Full wwPDB NMR Structure Validation Report (i)

Feb 8, 2022 – 04:03 PM EST

PDB ID	:	1CMO
Title	:	IMMUNOGLOBULIN MOTIF DNA-RECOGNITION AND HETERODIMERIZATION FOR THE PEBP2/CBF RUNT-DOMAIN
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Deposited on	:	1999-05-11

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:

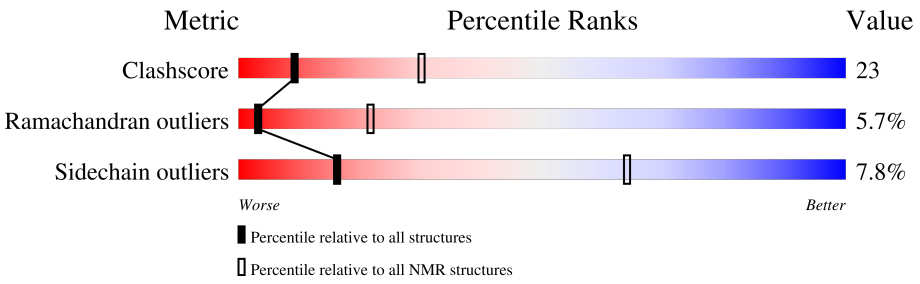
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.26
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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	127	54% 25% • 17%

2 Ensemble composition and analysis (i)

This entry contains 43 models. Model 21 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:62-A:166 (105)	0.35	21

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 5 clusters. No single-model clusters were found.

Cluster number	Models
1	3, 4, 6, 9, 11, 12, 13, 14, 16, 17, 18, 19, 20, 21, 22, 23, 24, 25, 26, 27, 28, 29, 30, 32, 33, 35, 37, 38, 39, 41
2	2, 8, 10, 31, 36, 42
3	7, 15, 34
4	40, 43
5	1, 5

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1977 atoms, of which 992 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called POLYOMAVIRUS ENHANCER BINDING PROTEIN 2.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	127	1977	619	992	182	181	3	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	81	SER	CYS	SEE REMARK 999	UNP Q01196

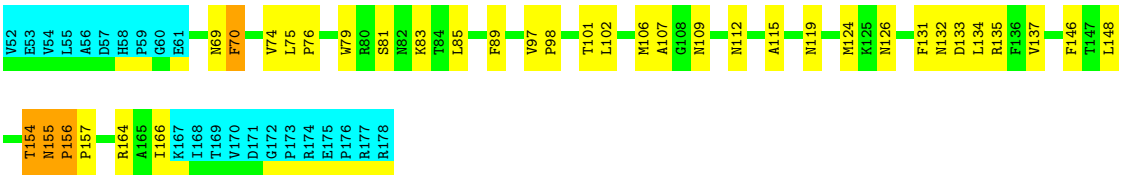
4 Residue-property plots (i)

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: POLYOMAVIRUS ENHANCER BINDING PROTEIN 2

Chain A: 54% 25% • 17%



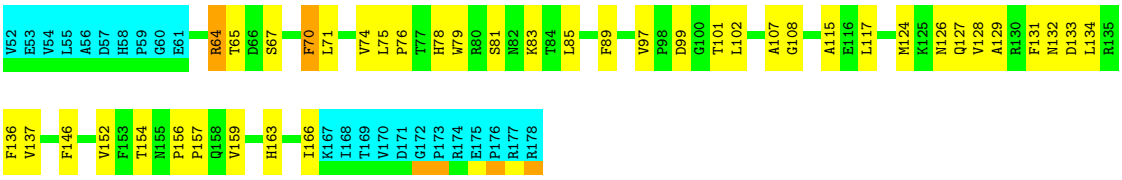
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: POLYOMAVIRUS ENHANCER BINDING PROTEIN 2

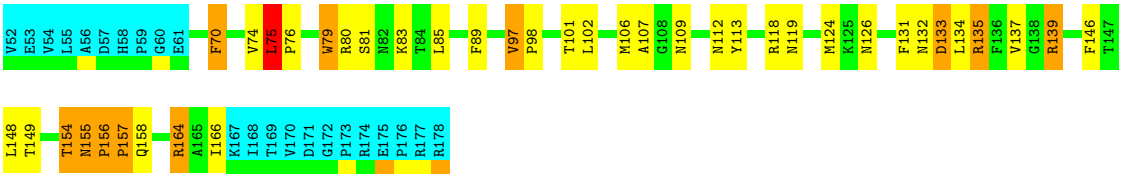
Chain A: 50% 31% • 17%



4.2.2 Score per residue for model 2

• Molecule 1: POLYOMAVIRUS ENHANCER BINDING PROTEIN 2

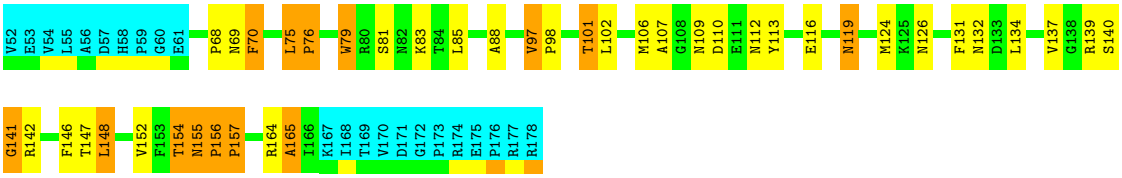
Chain A: 51% 22% 9% • 17%



4.2.3 Score per residue for model 3

- Molecule 1: POLYOMAVIRUS ENHANCER BINDING PROTEIN 2

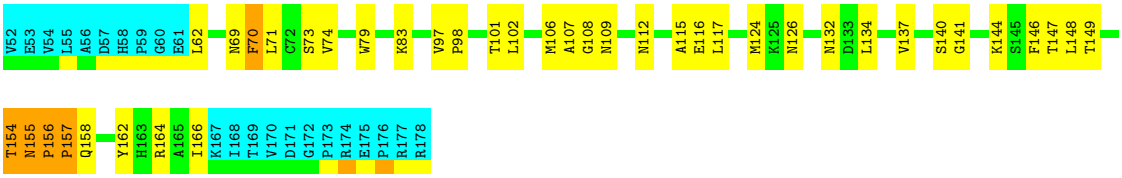
Chain A: 50% 22% 11% 17%



4.2.4 Score per residue for model 4

- Molecule 1: POLYOMAVIRUS ENHANCER BINDING PROTEIN 2

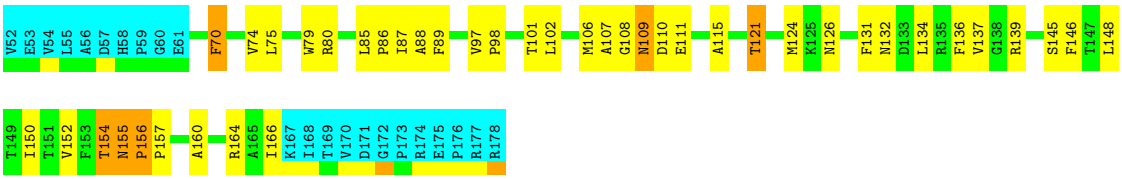
Chain A: 51% 28% • 17%



4.2.5 Score per residue for model 5

- Molecule 1: POLYOMAVIRUS ENHANCER BINDING PROTEIN 2

Chain A: 50% 28% 5% 17%



4.2.6 Score per residue for model 6

- Molecule 1: POLYOMAVIRUS ENHANCER BINDING PROTEIN 2

Chain A: 47% 28% 6% • 17%

V52 E53 V54 L55 A56 D57 H58 P59 G60 E61 S67 P68 N69 F70 L71 C72 S73 V74 W79 R80 S81 N82 K83 P86 I87 A88 F89 V97 T101 L102 A107 G108 N109 N112 Y113 R118 N119 A122 A123 M124 K125 N126 R130 F131 N132 D133 L134 R135 F136 V137

G138 R139 K144 S145 F146 T147 L148 V152 F153 T154 N155 P156 P157 Q158 V159 R164 K167 I168 T169 V170 D171 G172 P173 R174 E175 P176 R177 R178

4.2.7 Score per residue for model 7

- Molecule 1: POLYOMAVIRUS ENHANCER BINDING PROTEIN 2

Chain A: 53% 24% 6% 17%

V52 E53 V54 L55 A56 D57 H58 P59 G60 E61 D66 N69 F70 L71 L75 H78 W79 R80 S81 N82 K83 F89 V97 A107 G108 N109 D110 E111 A115 E116 N119 M124 K125 N126 F131 N132 D133 L134 R135 F136 V137 G141 S145 F146 T147 T154

N155 P156 P157 Q158 H163 K167 I168 T169 V170 D171 G172 P173 R174 E175 P176 R177 R178

4.2.8 Score per residue for model 8

- Molecule 1: POLYOMAVIRUS ENHANCER BINDING PROTEIN 2

Chain A: 46% 27% 10% 17%

V52 E53 V54 L55 A56 D57 H58 P59 G60 E61 R64 F70 L71 C72 S73 V74 W79 R80 S81 T84 L85 P86 F89 V97 P98 D99 G100 T101 M106 A107 G108 N109 D110 E111 S114 A115 E116 L117 R118 N119 M124 A129 R130 F131 N132 D133 L134 R135 F136 V137

R142 S145 F146 T147 L148 T149 I150 T151 V152 F153 T154 N155 P156 P157 A160 H163 I166 K167 I168 T169 V170 D171 G172 P173 R174 E175 P176 R177 R178

4.2.9 Score per residue for model 9

- Molecule 1: POLYOMAVIRUS ENHANCER BINDING PROTEIN 2

Chain A: 42% 31% 10% 17%

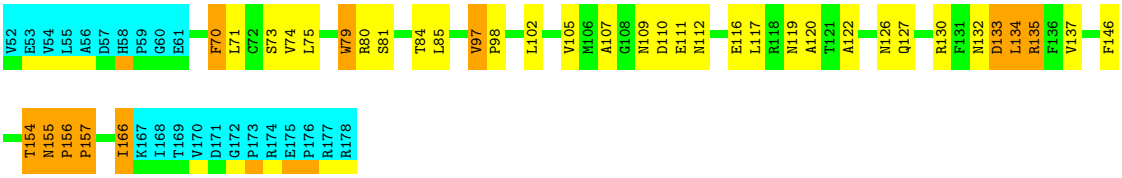
V52 E53 V54 L55 A56 D57 H58 P59 G60 E61 L62 S67 P68 N69 F70 L71 V74 L75 P76 T77 H78 W79 R80 S81 N82 K83 T84 L85 F89 V97 P98 D99 G100 T101 L102 M106 A107 G108 N109 N112 A115 E116 N119 A120 T121 A122 A123 M124 K125 N126 R130

