



# Full wwPDB NMR Structure Validation Report ⓘ

Mar 6, 2022 – 06:11 PM EST

PDB ID : 2ORC  
Title : CRO REPRESSOR INSERTION MUTANT K56-[DGEVK], NMR, 32  
STRUCTURES  
Authors : Mossing, M.C.  
Deposited on : 1998-01-20

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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 ⓘ symbol.

---

The following versions of software and data (see [references ⓘ](#)) 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

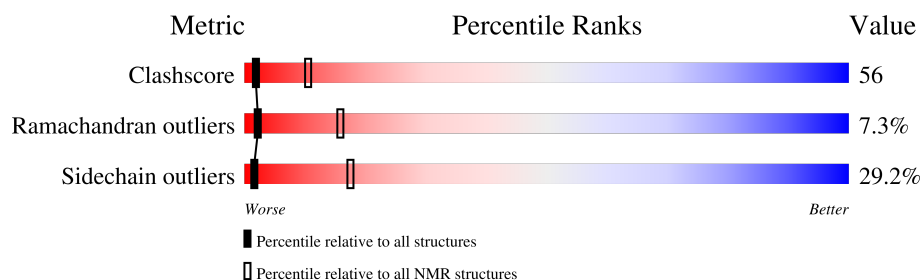
# 1 Overall quality at a glance

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  $\geq 3$ , 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  $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	71	<div> <div>15%</div> <div>59%</div> <div>14%</div> <div>11%</div> </div>

## 2 Ensemble composition and analysis

This entry contains 32 models. Model 26 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:3-A:60 (58)	0.73	26

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 1 single-model cluster was found.

Cluster number	Models
1	1, 2, 3, 4, 5, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 23, 24, 26, 27, 28, 29, 30, 31, 32
2	6, 22
Single-model clusters	25

### 3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1124 atoms, of which 569 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called CRO REPRESSOR.

Mol	Chain	Residues	Atoms						Trace
1	A	71	Total	C	H	N	O	S	0
			1124	350	569	97	106	2	

There are 5 discrepancies between the modelled and reference sequences:

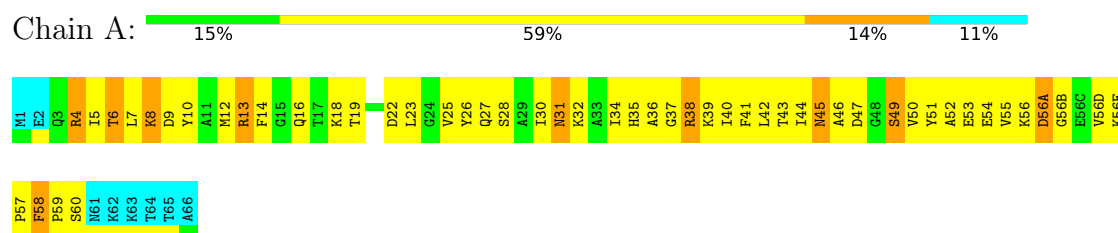
Chain	Residue	Modelled	Actual	Comment	Reference
A	54	GLU	-	insertion	UNP P03040
A	55	VAL	-	insertion	UNP P03040
A	56	LYS	-	insertion	UNP P03040
A	56A	ASP	-	insertion	UNP P03040
A	56B	GLY	-	insertion	UNP P03040

## 4 Residue-property plots

### 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: CRO REPRESSOR

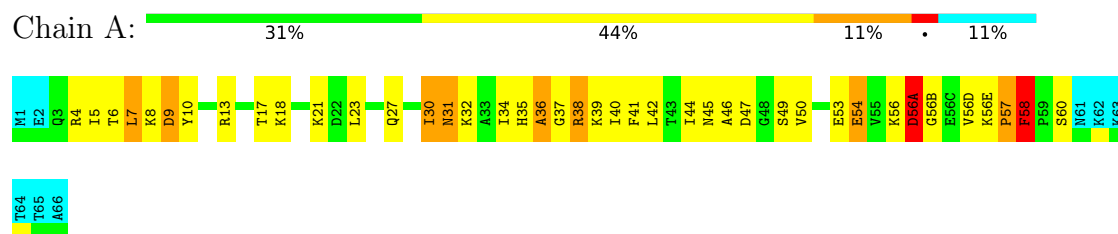


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

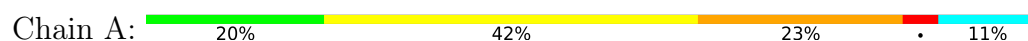
#### 4.2.1 Score per residue for model 1

