Full wwPDB NMR Structure Validation Report (i)

Oct 11, 2021 – 07:06 AM EDT

PDB ID	:	2JYW
Title	:	Solution structure of C-terminal domain of APOBEC3G
Authors	:	Chen, K.; Harjes, E.; Gross, P.J.; Fahmy, A.; Lu, Y.; Shindo, K.; Harris, R.S.; Matsuo, H.
Deposited on	:	2007-12-20

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:

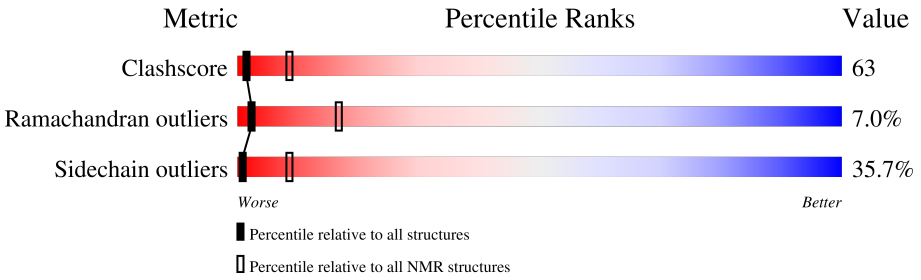
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.23.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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	195	18% 44% 20% 14% .

2 Ensemble composition and analysis (i)

This entry contains 10 models. Model 3 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *closest to the average*.

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:8-A:37, A:42-A:47, A:59-A:119, A:124-A:185 (159)	0.35	3

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

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

The models can be grouped into 2 clusters. No single-model clusters were found.

Cluster number	Models
1	1, 2, 3, 4, 5, 7, 8, 10
2	6, 9

3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 3003 atoms, of which 1458 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called DNA dC->dU-editing enzyme APOBEC-3G.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	187	3002	977	1458	276	281	10	0

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	GLY	-	expression tag	UNP Q9HC16
A	-6	PRO	-	expression tag	UNP Q9HC16
A	-5	LEU	-	expression tag	UNP Q9HC16
A	-4	GLY	-	expression tag	UNP Q9HC16
A	-3	SER	-	expression tag	UNP Q9HC16
A	-2	PRO	-	expression tag	UNP Q9HC16
A	-1	GLU	-	expression tag	UNP Q9HC16
A	0	PHE	-	expression tag	UNP Q9HC16
A	37	LYS	LEU	engineered mutation	UNP Q9HC16
A	46	ALA	CYS	engineered mutation	UNP Q9HC16
A	113	LYS	PHE	engineered mutation	UNP Q9HC16
A	124	ALA	CYS	engineered mutation	UNP Q9HC16
A	159	ALA	CYS	engineered mutation	UNP Q9HC16

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

Mol	Chain	Residues	Atoms	
			Total	Zn
2	A	1	1	1

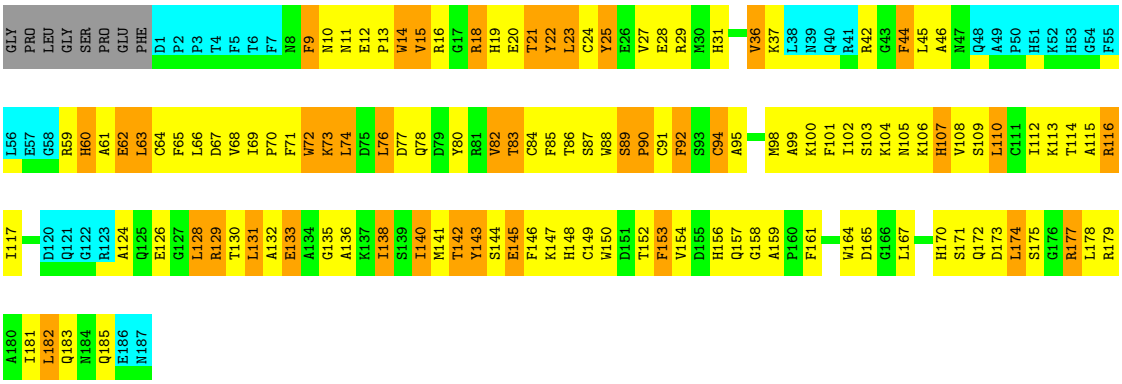
4 Residue-property plots (i)

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: DNA dC->dU-editing enzyme APOBEC-3G

Chain A: 18% 44% 20% 14% •



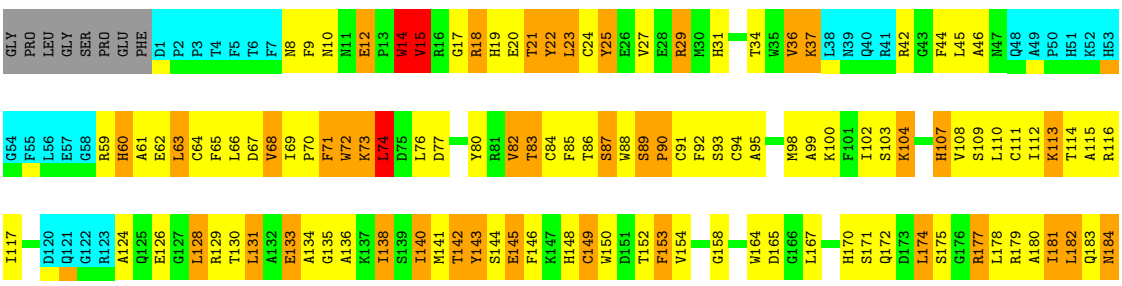
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

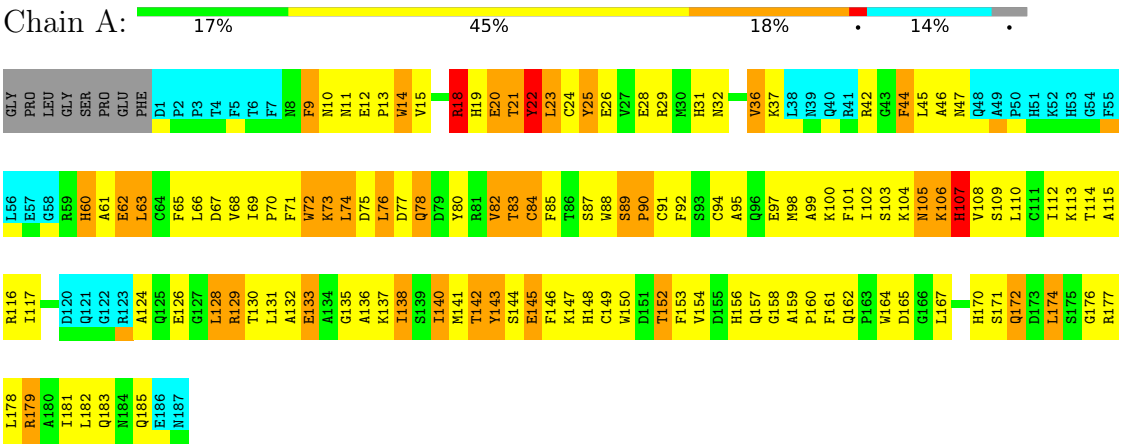
• Molecule 1: DNA dC->dU-editing enzyme APOBEC-3G

Chain A: 22% 38% 20% • 14% •



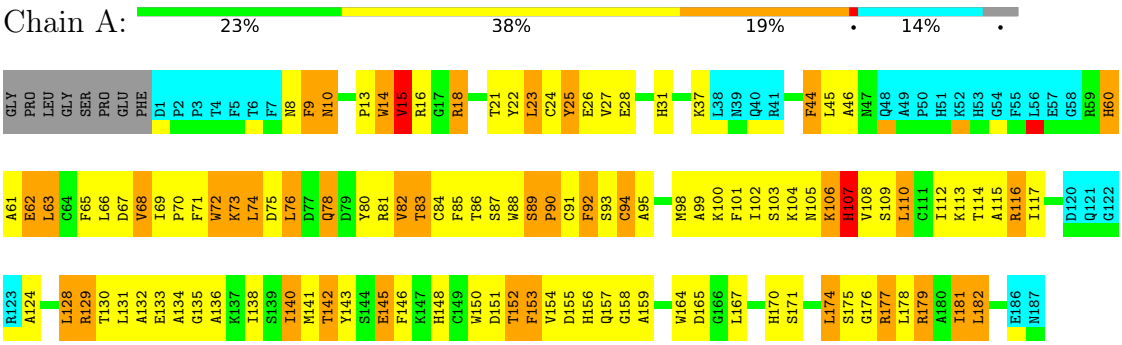
4.2.2 Score per residue for model 2

• Molecule 1: DNA dC->dU-editing enzyme APOBEC-3G



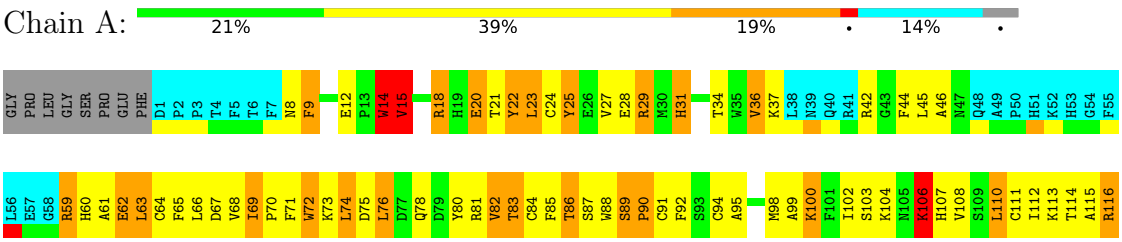
4.2.3 Score per residue for model 3 (medoid)