F131 N132 D133 L134 R135 F136 V137 F146 T147 L148 T149 I150 T151 V152 F153 T154 N155 P156 P157 Q158 V159 A160 R164 K167 I168 T169 V170 D171 G172 P173 R174 E175 P176 R177 R178

4.2.10 Score per residue for model 10

• Molecule 1: POLYOMAVIRUS ENHANCER BINDING PROTEIN 2

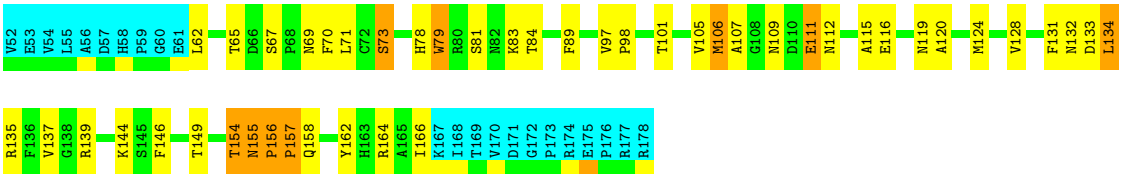
Chain A: 53% 21% 9% 17%



4.2.11 Score per residue for model 11

• Molecule 1: POLYOMAVIRUS ENHANCER BINDING PROTEIN 2

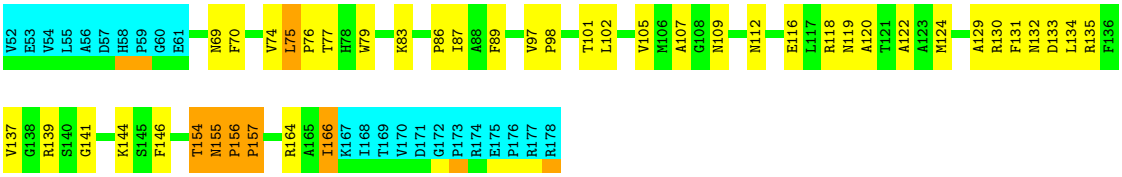
Chain A: 46% 29% 7% 17%



4.2.12 Score per residue for model 12

• Molecule 1: POLYOMAVIRUS ENHANCER BINDING PROTEIN 2

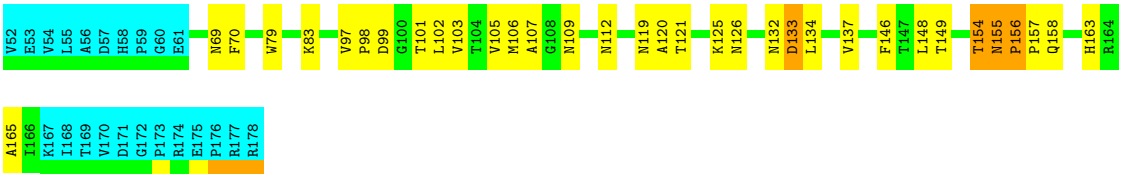
Chain A: 49% 29% 5% 17%



4.2.13 Score per residue for model 13

• Molecule 1: POLYOMAVIRUS ENHANCER BINDING PROTEIN 2

Chain A: 56% 24% • 17%



4.2.14 Score per residue for model 14

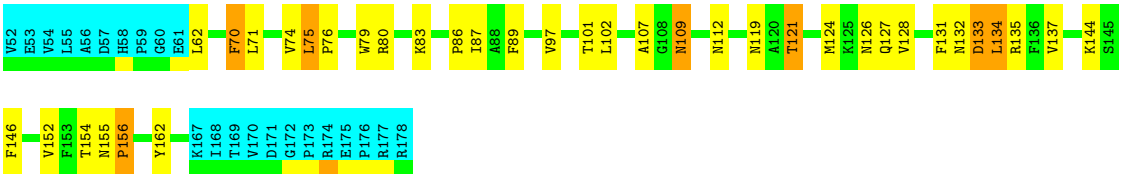
• Molecule 1: POLYOMAVIRUS ENHANCER BINDING PROTEIN 2

Chain A: 42% 35% 6% 17%

4.2.15 Score per residue for model 15

• Molecule 1: POLYOMAVIRUS ENHANCER BINDING PROTEIN 2

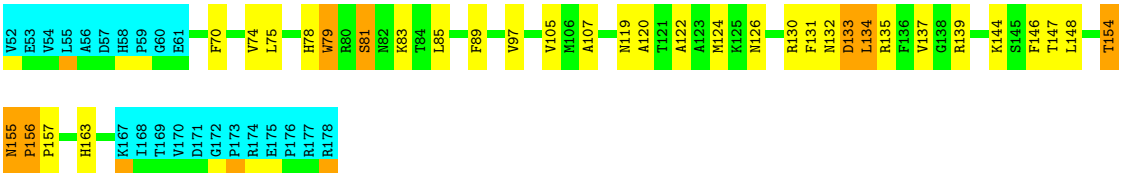
Chain A: 54% 24% 6% 17%



4.2.16 Score per residue for model 16

• Molecule 1: POLYOMAVIRUS ENHANCER BINDING PROTEIN 2

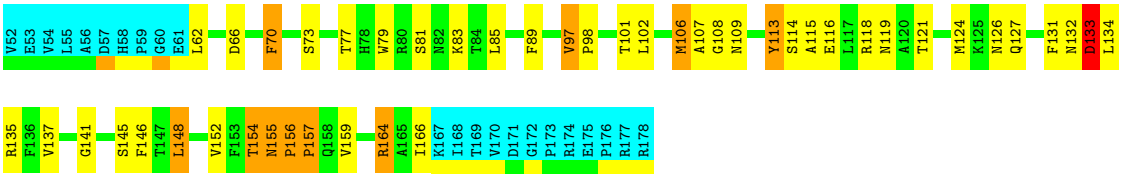
Chain A: 56% 21% 6% 17%



4.2.17 Score per residue for model 17

• Molecule 1: POLYOMAVIRUS ENHANCER BINDING PROTEIN 2

Chain A: 46% 28% 8% • 17%



4.2.18 Score per residue for model 18

• Molecule 1: POLYOMAVIRUS ENHANCER BINDING PROTEIN 2

Chain A: 48% 28% 7% 17%

V52 E53 V54 L55 A56 D57 H58 P59 G60 E61 R64 T65 F70 V74 W79 R80 S81 N82 K83 P86 F89 V97 T101 L102 V103 T104 V105 M106 A107 D110 E111 S114 A115 E116 N119 A120 N126 Q127 F131 N132 D133 L134 R135 F136 V137 F146

T147 L148 T149 I150 T151 V152 F153 T154 N155 P156 P157 A160 R164 K167 I168 T169 V170 D171 G172 P173 R174 E175 P176 R177 R178

4.2.19 Score per residue for model 19

• Molecule 1: POLYOMAVIRUS ENHANCER BINDING PROTEIN 2

Chain A: 50% 26% 7% 17%

V52 E53 V54 L55 A56 D57 H58 P59 G60 E61 D66 S67 F70 L71 L75 P76 W79 R80 S81 N82 K83 P86 V97 P98 T101 L102 V105 M106 A107 G108 N109 A115 R118 N119 A120 M124 K125 N126 F131 N132 D133 L134 V137 G138 R139 S140 G141

K144 S145 F146 T147 L148 T154 N155 P156 P157 Y162 H163 R164 A165 I166 K167 I168 T169 V170 D171 G172 P173 R174 E175 P176 R177 R178

4.2.20 Score per residue for model 20

• Molecule 1: POLYOMAVIRUS ENHANCER BINDING PROTEIN 2

Chain A: 51% 26% 5% • 17%

V52 E53 V54 L55 A56 D57 H58 P59 G60 E61 P68 N69 F70 L75 P76 K83 P86 I87 A88 V97 T101 L102 M106 A107 G108 N109 N112 Y113 S114 A115 E116 M124 K125 N126 F131 N132 D133 L134 V137 G138 R139 S140 G141 R142 F146 T147 L148 T149

T154 N155 P156 P157 Y162 H163 R164 A165 I166 K167 I168 T169 V170 D171 G172 P173 R174 E175 P176 R177 R178

4.2.21 Score per residue for model 21 (medoid)

• Molecule 1: POLYOMAVIRUS ENHANCER BINDING PROTEIN 2

Chain A: 46% 26% 11% 17%

V52 E53 V54 L55 A56 D57 H58 P59 G60 E61 R64 T65 D66 S67 P68 N69 F70 L71 C72 S73 V74 L75 W79 R80 S81 N82 K83 I87 A88 F89 V97 P98 T101 L102 M106 A107 G108 N112 Y113 S114 A115 E116 L117 R118 T121 M124 K125 N126 F131 N132

D133 L134 R135 F136 V137 K144 S145 F146 T147 L148 T149 V152 F153 T154 N155 P156 P157 K167 I168 T169 V170 D171 G172 P173 R174 E175 P176 R177 R178

4.2.22 Score per residue for model 22

• Molecule 1: POLYOMAVIRUS ENHANCER BINDING PROTEIN 2

Chain A: 49% 24% 9% 17%

V52 E53 V54 L55 A56 D57 H58 P59 G60 E61 T65 N69 F70 S73 V74 L75 W79 R80 S81 N82 K83 I87 A88 F89 V97 P98 D99 G100 T101 L102 M106 A107 G108 N109 N112 A115 N119 M124 A129 N132 D133 L134 R135 F136 V137 S140

G141 R142 F146 T149 V152 F153 T154 N155 P156 P157 Q158 R164 A165 I166 K167 I168 T169 V170 D171 G172 P173 R174 E175 P176 R177 R178

4.2.23 Score per residue for model 23

• Molecule 1: POLYOMAVIRUS ENHANCER BINDING PROTEIN 2

Chain A: 48% 26% 9% 17%

V52 E53 V54 L55 A56 D57 H58 P59 G60 E61 L62 F70 L71 L75 W79 K83 T84 L85 P86 I87 A88 F89 V97 T101 L102 V105 M106 A107 G108 N109 N112 Y113 L117 R118 N119 A120 T121 A122 A123 M124 K125 N126 Q127 R130 F131 N132 D133 L134 R135 F136