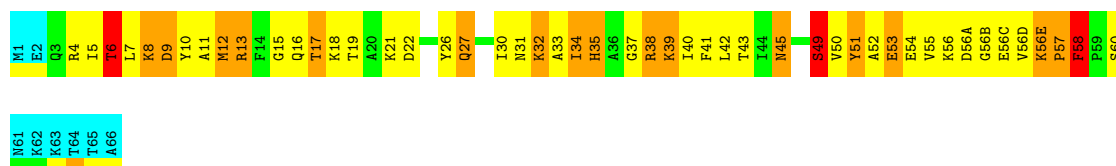
#### • Molecule 1: CRO REPRESSOR



#### 4.2.2 Score per residue for model 2

#### • Molecule 1: CRO REPRESSOR

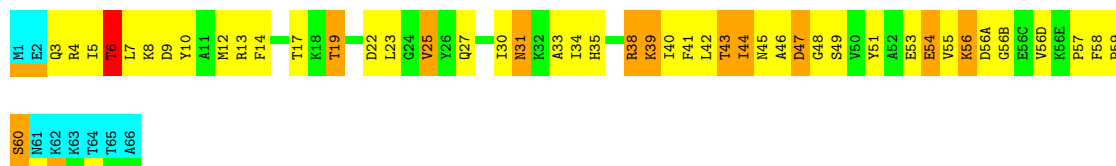




#### 4.2.3 Score per residue for model 3

- Molecule 1: CRO REPRESSOR

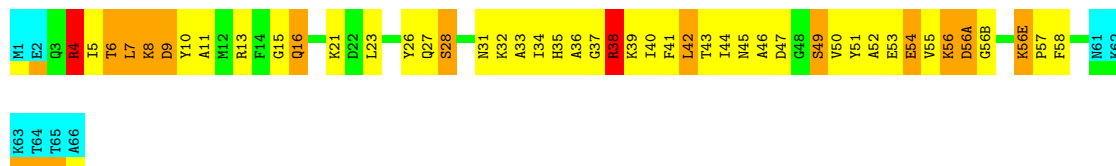
Chain A: 24% 48% 15% 11%



#### 4.2.4 Score per residue for model 4

- Molecule 1: CRO REPRESSOR

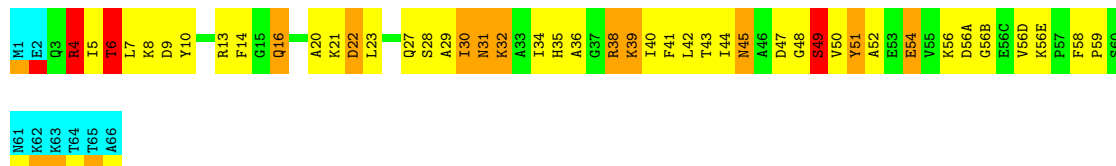
Chain A: 24% 45% 17% 11%



#### 4.2.5 Score per residue for model 5

- Molecule 1: CRO REPRESSOR

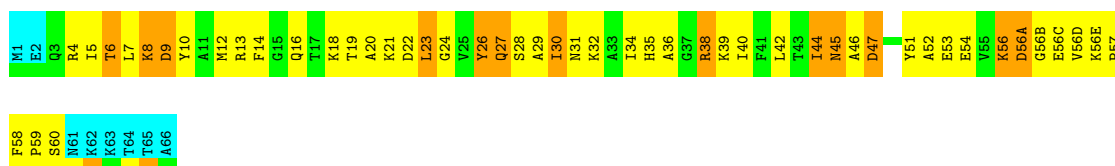
Chain A: 25% 45% 14% 11%



#### 4.2.6 Score per residue for model 6

- Molecule 1: CRO REPRESSOR

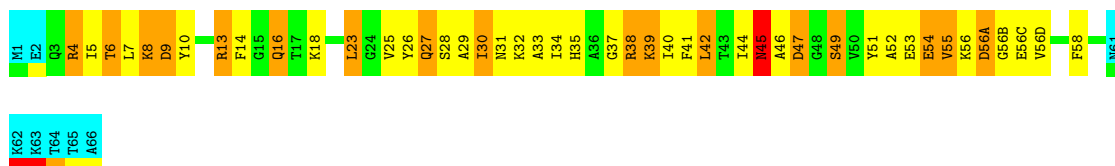
Chain A: 18% 52% 18% 11%



#### 4.2.7 Score per residue for model 7

- Molecule 1: CRO REPRESSOR

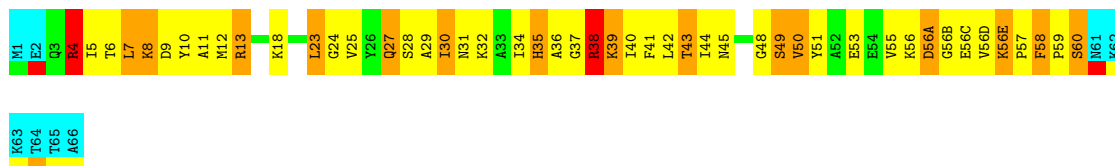
Chain A: 25% 38% 24% 11%



#### 4.2.8 Score per residue for model 8

- Molecule 1: CRO REPRESSOR

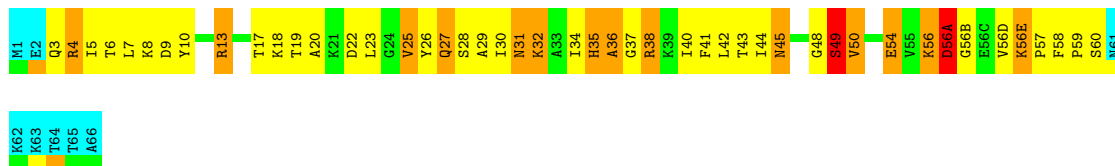
Chain A: 21% 44% 21% 11%



#### 4.2.9 Score per residue for model 9

- Molecule 1: CRO REPRESSOR

