Full wwPDB NMR Structure Validation Report (i)

Mar 1, 2022 – 10:52 AM EST

PDB ID	:	2G7H
Title	:	Structure of an O6-Methylguanine DNA Methyltransferase from Methanococcus jannaschii (MJ1529)
Authors	:	Roberts, A.
Deposited on	:	2006-02-28

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:

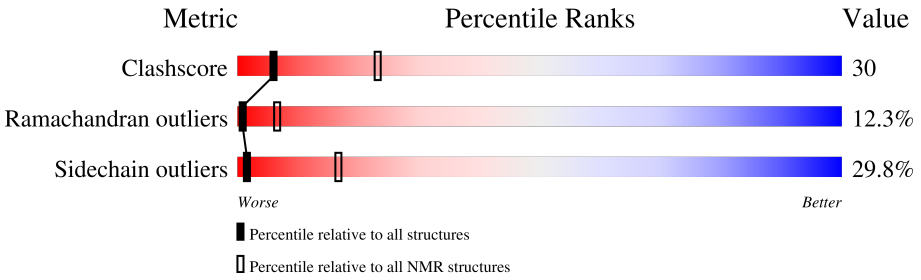
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.27
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.27

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	167	25% 47% 8% • 19%

2 Ensemble composition and analysis (i)

This entry contains 10 models. Model 7 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:1-A:27, A:48-A:156 (136)	0.74	7

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

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

The models can be grouped into 2 clusters and 5 single-model clusters were found.

Cluster number	Models
1	3, 4, 7
2	2, 10
Single-model clusters	1; 5; 6; 8; 9

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 2807 atoms, of which 1439 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Methylated-DNA--protein-cysteine methyltransferase.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	167	2807	892	1439	228	242	6	0

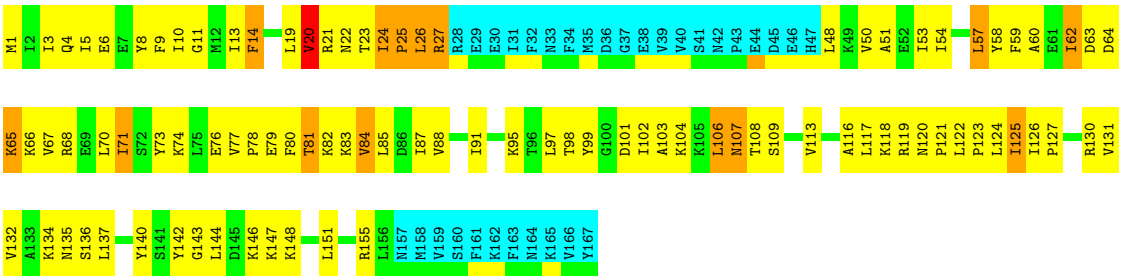
4 Residue-property plots (i)

4.1 Average score per residue in the NMR ensemble

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

• Molecule 1: Methylated-DNA--protein-cysteine methyltransferase

Chain A: 25% 47% 8% • 19%



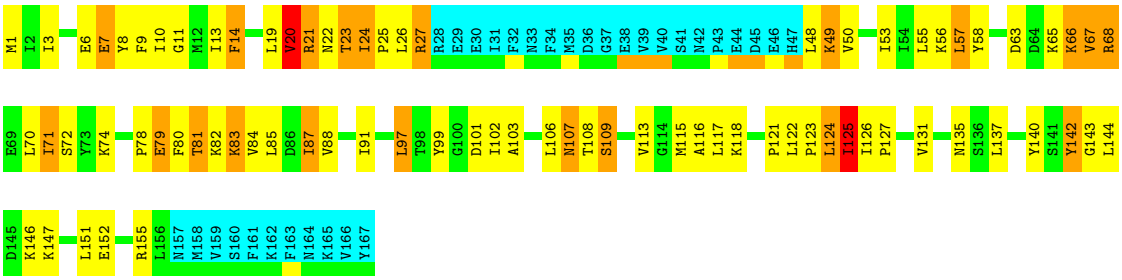
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: Methylated-DNA--protein-cysteine methyltransferase

