:11:GLN:O	1:A:15:ASP:OD1	1.10	1.65	15	1
1:A:15:ASP:O	1:A:19:GLU:OE2	1.06	1.71	17	1
1:A:19:GLU:OE2	1:A:66:VAL:HG21	1.06	1.51	10	2
1:A:20:GLU:OE2	1:A:91:PHE:CA	1.05	2.03	6	1
1:A:26:LYS:HE2	1:A:55:GLU:OE2	1.04	0.82	8	1
1:A:19:GLU:OE2	1:A:63:ILE:HD13	1.04	1.53	20	1
1:A:93:ASP:OD1	1:A:94:HIS:N	1.03	1.92	9	8
1:A:16:MET:HA	1:A:19:GLU:OE1	1.02	0.80	10	1
1:A:14:ARG:O	1:A:18:ASP:OD2	1.02	1.76	5	2
1:A:20:GLU:OE1	1:A:91:PHE:CD1	1.02	2.12	6	2
1:A:59:HIS:CE1	1:A:63:ILE:HD11	1.00	1.92	4	1
1:A:20:GLU:CD	1:A:91:PHE:CD1	0.98	2.36	6	2
1:A:20:GLU:CD	1:A:91:PHE:HD1	0.98	1.61	6	1
1:A:23:ILE:HG23	1:A:98:LEU:HD11	0.97	1.36	5	2
1:A:20:GLU:OE2	1:A:91:PHE:CD1	0.97	2.16	4	2
1:A:14:ARG:HA	1:A:17:ASP:OD2	0.96	1.59	11	2
1:A:16:MET:CA	1:A:19:GLU:OE2	0.96	2.13	17	1
1:A:16:MET:HA	1:A:19:GLU:OE2	0.95	1.61	17	1
1:A:59:HIS:NE2	1:A:63:ILE:HD11	0.94	1.76	4	2
1:A:15:ASP:C	1:A:19:GLU:OE2	0.94	2.05	17	1
1:A:20:GLU:OE1	1:A:91:PHE:CG	0.93	2.20	6	2
1:A:22:TRP:CD2	1:A:59:HIS:CE1	0.92	2.57	4	3
1:A:72:LYS:O	1:A:76:ASP:OD1	0.88	1.90	13	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:97:GLU:OE1	1:A:101:LEU:HD11	0.86	1.69	12	2
1:A:14:ARG:NH2	1:A:18:ASP:OD2	0.86	2.06	13	1
1:A:78:THR:HG22	1:A:82:GLU:OE2	0.86	1.71	17	1
1:A:15:ASP:HA	1:A:18:ASP:CG	0.85	1.92	16	3
1:A:20:GLU:CD	1:A:91:PHE:CB	0.85	2.44	6	1
1:A:22:TRP:CZ2	1:A:59:HIS:NE2	0.84	2.45	16	10
1:A:20:GLU:CD	1:A:91:PHE:HA	0.84	1.92	6	1
1:A:78:THR:CG2	1:A:82:GLU:OE2	0.84	2.25	17	1
1:A:20:GLU:OE1	1:A:23:ILE:HD12	0.84	1.72	16	1
1:A:68:ASP:OD1	1:A:69:THR:N	0.84	2.10	20	1
1:A:26:LYS:HE2	1:A:55:GLU:CD	0.84	1.93	8	1
1:A:20:GLU:OE2	1:A:91:PHE:HB2	0.83	1.73	4	2
1:A:53:GLU:OE1	1:A:53:GLU:N	0.82	2.13	19	1
1:A:93:ASP:OD1	1:A:93:ASP:C	0.82	2.17	10	7
1:A:22:TRP:CD1	1:A:25:GLU:OE2	0.80	2.34	6	1
1:A:55:GLU:HA	1:A:55:GLU:OE1	0.80	1.75	11	4
1:A:19:GLU:OE2	1:A:63:ILE:CD1	0.80	2.30	20	1
1:A:12:PHE:O	1:A:15:ASP:CG	0.80	2.20	15	1
1:A:12:PHE:CA	1:A:15:ASP:OD1	0.79	2.29	15	1
1:A:64:GLN:O	1:A:68:ASP:OD2	0.79	2.01	12	2
1:A:20:GLU:OE1	1:A:91:PHE:HA	0.79	1.78	10	1