Chain A: 23% 44% 20% 11%



#### 4.2.10 Score per residue for model 10

- Molecule 1: CRO REPRESSOR

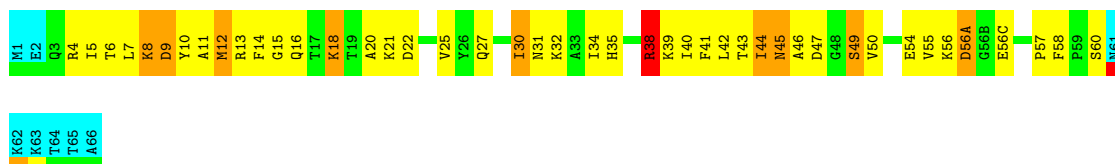
Chain A: 32% 38% 18% 11%



#### 4.2.11 Score per residue for model 11

- Molecule 1: CRO REPRESSOR

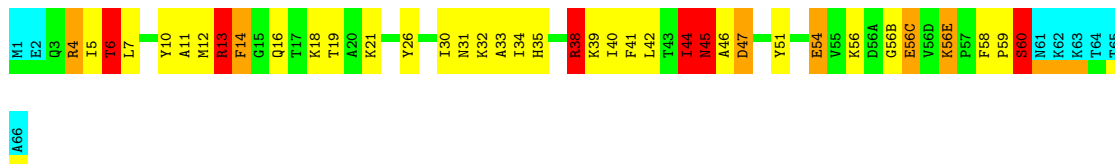
Chain A: 27% 48% 13% 11%



#### 4.2.12 Score per residue for model 12

- Molecule 1: CRO REPRESSOR

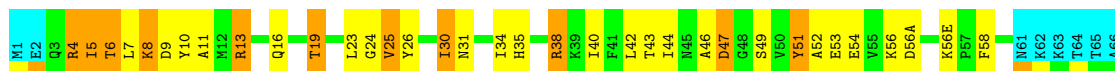
Chain A: 35% 37% 8% 8% 11%



#### 4.2.13 Score per residue for model 13

- Molecule 1: CRO REPRESSOR

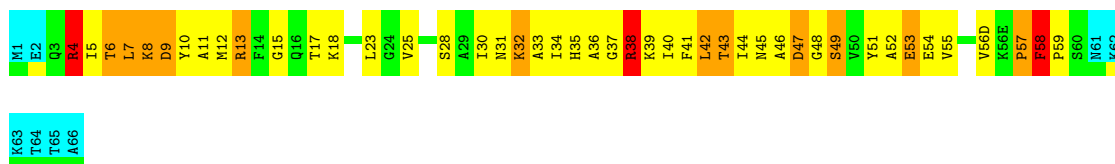
Chain A: 39% 34% 15% 11%



#### 4.2.14 Score per residue for model 14

- Molecule 1: CRO REPRESSOR

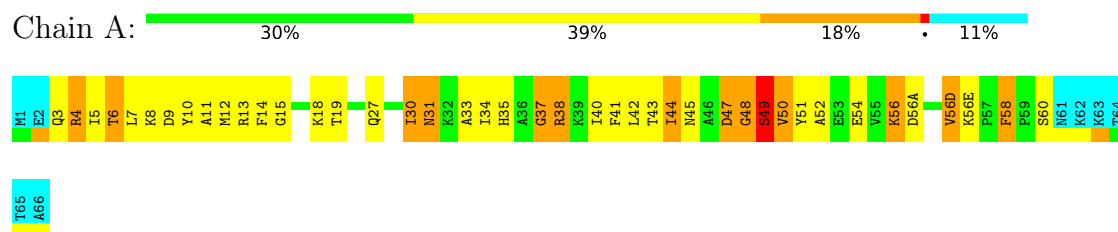
Chain A: 25% 42% 17% 11%





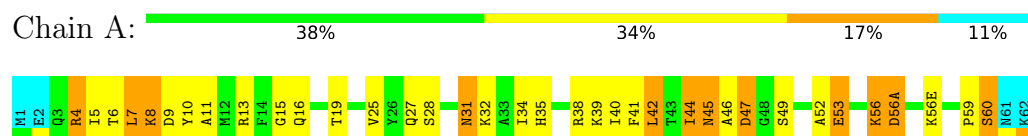
#### 4.2.15 Score per residue for model 15

- Molecule 1: CRO REPRESSOR



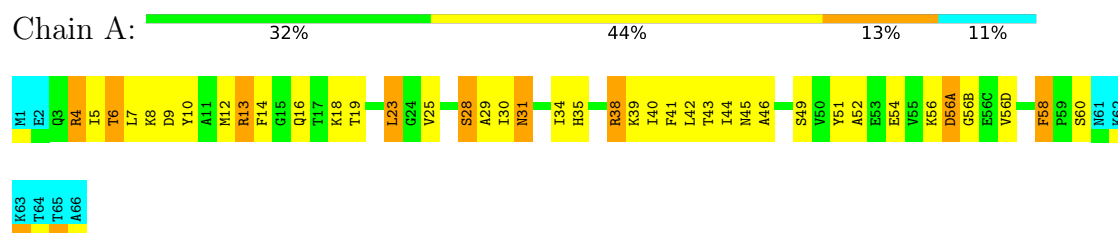
#### 4.2.16 Score per residue for model 16

- Molecule 1: CRO REPRESSOR



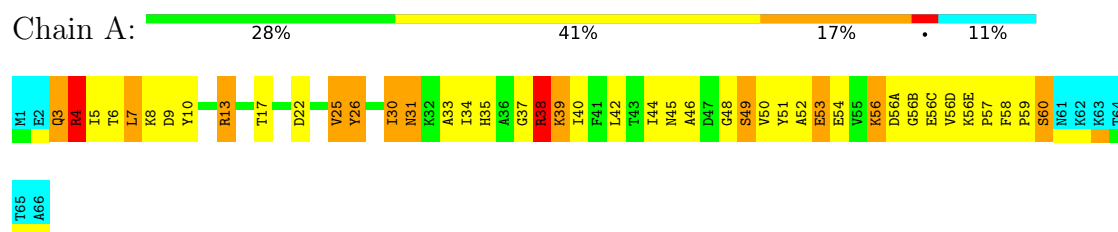
#### 4.2.17 Score per residue for model 17