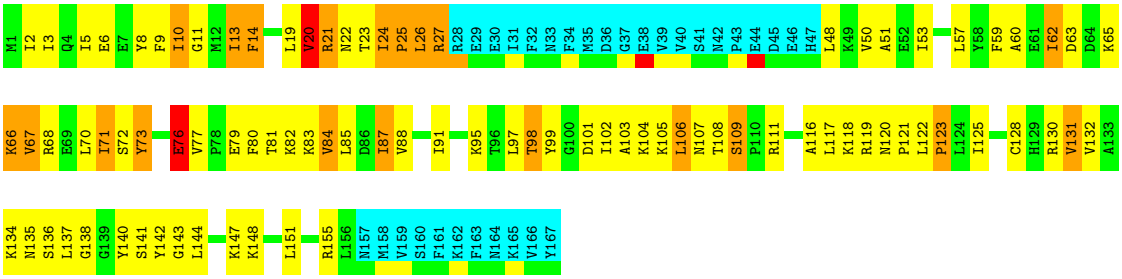
Chain A: 34% 34% 13% • 19%



4.2.2 Score per residue for model 2

• Molecule 1: Methylated-DNA--protein-cysteine methyltransferase

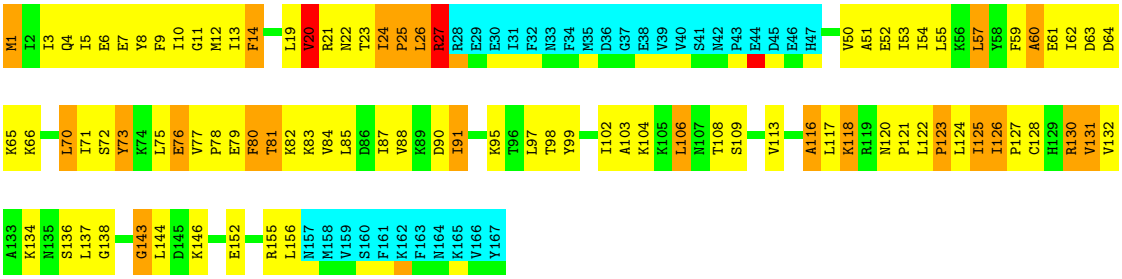
Chain A: 28% 40% 12% • 19%



4.2.3 Score per residue for model 3

• Molecule 1: Methylated-DNA--protein-cysteine methyltransferase

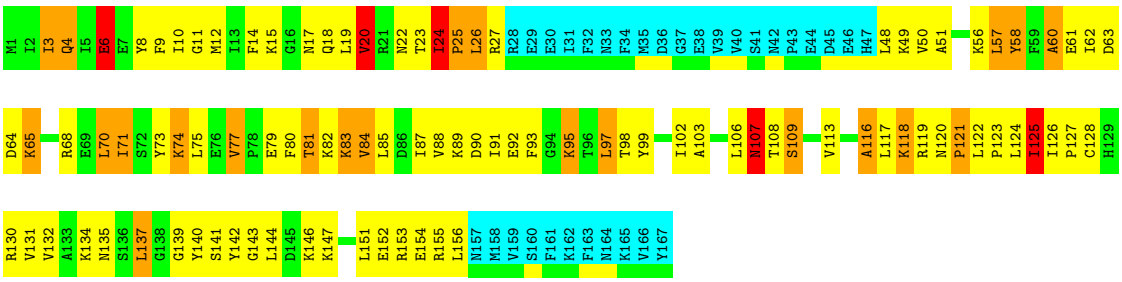
Chain A: 26% 41% 13% • 19%



4.2.4 Score per residue for model 4

• Molecule 1: Methylated-DNA--protein-cysteine methyltransferase

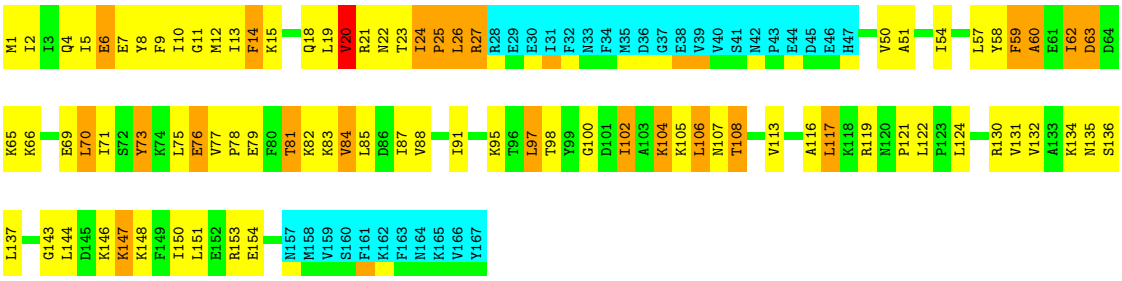
Chain A: 23% 43% 13% • 19%



4.2.5 Score per residue for model 5

• Molecule 1: Methylated-DNA--protein-cysteine methyltransferase

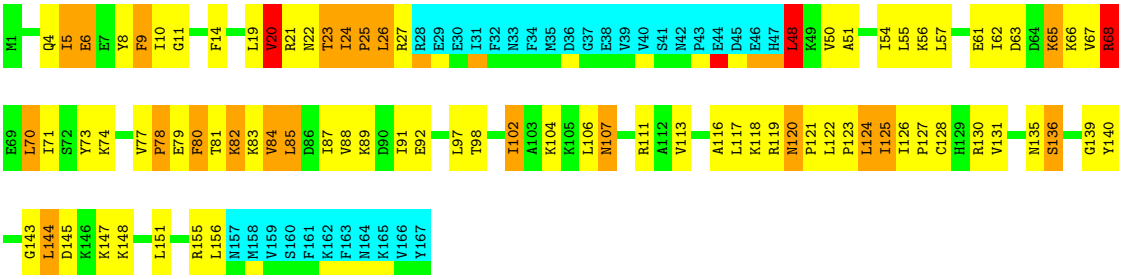
Chain A: 31% 37% 13% • 19%



4.2.6 Score per residue for model 6

• Molecule 1: Methylated-DNA--protein-cysteine methyltransferase

Chain A: 31% 36% 13% • 19%



4.2.7 Score per residue for model 7 (medoid)

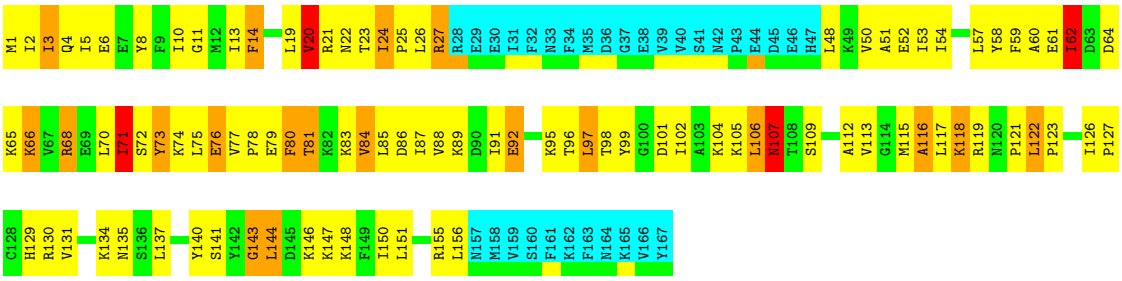
• Molecule 1: Methylated-DNA--protein-cysteine methyltransferase

Chain A: 25% 44% 10% • 19%

4.2.8 Score per residue for model 8

- Molecule 1: Methylated-DNA--protein-cysteine methyltransferase

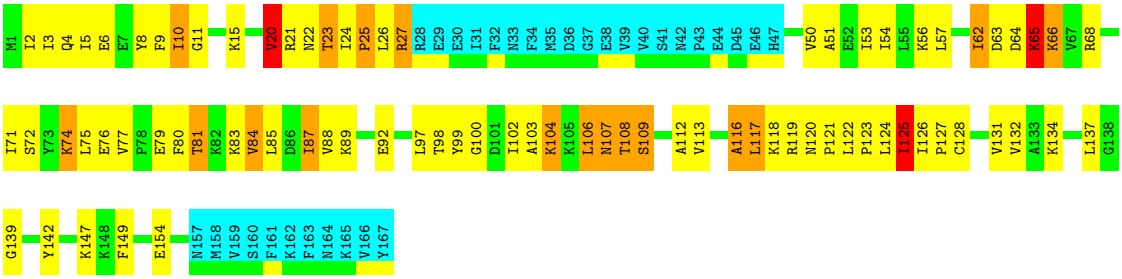
Chain A: 23% 45% 11% • 19%



4.2.9 Score per residue for model 9

- Molecule 1: Methylated-DNA--protein-cysteine methyltransferase

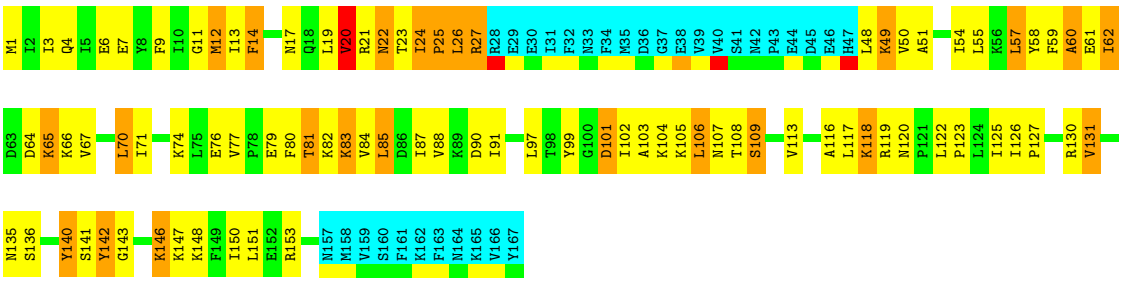
Chain A: 33% 37% 10% • 19%



4.2.10 Score per residue for model 10

- Molecule 1: Methylated-DNA--protein-cysteine methyltransferase

Chain A: 29% 38% 14% • 19%



5 Refinement protocol and experimental data overview (i)

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

Of the 150 calculated structures, 10 were deposited, based on the following criterion: *structures with the lowest energy.*

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

Software name	Classification	Version
CNS	structure solution	1.1
CNS	refinement	1.1

No chemical shift data was provided.