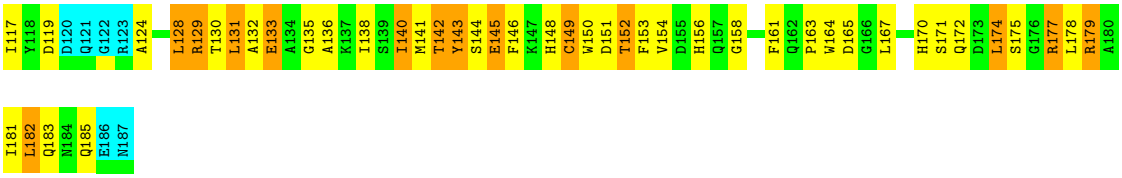
• Molecule 1: DNA dC->dU-editing enzyme APOBEC-3G



4.2.4 Score per residue for model 4

• Molecule 1: DNA dC->dU-editing enzyme APOBEC-3G

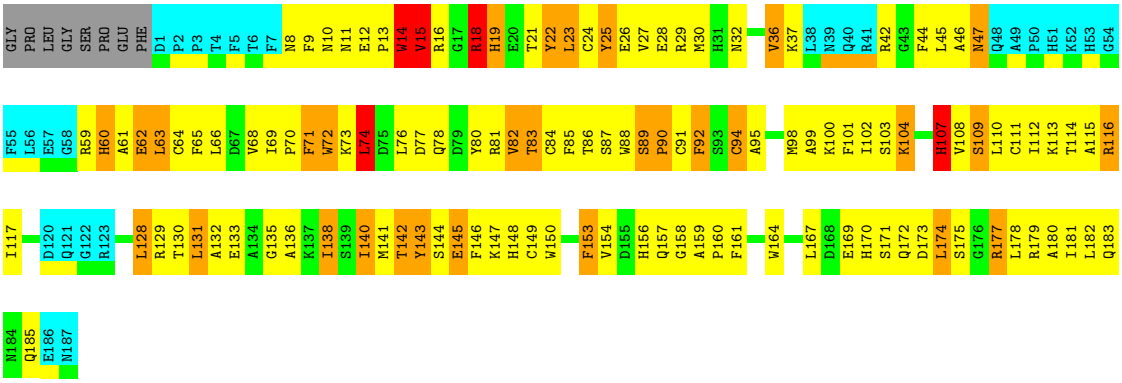




4.2.5 Score per residue for model 5

• Molecule 1: DNA dC->dU-editing enzyme APOBEC-3G

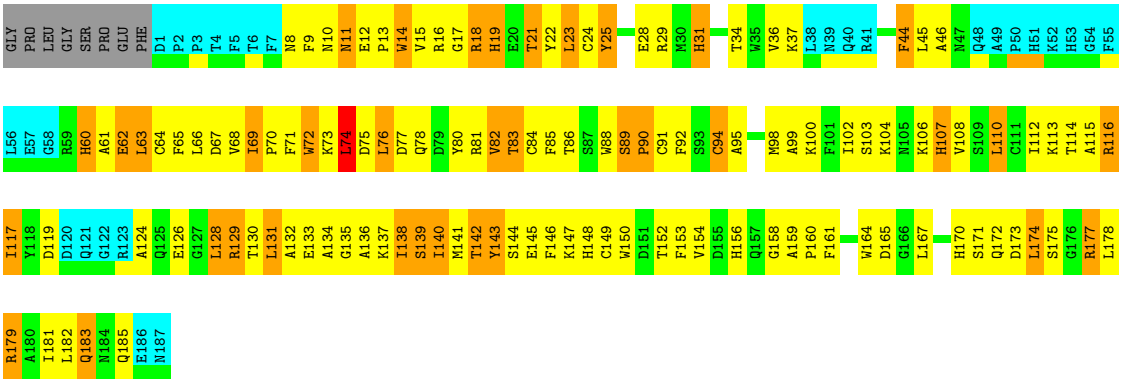
Chain A: 17% 46% 15% • 14% •



4.2.6 Score per residue for model 6

• Molecule 1: DNA dC->dU-editing enzyme APOBEC-3G

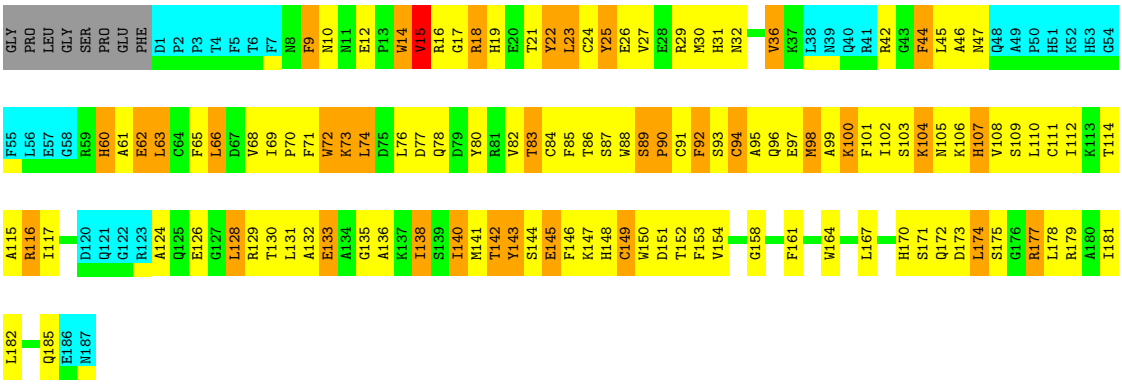
Chain A: 17% 45% 18% • 14% •



4.2.7 Score per residue for model 7

• Molecule 1: DNA dC->dU-editing enzyme APOBEC-3G

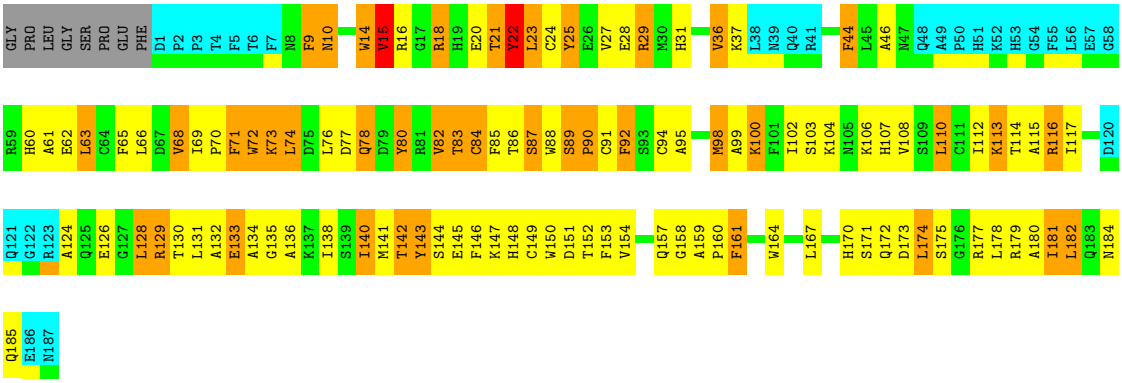
Chain A: 20% 43% 18% • 14% •



4.2.8 Score per residue for model 8

- Molecule 1: DNA dC->dU-editing enzyme APOBEC-3G

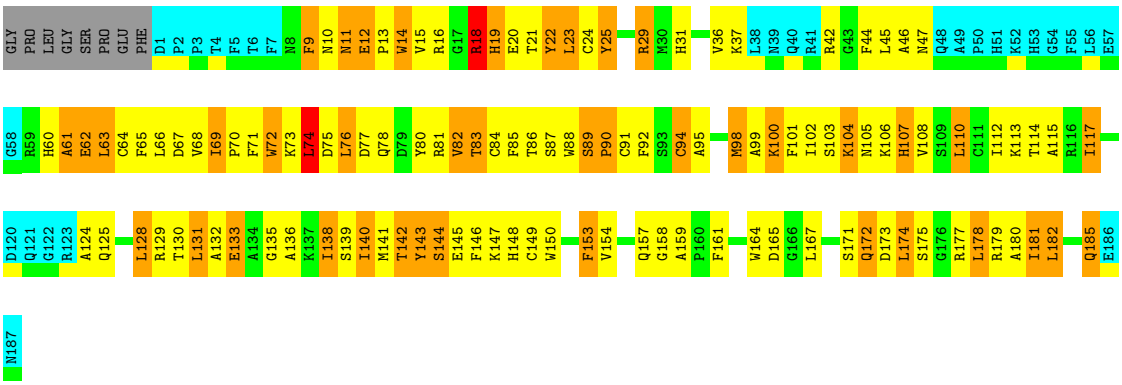
Chain A: 23% 37% 21% 14%



4.2.9 Score per residue for model 9

- Molecule 1: DNA dC->dU-editing enzyme APOBEC-3G

Chain A: 20% 39% 21% 14%



4.2.10 Score per residue for model 10

- Molecule 1: DNA dC->dU-editing enzyme APOBEC-3G

Chain A: 19% 42% 19% • 14% •

GLY PRO LEU GLY SER PRO GLU PHE D1 P2 P3 T4 F5 T6 F7 N8 F9 N10 N11 E12 P13 W14 V15 R16 G17 R18 H19 E20 T21 Y22 L23 C24 Y25 E26 V27 E28 R29 M30 H31 T34 W35 V36 K37 L38 N39 Q40 R41 F44 L45 A46 N47 Q48 A49 P50 H51 K52 H53 C54