1:A:14:ARG:NE	1:A:17:ASP:OD2	0.78	2.16	11	1
1:A:93:ASP:OD1	1:A:94:HIS:HD2	0.78	1.61	9	1
1:A:72:LYS:O	1:A:76:ASP:CG	0.77	2.23	13	1
1:A:17:ASP:C	1:A:17:ASP:OD1	0.77	2.23	12	1
1:A:62:ALA:O	1:A:66:VAL:HG23	0.76	1.81	6	3
1:A:56:LEU:O	1:A:60:GLU:OE1	0.75	2.03	10	2
1:A:22:TRP:CD1	1:A:23:ILE:N	0.74	2.56	4	1
1:A:20:GLU:CD	1:A:91:PHE:HB2	0.73	2.04	6	2
1:A:33:GLU:HA	1:A:33:GLU:OE1	0.72	1.84	6	2
1:A:16:MET:N	1:A:19:GLU:OE2	0.72	2.22	17	1
1:A:20:GLU:OE2	1:A:91:PHE:HD1	0.72	1.65	4	1
1:A:12:PHE:HA	1:A:15:ASP:OD1	0.72	1.84	15	1
1:A:20:GLU:CD	1:A:91:PHE:CA	0.72	2.55	6	1
1:A:59:HIS:O	1:A:63:ILE:HD12	0.72	1.85	15	4
1:A:52:LEU:HD21	1:A:102:ALA:HB1	0.72	1.62	12	2
1:A:16:MET:HA	1:A:19:GLU:CD	0.72	2.05	17	2
1:A:19:GLU:OE1	1:A:66:VAL:CG1	0.71	2.29	17	1
1:A:63:ILE:HG23	1:A:91:PHE:CE2	0.70	2.21	1	2
1:A:89:ALA:O	1:A:92:VAL:HG12	0.70	1.87	14	2
1:A:32:SER:OG	1:A:33:GLU:OE2	0.70	2.08	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:88:LEU:O	1:A:92:VAL:HG23	0.70	1.85	11	4
1:A:55:GLU:OE2	1:A:59:HIS:CE1	0.69	2.45	18	1
1:A:20:GLU:N	1:A:20:GLU:OE1	0.69	2.25	4	1
1:A:97:GLU:CA	1:A:97:GLU:OE1	0.69	2.40	7	1
1:A:97:GLU:CD	1:A:101:LEU:CD1	0.69	2.61	12	1
1:A:59:HIS:CE1	1:A:63:ILE:CD1	0.69	2.75	4	1
1:A:22:TRP:CE3	1:A:59:HIS:ND1	0.68	2.61	4	1
1:A:15:ASP:CA	1:A:18:ASP:CG	0.68	2.55	16	3
1:A:16:MET:C	1:A:19:GLU:OE1	0.68	2.32	10	2
1:A:14:ARG:C	1:A:18:ASP:OD2	0.68	2.32	5	2
1:A:12:PHE:O	1:A:15:ASP:OD2	0.68	2.12	15	1
1:A:53:GLU:HA	1:A:53:GLU:OE1	0.67	1.90	7	3
1:A:97:GLU:OE1	1:A:97:GLU:HA	0.67	1.90	7	1
1:A:71:LYS:O	1:A:75:ASP:OD2	0.66	2.12	9	1
1:A:11:GLN:O	1:A:15:ASP:OD2	0.66	2.14	2	1
1:A:19:GLU:N	1:A:19:GLU:CD	0.66	2.49	8	2
1:A:22:TRP:CH2	1:A:59:HIS:CD2	0.66	2.84	10	6
1:A:12:PHE:CD2	1:A:73:LEU:HD11	0.66	2.26	9	4
1:A:71:LYS:C	1:A:75:ASP:OD1	0.66	2.35	15	1
1:A:14:ARG:NH1	1:A:17:ASP:OD2	0.65	2.30	8	1
1:A:20:GLU:OE2	1:A:91:PHE:CB	0.65	2.44	4	2
1:A:22:TRP:CZ2	1:A:59:HIS:CD2	0.65	2.84	8	13
1:A:22:TRP:CZ3	1:A:59:HIS:CG	0.65	2.85	4	1
1:A:26:LYS:O	1:A:30:VAL:HG23	0.64	1.90	9	1