6 Model quality (i)

6.1 Standard geometry (i)

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	1105	1200	1199	68±9
All	All	11050	12000	11990	683

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 30.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:77:VAL:HG11	1:A:81:THR:HG22	1.10	1.22	6	3
1:A:87:ILE:HD11	1:A:102:ILE:HG21	0.98	1.28	6	1
1:A:70:LEU:HD22	1:A:125:ILE:HD13	0.89	1.40	10	1
1:A:87:ILE:CD1	1:A:102:ILE:HG21	0.85	2.01	6	1
1:A:73:TYR:CD2	1:A:122:LEU:HD22	0.84	2.07	3	1
1:A:121:PRO:O	1:A:122:LEU:HD13	0.84	1.72	1	1
1:A:70:LEU:HD12	1:A:122:LEU:HD13	0.81	1.50	5	1
1:A:124:LEU:O	1:A:125:ILE:HG23	0.81	1.76	9	1
1:A:60:ALA:HB2	1:A:153:ARG:NH1	0.80	1.91	5	1
1:A:48:LEU:HD12	1:A:49:LYS:N	0.80	1.92	4	3
1:A:85:LEU:O	1:A:88:VAL:HG12	0.80	1.76	9	9
1:A:87:ILE:HG12	1:A:91:ILE:HD12	0.80	1.53	5	2
1:A:20:VAL:HG23	1:A:74:LYS:CB	0.79	2.06	9	1
1:A:70:LEU:HD22	1:A:125:ILE:HG12	0.79	1.55	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:117:LEU:HD12	1:A:118:LYS:N	0.78	1.93	6	7
1:A:1:MET:CG	1:A:13:ILE:HG22	0.77	2.09	3	1
1:A:26:LEU:HD21	1:A:142:TYR:O	0.77	1.78	10	1
1:A:11:GLY:N	1:A:24:ILE:HG22	0.77	1.95	7	2
1:A:19:LEU:HD21	1:A:22:ASN:CG	0.76	2.01	2	2
1:A:121:PRO:O	1:A:122:LEU:HD23	0.76	1.80	5	3
1:A:84:VAL:HG11	1:A:117:LEU:HD21	0.75	1.57	5	1
1:A:19:LEU:HD23	1:A:122:LEU:HD11	0.75	1.56	6	1
1:A:121:PRO:C	1:A:122:LEU:HD22	0.74	2.03	9	2
1:A:103:ALA:HB1	1:A:108:THR:HG23	0.73	1.60	7	5
1:A:77:VAL:CG1	1:A:81:THR:HG22	0.73	2.11	6	2
1:A:70:LEU:CD2	1:A:125:ILE:HD13	0.73	2.13	10	1
1:A:117:LEU:HD13	1:A:128:CYS:SG	0.73	2.23	9	1
1:A:97:LEU:N	1:A:97:LEU:HD13	0.73	1.98	1	1
1:A:11:GLY:O	1:A:22:ASN:HA	0.72	1.84	5	10
1:A:147:LYS:O	1:A:151:LEU:HD13	0.72	1.85	2	3
1:A:139:GLY:O	1:A:144:LEU:HD21	0.72	1.84	4	1
1:A:84:VAL:O	1:A:87:ILE:HB	0.72	1.83	6	2
1:A:122:LEU:O	1:A:126:ILE:HD12	0.72	1.85	8	2
1:A:1:MET:HG3	1:A:13:ILE:HG22	0.71	1.59	3	1
1:A:91:ILE:HG21	1:A:130:ARG:NE	0.71	1.99	7	1
1:A:91:ILE:HG21	1:A:130:ARG:HD2	0.71	1.60	8	2
1:A:102:ILE:HG22	1:A:106:LEU:HD11	0.71	1.60	4	3
1:A:23:THR:HG21	1:A:123:PRO:HD2	0.71	1.63	8	4
1:A:7:GLU:O	1:A:26:LEU:HD23	0.70	1.86	1	1
1:A:26:LEU:O	1:A:26:LEU:HD12	0.70	1.87	1	1
1:A:57:LEU:HD23	1:A:62:ILE:HG21	0.70	1.61	9	2
1:A:57:LEU:HB3	1:A:62:ILE:HD11	0.70	1.64	10	2
1:A:147:LYS:O	1:A:151:LEU:HD12	0.69	1.87	8	1
1:A:66:LYS:CD	1:A:125:ILE:HG22	0.69	2.18	9	1
1:A:79:GLU:O	1:A:80:PHE:HB2	0.69	1.88	7	1
1:A:14:PHE:HB3	1:A:19:LEU:HD12	0.69	1.65	4	4
1:A:147:LYS:O	1:A:151:LEU:HD23	0.69	1.88	7	2
1:A:124:LEU:O	1:A:125:ILE:HD13	0.68	1.87	1	1
1:A:87:ILE:HD12	1:A:102:ILE:HG12	0.68	1.63	5	2
1:A:8:TYR:CE2	1:A:10:ILE:HD11	0.68	2.24	3	2
1:A:60:ALA:HB2	1:A:154:GLU:OE1	0.68	1.89	4	1
1:A:51:ALA:HA	1:A:54:ILE:HD12	0.67	1.66	7	4
1:A:77:VAL:HG11	1:A:81:THR:CG2	0.67	2.12	6	2
1:A:15:LYS:HD2	1:A:20:VAL:HG21	0.67	1.65	9	1
1:A:117:LEU:HD13	1:A:128:CYS:HB2	0.67	1.65	6	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:58:TYR:CE2	1:A:124:LEU:HD11	0.67	2.25	4	1
1:A:70:LEU:HD22	1:A:125:ILE:HG21	0.66	1.67	1	1
1:A:3:ILE:HD11	1:A:10:ILE:HD12	0.66	1.66	4	1
1:A:102:ILE:CD1	1:A:131:VAL:HG13	0.66	2.19	3	7
1:A:70:LEU:HD22	1:A:125:ILE:CD1	0.66	2.17	10	1
1:A:10:ILE:HG12	1:A:54:ILE:HD13	0.66	1.67	3	1
1:A:83:LYS:HE3	1:A:84:VAL:HG13	0.66	1.67	10	1
1:A:61:GLU:O	1:A:62:ILE:HG23	0.65	1.90	3	3
1:A:70:LEU:CD1	1:A:122:LEU:HD13	0.65	2.22	5	1
1:A:8:TYR:OH	1:A:55:LEU:HD13	0.64	1.90	7	2
1:A:87:ILE:HD11	1:A:102:ILE:CG2	0.64	2.15	6	1
1:A:70:LEU:HD22	1:A:125:ILE:CG1	0.64	2.21	7	1
1:A:57:LEU:HD23	1:A:62:ILE:HG12	0.64	1.69	2	1
1:A:83:LYS:CB	1:A:106:LEU:HD13	0.64	2.23	10	2
1:A:98:THR:HG23	1:A:132:VAL:O	0.64	1.91	3	1
1:A:14:PHE:HA	1:A:20:VAL:HG23	0.64	1.70	4	6
1:A:26:LEU:HD12	1:A:27:ARG:N	0.64	2.08	2	4
1:A:98:THR:HG22	1:A:132:VAL:HG23	0.64	1.70	9	1
1:A:77:VAL:HG12	1:A:81:THR:CG2	0.64	2.23	8	1
1:A:19:LEU:HD22	1:A:70:LEU:O	0.64	1.93	4	2
1:A:70:LEU:HD13	1:A:70:LEU:O	0.63	1.93	8	3
1:A:57:LEU:CD2	1:A:62:ILE:HG21	0.63	2.23	9	2
1:A:120:ASN:OD1	1:A:126:ILE:HG21	0.62	1.94	3	2
1:A:88:VAL:HG23	1:A:127:PRO:HG3	0.62	1.71	1	1
1:A:84:VAL:CG1	1:A:113:VAL:HG13	0.62	2.25	3	3
1:A:99:TYR:CE2	1:A:117:LEU:HD21	0.62	2.30	1	2
1:A:91:ILE:HG21	1:A:130:ARG:CD	0.62	2.24	7	1
1:A:23:THR:HG21	1:A:123:PRO:CD	0.62	2.24	8	2
1:A:84:VAL:O	1:A:87:ILE:HG22	0.62	1.95	7	7
1:A:97:LEU:HD22	1:A:130:ARG:NH1	0.61	2.10	7	1
1:A:61:GLU:C	1:A:62:ILE:HD13	0.61	2.15	8	1
1:A:83:LYS:HE3	1:A:113:VAL:HG13	0.61	1.70	10	1
1:A:62:ILE:HD12	1:A:66:LYS:HB2	0.61	1.72	3	1
1:A:87:ILE:HG23	1:A:91:ILE:HD11	0.61	1.71	7	3
1:A:24:ILE:HD13	1:A:25:PRO:HD2	0.61	1.73	4	1
1:A:60:ALA:HB2	1:A:153:ARG:CZ	0.61	2.24	5	1
1:A:73:TYR:HB3	1:A:122:LEU:HD13	0.61	1.71	3	1
1:A:77:VAL:HG12	1:A:81:THR:HB	0.61	1.73	8	1
1:A:8:TYR:CZ	1:A:55:LEU:HD13	0.61	2.31	3	2
1:A:124:LEU:O	1:A:125:ILE:HD12	0.61	1.95	4	1
1:A:147:LYS:HA	1:A:150:ILE:HD12	0.61	1.73	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:20:VAL:HG12	1:A:121:PRO:CB	0.60	2.26	8	1
1:A:83:LYS:CG	1:A:106:LEU:HD22	0.60	2.27	1	1