F55 L56 E57 G58 R59 H60 A61 E62 L63 C64 F65 L66 D67 V68 I69 P70 F71 W72 K73 L74 D75 L76 D77 Q78 D79 Y80 R81 V82 T83 C84 F85 T86 S87 W88 S89 P90 C91 F92 S93 C94 M98 A99 K100 F101 I102 S103 K104 N105 K106 H107 V108 S109 L110 C111 I112 K113 T114 A115 R116

I117 Y118 D119 D120 Q121 G122 R123 E126 G127 L128 R129 T130 L131 A132 E133 A134 G135 A136 K137 I138 S139 I140 M141 T142 Y143 S144 E145 F146 K147 H148 C149 W150 D151 T152 F153 V154 D155 H156 Q157 G158 A159 P160 F161 W164 D165 G166 L167 H170 S171 Q172 D173 L174 S175 G176 R177 L178 R179

A180 I181 L182 Q183 N184 Q185 E186 N187

5 Refinement protocol and experimental data overview (i)

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

Of the 100 calculated structures, 10 were deposited, based on the following criterion: *lowest energy, ramachandran parameters.*

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

Software name	Classification	Version
CNS	refinement	1.2
Atnos/Candid	structure solution	1.1

No chemical shift data was provided.

6 Model quality (i)

6.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts (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	1315	1249	1243	162±7
All	All	13160	12490	12430	1621

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 63.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:128:LEU:HD13	1:A:181:ILE:HG21	1.01	1.31	6	7
1:A:89:SER:HA	1:A:114:THR:HG21	0.96	1.36	2	9
1:A:69:ILE:HG22	1:A:74:LEU:HD21	0.96	1.33	8	1
1:A:72:TRP:CH2	1:A:74:LEU:HD23	0.91	2.00	8	1
1:A:65:PHE:CD1	1:A:82:VAL:HG11	0.88	2.03	1	10
1:A:108:VAL:HG22	1:A:110:LEU:HD11	0.87	1.45	4	3
1:A:178:LEU:HD22	1:A:181:ILE:HD11	0.86	1.45	6	1
1:A:99:ALA:CB	1:A:130:THR:HG22	0.86	2.01	6	10
1:A:102:ILE:HG23	1:A:108:VAL:CG1	0.86	2.01	9	10
1:A:72:TRP:CZ3	1:A:74:LEU:HD23	0.85	2.06	8	1
1:A:65:PHE:O	1:A:68:VAL:HG22	0.85	1.70	10	2
1:A:154:VAL:HG11	1:A:159:ALA:HB2	0.85	1.45	5	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:89:SER:CB	1:A:114:THR:HG21	0.84	2.03	10	1
1:A:92:PHE:CE1	1:A:124:ALA:HB2	0.84	2.07	6	5
1:A:89:SER:HB2	1:A:114:THR:HG21	0.82	1.52	10	1
1:A:102:ILE:HG23	1:A:108:VAL:HG11	0.81	1.51	9	6
1:A:150:TRP:HB2	1:A:158:GLY:HA2	0.81	1.53	8	10
1:A:108:VAL:HG22	1:A:110:LEU:HD13	0.81	1.52	2	4
1:A:65:PHE:O	1:A:68:VAL:HG12	0.80	1.76	2	7
1:A:142:THR:HG21	1:A:171:SER:CA	0.80	2.07	2	10
1:A:66:LEU:HD21	1:A:101:PHE:CG	0.80	2.11	9	4
1:A:69:ILE:HG23	1:A:72:TRP:CH2	0.79	2.13	2	6
1:A:74:LEU:HD13	1:A:78:GLN:HG2	0.78	1.55	4	4
1:A:131:LEU:HD22	1:A:135:GLY:HA3	0.78	1.55	7	1
1:A:92:PHE:CZ	1:A:124:ALA:HB2	0.78	2.13	2	2
1:A:66:LEU:HD21	1:A:101:PHE:CD1	0.78	2.14	7	4
1:A:15:VAL:HG23	1:A:21:THR:HG22	0.78	1.52	10	1
1:A:62:GLU:OE1	1:A:63:LEU:HD22	0.78	1.78	6	4
1:A:114:THR:OG1	1:A:174:LEU:HD11	0.77	1.80	10	10
1:A:115:ALA:O	1:A:142:THR:HG23	0.77	1.78	4	8
1:A:63:LEU:HD21	1:A:94:CYS:HA	0.76	1.57	8	9
1:A:128:LEU:CD1	1:A:181:ILE:HG21	0.75	2.12	10	5
1:A:82:VAL:CG2	1:A:110:LEU:HD23	0.74	2.12	3	5
1:A:181:ILE:HD13	1:A:182:LEU:N	0.74	1.98	3	2
1:A:102:ILE:HG21	1:A:135:GLY:O	0.74	1.83	4	9
1:A:117:ILE:HD12	1:A:117:ILE:O	0.74	1.81	7	2
1:A:98:MET:O	1:A:102:ILE:HD12	0.74	1.83	4	10
1:A:25:TYR:OH	1:A:68:VAL:HG21	0.73	1.84	8	2
1:A:178:LEU:HA	1:A:181:ILE:HD12	0.73	1.58	8	2
1:A:69:ILE:HG23	1:A:72:TRP:CZ3	0.72	2.18	1	6
1:A:164:TRP:CZ2	1:A:167:LEU:HD21	0.72	2.20	6	9
1:A:89:SER:CB	1:A:90:PRO:HD3	0.71	2.16	7	9
1:A:102:ILE:HG23	1:A:108:VAL:HG13	0.71	1.60	7	7
1:A:108:VAL:HG22	1:A:110:LEU:CD1	0.71	2.16	9	6
1:A:110:LEU:N	1:A:110:LEU:HD12	0.71	1.99	4	4
1:A:128:LEU:HD22	1:A:181:ILE:HG13	0.71	1.60	3	3
1:A:27:VAL:HG11	1:A:68:VAL:HG11	0.71	1.62	1	5
1:A:29:ARG:O	1:A:36:VAL:HG23	0.70	1.85	4	8
1:A:181:ILE:HD13	1:A:182:LEU:H	0.70	1.47	3	2
1:A:109:SER:O	1:A:110:LEU:HD12	0.70	1.87	7	4
1:A:98:MET:HE1	1:A:131:LEU:HD21	0.70	1.63	7	1
1:A:99:ALA:HB1	1:A:130:THR:HG22	0.69	1.64	5	8
1:A:69:ILE:HB	1:A:70:PRO:HD3	0.69	1.62	7	8