- Molecule 1: CRO REPRESSOR



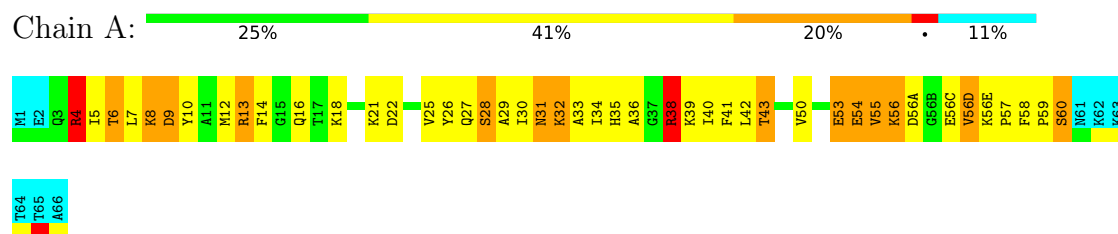
#### 4.2.18 Score per residue for model 18

- Molecule 1: CRO REPRESSOR



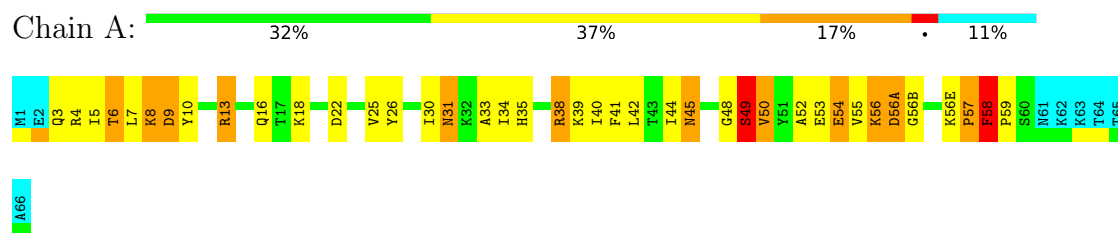
### 4.2.19 Score per residue for model 19

- Molecule 1: CRO REPRESSOR



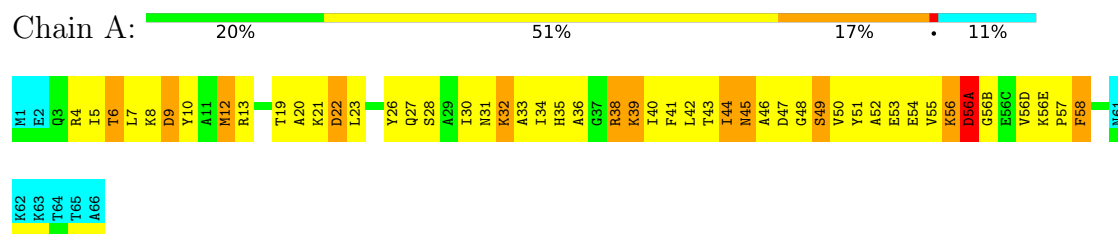
### 4.2.20 Score per residue for model 20

- Molecule 1: CRO REPRESSOR



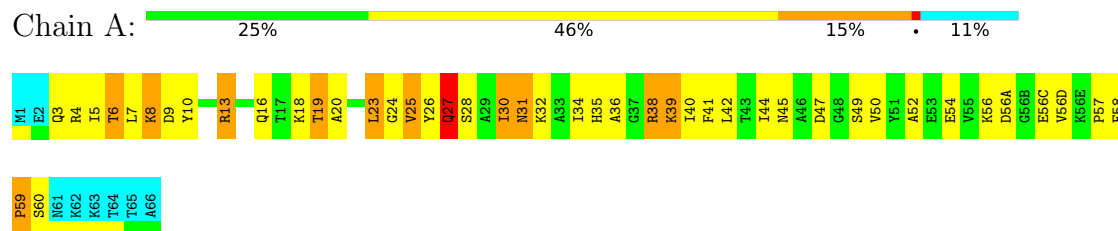
### 4.2.21 Score per residue for model 21

- Molecule 1: CRO REPRESSOR



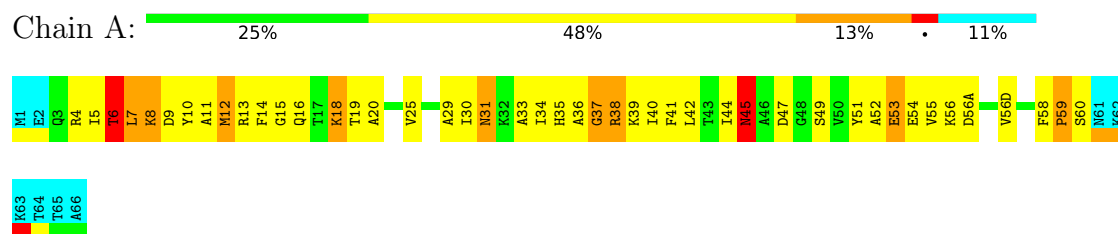
### 4.2.22 Score per residue for model 22

- Molecule 1: CRO REPRESSOR



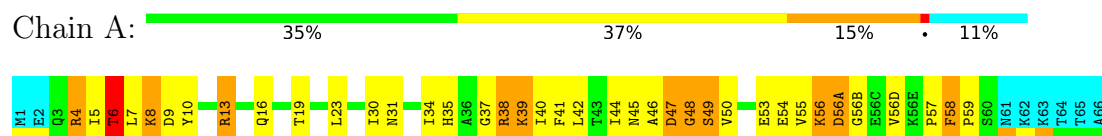
### 4.2.23 Score per residue for model 23