1:A:5:ILE:HD12	1:A:8:TYR:CE2	0.60	2.32	5	1
1:A:50:VAL:HA	1:A:53:ILE:HD12	0.60	1.71	2	5
1:A:97:LEU:O	1:A:131:VAL:HA	0.60	1.97	8	10
1:A:57:LEU:HD22	1:A:66:LYS:HG3	0.60	1.72	3	1
1:A:83:LYS:HB3	1:A:106:LEU:HD13	0.60	1.74	10	5
1:A:20:VAL:HG23	1:A:74:LYS:HB2	0.60	1.72	9	1
1:A:70:LEU:HD13	1:A:125:ILE:CD1	0.59	2.27	10	1
1:A:87:ILE:HG23	1:A:91:ILE:HD12	0.59	1.73	6	1
1:A:124:LEU:C	1:A:125:ILE:HD13	0.59	2.18	1	1
1:A:91:ILE:HG22	1:A:95:LYS:HD3	0.59	1.74	3	1
1:A:3:ILE:HD11	1:A:12:MET:HG2	0.59	1.75	10	1
1:A:98:THR:HG22	1:A:132:VAL:O	0.59	1.97	2	3
1:A:20:VAL:HG23	1:A:74:LYS:HB3	0.59	1.73	9	3
1:A:70:LEU:HD13	1:A:125:ILE:HD13	0.59	1.73	10	1
1:A:77:VAL:HG23	1:A:81:THR:HB	0.59	1.75	10	1
1:A:83:LYS:CE	1:A:84:VAL:HG13	0.59	2.28	10	1
1:A:14:PHE:HB3	1:A:19:LEU:HA	0.59	1.72	8	4
1:A:121:PRO:O	1:A:122:LEU:HD22	0.59	1.97	7	2
1:A:57:LEU:HD23	1:A:62:ILE:HD12	0.58	1.75	7	1
1:A:54:ILE:HG23	1:A:124:LEU:HD22	0.58	1.73	6	1
1:A:91:ILE:HD13	1:A:130:ARG:HD2	0.58	1.74	7	1
1:A:58:TYR:CE2	1:A:150:ILE:HD11	0.58	2.34	5	1
1:A:98:THR:HG22	1:A:132:VAL:CG2	0.58	2.28	9	1
1:A:9:PHE:O	1:A:24:ILE:O	0.58	2.22	10	6
1:A:121:PRO:C	1:A:122:LEU:HD12	0.58	2.19	3	1
1:A:97:LEU:H	1:A:97:LEU:HD13	0.57	1.59	4	2
1:A:70:LEU:HG	1:A:125:ILE:HG21	0.57	1.74	3	1
1:A:66:LYS:HD2	1:A:70:LEU:HD23	0.57	1.76	2	1
1:A:84:VAL:HG11	1:A:117:LEU:HD23	0.57	1.75	7	1
1:A:67:VAL:HG22	1:A:125:ILE:HG13	0.57	1.75	10	1
1:A:8:TYR:HB2	1:A:25:PRO:HA	0.57	1.75	4	1
1:A:109:SER:O	1:A:113:VAL:HG23	0.57	1.99	10	1
1:A:57:LEU:HD23	1:A:62:ILE:CD1	0.57	2.30	8	2
1:A:5:ILE:HG21	1:A:8:TYR:OH	0.56	2.00	3	5
1:A:70:LEU:HD13	1:A:125:ILE:HG12	0.56	1.75	2	1
1:A:81:THR:OG1	1:A:116:ALA:HB1	0.56	2.00	9	1
1:A:23:THR:O	1:A:24:ILE:HB	0.56	2.01	6	9
1:A:76:GLU:O	1:A:77:VAL:HG22	0.56	2.00	8	1
1:A:67:VAL:O	1:A:67:VAL:HG13	0.56	2.00	1	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:48:LEU:C	1:A:48:LEU:HD12	0.56	2.20	2	1
1:A:11:GLY:H	1:A:24:ILE:HG22	0.56	1.60	6	1
1:A:99:TYR:CD1	1:A:131:VAL:HG11	0.56	2.36	8	1
1:A:70:LEU:HD12	1:A:71:ILE:O	0.56	2.01	7	3
1:A:77:VAL:HB	1:A:81:THR:HG22	0.56	1.78	5	1
1:A:73:TYR:OH	1:A:85:LEU:HD21	0.56	2.01	2	1
1:A:91:ILE:HG23	1:A:95:LYS:CB	0.56	2.30	8	2
1:A:2:ILE:O	1:A:3:ILE:HD13	0.56	2.00	2	3
1:A:85:LEU:O	1:A:85:LEU:HD13	0.56	2.01	10	3
1:A:99:TYR:CE1	1:A:117:LEU:HD21	0.56	2.37	3	1
1:A:65:LYS:HG3	1:A:67:VAL:HG23	0.56	1.77	10	1
1:A:73:TYR:OH	1:A:85:LEU:HD11	0.55	2.00	2	1
1:A:84:VAL:CG1	1:A:102:ILE:HG21	0.55	2.31	5	1
1:A:97:LEU:N	1:A:97:LEU:CD1	0.55	2.70	1	1
1:A:23:THR:O	1:A:24:ILE:HD12	0.55	2.01	3	2
1:A:125:ILE:HD12	1:A:126:ILE:HG12	0.55	1.78	9	1
1:A:117:LEU:HD22	1:A:128:CYS:HA	0.55	1.78	6	3
1:A:62:ILE:H	1:A:62:ILE:HD13	0.55	1.60	5	1
1:A:5:ILE:HG22	1:A:6:GLU:HG2	0.55	1.78	5	1
1:A:26:LEU:HD12	1:A:26:LEU:C	0.55	2.21	1	1
1:A:53:ILE:O	1:A:62:ILE:HD11	0.55	2.01	7	1
1:A:77:VAL:HG12	1:A:81:THR:CB	0.55	2.32	8	1
1:A:103:ALA:CB	1:A:108:THR:HG23	0.55	2.32	4	3
1:A:113:VAL:O	1:A:116:ALA:HB3	0.55	2.02	5	4
1:A:58:TYR:CZ	1:A:124:LEU:HD11	0.54	2.36	4	1
1:A:83:LYS:HG3	1:A:106:LEU:HD13	0.54	1.77	2	1
1:A:24:ILE:O	1:A:24:ILE:HG23	0.54	2.02	6	2
1:A:59:PHE:O	1:A:60:ALA:HB3	0.54	2.03	2	4
1:A:81:THR:HG23	1:A:82:LYS:NZ	0.54	2.17	6	1
1:A:122:LEU:O	1:A:124:LEU:N	0.54	2.40	7	1
1:A:146:LYS:O	1:A:150:ILE:HD12	0.54	2.02	10	1
1:A:83:LYS:HB3	1:A:106:LEU:HD22	0.54	1.80	4	5
1:A:99:TYR:CD1	1:A:131:VAL:CG1	0.54	2.91	8	1
1:A:65:LYS:O	1:A:66:LYS:HB3	0.54	2.03	1	2
1:A:143:GLY:O	1:A:144:LEU:HB2	0.54	2.03	6	4
1:A:108:THR:HG23	1:A:112:ALA:HB3	0.54	1.79	9	1
1:A:19:LEU:HD21	1:A:22:ASN:CB	0.53	2.33	3	1
1:A:10:ILE:HG23	1:A:23:THR:HA	0.53	1.79	4	1
1:A:19:LEU:HD21	1:A:22:ASN:ND2	0.53	2.18	10	2
1:A:91:ILE:HG23	1:A:95:LYS:HB2	0.53	1.79	8	1
1:A:122:LEU:CB	1:A:125:ILE:HD11	0.53	2.33	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:8:TYR:OH	1:A:55:LEU:HD11	0.53	2.04	6	1
1:A:73:TYR:HD2	1:A:122:LEU:HD22	0.53	1.56	3	1
1:A:120:ASN:HD22	1:A:126:ILE:HD13	0.53	1.64	10	1
1:A:106:LEU:HD12	1:A:108:THR:CG2	0.52	2.34	9	1
1:A:26:LEU:HD23	1:A:146:LYS:HE2	0.52	1.80	10	1
1:A:58:TYR:HB2	1:A:124:LEU:HD21	0.52	1.81	1	1
1:A:129:HIS:CD2	1:A:150:ILE:HG21	0.52	2.39	7	1
1:A:66:LYS:CE	1:A:125:ILE:HG22	0.52	2.34	1	2
1:A:70:LEU:HD13	1:A:71:ILE:O	0.52	2.04	8	1
1:A:23:THR:HG21	1:A:123:PRO:HD3	0.52	1.82	1	1
1:A:27:ARG:CD	1:A:27:ARG:N	0.52	2.73	7	2
1:A:53:ILE:O	1:A:57:LEU:HD23	0.52	2.05	1	2
1:A:87:ILE:HD11	1:A:130:ARG:HH11	0.52	1.63	8	2
1:A:84:VAL:HG13	1:A:113:VAL:HG13	0.52	1.82	1	2
1:A:23:THR:CG2	1:A:123:PRO:HD2	0.52	2.35	9	1
1:A:23:THR:OG1	1:A:24:ILE:N	0.51	2.42	4	3
1:A:50:VAL:HG22	1:A:54:ILE:HD11	0.51	1.80	5	1
1:A:81:THR:O	1:A:84:VAL:CG2	0.51	2.58	8	5
1:A:23:THR:O	1:A:24:ILE:CB	0.51	2.58	2	9
1:A:50:VAL:HG13	1:A:51:ALA:N	0.51	2.21	6	4
1:A:84:VAL:HG21	1:A:117:LEU:CD2	0.51	2.36	5	1
1:A:106:LEU:HB2	1:A:108:THR:HG22	0.51	1.82	5	1
1:A:77:VAL:O	1:A:77:VAL:HG23	0.51	2.05	2	2
1:A:10:ILE:HD11	1:A:54:ILE:HG21	0.51	1.82	9	1
1:A:135:ASN:O	1:A:136:SER:CB	0.51	2.58	6	1
1:A:70:LEU:CD1	1:A:125:ILE:HD13	0.51	2.35	10	1