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:140:ILE:HG22	1:A:142:THR:OG1	0.69	1.88	5	10
1:A:15:VAL:HG13	1:A:88:TRP:NE1	0.68	2.02	10	4
1:A:102:ILE:HA	1:A:108:VAL:HG11	0.68	1.65	7	2
1:A:138:ILE:HB	1:A:178:LEU:HD11	0.68	1.63	3	7
1:A:142:THR:HG21	1:A:171:SER:N	0.68	2.03	6	10
1:A:89:SER:HA	1:A:114:THR:CG2	0.68	2.18	6	9
1:A:63:LEU:HD11	1:A:94:CYS:O	0.68	1.89	1	9
1:A:65:PHE:CZ	1:A:110:LEU:HD21	0.68	2.24	7	4
1:A:102:ILE:CG1	1:A:108:VAL:HG11	0.68	2.19	3	2
1:A:80:TYR:HB2	1:A:108:VAL:HG23	0.68	1.64	2	6
1:A:140:ILE:HD13	1:A:140:ILE:N	0.67	2.05	9	10
1:A:27:VAL:HG11	1:A:68:VAL:HG21	0.67	1.65	5	2
1:A:91:CYS:O	1:A:95:ALA:HB3	0.67	1.89	6	9
1:A:21:THR:HG21	1:A:60:HIS:HB3	0.67	1.65	10	1
1:A:99:ALA:HB3	1:A:130:THR:HG22	0.67	1.67	6	8
1:A:23:LEU:HD22	1:A:61:ALA:N	0.67	2.05	3	5
1:A:110:LEU:HD13	1:A:136:ALA:HB2	0.66	1.65	8	3
1:A:23:LEU:HD22	1:A:61:ALA:CA	0.66	2.20	5	5
1:A:66:LEU:HD13	1:A:98:MET:SD	0.66	2.30	2	2
1:A:177:ARG:O	1:A:181:ILE:HG23	0.66	1.89	8	4
1:A:10:ASN:HA	1:A:164:TRP:CZ3	0.66	2.26	1	3
1:A:98:MET:CE	1:A:131:LEU:HD21	0.66	2.21	7	1
1:A:63:LEU:HD21	1:A:94:CYS:CA	0.66	2.21	9	8
1:A:176:GLY:O	1:A:179:ARG:HG2	0.66	1.90	2	1
1:A:65:PHE:CG	1:A:82:VAL:HG11	0.65	2.26	7	7
1:A:128:LEU:HD22	1:A:181:ILE:HD13	0.65	1.66	4	6
1:A:23:LEU:HD22	1:A:61:ALA:H	0.65	1.52	10	1
1:A:90:PRO:HG3	1:A:117:ILE:HD13	0.64	1.67	10	1
1:A:82:VAL:HG21	1:A:110:LEU:HD23	0.64	1.69	3	3
1:A:175:SER:O	1:A:179:ARG:HG2	0.64	1.92	3	9
1:A:15:VAL:HG21	1:A:21:THR:HG23	0.64	1.67	6	2
1:A:112:ILE:HG22	1:A:114:THR:CG2	0.63	2.24	2	6
1:A:65:PHE:CE1	1:A:110:LEU:HD21	0.63	2.28	1	4
1:A:10:ASN:HA	1:A:164:TRP:CH2	0.63	2.28	3	7
1:A:108:VAL:HG22	1:A:110:LEU:HG	0.63	1.70	10	2
1:A:27:VAL:HG23	1:A:82:VAL:HG22	0.63	1.69	7	1
1:A:82:VAL:HG23	1:A:110:LEU:HD11	0.63	1.69	1	3
1:A:84:CYS:HB3	1:A:112:ILE:HG23	0.63	1.70	2	7
1:A:98:MET:HB3	1:A:131:LEU:HD13	0.63	1.70	2	1
1:A:9:PHE:HA	1:A:14:TRP:NE1	0.62	2.09	1	4
1:A:98:MET:HE2	1:A:102:ILE:HD13	0.62	1.70	9	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:25:TYR:CD1	1:A:44:PHE:CD2	0.62	2.88	6	5
1:A:15:VAL:HG11	1:A:87:SER:HB3	0.62	1.71	7	2
1:A:15:VAL:CG2	1:A:21:THR:HG22	0.62	2.25	10	1
1:A:181:ILE:HD12	1:A:182:LEU:N	0.61	2.10	6	6
1:A:90:PRO:HD3	1:A:117:ILE:HD13	0.61	1.72	4	3
1:A:131:LEU:HD23	1:A:132:ALA:N	0.61	2.10	9	3
1:A:86:THR:HG21	1:A:88:TRP:CZ2	0.61	2.30	8	7
1:A:22:TYR:CD1	1:A:46:ALA:HB1	0.61	2.30	3	1
1:A:9:PHE:CD1	1:A:146:PHE:CZ	0.61	2.88	4	2
1:A:90:PRO:CD	1:A:117:ILE:HD13	0.60	2.26	4	4
1:A:22:TYR:HA	1:A:46:ALA:HA	0.60	1.73	5	10
1:A:23:LEU:HD12	1:A:24:CYS:N	0.60	2.11	1	6
1:A:66:LEU:HA	1:A:69:ILE:HD11	0.60	1.71	9	3
1:A:98:MET:CE	1:A:102:ILE:HD13	0.60	2.26	2	3
1:A:108:VAL:HG13	1:A:108:VAL:O	0.60	1.97	2	10
1:A:69:ILE:HG22	1:A:72:TRP:CH2	0.60	2.30	4	2
1:A:63:LEU:N	1:A:63:LEU:HD13	0.60	2.10	1	7
1:A:88:TRP:HB2	1:A:117:ILE:CG2	0.60	2.26	1	10
1:A:15:VAL:HG13	1:A:88:TRP:HE1	0.60	1.57	10	1
1:A:159:ALA:HB1	1:A:160:PRO:HD2	0.60	1.74	2	1
1:A:23:LEU:HD22	1:A:61:ALA:HB2	0.59	1.74	2	8
1:A:74:LEU:HD13	1:A:78:GLN:HG3	0.59	1.74	2	2
1:A:100:LYS:O	1:A:104:LYS:N	0.59	2.35	4	10
1:A:69:ILE:CG2	1:A:74:LEU:HD21	0.59	2.21	8	1
1:A:14:TRP:CD2	1:A:87:SER:HB2	0.59	2.32	10	4
1:A:99:ALA:HB2	1:A:131:LEU:HA	0.59	1.74	6	10
1:A:150:TRP:CB	1:A:158:GLY:HA2	0.59	2.28	10	9
1:A:150:TRP:CH2	1:A:161:PHE:HB3	0.59	2.33	8	4
1:A:25:TYR:OH	1:A:68:VAL:HG11	0.59	1.97	5	1
1:A:80:TYR:CB	1:A:108:VAL:HG23	0.59	2.28	7	2
1:A:98:MET:SD	1:A:131:LEU:HD12	0.58	2.37	5	2
1:A:181:ILE:HD11	1:A:182:LEU:HD13	0.58	1.74	3	4
1:A:129:ARG:HG3	1:A:181:ILE:HG12	0.58	1.74	3	1
1:A:163:PRO:HB3	1:A:167:LEU:HD12	0.58	1.75	4	1
1:A:66:LEU:HD21	1:A:101:PHE:CD2	0.58	2.33	3	2
1:A:15:VAL:HB	1:A:21:THR:HA	0.58	1.75	3	3
1:A:15:VAL:O	1:A:21:THR:HG23	0.58	1.98	8	1
1:A:27:VAL:CG2	1:A:82:VAL:HG13	0.58	2.29	1	5
1:A:31:HIS:O	1:A:34:THR:HG22	0.58	1.98	6	4
1:A:140:ILE:N	1:A:140:ILE:CD1	0.58	2.67	3	10
1:A:74:LEU:HD22	1:A:78:GLN:HG3	0.58	1.74	3	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:68:VAL:O	1:A:71:PHE:HB2	0.58	1.98	9	3
1:A:114:THR:O	1:A:141:MET:N	0.58	2.37	3	10
1:A:86:THR:HG21	1:A:88:TRP:CE2	0.58	2.33	5	6
1:A:22:TYR:CD1	1:A:46:ALA:HB2	0.58	2.34	7	2
1:A:68:VAL:O	1:A:71:PHE:HB3	0.58	1.99	8	7
1:A:74:LEU:HD12	1:A:74:LEU:N	0.58	2.14	9	4
1:A:69:ILE:HB	1:A:70:PRO:CD	0.58	2.28	2	7
1:A:110:LEU:HD13	1:A:136:ALA:CB	0.57	2.29	3	1
1:A:146:PHE:CE2	1:A:164:TRP:CZ3	0.57	2.92	5	2
1:A:89:SER:HB3	1:A:90:PRO:HD3	0.57	1.75	7	6
1:A:76:LEU:HD12	1:A:76:LEU:O	0.57	2.00	9	5
1:A:110:LEU:HD12	1:A:110:LEU:H	0.57	1.58	3	4
1:A:142:THR:HG21	1:A:171:SER:CB	0.57	2.29	2	10
1:A:142:THR:O	1:A:146:PHE:N	0.57	2.38	3	10
1:A:9:PHE:CD1	1:A:146:PHE:CE1	0.57	2.93	7	6
1:A:178:LEU:CD2	1:A:181:ILE:HD11	0.57	2.24	6	1
1:A:24:CYS:HA	1:A:44:PHE:N	0.56	2.14	10	10
1:A:69:ILE:CG2	1:A:72:TRP:CH2	0.56	2.88	4	1
1:A:67:ASP:O	1:A:71:PHE:CD1	0.56	2.58	4	3
1:A:140:ILE:HD11	1:A:178:LEU:HD13	0.56	1.75	1	3
1:A:150:TRP:HA	1:A:154:VAL:HG23	0.56	1.76	5	9
1:A:141:MET:HA	1:A:145:GLU:HB2	0.56	1.77	6	2
1:A:27:VAL:HG23	1:A:82:VAL:HG13	0.56	1.78	10	5
1:A:69:ILE:CG1	1:A:70:PRO:HD3	0.56	2.31	4	1
1:A:140:ILE:HG21	1:A:175:SER:OG	0.56	2.00	1	3
1:A:112:ILE:HD12	1:A:138:ILE:HD12	0.56	1.77	6	3
1:A:60:HIS:N	1:A:60:HIS:CD2	0.56	2.72	3	7
1:A:148:HIS:NE2	1:A:152:THR:HG23	0.56	2.16	4	5
1:A:15:VAL:HG22	1:A:16:ARG:N	0.56	2.16	5	2
1:A:143:TYR:CD1	1:A:144:SER:N	0.55	2.74	4	9
1:A:9:PHE:HA	1:A:14:TRP:CD1	0.55	2.36	8	3
1:A:99:ALA:HB2	1:A:131:LEU:CA	0.55	2.31	8	10
1:A:103:SER:HB2	1:A:134:ALA:HB1	0.55	1.78	6	2