V137 G138 R139 S140 G141 F146 T147 L148 T154 N155 P156 P157 R164 K167 I168 T169 V170 D171 G172 P173 R174 E175 P176 R177 R178

4.2.24 Score per residue for model 24

• Molecule 1: POLYOMAVIRUS ENHANCER BINDING PROTEIN 2

Chain A: 53% 25% 5% 17%

V52 E53 V54 L55 A56 D57 H58 P59 G60 E61 S73 V74 L75 P76 T77 H78 W79 N82 K83 T84 L85 P86 F89 V97 P98 T101 L102 M106 A107 R118 N119 M124 K125 N126 Q127 V128 F131 N132 D133 L134 R135 F136 V137 G138 R139 K144 S145 F146 T147 L148

T149 T154 N155 P156 P157 R164 A165 I166 K167 I168 T169 V170 D171 G172 P173 R174 E175 P176 R177 R178

4.2.25 Score per residue for model 25

• Molecule 1: POLYOMAVIRUS ENHANCER BINDING PROTEIN 2

Chain A: 53% 25% 5% 17%

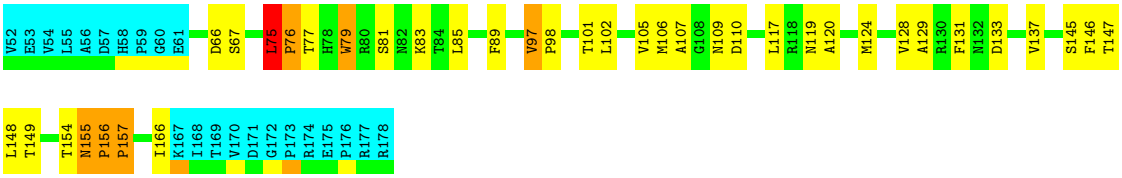
V52 E53 V54 L55 A56 D57 H58 P59 G60 E61 L62 V63 F70 S73 V74 L75 P76 W79 R80 K83 P86 F89 V97 P98 D99 A107 G108 N109 N112 L117 R118 M124 K125 N126 N132 D133 L134 V137 G138 R139 R142 S145 F146 T147 L148

T149 I150 T154 N155 P156 P157 A160 H163 K167 I168 T169 V170 D171 G172 P173 R174 E175 P176 R177 R178

4.2.26 Score per residue for model 26

• Molecule 1: POLYOMAVIRUS ENHANCER BINDING PROTEIN 2

Chain A: 53% 24% 5% • 17%



4.2.27 Score per residue for model 27

• Molecule 1: POLYOMAVIRUS ENHANCER BINDING PROTEIN 2

Chain A: 53% 20% 9% • 17%

4.2.28 Score per residue for model 28

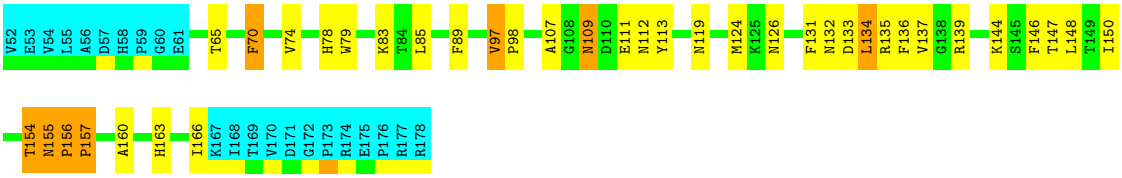
• Molecule 1: POLYOMAVIRUS ENHANCER BINDING PROTEIN 2