1:A:87:ILE:CG2	1:A:88:VAL:N	0.51	2.73	5	8
1:A:121:PRO:HB2	1:A:122:LEU:HD22	0.51	1.82	4	1
1:A:70:LEU:HD13	1:A:125:ILE:CG1	0.50	2.36	2	1
1:A:87:ILE:CG1	1:A:102:ILE:HG21	0.50	2.36	6	1
1:A:126:ILE:HG23	1:A:127:PRO:HD2	0.50	1.83	7	3
1:A:10:ILE:CD1	1:A:54:ILE:HG21	0.50	2.36	9	1
1:A:91:ILE:HG21	1:A:130:ARG:CZ	0.50	2.36	7	1
1:A:76:GLU:O	1:A:77:VAL:CG2	0.50	2.59	8	1
1:A:9:PHE:O	1:A:25:PRO:HA	0.50	2.07	9	2
1:A:79:GLU:O	1:A:80:PHE:CB	0.50	2.59	7	1
1:A:121:PRO:C	1:A:122:LEU:HD13	0.50	2.27	1	1
1:A:67:VAL:HA	1:A:70:LEU:HD21	0.50	1.84	2	1
1:A:126:ILE:HB	1:A:127:PRO:HD2	0.50	1.84	3	1
1:A:91:ILE:HG23	1:A:95:LYS:HB3	0.49	1.84	4	1
1:A:9:PHE:N	1:A:25:PRO:HA	0.49	2.21	5	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:24:ILE:HD13	1:A:25:PRO:CD	0.49	2.37	4	1
1:A:7:GLU:O	1:A:26:LEU:CD2	0.49	2.59	1	1
1:A:23:THR:O	1:A:24:ILE:HG22	0.49	2.08	4	1
1:A:20:VAL:HG12	1:A:76:GLU:OE1	0.49	2.07	5	1
1:A:26:LEU:C	1:A:26:LEU:HD12	0.49	2.27	4	2
1:A:4:GLN:CB	1:A:9:PHE:CE1	0.49	2.95	10	1
1:A:24:ILE:O	1:A:25:PRO:O	0.49	2.30	3	4
1:A:8:TYR:HE2	1:A:10:ILE:HD11	0.49	1.68	7	2
1:A:83:LYS:NZ	1:A:113:VAL:HG22	0.49	2.23	10	1
1:A:103:ALA:HB1	1:A:109:SER:N	0.49	2.23	4	3
1:A:48:LEU:O	1:A:51:ALA:HB3	0.49	2.07	8	2
1:A:80:PHE:O	1:A:81:THR:CB	0.49	2.60	7	1
1:A:97:LEU:HD13	1:A:97:LEU:N	0.49	2.23	4	2
1:A:77:VAL:N	1:A:78:PRO:CD	0.48	2.76	3	2
1:A:48:LEU:HD12	1:A:48:LEU:C	0.48	2.28	4	1
1:A:22:ASN:CG	1:A:22:ASN:O	0.48	2.50	10	1
1:A:57:LEU:HD13	1:A:66:LYS:HE3	0.48	1.84	3	1
1:A:62:ILE:HD13	1:A:62:ILE:N	0.48	2.23	5	1
1:A:77:VAL:O	1:A:77:VAL:HG13	0.48	2.08	7	2
1:A:129:HIS:NE2	1:A:150:ILE:HD12	0.48	2.24	8	1
1:A:64:ASP:O	1:A:65:LYS:CB	0.48	2.62	4	3
1:A:66:LYS:HD2	1:A:125:ILE:HG22	0.48	1.85	9	1
1:A:19:LEU:HD21	1:A:22:ASN:HB2	0.47	1.84	3	1
1:A:27:ARG:CD	1:A:27:ARG:H	0.47	2.22	5	1
1:A:60:ALA:HB2	1:A:153:ARG:NE	0.47	2.23	7	1
1:A:77:VAL:HG22	1:A:77:VAL:O	0.47	2.09	10	1
1:A:85:LEU:HD23	1:A:126:ILE:CD1	0.47	2.38	1	1
1:A:87:ILE:HG22	1:A:127:PRO:CG	0.47	2.38	7	2
1:A:58:TYR:CD2	1:A:124:LEU:HD11	0.47	2.44	4	1
1:A:8:TYR:OH	1:A:55:LEU:HD21	0.47	2.08	6	1
1:A:97:LEU:O	1:A:130:ARG:O	0.47	2.33	5	1
1:A:103:ALA:HB1	1:A:109:SER:CA	0.47	2.40	10	1
1:A:13:ILE:O	1:A:13:ILE:HG23	0.47	2.10	10	3
1:A:4:GLN:HB3	1:A:9:PHE:CZ	0.47	2.45	6	2
1:A:84:VAL:HG13	1:A:102:ILE:HG21	0.47	1.86	5	1
1:A:57:LEU:HD22	1:A:66:LYS:HE2	0.47	1.87	8	1
1:A:57:LEU:HA	1:A:62:ILE:HD11	0.47	1.86	2	1
1:A:4:GLN:CB	1:A:9:PHE:CZ	0.47	2.97	4	2
1:A:19:LEU:O	1:A:73:TYR:HA	0.47	2.09	8	1
1:A:117:LEU:HD23	1:A:117:LEU:N	0.47	2.25	5	1
1:A:87:ILE:HD12	1:A:102:ILE:CG1	0.47	2.38	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:25:PRO:O	1:A:26:LEU:O	0.46	2.33	10	3
1:A:9:PHE:CE2	1:A:25:PRO:O	0.46	2.68	9	1
1:A:75:LEU:HD23	1:A:75:LEU:O	0.46	2.10	4	1
1:A:129:HIS:NE2	1:A:150:ILE:HG21	0.46	2.26	7	1
1:A:122:LEU:O	1:A:125:ILE:HD13	0.46	2.11	6	1
1:A:91:ILE:HD13	1:A:130:ARG:CB	0.46	2.41	7	1
1:A:20:VAL:HG12	1:A:121:PRO:CG	0.46	2.40	8	1
1:A:80:PHE:O	1:A:81:THR:HG22	0.46	2.11	7	1
1:A:93:PHE:O	1:A:93:PHE:CD2	0.46	2.68	7	1
1:A:108:THR:HG23	1:A:109:SER:N	0.46	2.25	2	2
1:A:8:TYR:CG	1:A:8:TYR:O	0.46	2.69	5	1
1:A:8:TYR:CD2	1:A:10:ILE:HD11	0.46	2.46	3	1
1:A:88:VAL:HB	1:A:127:PRO:HD3	0.46	1.88	8	3
1:A:24:ILE:O	1:A:24:ILE:HG22	0.46	2.11	10	2
1:A:5:ILE:HD12	1:A:10:ILE:CD1	0.46	2.40	3	1
1:A:98:THR:O	1:A:102:ILE:HD12	0.46	2.11	6	2
1:A:21:ARG:NH1	1:A:24:ILE:HD11	0.46	2.26	2	1
1:A:99:TYR:HA	1:A:102:ILE:HD12	0.45	1.87	8	1
1:A:7:GLU:HB3	1:A:26:LEU:HD23	0.45	1.86	1	1
1:A:102:ILE:HD12	1:A:131:VAL:HG13	0.45	1.85	3	3
1:A:70:LEU:HD12	1:A:122:LEU:HD23	0.45	1.88	3	1
1:A:102:ILE:HG22	1:A:106:LEU:CD1	0.45	2.40	7	2
1:A:122:LEU:N	1:A:123:PRO:CD	0.45	2.79	4	2
1:A:132:VAL:HG12	1:A:137:LEU:HB3	0.45	1.89	5	1
1:A:8:TYR:CE1	1:A:55:LEU:HD13	0.45	2.47	3	1
1:A:120:ASN:ND2	1:A:126:ILE:HD13	0.45	2.26	10	1
1:A:103:ALA:HB2	1:A:113:VAL:HG21	0.45	1.87	1	3
1:A:70:LEU:HD22	1:A:125:ILE:HG13	0.45	1.89	2	1
1:A:143:GLY:O	1:A:144:LEU:CB	0.45	2.65	3	2
1:A:87:ILE:HG22	1:A:127:PRO:HG3	0.45	1.88	7	1
1:A:88:VAL:HG23	1:A:130:ARG:NH2	0.45	2.27	3	1
1:A:19:LEU:HD11	1:A:22:ASN:HB2	0.45	1.89	3	1
1:A:80:PHE:CE1	1:A:83:LYS:CD	0.45	3.00	3	1
1:A:106:LEU:O	1:A:107:ASN:CB	0.45	2.63	4	5
1:A:8:TYR:O	1:A:8:TYR:CD2	0.45	2.69	5	2
1:A:120:ASN:ND2	1:A:126:ILE:HD12	0.45	2.27	7	1
1:A:80:PHE:CD2	1:A:80:PHE:O	0.45	2.70	8	1
1:A:106:LEU:HD23	1:A:106:LEU:N	0.45	2.27	8	1
1:A:13:ILE:HG22	1:A:21:ARG:O	0.45	2.11	1	1
1:A:142:TYR:CE1	1:A:146:LYS:CE	0.45	2.99	1	1
1:A:103:ALA:HB1	1:A:109:SER:C	0.45	2.32	9	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:14:PHE:CB	1:A:19:LEU:HD12	0.45	2.41	4	1
1:A:91:ILE:HD13	1:A:130:ARG:NE	0.45	2.26	8	1
1:A:70:LEU:HD22	1:A:125:ILE:CG2	0.45	2.39	1	1
1:A:56:LYS:HD2	1:A:62:ILE:HD12	0.44	1.89	9	1
1:A:57:LEU:HD22	1:A:66:LYS:HD2	0.44	1.88	1	1
1:A:83:LYS:HZ2	1:A:113:VAL:HG22	0.44	1.71	10	1
1:A:80:PHE:O	1:A:81:THR:HB	0.44	2.12	7	1
1:A:10:ILE:O	1:A:10:ILE:HG22	0.44	2.12	2	1
1:A:19:LEU:O	1:A:74:LYS:N	0.44	2.51	6	2
1:A:57:LEU:HA	1:A:62:ILE:HD12	0.44	1.88	5	1