1:A:22:TRP:CE3	1:A:59:HIS:NE2	0.64	2.65	2	2
1:A:59:HIS:CD2	1:A:95:TRP:NE1	0.64	2.66	13	6
1:A:52:LEU:HD11	1:A:102:ALA:HB1	0.64	1.69	5	1
1:A:97:GLU:CD	1:A:101:LEU:HD11	0.63	2.13	12	2
1:A:19:GLU:CD	1:A:19:GLU:H	0.63	1.96	13	1
1:A:59:HIS:CD2	1:A:63:ILE:HD11	0.62	2.28	5	3
1:A:22:TRP:CD2	1:A:59:HIS:NE2	0.62	2.68	2	2
1:A:67:LEU:HD22	1:A:88:LEU:HD12	0.62	1.69	2	1
1:A:72:LYS:HA	1:A:75:ASP:OD2	0.62	1.95	9	1
1:A:20:GLU:OE2	1:A:91:PHE:CG	0.62	2.52	4	2
1:A:22:TRP:CE3	1:A:59:HIS:CE1	0.62	2.88	4	1
1:A:23:ILE:HG23	1:A:98:LEU:CD1	0.61	2.21	5	1
1:A:52:LEU:HD22	1:A:52:LEU:O	0.61	1.95	16	1
1:A:26:LYS:NZ	1:A:55:GLU:OE2	0.61	2.34	8	1
1:A:22:TRP:CE2	1:A:59:HIS:NE2	0.60	2.65	16	4
1:A:59:HIS:O	1:A:63:ILE:CG1	0.60	2.48	17	2
1:A:11:GLN:C	1:A:15:ASP:OD1	0.60	2.37	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:93:ASP:OD1	1:A:94:HIS:CD2	0.60	2.51	9	1
1:A:19:GLU:OE2	1:A:66:VAL:CG2	0.60	2.50	13	2
1:A:72:LYS:O	1:A:76:ASP:OD2	0.60	2.19	11	3
1:A:19:GLU:HB2	1:A:91:PHE:CE2	0.59	2.32	11	2
1:A:11:GLN:NE2	1:A:11:GLN:H	0.59	1.94	1	1
1:A:49:HIS:CE1	1:A:53:GLU:OE2	0.59	2.56	19	1
1:A:55:GLU:OE1	1:A:55:GLU:CA	0.58	2.51	5	3
1:A:17:ASP:OD1	1:A:17:ASP:N	0.58	2.36	8	1
1:A:12:PHE:C	1:A:15:ASP:OD1	0.58	2.41	15	1
1:A:79:ILE:HG22	1:A:80:GLY:N	0.58	2.14	14	2
1:A:33:GLU:OE1	1:A:45:LEU:HD21	0.58	1.99	20	1
1:A:20:GLU:OE1	1:A:20:GLU:HA	0.58	1.99	16	1
1:A:20:GLU:OE1	1:A:91:PHE:CA	0.57	2.51	10	1
1:A:52:LEU:HD13	1:A:53:GLU:N	0.57	2.14	16	1
1:A:14:ARG:CZ	1:A:17:ASP:OD2	0.57	2.52	8	1
1:A:26:LYS:HG3	1:A:59:HIS:NE2	0.57	2.14	12	1
1:A:19:GLU:HB3	1:A:91:PHE:CE2	0.57	2.34	18	1
1:A:59:HIS:CD2	1:A:95:TRP:HE1	0.57	2.18	14	3
1:A:63:ILE:HG12	1:A:91:PHE:CZ	0.57	2.34	1	4
1:A:12:PHE:HA	1:A:15:ASP:CG	0.57	2.19	15	1
1:A:33:GLU:CD	1:A:51:ARG:HH12	0.57	2.01	19	1
1:A:97:GLU:OE1	1:A:101:LEU:CG	0.56	2.52	8	1
1:A:15:ASP:N	1:A:18:ASP:OD2	0.56	2.37	16	1
1:A:12:PHE:CG	1:A:73:LEU:HD11	0.56	2.35	9	1
1:A:25:GLU:HG2	1:A:26:LYS:N	0.56	2.14	6	1
1:A:19:GLU:HG3	1:A:91:PHE:CZ	0.56	2.35	4	1
1:A:80:GLY:O	1:A:83:GLU:OE1	0.56	2.23	5	1