1:A:24:CYS:HA	1:A:44:PHE:HB2	0.55	1.78	8	5
1:A:68:VAL:O	1:A:72:TRP:CD1	0.55	2.60	8	8
1:A:69:ILE:HA	1:A:72:TRP:CE2	0.55	2.36	9	4
1:A:92:PHE:HE1	1:A:124:ALA:HB2	0.55	1.60	4	3
1:A:27:VAL:HG11	1:A:68:VAL:CG1	0.54	2.33	8	3
1:A:82:VAL:CG2	1:A:110:LEU:HD11	0.54	2.32	1	3
1:A:110:LEU:HB3	1:A:136:ALA:HB1	0.54	1.79	2	4
1:A:74:LEU:HD13	1:A:78:GLN:CG	0.54	2.32	3	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:154:VAL:CG1	1:A:159:ALA:HB2	0.54	2.28	5	1
1:A:65:PHE:CD1	1:A:66:LEU:N	0.54	2.76	8	10
1:A:73:LYS:O	1:A:74:LEU:C	0.54	2.46	6	1
1:A:142:THR:HG21	1:A:171:SER:HA	0.54	1.77	4	9
1:A:65:PHE:CE1	1:A:110:LEU:CD2	0.54	2.90	3	2
1:A:14:TRP:O	1:A:15:VAL:HG23	0.54	2.02	8	1
1:A:100:LYS:O	1:A:103:SER:N	0.54	2.41	10	10
1:A:74:LEU:HD22	1:A:78:GLN:CG	0.54	2.33	4	2
1:A:145:GLU:O	1:A:149:CYS:N	0.54	2.41	6	5
1:A:112:ILE:O	1:A:114:THR:HG23	0.54	2.03	6	5
1:A:90:PRO:HD2	1:A:117:ILE:HG21	0.53	1.80	10	5
1:A:15:VAL:HG11	1:A:87:SER:HB2	0.53	1.81	1	1
1:A:108:VAL:HG22	1:A:110:LEU:CG	0.53	2.33	3	3
1:A:128:LEU:HD22	1:A:181:ILE:CD1	0.53	2.33	9	1
1:A:88:TRP:CB	1:A:117:ILE:CG2	0.53	2.86	2	9
1:A:80:TYR:HB2	1:A:108:VAL:HA	0.53	1.78	6	3
1:A:23:LEU:HD22	1:A:61:ALA:CB	0.53	2.33	5	3
1:A:99:ALA:O	1:A:103:SER:N	0.53	2.41	2	10
1:A:82:VAL:O	1:A:110:LEU:HA	0.52	2.03	9	9
1:A:15:VAL:HG21	1:A:21:THR:CB	0.52	2.34	2	2
1:A:74:LEU:CD1	1:A:78:GLN:HG2	0.52	2.33	4	1
1:A:143:TYR:CE1	1:A:144:SER:OG	0.52	2.62	9	1
1:A:65:PHE:CZ	1:A:110:LEU:CD2	0.52	2.92	1	5
1:A:10:ASN:O	1:A:12:GLU:N	0.52	2.43	9	2
1:A:61:ALA:HB1	1:A:84:CYS:SG	0.52	2.45	4	2
1:A:26:GLU:HB2	1:A:83:THR:HG22	0.52	1.82	2	4
1:A:88:TRP:CB	1:A:117:ILE:HG23	0.52	2.35	2	2
1:A:140:ILE:HG23	1:A:174:LEU:HD13	0.52	1.80	2	1
1:A:82:VAL:O	1:A:110:LEU:HB3	0.52	2.05	6	5
1:A:177:ARG:NH1	1:A:181:ILE:HG23	0.52	2.20	5	1
1:A:148:HIS:CD2	1:A:152:THR:HG23	0.51	2.39	8	2
1:A:143:TYR:HA	1:A:167:LEU:HD13	0.51	1.82	6	2
1:A:149:CYS:O	1:A:152:THR:HG22	0.51	2.06	1	1
1:A:18:ARG:HB3	1:A:60:HIS:CD2	0.51	2.40	10	6
1:A:148:HIS:O	1:A:148:HIS:CD2	0.51	2.64	6	8
1:A:139:SER:C	1:A:140:ILE:HD13	0.51	2.26	6	2
1:A:25:TYR:CD2	1:A:65:PHE:HB3	0.51	2.40	4	5
1:A:116:ARG:HA	1:A:174:LEU:HD12	0.51	1.82	5	9
1:A:178:LEU:O	1:A:182:LEU:HB2	0.51	2.05	2	3
1:A:19:HIS:O	1:A:21:THR:HG22	0.51	2.06	1	1
1:A:102:ILE:HG13	1:A:108:VAL:HG11	0.51	1.83	3	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:22:TYR:CG	1:A:46:ALA:HB2	0.51	2.41	4	1
1:A:69:ILE:CB	1:A:70:PRO:HD3	0.51	2.36	4	3
1:A:21:THR:O	1:A:21:THR:HG23	0.51	2.06	4	1
1:A:102:ILE:HG21	1:A:135:GLY:C	0.51	2.26	7	4
1:A:66:LEU:HD13	1:A:98:MET:HG2	0.51	1.82	1	1
1:A:164:TRP:CH2	1:A:167:LEU:HD21	0.51	2.40	10	3
1:A:83:THR:CG2	1:A:85:PHE:CZ	0.50	2.95	8	6
1:A:177:ARG:O	1:A:181:ILE:HG13	0.50	2.06	2	6
1:A:60:HIS:O	1:A:61:ALA:HB3	0.50	2.06	3	1
1:A:106:LYS:O	1:A:107:HIS:CG	0.50	2.64	4	2
1:A:24:CYS:HA	1:A:44:PHE:CB	0.50	2.36	1	8
1:A:65:PHE:HB2	1:A:82:VAL:HG11	0.50	1.82	5	2
1:A:27:VAL:HB	1:A:82:VAL:HG13	0.50	1.82	7	2
1:A:65:PHE:CZ	1:A:110:LEU:HD13	0.50	2.42	10	1
1:A:103:SER:CB	1:A:134:ALA:HB1	0.50	2.36	8	2
1:A:116:ARG:CB	1:A:170:HIS:HB3	0.50	2.36	6	7
1:A:15:VAL:CG2	1:A:21:THR:HA	0.50	2.36	9	3
1:A:25:TYR:CE1	1:A:44:PHE:CE2	0.50	3.00	7	1
1:A:109:SER:C	1:A:110:LEU:HD12	0.50	2.26	1	4
1:A:178:LEU:HA	1:A:181:ILE:HD11	0.50	1.83	4	5
1:A:143:TYR:N	1:A:167:LEU:HD22	0.49	2.22	2	1
1:A:112:ILE:HG22	1:A:114:THR:HG22	0.49	1.84	1	2
1:A:89:SER:H	1:A:90:PRO:HD2	0.49	1.67	10	1
1:A:15:VAL:CB	1:A:21:THR:HA	0.49	2.37	3	2
1:A:68:VAL:HG22	1:A:72:TRP:HE1	0.49	1.67	4	1
1:A:110:LEU:HB2	1:A:136:ALA:CB	0.49	2.37	10	1
1:A:83:THR:CG2	1:A:85:PHE:CE2	0.49	2.96	3	5
1:A:153:PHE:CD1	1:A:153:PHE:O	0.49	2.65	6	3
1:A:65:PHE:CD1	1:A:65:PHE:C	0.49	2.85	6	8
1:A:72:TRP:CE3	1:A:74:LEU:HD21	0.49	2.43	7	5
1:A:66:LEU:HD12	1:A:69:ILE:HD11	0.49	1.84	6	1
1:A:9:PHE:CE1	1:A:146:PHE:CE1	0.49	3.00	4	3
1:A:141:MET:HA	1:A:145:GLU:CB	0.49	2.38	7	8
1:A:68:VAL:HA	1:A:71:PHE:HB3	0.49	1.84	5	3
1:A:153:PHE:O	1:A:153:PHE:CG	0.49	2.66	10	6
1:A:14:TRP:CH2	1:A:115:ALA:HB1	0.49	2.43	9	3
1:A:178:LEU:O	1:A:181:ILE:HD13	0.49	2.08	8	2
1:A:25:TYR:CD1	1:A:44:PHE:CE2	0.48	3.01	8	4
1:A:66:LEU:CD2	1:A:101:PHE:CD1	0.48	2.95	7	2
1:A:44:PHE:CZ	1:A:64:CYS:SG	0.48	3.06	1	5
1:A:140:ILE:HD12	1:A:174:LEU:HD22	0.48	1.85	5	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:102:ILE:CG2	1:A:108:VAL:HG11	0.48	2.36	10	2
1:A:74:LEU:HD21	1:A:80:TYR:CE1	0.48	2.43	9	2
1:A:175:SER:O	1:A:179:ARG:CG	0.48	2.61	3	1
1:A:44:PHE:CE1	1:A:64:CYS:SG	0.48	3.06	5	3
1:A:164:TRP:CE2	1:A:167:LEU:HG	0.48	2.43	3	4
1:A:110:LEU:O	1:A:136:ALA:HB1	0.48	2.09	4	3
1:A:15:VAL:O	1:A:17:GLY:N	0.48	2.47	7	2
1:A:69:ILE:CG2	1:A:80:TYR:CE1	0.48	2.97	7	2
1:A:63:LEU:CD2	1:A:94:CYS:HB3	0.48	2.38	10	4
1:A:132:ALA:HA	1:A:138:ILE:CG1	0.48	2.39	5	5
1:A:143:TYR:HB2	1:A:167:LEU:CB	0.48	2.39	3	1
1:A:89:SER:HB3	1:A:117:ILE:HG12	0.48	1.86	4	1
1:A:72:TRP:CE3	1:A:74:LEU:HD11	0.47	2.44	2	2
1:A:143:TYR:C	1:A:143:TYR:CD1	0.47	2.87	3	1
1:A:69:ILE:HD12	1:A:72:TRP:CH2	0.47	2.45	2	2
1:A:14:TRP:CG	1:A:87:SER:HB2	0.47	2.43	2	2
1:A:63:LEU:HD22	1:A:63:LEU:H	0.47	1.69	10	2
1:A:113:LYS:HB2	1:A:141:MET:HB2	0.47	1.86	1	1
1:A:66:LEU:HD22	1:A:98:MET:SD	0.47	2.50	2	1
1:A:181:ILE:CD1	1:A:182:LEU:HD13	0.47	2.40	6	2
1:A:23:LEU:HD11	1:A:44:PHE:CD2	0.47	2.44	6	3
1:A:65:PHE:CZ	1:A:110:LEU:HD22	0.47	2.43	3	2
1:A:60:HIS:O	1:A:61:ALA:C	0.47	2.53	9	2
1:A:148:HIS:CD2	1:A:148:HIS:O	0.47	2.68	8	2
1:A:164:TRP:CZ3	1:A:167:LEU:HD11	0.47	2.45	4	2
1:A:18:ARG:O	1:A:19:HIS:CB	0.47	2.62	9	4
1:A:69:ILE:HG13	1:A:70:PRO:HD2	0.47	1.86	6	2