Chain A: 50% 24% 8% 17%

4.2.29 Score per residue for model 29

• Molecule 1: POLYOMAVIRUS ENHANCER BINDING PROTEIN 2

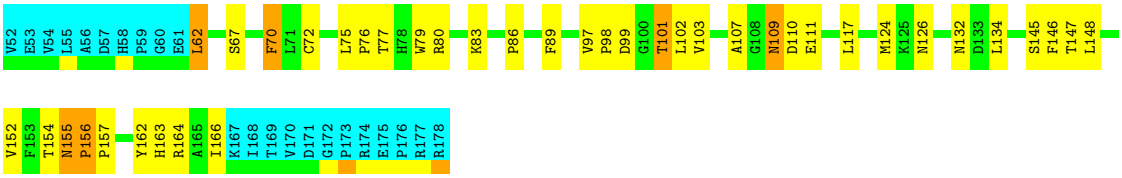
Chain A: 53% 24% 6% 17%



4.2.30 Score per residue for model 30

• Molecule 1: POLYOMAVIRUS ENHANCER BINDING PROTEIN 2

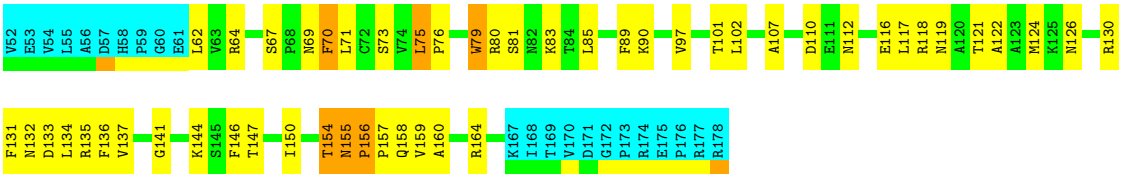
Chain A: 51% 27% 5% 17%



4.2.31 Score per residue for model 31

• Molecule 1: POLYOMAVIRUS ENHANCER BINDING PROTEIN 2

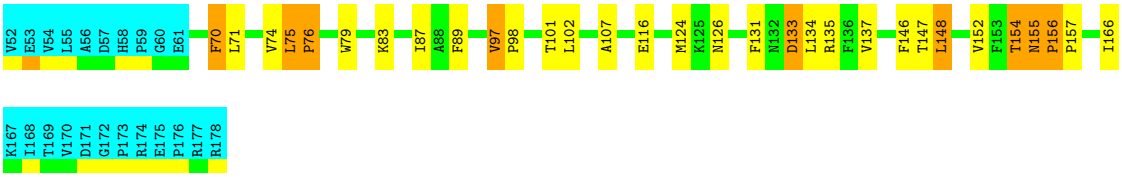
Chain A: 43% 35% 5% 17%



4.2.32 Score per residue for model 32

• Molecule 1: POLYOMAVIRUS ENHANCER BINDING PROTEIN 2

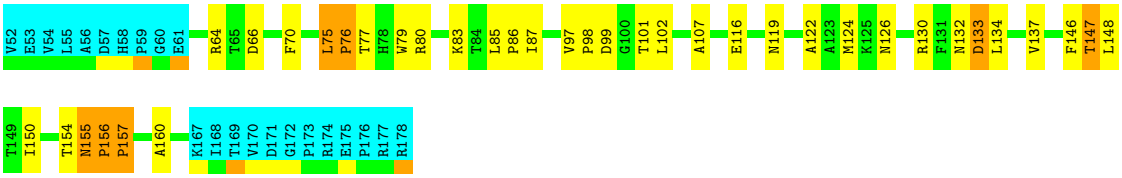
Chain A: 58% 17% 7% 17%



4.2.33 Score per residue for model 33

• Molecule 1: POLYOMAVIRUS ENHANCER BINDING PROTEIN 2

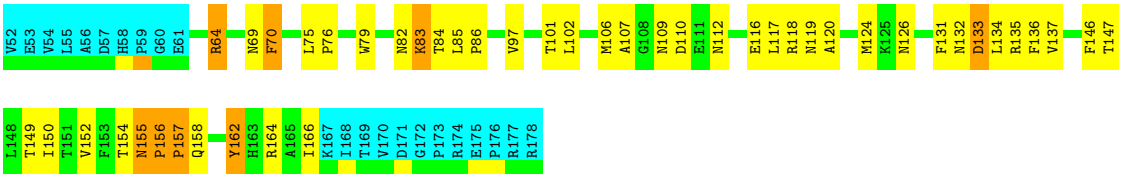
Chain A: 54% 24% 6% 17%



4.2.34 Score per residue for model 34

• Molecule 1: POLYOMAVIRUS ENHANCER BINDING PROTEIN 2

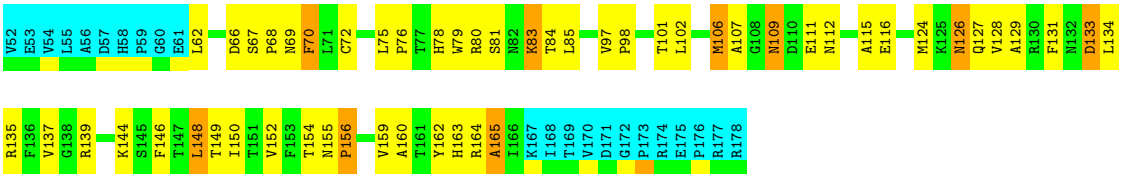
Chain A: 46% 30% 6% 17%



4.2.35 Score per residue for model 35

• Molecule 1: POLYOMAVIRUS ENHANCER BINDING PROTEIN 2

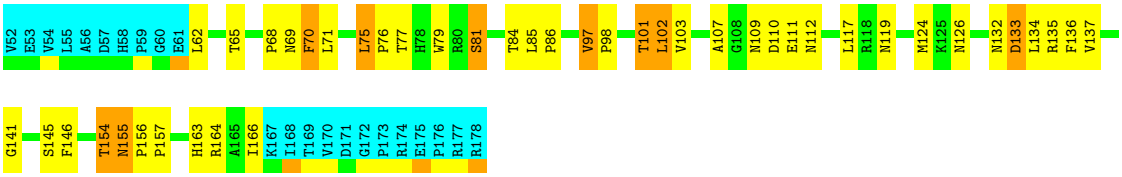
Chain A: 41% 35% 7% 17%



4.2.36 Score per residue for model 36

• Molecule 1: POLYOMAVIRUS ENHANCER BINDING PROTEIN 2

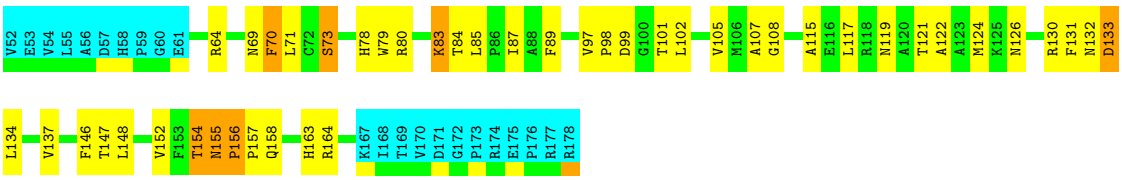
Chain A: 48% 28% 7% 17%



4.2.37 Score per residue for model 37

• Molecule 1: POLYOMAVIRUS ENHANCER BINDING PROTEIN 2

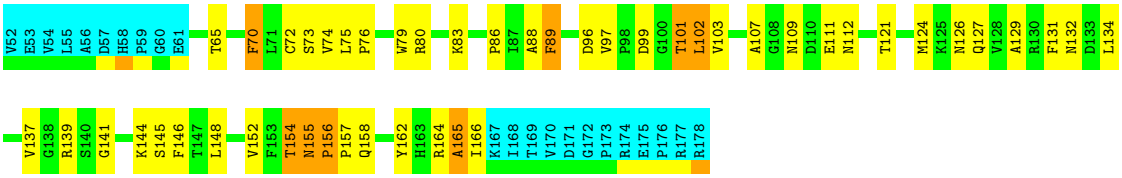
Chain A: 47% 30% 6% 17%



4.2.38 Score per residue for model 38

• Molecule 1: POLYOMAVIRUS ENHANCER BINDING PROTEIN 2

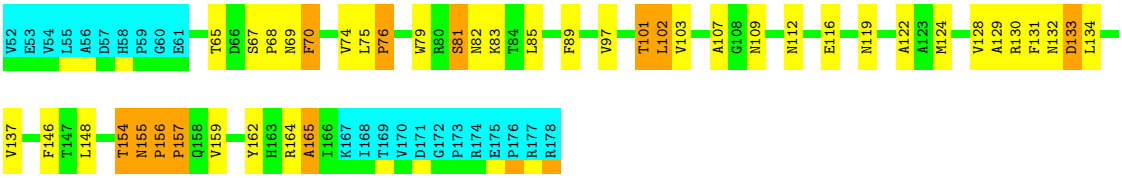
Chain A: 45% 31% 6% 17%



4.2.39 Score per residue for model 39

• Molecule 1: POLYOMAVIRUS ENHANCER BINDING PROTEIN 2

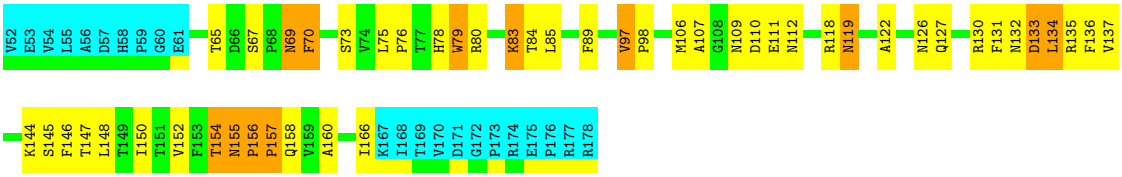
Chain A: 49% 25% 9% 17%



4.2.40 Score per residue for model 40

• Molecule 1: POLYOMAVIRUS ENHANCER BINDING PROTEIN 2

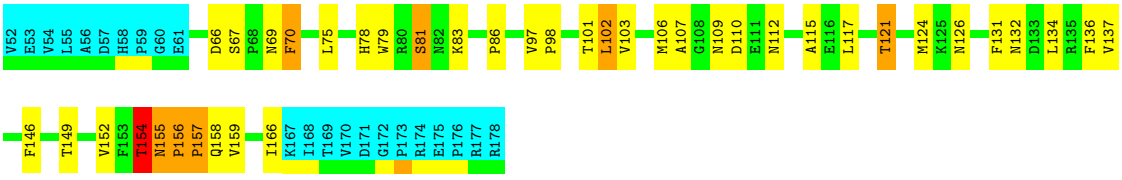
Chain A: 44% 29% 9% 17%



4.2.41 Score per residue for model 41

• Molecule 1: POLYOMAVIRUS ENHANCER BINDING PROTEIN 2

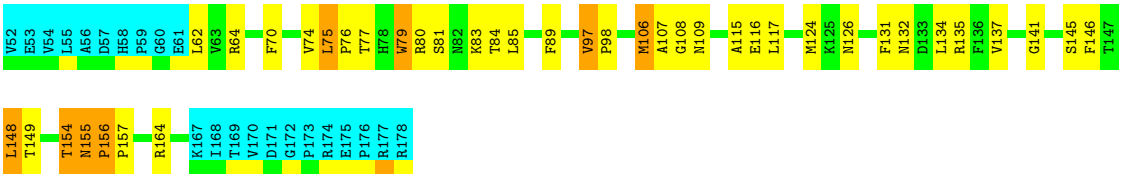
Chain A: 51% 25% 6% • 17%



4.2.42 Score per residue for model 42

- Molecule 1: POLYOMAVIRUS ENHANCER BINDING PROTEIN 2

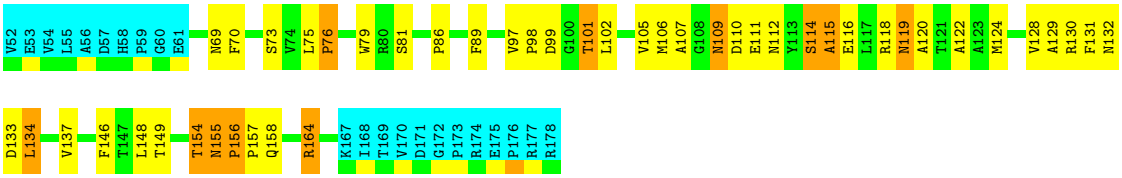
Chain A: 51% 25% 6% 17%



4.2.43 Score per residue for model 43

- Molecule 1: POLYOMAVIRUS ENHANCER BINDING PROTEIN 2

Chain A: 46% 28% 9% 17%



5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *HYBRID DISTANCE GEOMETRY/SIMULATED ANNEALING*.

Of the 300 calculated structures, 43 were deposited, based on the following criterion: *structures with the least restraint violations*.

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

Software name	Classification	Version
NMRPipe	structure solution	
PIPP	structure solution	
STAPP	structure solution	
X-PLOR	structure solution	
X-PLOR	refinement	3.843

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	812	819	819	37±7
All	All	34916	35217	35217	1597