1:A:15:ASP:C	1:A:18:ASP:OD2	0.56	2.42	16	1
1:A:19:GLU:HB3	1:A:91:PHE:CZ	0.55	2.35	18	1
1:A:23:ILE:HD11	1:A:91:PHE:CD2	0.55	2.36	16	2
1:A:22:TRP:CG	1:A:59:HIS:CE1	0.55	2.94	4	1
1:A:14:ARG:CA	1:A:17:ASP:OD2	0.55	2.45	11	1
1:A:90:GLN:HE21	1:A:94:HIS:CE1	0.55	2.20	15	2
1:A:67:LEU:HD13	1:A:68:ASP:N	0.54	2.17	11	1
1:A:53:GLU:OE1	1:A:53:GLU:CA	0.54	2.55	7	4
1:A:60:GLU:CB	1:A:61:PRO:HD3	0.54	2.33	14	15
1:A:18:ASP:OD1	1:A:19:GLU:N	0.54	2.40	4	1
1:A:30:VAL:HG13	1:A:48:LYS:HD2	0.54	1.79	1	1
1:A:45:LEU:HD12	1:A:105:ARG:NH2	0.54	2.18	20	1
1:A:67:LEU:HD23	1:A:88:LEU:HD22	0.54	1.79	11	1
1:A:14:ARG:CZ	1:A:18:ASP:OD2	0.54	2.56	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:32:SER:O	1:A:33:GLU:CB	0.53	2.56	2	2
1:A:19:GLU:HG3	1:A:20:GLU:N	0.53	2.18	19	4
1:A:63:ILE:HG12	1:A:91:PHE:CE2	0.53	2.39	10	1
1:A:19:GLU:CG	1:A:20:GLU:N	0.53	2.72	11	1
1:A:95:TRP:HA	1:A:98:LEU:HD12	0.53	1.81	5	1
1:A:96:LYS:HG3	1:A:97:GLU:N	0.53	2.18	16	2
1:A:23:ILE:HG22	1:A:24:LYS:N	0.53	2.19	9	1
1:A:59:HIS:CD2	1:A:95:TRP:CZ2	0.52	2.97	8	2
1:A:16:MET:O	1:A:19:GLU:HG2	0.52	2.04	16	5
1:A:19:GLU:HB2	1:A:91:PHE:CD2	0.52	2.39	11	1
1:A:19:GLU:HG2	1:A:91:PHE:CZ	0.52	2.40	9	2
1:A:57:ALA:O	1:A:61:PRO:CD	0.52	2.58	10	5
1:A:52:LEU:HD21	1:A:102:ALA:CB	0.52	2.35	5	1
1:A:67:LEU:HD12	1:A:67:LEU:C	0.51	2.25	7	1
1:A:93:ASP:CG	1:A:94:HIS:N	0.51	2.63	8	1
1:A:33:GLU:CA	1:A:33:GLU:OE1	0.51	2.57	19	1
1:A:12:PHE:CD2	1:A:73:LEU:HD22	0.51	2.41	2	3
1:A:59:HIS:NE2	1:A:63:ILE:CD1	0.51	2.66	4	1
1:A:20:GLU:CD	1:A:91:PHE:CG	0.51	2.75	6	1
1:A:63:ILE:CG1	1:A:91:PHE:CZ	0.51	2.93	1	4
1:A:23:ILE:CG2	1:A:24:LYS:N	0.51	2.72	9	4
1:A:59:HIS:CD2	1:A:63:ILE:CD1	0.51	2.93	4	1
1:A:26:LYS:HG2	1:A:59:HIS:NE2	0.51	2.21	15	2
1:A:63:ILE:HG13	1:A:91:PHE:CZ	0.51	2.41	11	1
1:A:59:HIS:O	1:A:63:ILE:HD13	0.50	2.06	4	1
1:A:56:LEU:HA	1:A:59:HIS:CE1	0.50	2.42	14	2
1:A:12:PHE:HA	1:A:15:ASP:OD2	0.50	2.06	15	1
1:A:97:GLU:OE1	1:A:101:LEU:HG	0.50	2.06	8	1
1:A:59:HIS:O	1:A:63:ILE:HG12	0.50	2.07	20	2
1:A:19:GLU:O	1:A:22:TRP:HB3	0.50	2.07	4	1