1:A:15:VAL:HG21	1:A:87:SER:HB3	0.47	1.85	7	1
1:A:8:ASN:O	1:A:14:TRP:CG	0.47	2.68	1	2
1:A:153:PHE:CD2	1:A:153:PHE:O	0.47	2.67	7	2
1:A:181:ILE:CD1	1:A:182:LEU:N	0.47	2.74	3	2
1:A:74:LEU:HD22	1:A:78:GLN:HG2	0.47	1.86	5	4
1:A:128:LEU:HD22	1:A:181:ILE:HD12	0.47	1.85	9	1
1:A:19:HIS:O	1:A:21:THR:N	0.47	2.48	1	1
1:A:146:PHE:O	1:A:149:CYS:HB3	0.47	2.10	8	6
1:A:181:ILE:HG12	1:A:182:LEU:N	0.47	2.25	9	2
1:A:80:TYR:CD1	1:A:80:TYR:N	0.47	2.82	8	1
1:A:90:PRO:HG3	1:A:128:LEU:HG	0.47	1.87	9	7
1:A:63:LEU:HD13	1:A:98:MET:HG3	0.47	1.86	8	1
1:A:108:VAL:CG2	1:A:110:LEU:HD21	0.47	2.39	9	1
1:A:90:PRO:HB3	1:A:128:LEU:HG	0.47	1.87	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:89:SER:CB	1:A:90:PRO:CD	0.47	2.92	3	8
1:A:142:THR:HG21	1:A:171:SER:HB3	0.47	1.87	10	10
1:A:147:LYS:HA	1:A:150:TRP:CE3	0.47	2.46	8	2
1:A:74:LEU:HD13	1:A:78:GLN:CD	0.47	2.30	10	1
1:A:179:ARG:O	1:A:183:GLN:HB2	0.46	2.10	2	3
1:A:177:ARG:O	1:A:180:ALA:N	0.46	2.48	9	3
1:A:69:ILE:CB	1:A:70:PRO:CD	0.46	2.92	4	2
1:A:9:PHE:O	1:A:14:TRP:NE1	0.46	2.49	3	4
1:A:25:TYR:CD1	1:A:25:TYR:C	0.46	2.89	2	3
1:A:9:PHE:HB3	1:A:161:PHE:CZ	0.46	2.46	7	1
1:A:14:TRP:CG	1:A:14:TRP:O	0.46	2.68	1	2
1:A:17:GLY:O	1:A:21:THR:HG21	0.46	2.09	1	1
1:A:91:CYS:HB3	1:A:94:CYS:HB2	0.46	1.87	1	5
1:A:17:GLY:O	1:A:18:ARG:O	0.46	2.33	6	1
1:A:65:PHE:CG	1:A:66:LEU:N	0.46	2.84	7	1
1:A:159:ALA:HB1	1:A:160:PRO:CD	0.46	2.41	10	1
1:A:69:ILE:HA	1:A:72:TRP:CZ2	0.46	2.46	2	4
1:A:66:LEU:HD22	1:A:98:MET:HG2	0.46	1.87	4	1
1:A:82:VAL:HB	1:A:110:LEU:HD23	0.46	1.88	4	3
1:A:69:ILE:CG2	1:A:72:TRP:CZ3	0.46	2.97	5	3
1:A:82:VAL:HB	1:A:110:LEU:HG	0.46	1.88	1	1
1:A:129:ARG:O	1:A:133:GLU:HB2	0.46	2.10	7	10
1:A:108:VAL:CG2	1:A:110:LEU:HD11	0.46	2.30	9	1
1:A:24:CYS:O	1:A:85:PHE:N	0.46	2.49	5	9
1:A:69:ILE:CD1	1:A:72:TRP:CZ2	0.46	2.99	2	1
1:A:15:VAL:HG13	1:A:88:TRP:CD1	0.46	2.46	6	2
1:A:69:ILE:HD12	1:A:70:PRO:HD3	0.46	1.86	6	2
1:A:65:PHE:CE1	1:A:66:LEU:HD12	0.46	2.45	7	1
1:A:65:PHE:HD1	1:A:82:VAL:HG11	0.46	1.69	4	2
1:A:66:LEU:HD13	1:A:102:ILE:HD11	0.46	1.87	4	1
1:A:14:TRP:CZ2	1:A:87:SER:OG	0.45	2.66	1	1
1:A:113:LYS:HG3	1:A:113:LYS:O	0.45	2.11	1	1
1:A:112:ILE:HD12	1:A:131:LEU:HD21	0.45	1.87	10	1
1:A:23:LEU:O	1:A:44:PHE:HB3	0.45	2.11	10	5
1:A:14:TRP:CE2	1:A:87:SER:HB2	0.45	2.46	3	2
1:A:18:ARG:HA	1:A:21:THR:HG22	0.45	1.87	4	1
1:A:69:ILE:HG21	1:A:80:TYR:CD2	0.45	2.46	4	1
1:A:29:ARG:HA	1:A:72:TRP:CZ3	0.45	2.47	6	1
1:A:14:TRP:C	1:A:15:VAL:HG22	0.45	2.32	1	2
1:A:69:ILE:HG22	1:A:72:TRP:CZ2	0.45	2.47	6	2
1:A:129:ARG:HG2	1:A:181:ILE:O	0.45	2.12	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:153:PHE:C	1:A:153:PHE:CD1	0.45	2.89	9	1
1:A:88:TRP:O	1:A:88:TRP:CE3	0.45	2.70	1	6
1:A:116:ARG:CG	1:A:170:HIS:HB3	0.45	2.42	4	8
1:A:164:TRP:CH2	1:A:167:LEU:HD11	0.45	2.46	4	1
1:A:31:HIS:CD2	1:A:78:GLN:CG	0.45	2.99	9	1
1:A:99:ALA:N	1:A:131:LEU:HD23	0.45	2.27	7	1
1:A:178:LEU:HA	1:A:181:ILE:CG1	0.45	2.42	2	1
1:A:25:TYR:CD2	1:A:65:PHE:CB	0.45	3.00	7	3
1:A:14:TRP:C	1:A:15:VAL:CG2	0.45	2.85	8	1
1:A:171:SER:OG	1:A:172:GLN:N	0.45	2.50	10	7
1:A:14:TRP:CD1	1:A:22:TYR:CB	0.45	3.00	4	1
1:A:9:PHE:O	1:A:14:TRP:CZ2	0.45	2.70	10	4
1:A:92:PHE:N	1:A:92:PHE:CD1	0.45	2.83	8	6
1:A:138:ILE:N	1:A:138:ILE:HD13	0.45	2.27	9	2
1:A:164:TRP:CZ2	1:A:167:LEU:CD2	0.45	3.00	10	3
1:A:99:ALA:HB2	1:A:131:LEU:N	0.45	2.26	8	1
1:A:62:GLU:CB	1:A:98:MET:HG3	0.44	2.41	10	2
1:A:66:LEU:HD22	1:A:98:MET:HA	0.44	1.88	5	1
1:A:164:TRP:CE3	1:A:164:TRP:N	0.44	2.85	3	2
1:A:89:SER:OG	1:A:90:PRO:HD3	0.44	2.13	7	1
1:A:72:TRP:CZ3	1:A:74:LEU:HD21	0.44	2.47	4	1
1:A:167:LEU:O	1:A:171:SER:CB	0.44	2.66	4	1
1:A:159:ALA:O	1:A:161:PHE:N	0.44	2.51	8	3
1:A:12:GLU:O	1:A:14:TRP:CE3	0.44	2.70	1	2
1:A:82:VAL:CB	1:A:110:LEU:HD23	0.44	2.41	4	2
1:A:154:VAL:HG11	1:A:159:ALA:CB	0.44	2.32	5	1
1:A:14:TRP:HE3	1:A:14:TRP:N	0.44	2.11	8	1
1:A:135:GLY:O	1:A:136:ALA:HB2	0.44	2.13	9	2
1:A:82:VAL:HG23	1:A:110:LEU:CD2	0.44	2.43	10	1
1:A:8:ASN:CB	1:A:22:TYR:CE2	0.44	3.00	3	1
1:A:150:TRP:O	1:A:154:VAL:HG23	0.44	2.13	6	6
1:A:22:TYR:CD2	1:A:46:ALA:HB2	0.44	2.48	4	2
1:A:82:VAL:HB	1:A:110:LEU:HB3	0.44	1.90	4	1
1:A:179:ARG:O	1:A:183:GLN:CB	0.44	2.66	6	1
1:A:86:THR:O	1:A:114:THR:HA	0.44	2.13	3	1
1:A:21:THR:O	1:A:46:ALA:HA	0.44	2.11	6	1
1:A:167:LEU:O	1:A:171:SER:HB3	0.44	2.12	1	5
1:A:63:LEU:HD13	1:A:98:MET:HG2	0.44	1.90	2	1
1:A:69:ILE:HD12	1:A:72:TRP:CZ2	0.44	2.48	2	1
1:A:74:LEU:HD12	1:A:74:LEU:H	0.44	1.71	4	1
1:A:83:THR:HG23	1:A:85:PHE:CE2	0.44	2.48	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:11:ASN:HB3	1:A:164:TRP:CG	0.44	2.47	9	1
1:A:60:HIS:CE1	1:A:94:CYS:SG	0.43	3.11	1	3
1:A:181:ILE:CG1	1:A:182:LEU:N	0.43	2.80	9	2
1:A:59:ARG:N	1:A:59:ARG:CD	0.43	2.81	4	1
1:A:113:LYS:HB3	1:A:141:MET:HE3	0.43	1.89	10	2
1:A:82:VAL:O	1:A:110:LEU:HG	0.43	2.14	2	1
1:A:69:ILE:CG1	1:A:70:PRO:CD	0.43	2.96	4	3
1:A:128:LEU:HD13	1:A:181:ILE:CG2	0.43	2.41	10	1
1:A:15:VAL:HB	1:A:88:TRP:CD1	0.43	2.49	7	2
1:A:29:ARG:N	1:A:36:VAL:O	0.43	2.52	6	1
1:A:95:ALA:HB1	1:A:131:LEU:CB	0.43	2.42	6	1
1:A:15:VAL:HG21	1:A:21:THR:OG1	0.43	2.13	2	1
1:A:174:LEU:O	1:A:174:LEU:CD2	0.43	2.66	3	1
1:A:92:PHE:CD1	1:A:92:PHE:N	0.43	2.86	5	2
1:A:150:TRP:CZ2	1:A:161:PHE:HB3	0.43	2.47	5	1
1:A:98:MET:CE	1:A:112:ILE:HD11	0.43	2.43	7	1
1:A:100:LYS:C	1:A:104:LYS:HG2	0.43	2.33	2	9
1:A:14:TRP:CD2	1:A:15:VAL:HG22	0.43	2.47	8	2
1:A:29:ARG:HB2	1:A:72:TRP:CZ3	0.43	2.48	8	1
1:A:25:TYR:CG	1:A:26:GLU:N	0.43	2.87	3	1
1:A:86:THR:HG22	1:A:87:SER:N	0.43	2.29	3	2
1:A:30:MET:O	1:A:78:GLN:HB2	0.43	2.14	7	1