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 23.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:62:LEU:H	1:A:62:LEU:HD22	0.84	1.33	23	1
1:A:166:ILE:H	1:A:166:ILE:HD13	0.82	1.35	12	2
1:A:148:LEU:N	1:A:148:LEU:HD23	0.81	1.89	42	2
1:A:62:LEU:HD22	1:A:62:LEU:N	0.80	1.92	23	1
1:A:62:LEU:N	1:A:62:LEU:HD22	0.79	1.92	30	6
1:A:116:GLU:O	1:A:137:VAL:HG12	0.79	1.78	31	12
1:A:109:ASN:HD21	1:A:144:LYS:HZ3	0.78	1.18	4	1
1:A:124:MET:SD	1:A:129:ALA:HB2	0.78	2.19	12	9
1:A:70:PHE:C	1:A:71:LEU:HD22	0.77	2.00	31	4
1:A:101:THR:HG21	1:A:154:THR:OG1	0.76	1.80	18	2
1:A:62:LEU:N	1:A:62:LEU:HD13	0.74	1.96	25	2
1:A:109:ASN:ND2	1:A:111:GLU:H	0.73	1.81	5	2
1:A:109:ASN:ND2	1:A:110:ASP:N	0.73	2.36	5	2
1:A:154:THR:HG22	1:A:155:ASN:N	0.72	1.99	18	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:70:PHE:C	1:A:71:LEU:HD12	0.71	2.06	15	8
1:A:102:LEU:HD23	1:A:103:VAL:N	0.71	2.01	13	1
1:A:137:VAL:HG13	1:A:137:VAL:O	0.69	1.85	4	5
1:A:102:LEU:HD13	1:A:103:VAL:N	0.69	2.03	30	6
1:A:97:VAL:HG22	1:A:97:VAL:O	0.68	1.87	35	30
1:A:85:LEU:HD22	1:A:85:LEU:N	0.68	2.03	5	3
1:A:75:LEU:N	1:A:76:PRO:CD	0.68	2.57	31	19
1:A:147:THR:HG1	1:A:163:HIS:CE1	0.68	2.07	16	2
1:A:132:ASN:O	1:A:134:LEU:N	0.68	2.27	36	24
1:A:75:LEU:HD22	1:A:75:LEU:N	0.68	2.04	5	1
1:A:70:PHE:CE2	1:A:152:VAL:HG21	0.68	2.24	34	13
1:A:109:ASN:ND2	1:A:145:SER:N	0.68	2.42	7	2
1:A:154:THR:HG22	1:A:155:ASN:H	0.68	1.46	18	5
1:A:70:PHE:CZ	1:A:152:VAL:HG21	0.67	2.24	34	20
1:A:166:ILE:C	1:A:166:ILE:HD12	0.67	2.10	19	4
1:A:154:THR:OG1	1:A:155:ASN:N	0.67	2.28	6	28
1:A:119:ASN:ND2	1:A:132:ASN:H	0.67	1.87	43	21
1:A:141:GLY:N	1:A:144:LYS:NZ	0.67	2.42	12	1
1:A:109:ASN:ND2	1:A:112:ASN:ND2	0.67	2.43	11	9
1:A:109:ASN:HD22	1:A:112:ASN:ND2	0.66	1.88	34	9
1:A:139:ARG:HH21	1:A:146:PHE:N	0.66	1.88	38	1
1:A:89:PHE:CE1	1:A:131:PHE:CE2	0.66	2.83	43	13
1:A:109:ASN:ND2	1:A:145:SER:H	0.66	1.87	7	2
1:A:150:ILE:CG2	1:A:160:ALA:HB3	0.66	2.20	5	4
1:A:109:ASN:HD21	1:A:144:LYS:NZ	0.66	1.88	4	1
1:A:109:ASN:ND2	1:A:144:LYS:HZ3	0.65	1.88	4	1
1:A:117:LEU:HD22	1:A:117:LEU:N	0.65	2.07	42	1
1:A:75:LEU:H	1:A:76:PRO:CD	0.65	2.05	2	17
1:A:79:TRP:NE1	1:A:81:SER:OG	0.65	2.30	42	9
1:A:117:LEU:HD12	1:A:117:LEU:N	0.64	2.07	14	11
1:A:89:PHE:CE1	1:A:131:PHE:CE1	0.64	2.84	7	9
1:A:89:PHE:CZ	1:A:131:PHE:CE1	0.64	2.85	17	10
1:A:70:PHE:O	1:A:71:LEU:HD12	0.64	1.92	9	1
1:A:109:ASN:ND2	1:A:112:ASN:N	0.64	2.46	15	1
1:A:109:ASN:HD21	1:A:139:ARG:NE	0.64	1.91	19	1
1:A:75:LEU:C	1:A:75:LEU:HD13	0.63	2.13	40	2
1:A:109:ASN:ND2	1:A:144:LYS:NZ	0.63	2.47	4	1
1:A:126:ASN:ND2	1:A:128:VAL:H	0.62	1.92	24	2
1:A:106:MET:SD	1:A:106:MET:N	0.62	2.72	27	5
1:A:107:ALA:O	1:A:146:PHE:CE1	0.62	2.53	1	43
1:A:101:THR:HG21	1:A:154:THR:CG2	0.62	2.24	33	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:137:VAL:HG22	1:A:137:VAL:O	0.61	1.95	15	32
1:A:89:PHE:CZ	1:A:131:PHE:CE2	0.61	2.88	24	13
1:A:74:VAL:HG13	1:A:74:VAL:O	0.61	1.94	9	10
1:A:97:VAL:HG23	1:A:154:THR:HG21	0.61	1.71	32	5
1:A:119:ASN:O	1:A:119:ASN:ND2	0.61	2.34	23	8
1:A:146:PHE:CD2	1:A:166:ILE:CG2	0.61	2.83	10	4
1:A:109:ASN:OD1	1:A:112:ASN:N	0.61	2.33	11	5
1:A:118:ARG:NH2	1:A:135:ARG:NH2	0.61	2.49	34	1
1:A:150:ILE:HG23	1:A:160:ALA:HB3	0.61	1.72	5	4
1:A:166:ILE:HD12	1:A:166:ILE:O	0.61	1.96	2	2
1:A:97:VAL:N	1:A:98:PRO:CD	0.60	2.64	26	25
1:A:109:ASN:ND2	1:A:145:SER:O	0.60	2.34	7	3
1:A:119:ASN:ND2	1:A:119:ASN:O	0.60	2.34	40	7
1:A:166:ILE:H	1:A:166:ILE:CD1	0.60	2.07	12	2
1:A:69:ASN:OD1	1:A:69:ASN:N	0.60	2.33	11	2
1:A:148:LEU:N	1:A:148:LEU:CD2	0.60	2.65	6	2
1:A:109:ASN:HD21	1:A:112:ASN:ND2	0.60	1.95	38	2
1:A:69:ASN:HD21	1:A:158:GLN:NE2	0.60	1.95	28	3
1:A:119:ASN:HD21	1:A:132:ASN:H	0.59	1.39	11	1
1:A:148:LEU:HD22	1:A:162:TYR:CE2	0.59	2.33	38	2
1:A:109:ASN:OD1	1:A:110:ASP:N	0.59	2.35	7	3
1:A:117:LEU:N	1:A:117:LEU:CD2	0.59	2.66	42	2
1:A:131:PHE:N	1:A:131:PHE:CD1	0.59	2.69	41	7
1:A:162:TYR:OH	1:A:164:ARG:NE	0.59	2.36	30	3
1:A:101:THR:OG1	1:A:102:LEU:N	0.59	2.34	33	32
1:A:107:ALA:O	1:A:146:PHE:CZ	0.59	2.55	15	34
1:A:109:ASN:HD22	1:A:109:ASN:N	0.58	1.95	27	1
1:A:109:ASN:ND2	1:A:112:ASN:HD22	0.58	1.96	9	6
1:A:79:TRP:CG	1:A:80:ARG:N	0.58	2.70	5	17
1:A:82:ASN:OD1	1:A:83:LYS:N	0.58	2.36	6	8
1:A:79:TRP:CH2	1:A:81:SER:O	0.58	2.56	36	1
1:A:84:THR:CG2	1:A:135:ARG:HE	0.58	2.12	10	1
1:A:148:LEU:HD12	1:A:148:LEU:N	0.58	2.14	14	8
1:A:64:ARG:CA	1:A:64:ARG:NE	0.58	2.66	34	1
1:A:79:TRP:CD2	1:A:87:ILE:CG2	0.58	2.87	5	2
1:A:145:SER:OG	1:A:163:HIS:NE2	0.58	2.37	8	2
1:A:75:LEU:O	1:A:77:THR:N	0.58	2.37	12	3
1:A:69:ASN:HD21	1:A:158:GLN:HE22	0.57	1.41	34	1
1:A:79:TRP:CZ2	1:A:136:PHE:CD2	0.57	2.91	1	1
1:A:109:ASN:ND2	1:A:111:GLU:N	0.57	2.52	5	1
1:A:118:ARG:NH1	1:A:135:ARG:HH21	0.57	1.96	34	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:107:ALA:HB1	1:A:146:PHE:CZ	0.57	2.34	38	29
1:A:77:THR:OG1	1:A:164:ARG:NH1	0.57	2.36	14	1
1:A:139:ARG:HH21	1:A:144:LYS:NZ	0.57	1.97	24	2
1:A:77:THR:CB	1:A:164:ARG:NH2	0.57	2.67	42	1
1:A:155:ASN:N	1:A:156:PRO:CD	0.57	2.68	11	41
1:A:109:ASN:OD1	1:A:145:SER:N	0.57	2.38	30	2
1:A:110:ASP:OD1	1:A:111:GLU:N	0.57	2.37	10	3
1:A:69:ASN:OD1	1:A:158:GLN:NE2	0.57	2.37	11	4
1:A:139:ARG:O	1:A:144:LYS:NZ	0.57	2.37	12	1
1:A:166:ILE:O	1:A:166:ILE:HG23	0.57	1.99	22	4
1:A:109:ASN:OD1	1:A:111:GLU:N	0.57	2.37	8	7
1:A:166:ILE:HD13	1:A:166:ILE:N	0.57	2.12	12	2
1:A:85:LEU:N	1:A:85:LEU:HD12	0.57	2.15	14	2
1:A:109:ASN:OD1	1:A:112:ASN:ND2	0.57	2.38	15	5
1:A:84:THR:C	1:A:85:LEU:HD12	0.57	2.20	14	1
1:A:78:HIS:CD2	1:A:79:TRP:N	0.57	2.72	14	3
1:A:150:ILE:HD11	1:A:162:TYR:OH	0.57	2.00	34	1
1:A:126:ASN:ND2	1:A:126:ASN:H	0.56	1.98	35	2
1:A:119:ASN:HD22	1:A:132:ASN:H	0.56	1.41	16	2
1:A:64:ARG:N	1:A:64:ARG:CD	0.56	2.68	34	1
1:A:106:MET:O	1:A:148:LEU:HD23	0.56	2.00	3	5
1:A:133:ASP:N	1:A:133:ASP:OD1	0.56	2.39	17	1
1:A:162:TYR:OH	1:A:164:ARG:CZ	0.56	2.54	19	1
1:A:126:ASN:H	1:A:126:ASN:HD22	0.56	1.41	35	2
1:A:113:TYR:CE1	1:A:139:ARG:CZ	0.56	2.88	2	1
1:A:109:ASN:HD22	1:A:112:ASN:HD22	0.56	1.41	41	3
1:A:111:GLU:OE2	1:A:144:LYS:NZ	0.56	2.39	40	1
1:A:74:VAL:HG12	1:A:75:LEU:N	0.56	2.16	5	2
1:A:133:ASP:O	1:A:135:ARG:N	0.56	2.39	9	16
1:A:133:ASP:OD1	1:A:135:ARG:NH2	0.56	2.39	2	1
1:A:97:VAL:CG2	1:A:154:THR:HG21	0.56	2.30	33	2
1:A:97:VAL:O	1:A:97:VAL:HG13	0.56	2.01	15	8
1:A:75:LEU:O	1:A:75:LEU:HD12	0.55	2.00	19	1
1:A:109:ASN:HD22	1:A:111:GLU:H	0.55	1.44	30	1
1:A:117:LEU:N	1:A:117:LEU:HD22	0.55	2.16	10	1
1:A:68:PRO:O	1:A:69:ASN:ND2	0.55	2.40	20	1
1:A:71:LEU:N	1:A:71:LEU:HD22	0.55	2.15	23	1
1:A:119:ASN:ND2	1:A:132:ASN:N	0.55	2.54	43	5
1:A:147:THR:C	1:A:148:LEU:HD12	0.55	2.22	30	11
1:A:139:ARG:HH11	1:A:139:ARG:CG	0.55	2.14	27	1
1:A:108:GLY:N	1:A:115:ALA:H	0.55	2.00	20	13