#### • Molecule 1: CRO REPRESSOR



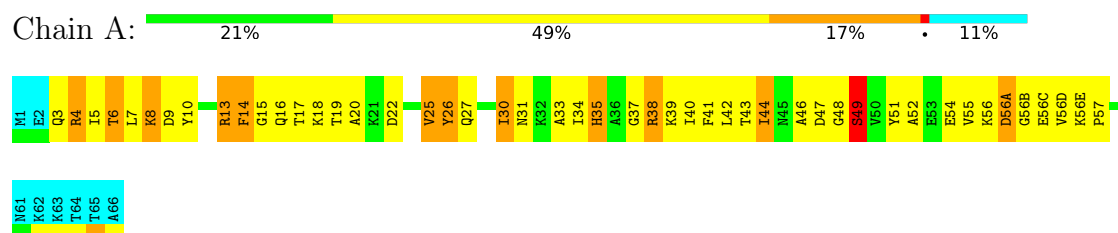
### 4.2.24 Score per residue for model 24

#### • Molecule 1: CRO REPRESSOR



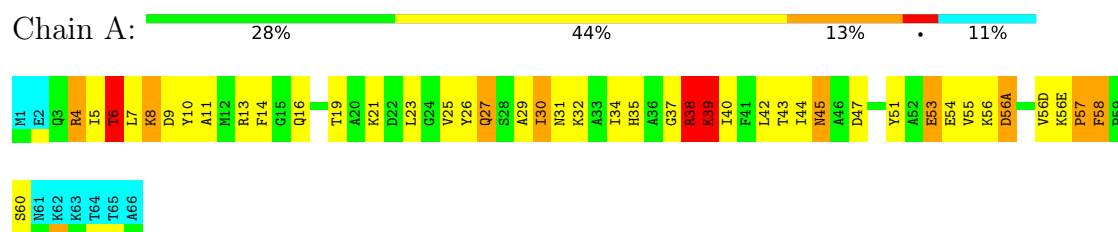
### 4.2.25 Score per residue for model 25

#### • Molecule 1: CRO REPRESSOR



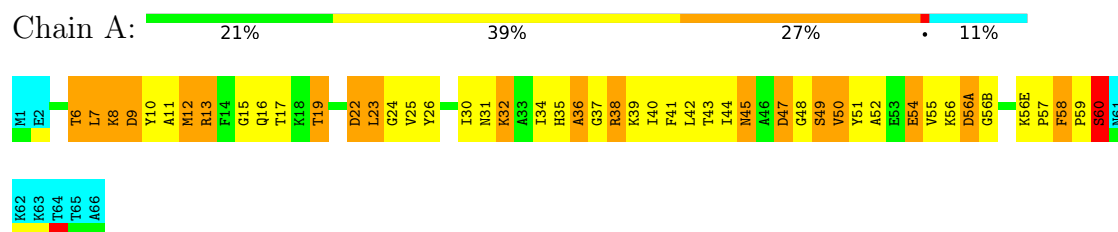
### 4.2.26 Score per residue for model 26 (medoid)

#### • Molecule 1: CRO REPRESSOR



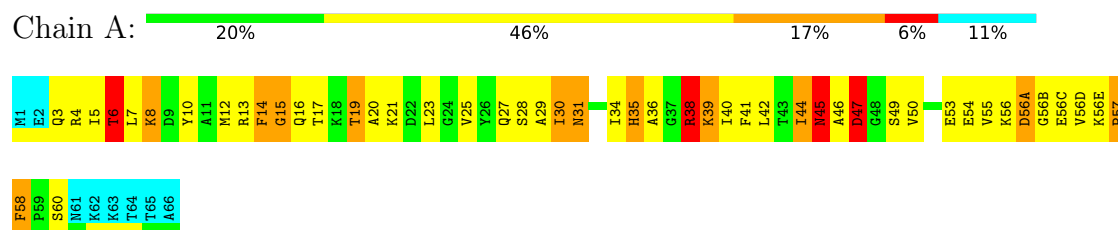
### 4.2.27 Score per residue for model 27

- Molecule 1: CRO REPRESSOR



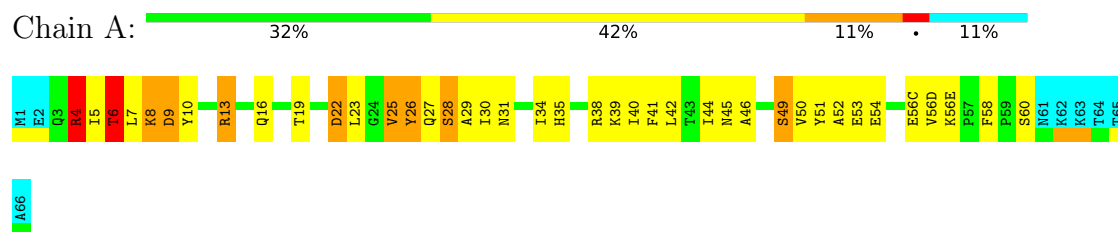
### 4.2.28 Score per residue for model 28

- Molecule 1: CRO REPRESSOR



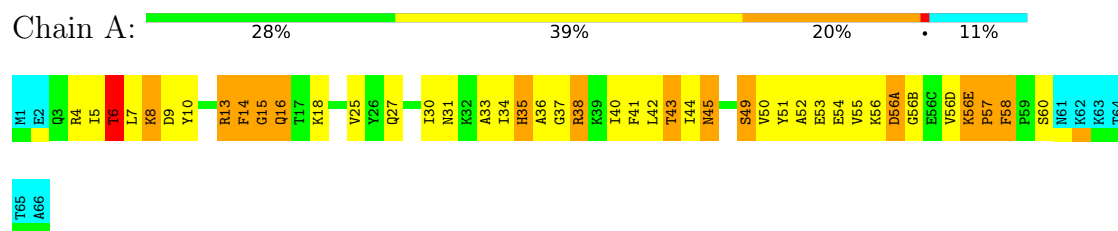
### 4.2.29 Score per residue for model 29