1:A:14:PHE:HD2	1:A:19:LEU:HD12	0.44	1.72	7	1
1:A:67:VAL:HG22	1:A:125:ILE:CG1	0.44	2.42	10	1
1:A:81:THR:O	1:A:84:VAL:HG23	0.44	2.13	1	6
1:A:19:LEU:HD13	1:A:71:ILE:HD12	0.44	1.89	7	1
1:A:87:ILE:CG2	1:A:127:PRO:CG	0.44	2.96	7	1
1:A:80:PHE:CD1	1:A:80:PHE:O	0.44	2.70	9	1
1:A:117:LEU:HD12	1:A:117:LEU:C	0.44	2.32	1	6
1:A:122:LEU:HB3	1:A:125:ILE:HD11	0.44	1.89	1	1
1:A:117:LEU:HA	1:A:120:ASN:OD1	0.44	2.13	7	1
1:A:99:TYR:HE1	1:A:117:LEU:HD11	0.43	1.73	2	2
1:A:23:THR:CG2	1:A:121:PRO:O	0.43	2.66	1	1
1:A:4:GLN:HB2	1:A:9:PHE:CZ	0.43	2.49	3	1
1:A:98:THR:C	1:A:102:ILE:HD12	0.43	2.33	3	1
1:A:120:ASN:CG	1:A:126:ILE:HD12	0.43	2.34	7	1
1:A:57:LEU:HD22	1:A:66:LYS:CD	0.43	2.42	9	1
1:A:126:ILE:HD12	1:A:128:CYS:HB3	0.43	1.89	3	1
1:A:70:LEU:HD13	1:A:70:LEU:C	0.43	2.32	8	1
1:A:9:PHE:CE1	1:A:27:ARG:O	0.43	2.71	10	2
1:A:5:ILE:CG2	1:A:8:TYR:CZ	0.43	3.01	9	2
1:A:83:LYS:CB	1:A:106:LEU:HD22	0.43	2.44	6	2
1:A:67:VAL:HG13	1:A:68:ARG:N	0.43	2.28	6	1
1:A:122:LEU:HB2	1:A:125:ILE:CD1	0.43	2.43	6	1
1:A:88:VAL:HB	1:A:127:PRO:CG	0.43	2.44	7	1
1:A:13:ILE:HG23	1:A:21:ARG:HB3	0.43	1.91	5	1
1:A:152:GLU:O	1:A:156:LEU:HD23	0.43	2.14	7	1
1:A:126:ILE:CG2	1:A:127:PRO:HD2	0.43	2.44	7	1
1:A:2:ILE:HG22	1:A:3:ILE:N	0.43	2.29	8	1
1:A:123:PRO:HB2	1:A:124:LEU:HD12	0.43	1.89	3	1
1:A:81:THR:CB	1:A:116:ALA:HB1	0.43	2.44	9	1
1:A:20:VAL:O	1:A:121:PRO:CB	0.42	2.67	2	1
1:A:59:PHE:O	1:A:60:ALA:CB	0.42	2.67	5	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:99:TYR:CE2	1:A:131:VAL:O	0.42	2.72	2	2
1:A:14:PHE:CB	1:A:19:LEU:HA	0.42	2.44	4	1
1:A:87:ILE:HG22	1:A:88:VAL:N	0.42	2.28	6	1
1:A:8:TYR:HA	1:A:26:LEU:N	0.42	2.29	7	1
1:A:9:PHE:CZ	1:A:27:ARG:HA	0.42	2.49	7	1
1:A:122:LEU:N	1:A:123:PRO:HD3	0.42	2.30	4	1
1:A:20:VAL:HG12	1:A:76:GLU:CD	0.42	2.34	5	1
1:A:80:PHE:O	1:A:80:PHE:CG	0.42	2.72	8	1
1:A:124:LEU:O	1:A:125:ILE:CG2	0.42	2.60	9	1
1:A:4:GLN:HB3	1:A:9:PHE:CE1	0.42	2.49	10	1
1:A:26:LEU:O	1:A:27:ARG:CB	0.42	2.67	4	1
1:A:81:THR:HG21	1:A:120:ASN:OD1	0.42	2.14	4	1
1:A:97:LEU:HD22	1:A:130:ARG:O	0.42	2.15	4	1
1:A:153:ARG:HD2	1:A:154:GLU:N	0.42	2.29	5	1
1:A:22:ASN:O	1:A:23:THR:CG2	0.42	2.68	7	2
1:A:91:ILE:HD12	1:A:130:ARG:NE	0.42	2.28	3	1
1:A:73:TYR:CE2	1:A:125:ILE:HD11	0.42	2.48	3	1
1:A:81:THR:OG1	1:A:120:ASN:ND2	0.42	2.53	6	1
1:A:87:ILE:HD11	1:A:130:ARG:NH1	0.42	2.29	8	1
1:A:57:LEU:HD22	1:A:66:LYS:CE	0.42	2.44	9	1
1:A:84:VAL:CG1	1:A:113:VAL:CG1	0.42	2.97	6	1
1:A:50:VAL:O	1:A:54:ILE:HD12	0.42	2.14	8	1
1:A:99:TYR:CZ	1:A:131:VAL:O	0.42	2.73	9	1
1:A:122:LEU:HB2	1:A:125:ILE:HD11	0.42	1.91	9	1
1:A:78:PRO:O	1:A:79:GLU:CB	0.42	2.66	5	2
1:A:91:ILE:HG22	1:A:130:ARG:HH11	0.42	1.73	2	1
1:A:22:ASN:C	1:A:23:THR:CG2	0.42	2.87	10	2
1:A:98:THR:CB	1:A:132:VAL:O	0.42	2.68	5	1
1:A:77:VAL:N	1:A:78:PRO:HD3	0.42	2.29	8	1
1:A:26:LEU:C	1:A:26:LEU:CD1	0.41	2.88	1	1
1:A:66:LYS:HE3	1:A:125:ILE:HG22	0.41	1.92	1	1
1:A:100:GLY:O	1:A:104:LYS:CB	0.41	2.67	9	2
1:A:80:PHE:O	1:A:116:ALA:HB1	0.41	2.15	3	1
1:A:27:ARG:O	1:A:27:ARG:HG2	0.41	2.15	9	1
1:A:9:PHE:O	1:A:24:ILE:HG23	0.41	2.14	4	1
1:A:23:THR:O	1:A:24:ILE:CG2	0.41	2.69	4	1
1:A:26:LEU:CD1	1:A:27:ARG:N	0.41	2.84	4	2
1:A:54:ILE:HA	1:A:57:LEU:HD21	0.41	1.93	10	1
1:A:3:ILE:HD11	1:A:10:ILE:HB	0.41	1.91	4	1
1:A:96:THR:O	1:A:97:LEU:HD12	0.41	2.16	8	1
1:A:10:ILE:HG23	1:A:23:THR:CA	0.41	2.46	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:56:LYS:HB2	1:A:62:ILE:HD11	0.41	1.92	7	1
1:A:65:LYS:O	1:A:66:LYS:CB	0.41	2.68	8	1
1:A:8:TYR:O	1:A:8:TYR:CG	0.41	2.74	9	1
1:A:125:ILE:N	1:A:125:ILE:HD12	0.41	2.30	2	1
1:A:13:ILE:HG23	1:A:13:ILE:O	0.41	2.15	5	1
1:A:91:ILE:CG2	1:A:95:LYS:CB	0.41	2.99	5	1
1:A:77:VAL:CG2	1:A:78:PRO:CD	0.41	2.98	6	1
1:A:58:TYR:O	1:A:58:TYR:CD1	0.41	2.73	8	1
1:A:5:ILE:O	1:A:8:TYR:CD1	0.41	2.73	9	1
1:A:97:LEU:HD23	1:A:101:ASP:HB3	0.41	1.92	10	1
1:A:76:GLU:O	1:A:77:VAL:CG1	0.41	2.69	2	1
1:A:19:LEU:CB	1:A:71:ILE:HB	0.41	2.46	8	1
1:A:9:PHE:O	1:A:24:ILE:CG2	0.41	2.69	4	1
1:A:22:ASN:OD1	1:A:122:LEU:CD1	0.41	2.69	4	1
1:A:141:SER:O	1:A:143:GLY:N	0.41	2.54	8	2
1:A:61:GLU:O	1:A:62:ILE:O	0.41	2.39	8	1
1:A:73:TYR:CD1	1:A:122:LEU:CD1	0.41	3.04	8	1
1:A:120:ASN:CG	1:A:126:ILE:HG21	0.41	2.35	3	1
1:A:93:PHE:CZ	1:A:154:GLU:OE2	0.41	2.74	4	1
1:A:9:PHE:CB	1:A:24:ILE:O	0.41	2.69	6	1
1:A:122:LEU:C	1:A:126:ILE:HD12	0.40	2.36	4	1
1:A:10:ILE:HG21	1:A:54:ILE:HD13	0.40	1.93	8	1
1:A:117:LEU:O	1:A:120:ASN:ND2	0.40	2.54	9	1
1:A:83:LYS:CB	1:A:106:LEU:CD1	0.40	2.99	10	1
1:A:120:ASN:CB	1:A:121:PRO:CD	0.40	2.99	4	1
1:A:84:VAL:HG13	1:A:113:VAL:CG1	0.40	2.46	6	1
1:A:96:THR:HA	1:A:130:ARG:HG2	0.40	1.93	8	1
1:A:6:GLU:HB2	1:A:8:TYR:CE1	0.40	2.52	4	1
1:A:85:LEU:O	1:A:88:VAL:CG1	0.40	2.65	7	1
1:A:73:TYR:CE2	1:A:85:LEU:HD22	0.40	2.52	5	1
1:A:99:TYR:CD2	1:A:132:VAL:O	0.40	2.75	7	1
1:A:77:VAL:CG2	1:A:81:THR:HG22	0.40	2.46	9	1
1:A:10:ILE:CG2	1:A:22:ASN:ND2	0.40	2.84	3	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	135/167 (81%)	90±3 (67±2%)	29±3 (21±3%)	17±3 (12±2%)	1 6
All	All	1350/1670 (81%)	898 (67%)	286 (21%)	166 (12%)	1 6