1:A:142:THR:O	1:A:144:SER:N	0.43	2.52	10	2
1:A:110:LEU:CB	1:A:136:ALA:HB1	0.43	2.44	5	2
1:A:128:LEU:O	1:A:132:ALA:HB3	0.43	2.14	4	4
1:A:89:SER:HA	1:A:114:THR:CB	0.43	2.43	7	1
1:A:68:VAL:O	1:A:72:TRP:NE1	0.43	2.52	5	3
1:A:10:ASN:HB3	1:A:161:PHE:CE1	0.43	2.49	2	1
1:A:90:PRO:CG	1:A:128:LEU:HG	0.43	2.44	6	2
1:A:14:TRP:N	1:A:14:TRP:CE3	0.43	2.87	8	1
1:A:108:VAL:CG1	1:A:108:VAL:O	0.43	2.67	2	2
1:A:69:ILE:HG21	1:A:80:TYR:CG	0.43	2.48	6	1
1:A:153:PHE:O	1:A:153:PHE:CD2	0.43	2.72	5	1
1:A:74:LEU:HD21	1:A:80:TYR:CD1	0.43	2.48	6	1
1:A:92:PHE:CZ	1:A:124:ALA:CB	0.42	2.98	2	1
1:A:131:LEU:HD12	1:A:135:GLY:HA3	0.42	1.91	2	1
1:A:154:VAL:HG12	1:A:156:HIS:H	0.42	1.73	4	2
1:A:107:HIS:O	1:A:107:HIS:CG	0.42	2.72	5	1
1:A:45:LEU:H	1:A:45:LEU:HD23	0.42	1.74	7	1
1:A:60:HIS:CD2	1:A:60:HIS:N	0.42	2.86	8	1
1:A:72:TRP:O	1:A:73:LYS:CE	0.42	2.67	7	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:142:THR:O	1:A:143:TYR:C	0.42	2.58	3	5
1:A:60:HIS:O	1:A:62:GLU:N	0.42	2.51	9	3
1:A:60:HIS:O	1:A:64:CYS:N	0.42	2.51	6	2
1:A:89:SER:OG	1:A:138:ILE:HG21	0.42	2.15	8	1
1:A:91:CYS:O	1:A:92:PHE:C	0.42	2.57	10	1
1:A:110:LEU:CB	1:A:136:ALA:CB	0.42	2.97	5	4
1:A:78:GLN:OE1	1:A:80:TYR:CE1	0.42	2.72	5	2
1:A:29:ARG:CB	1:A:72:TRP:CZ3	0.42	3.02	8	1
1:A:140:ILE:CD1	1:A:178:LEU:HD13	0.42	2.43	1	1
1:A:143:TYR:HE2	1:A:171:SER:HG	0.42	1.55	2	1
1:A:22:TYR:HA	1:A:46:ALA:CA	0.42	2.42	4	2
1:A:69:ILE:HG13	1:A:70:PRO:CD	0.42	2.45	6	2
1:A:150:TRP:HA	1:A:154:VAL:CG2	0.42	2.45	2	3
1:A:86:THR:HG22	1:A:87:SER:H	0.42	1.75	3	2
1:A:174:LEU:O	1:A:174:LEU:HD23	0.42	2.14	3	1
1:A:82:VAL:HB	1:A:110:LEU:HD22	0.42	1.91	10	1
1:A:65:PHE:HB2	1:A:82:VAL:CG1	0.42	2.45	5	2
1:A:18:ARG:HB3	1:A:60:HIS:NE2	0.42	2.29	10	2
1:A:88:TRP:C	1:A:114:THR:HB	0.42	2.35	8	2
1:A:110:LEU:N	1:A:110:LEU:CD1	0.42	2.79	3	2
1:A:21:THR:HG22	1:A:23:LEU:HB3	0.42	1.91	6	1
1:A:148:HIS:NE2	1:A:152:THR:CG2	0.42	2.83	8	1
1:A:177:ARG:O	1:A:181:ILE:CG2	0.42	2.68	9	1
1:A:142:THR:O	1:A:146:PHE:HB2	0.42	2.15	7	1
1:A:110:LEU:CD1	1:A:110:LEU:N	0.42	2.78	9	1
1:A:115:ALA:HA	1:A:141:MET:O	0.42	2.15	1	1
1:A:22:TYR:HA	1:A:46:ALA:CB	0.42	2.45	4	1
1:A:66:LEU:CD1	1:A:102:ILE:HD11	0.42	2.45	8	2
1:A:12:GLU:O	1:A:14:TRP:N	0.42	2.52	6	2
1:A:15:VAL:CG2	1:A:16:ARG:N	0.42	2.83	9	2
1:A:98:MET:HB3	1:A:131:LEU:HD12	0.42	1.92	10	1
1:A:18:ARG:HB3	1:A:60:HIS:CE1	0.41	2.50	1	1
1:A:105:ASN:ND2	1:A:107:HIS:ND1	0.41	2.68	2	1
1:A:27:VAL:CB	1:A:82:VAL:HG13	0.41	2.44	5	1
1:A:150:TRP:CH2	1:A:161:PHE:CB	0.41	3.03	8	1
1:A:60:HIS:CD2	1:A:60:HIS:H	0.41	2.33	10	1
1:A:62:GLU:OE2	1:A:94:CYS:CB	0.41	2.67	6	2
1:A:176:GLY:HA2	1:A:179:ARG:HG3	0.41	1.92	3	1
1:A:86:THR:CG2	1:A:88:TRP:CE2	0.41	3.03	5	3
1:A:74:LEU:HB2	1:A:78:GLN:HG2	0.41	1.91	10	1
1:A:143:TYR:HB2	1:A:167:LEU:HB3	0.41	1.91	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:98:MET:O	1:A:102:ILE:CD1	0.41	2.68	7	1
1:A:69:ILE:CG2	1:A:80:TYR:CD1	0.41	3.03	1	1
1:A:142:THR:CB	1:A:171:SER:CB	0.41	2.99	3	3
1:A:140:ILE:CD1	1:A:174:LEU:HD22	0.41	2.45	9	6
1:A:62:GLU:HB2	1:A:98:MET:HG3	0.41	1.92	2	1
1:A:27:VAL:HG22	1:A:28:GLU:N	0.41	2.29	4	2
1:A:23:LEU:HD11	1:A:44:PHE:HD2	0.41	1.74	6	1
1:A:62:GLU:O	1:A:65:PHE:CE2	0.41	2.73	7	1
1:A:87:SER:HA	1:A:115:ALA:CB	0.41	2.46	8	2
1:A:37:LYS:N	1:A:37:LYS:CD	0.41	2.83	1	1
1:A:183:GLN:O	1:A:184:ASN:ND2	0.41	2.54	1	1
1:A:105:ASN:ND2	1:A:106:LYS:N	0.41	2.69	2	1
1:A:69:ILE:HB	1:A:80:TYR:CZ	0.41	2.51	9	2
1:A:8:ASN:O	1:A:14:TRP:CD1	0.41	2.74	1	1
1:A:62:GLU:HG3	1:A:63:LEU:HD22	0.41	1.92	4	1
1:A:14:TRP:CD1	1:A:87:SER:HB2	0.41	2.51	9	2
1:A:68:VAL:C	1:A:71:PHE:HB3	0.41	2.35	8	1
1:A:21:THR:HG21	1:A:60:HIS:CB	0.41	2.42	10	1
1:A:105:ASN:ND2	1:A:107:HIS:CG	0.41	2.89	2	1
1:A:68:VAL:HG22	1:A:71:PHE:CD2	0.41	2.51	1	1
1:A:68:VAL:HG22	1:A:71:PHE:HD2	0.41	1.76	1	1
1:A:75:ASP:O	1:A:78:GLN:HG3	0.41	2.16	4	1
1:A:98:MET:HE3	1:A:110:LEU:HD23	0.41	1.92	7	1
1:A:105:ASN:OD1	1:A:107:HIS:CE1	0.41	2.74	7	2
1:A:106:LYS:O	1:A:107:HIS:CD2	0.41	2.74	10	1
1:A:67:ASP:O	1:A:70:PRO:HG2	0.41	2.15	2	1
1:A:72:TRP:HE3	1:A:74:LEU:HG	0.41	1.74	4	1
1:A:62:GLU:OE1	1:A:95:ALA:N	0.41	2.54	7	1
1:A:69:ILE:N	1:A:69:ILE:HD13	0.41	2.32	7	1
1:A:31:HIS:CE1	1:A:78:GLN:OE1	0.41	2.74	8	1
1:A:94:CYS:O	1:A:98:MET:HB2	0.41	2.15	10	1
1:A:29:ARG:HG2	1:A:72:TRP:CD2	0.40	2.51	9	1
1:A:15:VAL:HG23	1:A:21:THR:CG2	0.40	2.35	10	1
1:A:21:THR:O	1:A:23:LEU:N	0.40	2.54	10	1
1:A:59:ARG:HB3	1:A:63:LEU:HB2	0.40	1.93	10	1
1:A:129:ARG:CG	1:A:181:ILE:O	0.40	2.69	3	1
1:A:129:ARG:O	1:A:133:GLU:CB	0.40	2.69	4	1
1:A:178:LEU:HD23	1:A:179:ARG:NH1	0.40	2.31	4	1
1:A:115:ALA:O	1:A:116:ARG:HB3	0.40	2.16	6	2
1:A:88:TRP:CA	1:A:117:ILE:HG23	0.40	2.46	6	1
1:A:105:ASN:OD1	1:A:107:HIS:CG	0.40	2.74	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:65:PHE:CD1	1:A:82:VAL:CG1	0.40	2.99	9	1
1:A:174:LEU:CD2	1:A:174:LEU:O	0.40	2.69	9	1
1:A:71:PHE:CD2	1:A:72:TRP:CD1	0.40	3.09	1	1
1:A:164:TRP:N	1:A:164:TRP:CE3	0.40	2.90	2	1
1:A:179:ARG:O	1:A:183:GLN:CG	0.40	2.69	2	1
1:A:14:TRP:CD1	1:A:87:SER:CB	0.40	3.04	5	1
1:A:25:TYR:CE2	1:A:27:VAL:CG1	0.40	3.05	5	1
1:A:62:GLU:HB3	1:A:98:MET:CG	0.40	2.46	5	1
1:A:107:HIS:O	1:A:107:HIS:ND1	0.40	2.54	6	1
1:A:128:LEU:O	1:A:132:ALA:CB	0.40	2.70	8	1
1:A:153:PHE:CD1	1:A:153:PHE:C	0.40	2.95	1	1
1:A:90:PRO:HG3	1:A:128:LEU:CD2	0.40	2.46	7	1
1:A:98:MET:SD	1:A:131:LEU:HD21	0.40	2.56	7	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	159/195 (82%)	117±3 (74±2%)	31±3 (19±2%)	11±2 (7±1%)	2	17
All	All	1590/1950 (82%)	1172 (74%)	307 (19%)	111 (7%)	2	17