- Molecule 1: CRO REPRESSOR



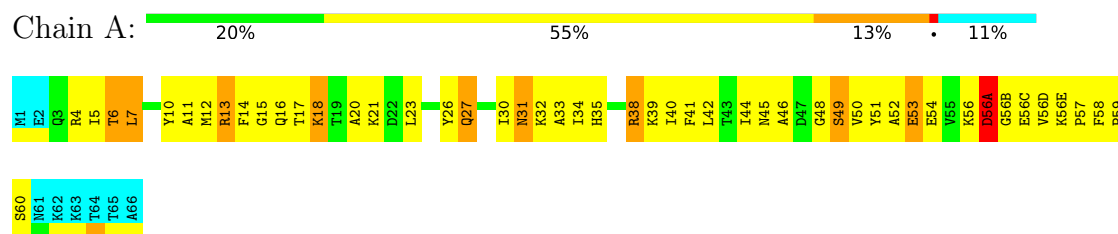
### 4.2.30 Score per residue for model 30

- Molecule 1: CRO REPRESSOR



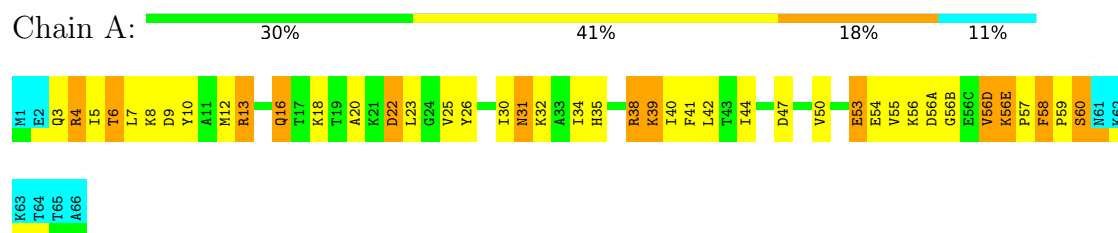
### 4.2.31 Score per residue for model 31

#### • Molecule 1: CRO REPRESSOR



### 4.2.32 Score per residue for model 32

#### • Molecule 1: CRO REPRESSOR



## 5 Refinement protocol and experimental data overview

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

Of the 50 calculated structures, 32 were deposited, based on the following criterion: *NO DISTANCE VIOLATION > 0.5Å, NO DIHEDRAL VIOLATION > 5 DEGREES*.

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

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

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.

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	2.8±0.6
All	All	0	88

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

All unique planar outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	13	ARG	Sidechain	31
1	A	38	ARG	Sidechain	29
1	A	4	ARG	Sidechain	28

### 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	492	501	501	56±11
All	All	15744	16032	16032	1783

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 56.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:23:LEU:HD12	1:A:25:VAL:HG21	1.04	1.23	7	2
1:A:7:LEU:HD12	1:A:40:ILE:HD13	0.97	1.32	23	2
1:A:7:LEU:CD1	1:A:42:LEU:HD11	0.96	1.91	4	5
1:A:22:ASP:OD2	1:A:50:VAL:HG11	0.95	1.62	19	1
1:A:23:LEU:HD22	1:A:42:LEU:HD22	0.93	1.36	22	1
1:A:7:LEU:HD23	1:A:40:ILE:HD12	0.92	1.38	18	3
1:A:7:LEU:HD22	1:A:40:ILE:HD13	0.92	1.40	21	1
1:A:44:ILE:HG23	1:A:49:SER:O	0.91	1.64	9	12
1:A:7:LEU:HD13	1:A:34:ILE:HG12	0.91	1.41	23	1
1:A:7:LEU:HD22	1:A:40:ILE:HD12	0.90	1.43	20	11
1:A:5:ILE:O	1:A:42:LEU:HD12	0.90	1.66	16	3
1:A:7:LEU:HD23	1:A:40:ILE:HD13	0.89	1.41	3	5
1:A:55:VAL:O	1:A:56(D):VAL:HG12	0.89	1.66	25	1
1:A:27:GLN:HA	1:A:30:ILE:HD12	0.88	1.45	3	1
1:A:23:LEU:HD11	1:A:25:VAL:CG2	0.88	1.99	8	2
1:A:23:LEU:HD12	1:A:25:VAL:CG2	0.86	1.99	7	2
1:A:37:GLY:O	1:A:40:ILE:HD11	0.86	1.69	2	4
1:A:7:LEU:HB2	1:A:34:ILE:HD11	0.85	1.47	4	1
1:A:7:LEU:HD12	1:A:42:LEU:HD11	0.85	1.47	21	3
1:A:22:ASP:HB3	1:A:50:VAL:HG11	0.83	1.47	32	2
1:A:5:ILE:HG22	1:A:10:TYR:HB2	0.82	1.49	14	20
1:A:46:ALA:HB3	1:A:49:SER:CB	0.82	2.03	25	5
1:A:7:LEU:HD23	1:A:40:ILE:CD1	0.82	2.05	28	2
1:A:23:LEU:HD22	1:A:42:LEU:CD2	0.81	2.03	22	2
1:A:7:LEU:HD12	1:A:19:THR:HG21	0.81	1.49	25	1
1:A:7:LEU:HD11	1:A:42:LEU:HD21	0.80	1.54	10	4
1:A:49:SER:O	1:A:50:VAL:HG23	0.79	1.77	9	6
1:A:42:LEU:HD12	1:A:42:LEU:N	0.77	1.95	27	17
1:A:7:LEU:CB	1:A:34:ILE:HD11	0.77	2.09	4	3
1:A:7:LEU:CD2	1:A:40:ILE:HD12	0.77	2.10	20	9
1:A:17:THR:HG23	1:A:27:GLN:OE1	0.76	1.81	2	1
1:A:7:LEU:HD21	1:A:40:ILE:HG21	0.76	1.57	18	5
1:A:7:LEU:CD1	1:A:42:LEU:HD21	0.76	2.11	10	5
1:A:46:ALA:HB3	1:A:49:SER:HB2	0.76	1.58	25	3
1:A:8:LYS:HB2	1:A:34:ILE:HD13	0.75	1.57	2	2
1:A:7:LEU:HD13	1:A:34:ILE:CG1	0.75	2.10	23	1
1:A:30:ILE:HG22	1:A:34:ILE:HD12	0.74	1.58	17	9
1:A:40:ILE:HG23	1:A:54:GLU:CA	0.74	2.12	30	1
1:A:40:ILE:HG23	1:A:54:GLU:HG3	0.74	1.59	13	1
1:A:7:LEU:HB3	1:A:34:ILE:HD11	0.74	1.59	16	4
1:A:7:LEU:HD13	1:A:40:ILE:HG21	0.73	1.58	21	1
1:A:7:LEU:HD21	1:A:40:ILE:CG2	0.73	2.14	8	5