All 41 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	20	VAL	10
1	A	25	PRO	10
1	A	71	ILE	10
1	A	6	GLU	9
1	A	24	ILE	9
1	A	81	THR	8
1	A	116	ALA	8
1	A	107	ASN	7
1	A	26	LEU	7
1	A	143	GLY	6
1	A	60	ALA	6
1	A	65	LYS	6
1	A	135	ASN	5
1	A	137	LEU	5
1	A	79	GLU	5
1	A	68	ARG	4
1	A	80	PHE	4
1	A	131	VAL	4
1	A	63	ASP	4
1	A	125	ILE	3
1	A	123	PRO	3
1	A	136	SER	3
1	A	27	ARG	2
1	A	67	VAL	2
1	A	142	TYR	2
1	A	76	GLU	2
1	A	138	GLY	2
1	A	140	TYR	2
1	A	92	GLU	2
1	A	139	GLY	2
1	A	112	ALA	2
1	A	62	ILE	2
1	A	64	ASP	2
1	A	141	SER	1

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Mol	Chain	Res	Type	Models (Total)
1	A	5	ILE	1
1	A	48	LEU	1
1	A	144	LEU	1
1	A	66	LYS	1
1	A	124	LEU	1
1	A	75	LEU	1
1	A	134	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	122/152 (80%)	86±4 (70±4%)	36±4 (30±4%)	1 17
All	All	1220/1520 (80%)	857 (70%)	363 (30%)	1 17