1:A:59:HIS:CD2	1:A:95:TRP:CE2	0.50	3.00	8	2
1:A:68:ASP:OD1	1:A:68:ASP:C	0.50	2.50	20	1
1:A:30:VAL:HG13	1:A:105:ARG:HG3	0.50	1.83	5	1
1:A:17:ASP:OD1	1:A:18:ASP:N	0.50	2.45	12	1
1:A:56:LEU:HD23	1:A:95:TRP:CH2	0.50	2.42	15	1
1:A:22:TRP:CD1	1:A:22:TRP:C	0.49	2.85	4	2
1:A:19:GLU:HG3	1:A:66:VAL:HG11	0.49	1.84	8	1
1:A:29:LEU:HD22	1:A:55:GLU:CD	0.49	2.28	8	1
1:A:33:GLU:OE1	1:A:33:GLU:N	0.49	2.45	19	1
1:A:66:VAL:CG1	1:A:67:LEU:N	0.49	2.76	3	3
1:A:10:HIS:ND1	1:A:11:GLN:N	0.49	2.60	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:12:PHE:HB2	1:A:73:LEU:HD21	0.49	1.85	11	1
1:A:63:ILE:CG1	1:A:91:PHE:CE2	0.49	2.96	10	1
1:A:52:LEU:HD22	1:A:52:LEU:C	0.49	2.27	16	1
1:A:19:GLU:HB3	1:A:91:PHE:CE1	0.49	2.42	13	1
1:A:79:ILE:O	1:A:81:LYS:N	0.49	2.46	2	2
1:A:97:GLU:HG2	1:A:98:LEU:N	0.49	2.22	4	1
1:A:49:HIS:CE1	1:A:105:ARG:HE	0.49	2.26	9	1
1:A:30:VAL:HG13	1:A:48:LYS:CD	0.48	2.38	1	1
1:A:66:VAL:HG12	1:A:88:LEU:HD11	0.48	1.85	13	1
1:A:22:TRP:HD1	1:A:25:GLU:OE2	0.48	1.88	6	1
1:A:63:ILE:HG23	1:A:91:PHE:CD2	0.48	2.43	1	2
1:A:67:LEU:C	1:A:67:LEU:HD13	0.48	2.28	3	1
1:A:67:LEU:HD13	1:A:67:LEU:C	0.48	2.29	11	1
1:A:60:GLU:HB2	1:A:61:PRO:HD3	0.48	1.86	9	4
1:A:86:GLN:HG3	1:A:87:ARG:N	0.48	2.24	13	1
1:A:22:TRP:HZ2	1:A:59:HIS:NE2	0.47	2.06	19	4
1:A:44:ASN:O	1:A:47:LYS:HG3	0.47	2.08	1	1
1:A:77:ASN:N	1:A:77:ASN:HD22	0.47	2.07	3	1
1:A:22:TRP:CE3	1:A:23:ILE:N	0.47	2.82	2	2
1:A:19:GLU:HG3	1:A:66:VAL:HG21	0.47	1.87	13	1
1:A:73:LEU:O	1:A:77:ASN:ND2	0.47	2.47	15	1
1:A:23:ILE:CG2	1:A:98:LEU:HD11	0.47	2.24	5	1
1:A:51:ARG:NH2	1:A:55:GLU:OE2	0.47	2.48	5	1
1:A:12:PHE:O	1:A:15:ASP:OD1	0.47	2.32	15	1
1:A:86:GLN:O	1:A:89:ALA:HB3	0.47	2.09	1	1
1:A:22:TRP:CE2	1:A:59:HIS:CE1	0.47	3.01	4	1
1:A:60:GLU:O	1:A:64:GLN:CB	0.47	2.62	19	1
1:A:12:PHE:CD2	1:A:73:LEU:CD1	0.47	2.98	12	1
1:A:27:LYS:HG3	1:A:28:LEU:N	0.47	2.24	18	1
1:A:93:ASP:O	1:A:96:LYS:CG	0.47	2.63	16	2
1:A:29:LEU:HD13	1:A:51:ARG:HH22	0.47	1.69	7	1
1:A:13:PHE:CZ	1:A:87:ARG:NH2	0.46	2.83	2	1
1:A:60:GLU:HB3	1:A:61:PRO:HD3	0.46	1.87	6	4