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:84:THR:CG2	1:A:135:ARG:HH11	0.55	2.15	34	2
1:A:163:HIS:CD2	1:A:163:HIS:O	0.55	2.59	14	1
1:A:133:ASP:O	1:A:134:LEU:C	0.55	2.45	43	7
1:A:119:ASN:OD1	1:A:134:LEU:N	0.55	2.40	43	4
1:A:124:MET:SD	1:A:126:ASN:O	0.55	2.64	34	26
1:A:146:PHE:CE2	1:A:166:ILE:HD11	0.55	2.36	34	1
1:A:67:SER:O	1:A:69:ASN:N	0.55	2.39	9	1
1:A:112:ASN:HD21	1:A:144:LYS:CE	0.55	2.15	29	2
1:A:79:TRP:CD2	1:A:79:TRP:C	0.55	2.80	8	5
1:A:84:THR:O	1:A:135:ARG:NH1	0.55	2.40	8	1
1:A:109:ASN:ND2	1:A:112:ASN:H	0.55	1.98	15	1
1:A:139:ARG:NH1	1:A:141:GLY:O	0.55	2.40	38	2
1:A:83:LYS:O	1:A:85:LEU:N	0.54	2.37	39	10
1:A:132:ASN:O	1:A:133:ASP:C	0.54	2.45	13	6
1:A:81:SER:OG	1:A:85:LEU:N	0.54	2.40	10	2
1:A:89:PHE:CZ	1:A:131:PHE:CZ	0.54	2.95	17	1
1:A:109:ASN:HD22	1:A:145:SER:N	0.54	2.00	7	1
1:A:164:ARG:NE	1:A:166:ILE:O	0.54	2.40	28	1
1:A:88:ALA:HB1	1:A:131:PHE:O	0.54	2.02	20	4
1:A:140:SER:O	1:A:142:ARG:N	0.54	2.41	3	4
1:A:147:THR:C	1:A:148:LEU:HD23	0.54	2.21	6	2
1:A:112:ASN:HD21	1:A:144:LYS:NZ	0.54	2.00	11	3
1:A:148:LEU:HD13	1:A:162:TYR:CD2	0.54	2.38	39	2
1:A:79:TRP:HE1	1:A:81:SER:CB	0.54	2.16	42	5
1:A:106:MET:SD	1:A:149:THR:OG1	0.54	2.66	28	16
1:A:109:ASN:HD21	1:A:112:ASN:N	0.54	2.00	15	1
1:A:118:ARG:CZ	1:A:135:ARG:HH21	0.54	2.15	34	1
1:A:163:HIS:O	1:A:163:HIS:CG	0.54	2.61	35	7
1:A:139:ARG:NH2	1:A:144:LYS:O	0.54	2.41	19	2
1:A:134:LEU:C	1:A:134:LEU:HD23	0.54	2.22	34	4
1:A:126:ASN:OD1	1:A:127:GLN:N	0.54	2.41	38	3
1:A:134:LEU:HD22	1:A:136:PHE:CE2	0.54	2.38	7	2
1:A:105:VAL:HG12	1:A:120:ALA:HB1	0.54	1.78	13	6
1:A:62:LEU:N	1:A:62:LEU:CD2	0.54	2.65	30	6
1:A:112:ASN:HD21	1:A:144:LYS:HZ3	0.54	1.46	11	1
1:A:77:THR:O	1:A:164:ARG:NH1	0.54	2.39	30	2
1:A:78:HIS:NE2	1:A:79:TRP:O	0.54	2.40	27	1
1:A:109:ASN:ND2	1:A:139:ARG:HE	0.53	2.02	19	1
1:A:162:TYR:OH	1:A:164:ARG:NH2	0.53	2.41	30	1
1:A:81:SER:OG	1:A:85:LEU:O	0.53	2.27	3	8
1:A:105:VAL:HG13	1:A:117:LEU:HD12	0.53	1.81	37	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:122:ALA:CB	1:A:130:ARG:O	0.53	2.57	43	12
1:A:137:VAL:O	1:A:137:VAL:CG1	0.53	2.57	4	5
1:A:79:TRP:CE2	1:A:87:ILE:CG2	0.53	2.92	6	5
1:A:105:VAL:CG1	1:A:120:ALA:HB1	0.53	2.32	43	9
1:A:139:ARG:CG	1:A:139:ARG:NH1	0.53	2.71	27	1
1:A:109:ASN:N	1:A:109:ASN:ND2	0.53	2.57	27	1
1:A:79:TRP:NE1	1:A:81:SER:CB	0.53	2.71	42	7
1:A:154:THR:CG2	1:A:155:ASN:H	0.52	2.16	18	2
1:A:79:TRP:CZ2	1:A:136:PHE:CG	0.52	2.98	1	1
1:A:81:SER:O	1:A:81:SER:OG	0.52	2.25	39	1
1:A:148:LEU:HD23	1:A:148:LEU:H	0.52	1.59	42	1
1:A:67:SER:OG	1:A:159:VAL:N	0.52	2.42	6	1
1:A:79:TRP:CZ2	1:A:81:SER:C	0.52	2.83	36	1
1:A:83:LYS:CG	1:A:84:THR:N	0.52	2.73	42	1
1:A:119:ASN:OD1	1:A:132:ASN:N	0.52	2.42	11	1
1:A:113:TYR:CE2	1:A:114:SER:O	0.52	2.62	20	3
1:A:105:VAL:HG22	1:A:150:ILE:HG23	0.52	1.82	27	1
1:A:147:THR:OG1	1:A:163:HIS:CE1	0.52	2.63	16	2
1:A:84:THR:C	1:A:85:LEU:HD22	0.52	2.25	34	2
1:A:118:ARG:CZ	1:A:135:ARG:NH2	0.52	2.73	34	1
1:A:79:TRP:C	1:A:79:TRP:CE3	0.51	2.84	8	5
1:A:146:PHE:CG	1:A:166:ILE:HG23	0.51	2.41	40	4
1:A:163:HIS:O	1:A:163:HIS:ND1	0.51	2.43	27	2
1:A:132:ASN:OD1	1:A:133:ASP:N	0.51	2.41	7	1
1:A:83:LYS:C	1:A:85:LEU:H	0.51	2.08	35	7
1:A:97:VAL:O	1:A:97:VAL:CG2	0.51	2.58	35	10
1:A:97:VAL:HG23	1:A:154:THR:OG1	0.51	2.05	36	8
1:A:118:ARG:HE	1:A:135:ARG:NH2	0.51	2.04	12	1
1:A:84:THR:CG2	1:A:135:ARG:NH1	0.51	2.73	40	3
1:A:101:THR:HG22	1:A:102:LEU:H	0.51	1.66	36	1
1:A:73:SER:O	1:A:74:VAL:C	0.51	2.49	14	2
1:A:79:TRP:CZ2	1:A:80:ARG:O	0.50	2.65	7	1
1:A:150:ILE:HG22	1:A:160:ALA:O	0.50	2.06	5	3
1:A:69:ASN:OD1	1:A:158:GLN:OE1	0.50	2.29	41	3
1:A:113:TYR:CE2	1:A:139:ARG:NH2	0.50	2.79	23	2
1:A:79:TRP:CE2	1:A:136:PHE:CD2	0.50	2.99	1	1
1:A:121:THR:O	1:A:121:THR:OG1	0.50	2.30	17	6
1:A:109:ASN:HD21	1:A:112:ASN:CG	0.50	2.10	11	2
1:A:85:LEU:N	1:A:85:LEU:CD2	0.50	2.74	5	2
1:A:164:ARG:O	1:A:165:ALA:O	0.50	2.30	35	4
1:A:106:MET:SD	1:A:149:THR:O	0.50	2.69	22	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:139:ARG:NH2	1:A:146:PHE:N	0.50	2.58	38	1
1:A:139:ARG:N	1:A:139:ARG:HE	0.50	2.05	2	1
1:A:118:ARG:O	1:A:119:ASN:OD1	0.50	2.29	6	6
1:A:116:GLU:OE2	1:A:118:ARG:NH2	0.50	2.45	8	1
1:A:117:LEU:N	1:A:117:LEU:CD1	0.50	2.74	14	4
1:A:142:ARG:NH1	1:A:142:ARG:CG	0.50	2.73	8	1
1:A:75:LEU:HD23	1:A:75:LEU:O	0.50	2.07	23	2
1:A:71:LEU:HD22	1:A:71:LEU:N	0.49	2.22	32	2
1:A:131:PHE:CD1	1:A:131:PHE:N	0.49	2.79	35	9
1:A:79:TRP:CE2	1:A:81:SER:N	0.49	2.78	31	2
1:A:118:ARG:NH2	1:A:133:ASP:OD2	0.49	2.45	34	1
1:A:79:TRP:CE3	1:A:79:TRP:C	0.49	2.86	2	1
1:A:113:TYR:CE2	1:A:139:ARG:CZ	0.49	2.95	23	1
1:A:64:ARG:CZ	1:A:65:THR:O	0.49	2.61	1	1
1:A:118:ARG:O	1:A:133:ASP:O	0.49	2.30	31	2
1:A:79:TRP:CE3	1:A:79:TRP:O	0.49	2.66	8	3
1:A:118:ARG:HH11	1:A:135:ARG:HH12	0.49	1.49	21	1
1:A:64:ARG:CD	1:A:64:ARG:H	0.49	2.20	34	1
1:A:75:LEU:N	1:A:75:LEU:CD2	0.49	2.76	5	1
1:A:112:ASN:ND2	1:A:139:ARG:HE	0.49	2.05	25	2
1:A:113:TYR:CD2	1:A:114:SER:O	0.49	2.65	21	2
1:A:109:ASN:CG	1:A:139:ARG:HE	0.49	2.11	19	1
1:A:99:ASP:OD1	1:A:101:THR:CG2	0.49	2.61	28	6
1:A:150:ILE:N	1:A:160:ALA:O	0.49	2.41	25	7
1:A:154:THR:CG2	1:A:155:ASN:N	0.49	2.69	18	2
1:A:106:MET:CG	1:A:149:THR:OG1	0.49	2.61	4	4
1:A:110:ASP:OD1	1:A:147:THR:OG1	0.49	2.31	3	4
1:A:89:PHE:CE2	1:A:131:PHE:CE1	0.49	3.00	15	1
1:A:109:ASN:ND2	1:A:109:ASN:H	0.49	2.04	25	1
1:A:146:PHE:CE2	1:A:148:LEU:HD11	0.49	2.42	40	2
1:A:109:ASN:HD22	1:A:111:GLU:N	0.49	2.05	5	2
1:A:155:ASN:N	1:A:155:ASN:OD1	0.49	2.45	10	1
1:A:65:THR:OG1	1:A:67:SER:OG	0.49	2.29	40	1
1:A:106:MET:CG	1:A:149:THR:HG1	0.48	2.21	4	2
1:A:105:VAL:HG13	1:A:150:ILE:HG12	0.48	1.85	28	1
1:A:124:MET:SD	1:A:128:VAL:C	0.48	2.91	35	7
1:A:109:ASN:HD21	1:A:145:SER:H	0.48	1.51	7	1
1:A:126:ASN:ND2	1:A:126:ASN:N	0.48	2.59	35	2
1:A:126:ASN:CG	1:A:127:GLN:N	0.48	2.67	15	7
1:A:66:ASP:OD1	1:A:67:SER:N	0.48	2.47	19	3
1:A:126:ASN:HD22	1:A:128:VAL:H	0.48	1.50	24	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:74:VAL:O	1:A:74:VAL:CG1	0.48	2.62	25	7
1:A:166:ILE:C	1:A:166:ILE:CD1	0.48	2.82	19	4
1:A:146:PHE:CG	1:A:166:ILE:CG2	0.48	2.96	40	5
1:A:64:ARG:NE	1:A:64:ARG:N	0.48	2.61	34	1
1:A:99:ASP:OD2	1:A:154:THR:CG2	0.48	2.62	25	2
1:A:79:TRP:CD2	1:A:80:ARG:N	0.48	2.82	7	3
1:A:118:ARG:HH11	1:A:135:ARG:NH1	0.48	2.06	24	1
1:A:119:ASN:ND2	1:A:132:ASN:OD1	0.48	2.47	7	1
1:A:109:ASN:HD21	1:A:112:ASN:HD22	0.48	1.52	25	1
1:A:78:HIS:CD2	1:A:79:TRP:H	0.48	2.26	7	1
1:A:79:TRP:C	1:A:79:TRP:CD2	0.47	2.87	2	1
1:A:164:ARG:NH1	1:A:164:ARG:CG	0.47	2.77	2	2
1:A:126:ASN:HD22	1:A:126:ASN:N	0.47	2.05	35	1
1:A:148:LEU:HD13	1:A:162:TYR:CE2	0.47	2.44	39	1
1:A:113:TYR:CE1	1:A:139:ARG:NH1	0.47	2.82	20	1
1:A:118:ARG:HH11	1:A:135:ARG:CZ	0.47	2.22	24	1
1:A:162:TYR:C	1:A:162:TYR:CD1	0.47	2.88	30	1
1:A:119:ASN:OD1	1:A:133:ASP:C	0.47	2.52	6	3
1:A:99:ASP:OD1	1:A:99:ASP:C	0.47	2.53	1	4
1:A:75:LEU:CB	1:A:76:PRO:CD	0.47	2.92	3	1
1:A:106:MET:C	1:A:106:MET:SD	0.47	2.93	4	2
1:A:111:GLU:H	1:A:111:GLU:CD	0.47	2.12	11	1
1:A:162:TYR:CD1	1:A:163:HIS:N	0.47	2.82	30	1
1:A:64:ARG:CA	1:A:64:ARG:HE	0.47	2.23	34	1
1:A:80:ARG:NH1	1:A:80:ARG:CG	0.47	2.77	40	1
1:A:119:ASN:CG	1:A:119:ASN:O	0.47	2.54	11	2
1:A:111:GLU:N	1:A:111:GLU:OE1	0.47	2.48	38	1
1:A:116:GLU:OE1	1:A:118:ARG:NH1	0.47	2.47	17	1
1:A:109:ASN:OD1	1:A:109:ASN:C	0.47	2.52	11	2
1:A:79:TRP:CE2	1:A:87:ILE:HG23	0.47	2.45	21	7
1:A:79:TRP:HE1	1:A:81:SER:HG	0.47	1.51	16	2
1:A:97:VAL:H	1:A:98:PRO:HD3	0.47	1.68	36	4
1:A:118:ARG:NH1	1:A:118:ARG:CG	0.46	2.74	25	1
1:A:142:ARG:CG	1:A:142:ARG:HH11	0.46	2.22	8	1
1:A:113:TYR:CE2	1:A:139:ARG:NE	0.46	2.83	3	2
1:A:65:THR:OG1	1:A:70:PHE:O	0.46	2.31	39	9
1:A:66:ASP:OD1	1:A:159:VAL:O	0.46	2.33	35	3
1:A:135:ARG:NH1	1:A:135:ARG:CG	0.46	2.78	18	2
1:A:152:VAL:HG12	1:A:154:THR:HG22	0.46	1.86	41	1