Continued on next page...



*Continued from previous page...*

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:25:VAL:CG1	1:A:30:ILE:HD11	0.73	2.12	17	1
1:A:22:ASP:CB	1:A:50:VAL:HG11	0.73	2.13	32	1
1:A:56(D):VAL:O	1:A:56(D):VAL:HG23	0.73	1.82	2	3
1:A:56(B):GLY:O	1:A:56(D):VAL:HG13	0.73	1.82	2	3
1:A:7:LEU:HD21	1:A:34:ILE:HG12	0.73	1.60	13	7
1:A:43:THR:HG22	1:A:48:GLY:HA2	0.73	1.60	15	1
1:A:33:ALA:HB1	1:A:40:ILE:CD1	0.73	2.14	31	2
1:A:45:ASN:O	1:A:46:ALA:HB3	0.73	1.84	1	12
1:A:30:ILE:HG22	1:A:31:ASN:N	0.73	1.98	11	13
1:A:7:LEU:HB2	1:A:42:LEU:HD11	0.72	1.62	3	5
1:A:23:LEU:HD21	1:A:52:ALA:HB2	0.72	1.61	21	1
1:A:7:LEU:HD11	1:A:30:ILE:CD1	0.71	2.16	25	3
1:A:44:ILE:HG12	1:A:50:VAL:HG22	0.71	1.62	24	2
1:A:46:ALA:O	1:A:47:ASP:CB	0.70	2.39	3	11
1:A:43:THR:HG23	1:A:43:THR:O	0.70	1.86	17	2
1:A:40:ILE:HG23	1:A:54:GLU:HA	0.70	1.62	30	1
1:A:7:LEU:HD23	1:A:34:ILE:CG1	0.70	2.17	21	1
1:A:50:VAL:HG12	1:A:50:VAL:O	0.70	1.84	15	3
1:A:22:ASP:OD1	1:A:50:VAL:HG21	0.70	1.87	18	4
1:A:7:LEU:HD13	1:A:42:LEU:HD11	0.70	1.63	10	3
1:A:26:TYR:O	1:A:30:ILE:HD12	0.70	1.87	10	4
1:A:30:ILE:HG22	1:A:34:ILE:CD1	0.70	2.16	17	3
1:A:32:LYS:O	1:A:36:ALA:HB3	0.69	1.87	19	2
1:A:23:LEU:HD13	1:A:42:LEU:HD21	0.69	1.63	6	2
1:A:16:GLN:NE2	1:A:30:ILE:HG21	0.69	2.02	31	1
1:A:48:GLY:O	1:A:50:VAL:HG23	0.69	1.87	18	2
1:A:7:LEU:HD12	1:A:40:ILE:CD1	0.69	2.15	23	2
1:A:30:ILE:HG23	1:A:34:ILE:HD12	0.69	1.63	29	4
1:A:7:LEU:HD12	1:A:19:THR:CG2	0.68	2.18	25	1
1:A:7:LEU:HD13	1:A:42:LEU:CD1	0.68	2.19	10	2
1:A:16:GLN:NE2	1:A:30:ILE:HG22	0.68	2.03	23	1
1:A:44:ILE:HG22	1:A:46:ALA:H	0.68	1.48	24	1
1:A:30:ILE:HD12	1:A:34:ILE:HD11	0.67	1.64	5	4
1:A:23:LEU:HD11	1:A:25:VAL:HG21	0.67	1.65	8	2
1:A:30:ILE:N	1:A:30:ILE:HD13	0.67	2.04	17	4
1:A:44:ILE:HG22	1:A:44:ILE:O	0.67	1.89	25	3
1:A:16:GLN:O	1:A:20:ALA:HB2	0.67	1.89	5	6
1:A:33:ALA:O	1:A:40:ILE:HD11	0.67	1.90	23	3
1:A:7:LEU:CD1	1:A:23:LEU:HD11	0.67	2.19	31	1
1:A:25:VAL:HG12	1:A:30:ILE:HD11	0.67	1.66	17	1
1:A:23:LEU:CD2	1:A:52:ALA:HB2	0.67	2.20	21	1