1:A:80:GLY:HA2	1:A:83:GLU:OE2	0.46	2.10	6	1
1:A:14:ARG:HA	1:A:14:ARG:NH1	0.46	2.26	12	1
1:A:12:PHE:CD2	1:A:73:LEU:CD2	0.46	2.99	1	2
1:A:19:GLU:OE2	1:A:91:PHE:CZ	0.46	2.57	6	1
1:A:59:HIS:HB3	1:A:95:TRP:CZ2	0.46	2.46	11	1
1:A:97:GLU:OE1	1:A:100:GLN:NE2	0.46	2.49	7	1
1:A:49:HIS:CE1	1:A:105:ARG:HG3	0.46	2.45	20	1
1:A:55:GLU:O	1:A:59:HIS:ND1	0.46	2.49	15	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:59:HIS:CG	1:A:95:TRP:CH2	0.46	3.04	11	1
1:A:60:GLU:CB	1:A:61:PRO:CD	0.46	2.94	20	2
1:A:30:VAL:HG13	1:A:48:LYS:CE	0.45	2.41	1	1
1:A:79:ILE:HG23	1:A:79:ILE:O	0.45	2.12	13	1
1:A:63:ILE:HG12	1:A:91:PHE:CE1	0.45	2.45	15	1
1:A:66:VAL:HG12	1:A:67:LEU:N	0.45	2.26	15	2
1:A:56:LEU:HA	1:A:59:HIS:ND1	0.45	2.25	14	2
1:A:32:SER:O	1:A:33:GLU:HB2	0.45	2.10	2	2
1:A:91:PHE:CD1	1:A:91:PHE:C	0.45	2.89	2	4
1:A:18:ASP:N	1:A:18:ASP:OD1	0.45	2.49	13	1
1:A:29:LEU:HD13	1:A:51:ARG:CZ	0.45	2.40	14	1
1:A:14:ARG:O	1:A:18:ASP:CG	0.45	2.54	14	1
1:A:23:ILE:HD11	1:A:91:PHE:CE2	0.45	2.47	19	1
1:A:90:GLN:NE2	1:A:94:HIS:CG	0.45	2.85	1	1
1:A:19:GLU:HG2	1:A:20:GLU:H	0.45	1.72	11	1
1:A:15:ASP:OD1	1:A:16:MET:N	0.44	2.50	20	1
1:A:95:TRP:CH2	1:A:99:LYS:NZ	0.44	2.86	4	1
1:A:56:LEU:HD12	1:A:59:HIS:CE1	0.44	2.46	14	1
1:A:79:ILE:O	1:A:80:GLY:C	0.44	2.56	20	1
1:A:19:GLU:CG	1:A:91:PHE:CE2	0.44	3.01	2	2
1:A:19:GLU:CG	1:A:91:PHE:CZ	0.44	3.01	5	1
1:A:64:GLN:C	1:A:68:ASP:OD2	0.44	2.55	12	1
1:A:72:LYS:HA	1:A:75:ASP:OD1	0.44	2.12	15	1
1:A:105:ARG:NE	1:A:106:GLY:N	0.44	2.65	10	1
1:A:20:GLU:O	1:A:23:ILE:HG22	0.44	2.13	15	1
1:A:22:TRP:CZ3	1:A:59:HIS:NE2	0.43	2.85	2	1
1:A:13:PHE:CD1	1:A:13:PHE:C	0.43	2.91	10	1
1:A:63:ILE:HG22	1:A:64:GLN:N	0.43	2.28	14	1
1:A:14:ARG:NH2	1:A:17:ASP:HB3	0.43	2.29	1	1
1:A:50:LYS:C	1:A:53:GLU:OE1	0.43	2.52	17	1
1:A:19:GLU:CB	1:A:91:PHE:CE2	0.43	3.02	18	1
1:A:96:LYS:HZ3	1:A:97:GLU:CD	0.43	2.17	16	1
1:A:100:GLN:HG2	1:A:101:LEU:N	0.43	2.29	1	1
1:A:19:GLU:HG2	1:A:20:GLU:N	0.43	2.28	11	1
1:A:20:GLU:OE1	1:A:20:GLU:CA	0.43	2.67	16	1
1:A:19:GLU:O	1:A:22:TRP:N	0.43	2.52	4	2