All 101 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	20	VAL	10
1	A	27	ARG	9
1	A	14	PHE	8
1	A	66	LYS	8
1	A	82	LYS	8
1	A	104	LYS	8
1	A	21	ARG	7
1	A	109	SER	7
1	A	73	TYR	7
1	A	119	ARG	7
1	A	57	LEU	6
1	A	68	ARG	6
1	A	83	LYS	6
1	A	140	TYR	6
1	A	155	ARG	6
1	A	76	GLU	6
1	A	84	VAL	6
1	A	106	LEU	6

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Mol	Chain	Res	Type	Models (Total)
1	A	148	LYS	6
1	A	1	MET	5
1	A	10	ILE	5
1	A	63	ASP	5
1	A	72	SER	5
1	A	74	LYS	5
1	A	79	GLU	5
1	A	80	PHE	5
1	A	101	ASP	5
1	A	125	ILE	5
1	A	62	ILE	5
1	A	134	LYS	5
1	A	70	LEU	5
1	A	118	LYS	5
1	A	146	LYS	5
1	A	7	GLU	4
1	A	97	LEU	4
1	A	107	ASN	4
1	A	124	LEU	4
1	A	105	LYS	4
1	A	142	TYR	4
1	A	144	LEU	4
1	A	12	MET	4
1	A	90	ASP	4
1	A	4	GLN	4
1	A	89	LYS	4
1	A	23	THR	3
1	A	56	LYS	3
1	A	87	ILE	3
1	A	152	GLU	3
1	A	111	ARG	3
1	A	52	GLU	3
1	A	75	LEU	3
1	A	130	ARG	3
1	A	137	LEU	3
1	A	6	GLU	3
1	A	18	GLN	3
1	A	65	LYS	3
1	A	156	LEU	3
1	A	26	LEU	3
1	A	59	PHE	3
1	A	102	ILE	3

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Mol	Chain	Res	Type	Models (Total)
1	A	135	ASN	3
1	A	147	LYS	3
1	A	85	LEU	3
1	A	92	GLU	3
1	A	49	LYS	2
1	A	115	MET	2
1	A	95	LYS	2
1	A	98	THR	2
1	A	120	ASN	2
1	A	136	SER	2
1	A	91	ILE	2
1	A	3	ILE	2
1	A	15	LYS	2
1	A	17	ASN	2
1	A	58	TYR	2
1	A	71	ILE	2
1	A	141	SER	2
1	A	153	ARG	2
1	A	108	THR	2
1	A	117	LEU	2
1	A	151	LEU	2
1	A	48	LEU	2
1	A	86	ASP	2
1	A	13	ILE	1
1	A	64	ASP	1
1	A	126	ILE	1
1	A	24	ILE	1
1	A	77	VAL	1
1	A	121	PRO	1
1	A	69	GLU	1
1	A	9	PHE	1
1	A	61	GLU	1
1	A	78	PRO	1
1	A	145	ASP	1
1	A	81	THR	1
1	A	96	THR	1
1	A	122	LEU	1
1	A	149	PHE	1
1	A	154	GLU	1
1	A	22	ASN	1
1	A	55	LEU	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