1:A:166:ILE:HD12	1:A:166:ILE:C	0.46	2.30	2	1
1:A:69:ASN:HD21	1:A:158:GLN:CD	0.46	2.13	7	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:66:ASP:O	1:A:66:ASP:OD1	0.46	2.33	7	1
1:A:107:ALA:HB1	1:A:146:PHE:CE2	0.46	2.44	25	3
1:A:130:ARG:NE	1:A:132:ASN:OD1	0.46	2.49	28	1
1:A:139:ARG:C	1:A:139:ARG:CD	0.46	2.84	19	1
1:A:79:TRP:CH2	1:A:136:PHE:CG	0.46	3.04	34	2
1:A:109:ASN:OD1	1:A:145:SER:O	0.46	2.32	30	3
1:A:72:CYS:O	1:A:73:SER:O	0.46	2.34	8	1
1:A:126:ASN:CG	1:A:127:GLN:H	0.46	2.15	15	6
1:A:62:LEU:N	1:A:62:LEU:CD1	0.46	2.68	25	1
1:A:63:VAL:HG23	1:A:74:VAL:O	0.45	2.10	25	1
1:A:77:THR:C	1:A:164:ARG:HH12	0.45	2.14	30	1
1:A:75:LEU:C	1:A:75:LEU:CD1	0.45	2.84	40	1
1:A:79:TRP:CZ3	1:A:136:PHE:CZ	0.45	3.04	1	1
1:A:78:HIS:C	1:A:78:HIS:CD2	0.45	2.90	1	1
1:A:139:ARG:C	1:A:144:LYS:HZ1	0.45	2.13	12	1
1:A:74:VAL:HG21	1:A:89:PHE:CD1	0.45	2.46	38	1
1:A:148:LEU:N	1:A:162:TYR:O	0.45	2.46	30	1
1:A:70:PHE:CD1	1:A:158:GLN:OE1	0.45	2.70	2	2
1:A:142:ARG:HH11	1:A:142:ARG:HG2	0.45	1.72	8	1
1:A:105:VAL:HG22	1:A:150:ILE:HG12	0.45	1.87	14	1
1:A:116:GLU:O	1:A:137:VAL:CG1	0.45	2.65	42	8
1:A:132:ASN:C	1:A:134:LEU:H	0.45	2.15	10	5
1:A:68:PRO:O	1:A:69:ASN:OD1	0.45	2.35	21	7
1:A:97:VAL:N	1:A:98:PRO:HD3	0.45	2.26	10	6
1:A:64:ARG:HE	1:A:64:ARG:H	0.45	1.55	37	1
1:A:139:ARG:HH21	1:A:145:SER:C	0.45	2.15	38	1
1:A:118:ARG:O	1:A:119:ASN:CG	0.45	2.55	43	4
1:A:109:ASN:OD1	1:A:144:LYS:NZ	0.45	2.48	4	1
1:A:109:ASN:HD22	1:A:145:SER:C	0.45	2.15	17	1
1:A:75:LEU:N	1:A:76:PRO:HD2	0.45	2.27	30	4
1:A:79:TRP:CH2	1:A:136:PHE:CD2	0.45	3.05	29	1
1:A:84:THR:O	1:A:84:THR:HG22	0.45	2.12	42	1
1:A:73:SER:OG	1:A:74:VAL:N	0.45	2.49	4	3
1:A:86:PRO:CG	1:A:134:LEU:O	0.45	2.65	5	1
1:A:73:SER:O	1:A:75:LEU:N	0.45	2.50	24	1
1:A:106:MET:O	1:A:148:LEU:CB	0.45	2.65	42	1
1:A:164:ARG:HG2	1:A:164:ARG:HH11	0.44	1.72	2	1
1:A:108:GLY:CA	1:A:115:ALA:H	0.44	2.26	4	4
1:A:79:TRP:NE1	1:A:81:SER:HB2	0.44	2.26	36	1
1:A:67:SER:OG	1:A:159:VAL:O	0.44	2.35	39	5
1:A:70:PHE:CE2	1:A:152:VAL:CG2	0.44	3.01	6	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:109:ASN:ND2	1:A:112:ASN:CG	0.44	2.71	11	1
1:A:109:ASN:ND2	1:A:145:SER:C	0.44	2.71	17	1
1:A:89:PHE:CD1	1:A:89:PHE:N	0.44	2.86	9	4
1:A:69:ASN:CG	1:A:158:GLN:HE22	0.44	2.16	11	1
1:A:77:THR:O	1:A:164:ARG:CD	0.44	2.65	28	1
1:A:146:PHE:O	1:A:164:ARG:O	0.44	2.36	43	1
1:A:119:ASN:HD21	1:A:132:ASN:N	0.44	2.10	40	1
1:A:70:PHE:CE1	1:A:158:GLN:OE1	0.44	2.71	38	2
1:A:117:LEU:CB	1:A:120:ALA:HB2	0.44	2.42	34	2
1:A:166:ILE:CD1	1:A:166:ILE:N	0.44	2.76	12	1
1:A:118:ARG:NH1	1:A:135:ARG:NH2	0.44	2.65	24	1
1:A:81:SER:OG	1:A:85:LEU:C	0.44	2.56	10	2
1:A:69:ASN:CG	1:A:158:GLN:NE2	0.44	2.71	11	1
1:A:139:ARG:C	1:A:144:LYS:NZ	0.44	2.71	12	1
1:A:150:ILE:HB	1:A:160:ALA:HB3	0.44	1.90	27	2
1:A:156:PRO:O	1:A:158:GLN:OE1	0.44	2.36	43	1
1:A:101:THR:CB	1:A:154:THR:HG22	0.44	2.42	17	1
1:A:119:ASN:O	1:A:119:ASN:CG	0.44	2.55	19	1
1:A:112:ASN:CB	1:A:139:ARG:HH11	0.44	2.25	2	1
1:A:145:SER:OG	1:A:163:HIS:CE1	0.44	2.71	8	1
1:A:67:SER:C	1:A:69:ASN:H	0.44	2.16	9	1
1:A:163:HIS:O	1:A:163:HIS:CD2	0.43	2.71	25	2
1:A:113:TYR:OH	1:A:139:ARG:CZ	0.43	2.66	6	1
1:A:83:LYS:C	1:A:85:LEU:N	0.43	2.72	35	4
1:A:84:THR:HG23	1:A:135:ARG:NH1	0.43	2.28	40	1
1:A:97:VAL:HG23	1:A:154:THR:CB	0.43	2.43	29	3
1:A:130:ARG:CD	1:A:132:ASN:OD1	0.43	2.66	28	1
1:A:75:LEU:C	1:A:75:LEU:HD12	0.43	2.33	31	1
1:A:146:PHE:CD2	1:A:166:ILE:HG23	0.43	2.48	11	1
1:A:141:GLY:N	1:A:144:LYS:HZ3	0.43	2.11	12	1
1:A:140:SER:O	1:A:141:GLY:C	0.43	2.55	3	2
1:A:113:TYR:OH	1:A:139:ARG:NE	0.43	2.51	6	1
1:A:77:THR:OG1	1:A:164:ARG:NH2	0.43	2.51	42	1
1:A:162:TYR:CD1	1:A:162:TYR:C	0.43	2.91	19	2
1:A:114:SER:O	1:A:115:ALA:O	0.43	2.37	18	2
1:A:139:ARG:CZ	1:A:141:GLY:O	0.43	2.67	19	1
1:A:146:PHE:CD1	1:A:166:ILE:CG2	0.43	3.01	8	1
1:A:74:VAL:HG22	1:A:75:LEU:N	0.43	2.29	12	1
1:A:109:ASN:ND2	1:A:139:ARG:NE	0.43	2.61	19	1
1:A:126:ASN:ND2	1:A:128:VAL:N	0.43	2.66	35	1
1:A:112:ASN:HD21	1:A:139:ARG:HE	0.43	1.54	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:102:LEU:HD13	1:A:102:LEU:C	0.43	2.33	30	1
1:A:71:LEU:N	1:A:71:LEU:CD2	0.43	2.81	23	1
1:A:62:LEU:CD1	1:A:71:LEU:HD13	0.43	2.43	28	1
1:A:75:LEU:H	1:A:76:PRO:HD3	0.43	1.72	15	1
1:A:156:PRO:O	1:A:157:PRO:C	0.43	2.57	34	22
1:A:78:HIS:CG	1:A:79:TRP:N	0.43	2.87	7	1
1:A:113:TYR:CZ	1:A:139:ARG:NE	0.43	2.87	23	1
1:A:83:LYS:HG3	1:A:84:THR:N	0.43	2.28	42	1
1:A:155:ASN:O	1:A:157:PRO:CD	0.42	2.67	4	1
1:A:109:ASN:CG	1:A:111:GLU:OE2	0.42	2.58	11	1
1:A:137:VAL:O	1:A:137:VAL:CG2	0.42	2.67	15	1
1:A:66:ASP:OD1	1:A:66:ASP:C	0.42	2.58	41	2
1:A:72:CYS:SG	1:A:162:TYR:OH	0.42	2.68	35	1
1:A:76:PRO:C	1:A:78:HIS:N	0.42	2.69	1	1
1:A:79:TRP:CE2	1:A:80:ARG:O	0.42	2.72	7	1
1:A:74:VAL:CG1	1:A:75:LEU:N	0.42	2.81	5	1
1:A:74:VAL:CG2	1:A:89:PHE:CG	0.42	3.02	15	1
1:A:75:LEU:HD13	1:A:75:LEU:O	0.42	2.15	32	2
1:A:126:ASN:ND2	1:A:127:GLN:N	0.42	2.67	35	1
1:A:74:VAL:O	1:A:74:VAL:HG13	0.42	2.14	2	1
1:A:102:LEU:HD13	1:A:103:VAL:H	0.42	1.74	18	1
1:A:132:ASN:CG	1:A:133:ASP:H	0.42	2.17	34	1
1:A:132:ASN:CG	1:A:133:ASP:N	0.42	2.73	34	1
1:A:97:VAL:H	1:A:98:PRO:CD	0.42	2.27	36	1
1:A:112:ASN:HD21	1:A:144:LYS:HE2	0.42	1.73	29	1
1:A:79:TRP:HE1	1:A:81:SER:HB2	0.42	1.75	10	2
1:A:69:ASN:ND2	1:A:158:GLN:NE2	0.42	2.65	28	2
1:A:144:LYS:HZ2	1:A:144:LYS:CB	0.42	2.27	4	1
1:A:85:LEU:N	1:A:85:LEU:CD1	0.42	2.83	14	1
1:A:70:PHE:CZ	1:A:152:VAL:CG2	0.42	3.03	18	2
1:A:99:ASP:N	1:A:99:ASP:OD1	0.42	2.53	33	2
1:A:73:SER:OG	1:A:90:LYS:NZ	0.42	2.48	31	1
1:A:75:LEU:O	1:A:76:PRO:C	0.41	2.59	3	1
1:A:109:ASN:ND2	1:A:109:ASN:C	0.41	2.72	5	1
1:A:109:ASN:CB	1:A:145:SER:O	0.41	2.68	25	1
1:A:141:GLY:N	1:A:144:LYS:HZ2	0.41	2.09	12	1
1:A:116:GLU:O	1:A:137:VAL:HG13	0.41	2.14	21	1
1:A:110:ASP:CG	1:A:111:GLU:N	0.41	2.74	43	1
1:A:79:TRP:CH2	1:A:136:PHE:CD1	0.41	3.09	1	1
1:A:98:PRO:CB	1:A:126:ASN:ND2	0.41	2.83	13	1
1:A:137:VAL:O	1:A:137:VAL:HG22	0.41	2.13	29	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:82:ASN:HD21	1:A:85:LEU:HD12	0.41	1.74	24	1
1:A:75:LEU:N	1:A:76:PRO:HD3	0.41	2.28	31	1
1:A:81:SER:OG	1:A:83:LYS:O	0.41	2.37	17	1
1:A:130:ARG:NH1	1:A:130:ARG:CG	0.41	2.83	28	1
1:A:112:ASN:HD21	1:A:144:LYS:HD3	0.41	1.75	31	1
1:A:97:VAL:HG23	1:A:154:THR:HB	0.41	1.92	11	2
1:A:97:VAL:O	1:A:97:VAL:HG22	0.41	2.15	27	3
1:A:146:PHE:CD2	1:A:148:LEU:HD11	0.41	2.51	9	1
1:A:62:LEU:HD12	1:A:62:LEU:N	0.41	2.31	15	1
1:A:126:ASN:OD1	1:A:128:VAL:N	0.41	2.47	15	1
1:A:78:HIS:O	1:A:78:HIS:CD2	0.41	2.74	37	1
1:A:97:VAL:O	1:A:126:ASN:O	0.41	2.39	25	1
1:A:118:ARG:CG	1:A:118:ARG:HH11	0.41	2.28	25	1
1:A:134:LEU:C	1:A:134:LEU:CD2	0.41	2.89	16	3
1:A:166:ILE:O	1:A:166:ILE:CG2	0.41	2.66	22	1
1:A:75:LEU:H	1:A:76:PRO:HD2	0.41	1.75	26	1
1:A:70:PHE:O	1:A:71:LEU:HD22	0.41	2.16	31	1
1:A:134:LEU:HD21	1:A:136:PHE:CZ	0.41	2.51	31	1
1:A:79:TRP:CE2	1:A:81:SER:CB	0.41	3.04	36	1
1:A:110:ASP:O	1:A:110:ASP:OD1	0.41	2.39	41	1
1:A:80:ARG:O	1:A:80:ARG:CG	0.41	2.69	7	1
1:A:139:ARG:NH2	1:A:144:LYS:HZ2	0.41	2.13	16	1
1:A:75:LEU:CD1	1:A:75:LEU:O	0.41	2.69	21	1
1:A:110:ASP:CG	1:A:147:THR:OG1	0.40	2.59	34	1
1:A:80:ARG:HG2	1:A:80:ARG:HH11	0.40	1.76	40	1
1:A:105:VAL:HG22	1:A:106:MET:N	0.40	2.31	13	1
1:A:164:ARG:HG2	1:A:165:ALA:H	0.40	1.77	20	1
1:A:141:GLY:N	1:A:144:LYS:CE	0.40	2.85	4	1
1:A:109:ASN:CG	1:A:110:ASP:N	0.40	2.74	5	1
1:A:81:SER:CB	1:A:85:LEU:O	0.40	2.70	31	1
1:A:79:TRP:CE3	1:A:136:PHE:CE2	0.40	3.10	1	1
1:A:71:LEU:HD12	1:A:71:LEU:N	0.40	2.31	11	1
1:A:97:VAL:HG13	1:A:97:VAL:O	0.40	2.16	16	1
1:A:77:THR:O	1:A:164:ARG:NH2	0.40	2.55	30	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	105/127 (83%)	84±2 (80±2%)	15±2 (14±2%)	6±2 (6±2%)	3 22
All	All	4515/5461 (83%)	3618 (80%)	638 (14%)	259 (6%)	3 22