1:A:67:LEU:C	1:A:67:LEU:HD23	0.43	2.33	17	1
1:A:12:PHE:CE2	1:A:73:LEU:HD22	0.43	2.49	20	1
1:A:28:LEU:O	1:A:28:LEU:HD13	0.42	2.14	5	1
1:A:14:ARG:HD2	1:A:17:ASP:OD2	0.42	2.14	8	1
1:A:12:PHE:CE2	1:A:16:MET:SD	0.42	3.13	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:22:TRP:CE3	1:A:23:ILE:HA	0.42	2.49	2	1
1:A:53:GLU:HG2	1:A:54:ALA:N	0.42	2.29	15	1
1:A:57:ALA:O	1:A:61:PRO:HD2	0.42	2.14	19	1
1:A:100:GLN:NE2	1:A:101:LEU:N	0.42	2.67	20	1
1:A:11:GLN:NE2	1:A:11:GLN:N	0.42	2.66	1	1
1:A:93:ASP:O	1:A:96:LYS:HG3	0.42	2.14	11	1
1:A:19:GLU:OE1	1:A:66:VAL:HG21	0.42	2.14	7	1
1:A:19:GLU:CG	1:A:66:VAL:HG21	0.42	2.44	13	1
1:A:77:ASN:ND2	1:A:80:GLY:N	0.42	2.68	2	1
1:A:16:MET:SD	1:A:87:ARG:NH2	0.42	2.92	4	1
1:A:22:TRP:CH2	1:A:59:HIS:CG	0.42	3.07	4	1
1:A:59:HIS:CG	1:A:95:TRP:CZ2	0.42	3.08	13	1
1:A:23:ILE:HD12	1:A:91:PHE:CZ	0.42	2.50	20	1
1:A:75:ASP:OD1	1:A:75:ASP:C	0.41	2.58	20	1
1:A:19:GLU:HG2	1:A:91:PHE:CE2	0.41	2.50	12	1
1:A:14:ARG:CZ	1:A:18:ASP:HB3	0.41	2.45	14	1
1:A:77:ASN:ND2	1:A:77:ASN:N	0.41	2.67	18	1
1:A:77:ASN:OD1	1:A:78:THR:N	0.41	2.53	11	1
1:A:19:GLU:HB3	1:A:91:PHE:CD1	0.41	2.49	13	1
1:A:19:GLU:HG3	1:A:91:PHE:CE2	0.41	2.51	2	1
1:A:59:HIS:O	1:A:60:GLU:C	0.41	2.59	3	2
1:A:30:VAL:CG1	1:A:31:SER:N	0.41	2.82	6	1
1:A:49:HIS:CE1	1:A:105:ARG:HH21	0.41	2.33	3	1
1:A:59:HIS:O	1:A:63:ILE:N	0.41	2.53	20	1
1:A:16:MET:SD	1:A:87:ARG:NH1	0.41	2.93	14	1
1:A:90:GLN:NE2	1:A:94:HIS:ND1	0.41	2.69	1	1
1:A:60:GLU:O	1:A:64:GLN:HB2	0.41	2.15	7	1
1:A:22:TRP:CZ3	1:A:23:ILE:CD1	0.41	3.03	12	1
1:A:23:ILE:HD13	1:A:94:HIS:HB3	0.41	1.92	19	1
1:A:23:ILE:HG23	1:A:24:LYS:N	0.41	2.29	15	1
1:A:45:LEU:HB3	1:A:46:ARG:CZ	0.41	2.46	15	1
1:A:92:VAL:CG1	1:A:93:ASP:N	0.41	2.84	15	1
1:A:16:MET:SD	1:A:66:VAL:CG1	0.41	3.09	19	1
1:A:12:PHE:CD1	1:A:69:THR:HB	0.41	2.51	14	1
1:A:12:PHE:C	1:A:15:ASP:CG	0.41	2.80	15	1
1:A:32:SER:O	1:A:33:GLU:CG	0.41	2.69	17	1
1:A:23:ILE:HD12	1:A:91:PHE:CE2	0.41	2.51	20	1
1:A:96:LYS:HG2	1:A:97:GLU:N	0.40	2.32	2	1
1:A:96:LYS:CD	1:A:97:GLU:N	0.40	2.84	3	1
1:A:11:GLN:HG3	1:A:12:PHE:N	0.40	2.31	17	1