All 25 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	18	ARG	10
1	A	76	LEU	10
1	A	90	PRO	9
1	A	143	TYR	9
1	A	107	HIS	8
1	A	15	VAL	6
1	A	13	PRO	6
1	A	20	GLU	5
1	A	22	TYR	5

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Mol	Chain	Res	Type	Models (Total)
1	A	157	GLN	5
1	A	74	LEU	4
1	A	11	ASN	4
1	A	75	ASP	4
1	A	14	TRP	3
1	A	106	LYS	3
1	A	89	SER	3
1	A	19	HIS	3
1	A	160	PRO	3
1	A	185	GLN	2
1	A	21	THR	2
1	A	16	ARG	2
1	A	61	ALA	2
1	A	124	ALA	1
1	A	47	ASN	1
1	A	73	LYS	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	141/171 (82%)	91±3 (64±2%)	50±3 (36±2%)	1 8
All	All	1410/1710 (82%)	906 (64%)	504 (36%)	1 8

All 103 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	14	TRP	10
1	A	23	LEU	10
1	A	25	TYR	10
1	A	62	GLU	10
1	A	63	LEU	10
1	A	72	TRP	10
1	A	74	LEU	10
1	A	83	THR	10
1	A	128	LEU	10

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Mol	Chain	Res	Type	Models (Total)
1	A	140	ILE	10
1	A	142	THR	10
1	A	174	LEU	10
1	A	37	LYS	9
1	A	73	LYS	9
1	A	82	VAL	9
1	A	185	GLN	9
1	A	36	VAL	8
1	A	77	ASP	8
1	A	89	SER	8
1	A	113	LYS	8
1	A	106	LYS	8
1	A	15	VAL	7
1	A	45	LEU	7
1	A	60	HIS	7
1	A	133	GLU	7
1	A	145	GLU	7
1	A	165	ASP	7
1	A	9	PHE	7
1	A	116	ARG	7
1	A	12	GLU	6
1	A	22	TYR	6
1	A	42	ARG	6
1	A	126	GLU	6
1	A	138	ILE	6
1	A	177	ARG	6
1	A	31	HIS	6
1	A	152	THR	6
1	A	94	CYS	6
1	A	173	ASP	6
1	A	29	ARG	5
1	A	107	HIS	5
1	A	111	CYS	5
1	A	131	LEU	5
1	A	149	CYS	5
1	A	153	PHE	5
1	A	182	LEU	5
1	A	18	ARG	5
1	A	44	PHE	5
1	A	78	GLN	5
1	A	129	ARG	5
1	A	81	ARG	5

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Mol	Chain	Res	Type	Models (Total)
1	A	92	PHE	5
1	A	110	LEU	5
1	A	151	ASP	5
1	A	100	LYS	5
1	A	21	THR	4
1	A	71	PHE	4
1	A	104	LYS	4
1	A	181	ILE	4
1	A	28	GLU	4
1	A	47	ASN	4
1	A	84	CYS	4
1	A	147	LYS	4
1	A	156	HIS	4
1	A	172	GLN	4
1	A	179	ARG	4
1	A	98	MET	4
1	A	59	ARG	3
1	A	68	VAL	3
1	A	93	SER	3
1	A	19	HIS	3
1	A	32	ASN	3
1	A	137	LYS	3
1	A	69	ILE	3
1	A	119	ASP	3
1	A	67	ASP	2
1	A	87	SER	2
1	A	184	ASN	2
1	A	20	GLU	2
1	A	97	GLU	2
1	A	105	ASN	2
1	A	10	ASN	2
1	A	109	SER	2
1	A	86	THR	2
1	A	117	ILE	2
1	A	183	GLN	2
1	A	178	LEU	2
1	A	162	GLN	1
1	A	155	ASP	1
1	A	8	ASN	1
1	A	30	MET	1
1	A	169	GLU	1
1	A	11	ASN	1

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Mol	Chain	Res	Type	Models (Total)
1	A	139	SER	1
1	A	66	LEU	1
1	A	96	GLN	1
1	A	80	TYR	1
1	A	161	PHE	1
1	A	125	GLN	1
1	A	144	SER	1
1	A	157	GLN	1
1	A	16	ARG	1
1	A	141	MET	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)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

6.7 Other polymers (i)

There are no such molecules in this entry.

6.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

7 Chemical shift validation (i)

No chemical shift data were provided