All 19 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	156	PRO	43
1	A	157	PRO	41
1	A	83	LYS	28
1	A	86	PRO	19
1	A	133	ASP	18
1	A	134	LEU	18
1	A	97	VAL	14
1	A	154	THR	13
1	A	141	GLY	11
1	A	164	ARG	10
1	A	76	PRO	9
1	A	115	ALA	8
1	A	75	LEU	7
1	A	165	ALA	6
1	A	73	SER	4
1	A	74	VAL	4
1	A	84	THR	3
1	A	166	ILE	2
1	A	68	PRO	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	89/108 (82%)	82±2 (92±2%)	7±2 (8±2%)	16 64
All	All	3827/4644 (82%)	3527 (92%)	300 (8%)	16 64

All 46 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	70	PHE	40
1	A	155	ASN	40
1	A	154	THR	28
1	A	79	TRP	18
1	A	148	LEU	16
1	A	75	LEU	13
1	A	101	THR	12
1	A	109	ASN	11
1	A	64	ARG	9
1	A	81	SER	9
1	A	106	MET	9
1	A	121	THR	8
1	A	102	LEU	8
1	A	119	ASN	7
1	A	135	ARG	5
1	A	164	ARG	5
1	A	62	LEU	5
1	A	166	ILE	4
1	A	72	CYS	4
1	A	114	SER	4
1	A	67	SER	4
1	A	139	ARG	3
1	A	136	PHE	3
1	A	131	PHE	3
1	A	69	ASN	3
1	A	113	TYR	3
1	A	89	PHE	3
1	A	142	ARG	2
1	A	162	TYR	2
1	A	147	THR	2
1	A	126	ASN	2
1	A	83	LYS	1
1	A	144	LYS	1
1	A	111	GLU	1
1	A	125	LYS	1
1	A	74	VAL	1
1	A	133	ASP	1
1	A	134	LEU	1
1	A	118	ARG	1
1	A	66	ASP	1
1	A	124	MET	1
1	A	156	PRO	1

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Mol	Chain	Res	Type	Models (Total)
1	A	163	HIS	1
1	A	130	ARG	1
1	A	80	ARG	1
1	A	96	ASP	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