1:A:97:GLU:OE1	1:A:97:GLU:N	0.40	2.54	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:59:HIS:HD2	1:A:95:TRP:NE1	0.40	2.14	4	1
1:A:52:LEU:HD13	1:A:52:LEU:C	0.40	2.37	16	1
1:A:82:GLU:H	1:A:82:GLU:HG2	0.40	1.38	6	1
1:A:19:GLU:CD	1:A:66:VAL:HG21	0.40	2.37	7	1
1:A:28:LEU:C	1:A:28:LEU:HD13	0.40	2.37	7	1
1:A:13:PHE:CE1	1:A:87:ARG:NH1	0.40	2.89	10	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	87/110 (79%)	84±1 (96±1%)	3±1 (3±1%)	1±1 (1±1%)	20	68
All	All	1740/2200 (79%)	1671 (96%)	52 (3%)	17 (1%)	20	68

All 6 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	79	ILE	6
1	A	80	GLY	3
1	A	77	ASN	3
1	A	33	GLU	2
1	A	78	THR	2
1	A	76	ASP	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	77/95 (81%)	52±4 (67±5%)	25±4 (33±5%)	1 12
All	All	1540/1900 (81%)	1032 (67%)	508 (33%)	1 12

All 73 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	96	LYS	16
1	A	60	GLU	15
1	A	93	ASP	15
1	A	21	SER	13
1	A	47	LYS	13
1	A	72	LYS	13
1	A	26	LYS	13
1	A	50	LYS	12
1	A	14	ARG	12
1	A	85	GLN	12
1	A	105	ARG	12
1	A	16	MET	11
1	A	25	GLU	11
1	A	18	ASP	11
1	A	13	PHE	10
1	A	81	LYS	10
1	A	71	LYS	9
1	A	87	ARG	9
1	A	100	GLN	9
1	A	20	GLU	9
1	A	33	GLU	9
1	A	46	ARG	9
1	A	27	LYS	8
1	A	48	LYS	8
1	A	99	LYS	8
1	A	24	LYS	8
1	A	51	ARG	8
1	A	97	GLU	8
1	A	83	GLU	7
1	A	29	LEU	7
1	A	68	ASP	7
1	A	98	LEU	7
1	A	28	LEU	7
1	A	49	HIS	7
1	A	53	GLU	7
1	A	31	SER	6

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Mol	Chain	Res	Type	Models (Total)
1	A	52	LEU	6
1	A	56	LEU	6
1	A	64	GLN	6
1	A	78	THR	6
1	A	82	GLU	6
1	A	86	GLN	6
1	A	88	LEU	6
1	A	55	GLU	6
1	A	19	GLU	6
1	A	17	ASP	5
1	A	67	LEU	5
1	A	74	SER	5
1	A	90	GLN	5
1	A	101	LEU	5
1	A	43	GLN	5
1	A	76	ASP	5
1	A	44	ASN	5
1	A	23	ILE	4
1	A	75	ASP	4
1	A	59	HIS	4
1	A	107	GLN	4
1	A	66	VAL	4
1	A	77	ASN	4
1	A	45	LEU	4
1	A	15	ASP	3
1	A	11	GLN	3
1	A	32	SER	3
1	A	73	LEU	3
1	A	30	VAL	3
1	A	92	VAL	3
1	A	91	PHE	3
1	A	94	HIS	2
1	A	63	ILE	2
1	A	79	ILE	2
1	A	10	HIS	1
1	A	22	TRP	1
1	A	12	PHE	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