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:23:LEU:CD1	1:A:42:LEU:HD21	0.66	2.20	6	1
1:A:19:THR:O	1:A:23:LEU:HD12	0.66	1.90	9	6
1:A:7:LEU:HA	1:A:42:LEU:HD13	0.66	1.68	29	6
1:A:23:LEU:HD21	1:A:42:LEU:HD23	0.66	1.67	4	1
1:A:45:ASN:O	1:A:46:ALA:CB	0.65	2.44	29	8
1:A:5:ILE:HD12	1:A:10:TYR:CE1	0.65	2.26	17	6
1:A:54:GLU:O	1:A:56(D):VAL:HA	0.65	1.92	25	16
1:A:33:ALA:CB	1:A:58:PHE:CZ	0.65	2.80	7	4
1:A:38:ARG:N	1:A:38:ARG:HD2	0.65	2.06	8	4
1:A:30:ILE:O	1:A:33:ALA:HB3	0.64	1.91	2	1
1:A:7:LEU:HD12	1:A:42:LEU:CD1	0.64	2.22	21	2
1:A:20:ALA:HB1	1:A:24:GLY:O	0.64	1.91	22	1
1:A:7:LEU:HG	1:A:34:ILE:HD11	0.64	1.68	12	3
1:A:7:LEU:HD11	1:A:34:ILE:HD11	0.64	1.66	1	6
1:A:38:ARG:HB2	1:A:40:ILE:HD11	0.63	1.69	22	1
1:A:10:TYR:CE1	1:A:44:ILE:CD1	0.63	2.82	28	1
1:A:32:LYS:O	1:A:36:ALA:HB2	0.63	1.94	14	7
1:A:10:TYR:CZ	1:A:14:PHE:CZ	0.63	2.87	25	2
1:A:3:GLN:CG	1:A:3:GLN:O	0.63	2.47	18	1
1:A:7:LEU:HD11	1:A:34:ILE:CD1	0.63	2.24	32	4
1:A:7:LEU:CD2	1:A:34:ILE:HD11	0.62	2.24	12	1
1:A:14:PHE:N	1:A:14:PHE:CD1	0.62	2.67	12	3
1:A:7:LEU:N	1:A:7:LEU:HD13	0.62	2.09	16	1
1:A:40:ILE:O	1:A:41:PHE:CG	0.61	2.54	2	21
1:A:7:LEU:CG	1:A:34:ILE:HD11	0.61	2.25	12	1
1:A:43:THR:HG22	1:A:48:GLY:CA	0.61	2.24	15	1
1:A:46:ALA:HB3	1:A:49:SER:OG	0.61	1.95	11	1
1:A:10:TYR:CE2	1:A:44:ILE:HD11	0.61	2.31	11	8
1:A:7:LEU:HD11	1:A:34:ILE:CG1	0.61	2.26	32	1
1:A:10:TYR:CE1	1:A:14:PHE:CZ	0.60	2.89	12	1
1:A:7:LEU:HD22	1:A:42:LEU:HD11	0.60	1.72	31	1
1:A:44:ILE:CD1	1:A:50:VAL:HG22	0.60	2.26	10	1
1:A:40:ILE:C	1:A:41:PHE:CG	0.60	2.75	3	22
1:A:5:ILE:HG21	1:A:10:TYR:CG	0.60	2.31	13	1
1:A:22:ASP:CG	1:A:50:VAL:HG21	0.60	2.16	11	4
1:A:50:VAL:O	1:A:51:TYR:CG	0.60	2.55	21	1
1:A:48:GLY:O	1:A:50:VAL:N	0.60	2.34	9	4
1:A:11:ALA:HB2	1:A:19:THR:HG21	0.60	1.71	13	2
1:A:33:ALA:HB1	1:A:40:ILE:HD12	0.60	1.73	31	1
1:A:6:THR:O	1:A:10:TYR:CB	0.60	2.50	31	30
1:A:23:LEU:CD1	1:A:25:VAL:CG2	0.60	2.79	8	1

Continued on next page...

*Continued from previous page...*

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:37:GLY:O	1:A:39:LYS:N	0.60	2.35	8	1
1:A:7:LEU:CD1	1:A:19:THR:HG21	0.59	2.25	25	1
1:A:30:ILE:N	1:A:30:ILE:CD1	0.59	2.66	27	8
1:A:31:ASN:O	1:A:35:HIS:CB	0.59	2.50	19	31
1:A:26:TYR:O	1:A:30:ILE:HD13	0.59	1.96	27	3
1:A:38:ARG:N	1:A:38:ARG:CD	0.59	2.63	8	1
1:A:11:ALA:HB2	1:A:19:THR:OG1	0.59	1.96	12	3
1:A:5:ILE:HG22	1:A:10:TYR:CB	0.59	2.25	14	9
1:A:38:ARG:CD	1:A:38:ARG:N	0.59	2.65	22	6
1:A:31:ASN:O	1:A:35:HIS:CG	0.59	2.55	8	2
1:A:43:THR:CG2	1:A:43:THR:O	0.59	2.51	8	1
1:A:7:LEU:CD1	1:A:19:THR:CG2	0.59	2.80	25	1
1:A:31:ASN:OD1	1:A:35:HIS:CE1	0.59	2.55	28	1
1:A:40:ILE:O	1:A:41:PHE:CD1	0.58	2.56	1	16
1:A:31:ASN:O	1:A:35:HIS:HB2	0.58	1.98	28	15
1:A:3:GLN:CB	1:A:45:ASN:ND2	0.58	2.66	15	1
1:A:40:ILE:O	1:A:41:PHE:CD2	0.58	2.56	8	2
1:A:4:ARG:NH1	1:A:41:PHE:CG	0.58	2.72	29	1
1:A:25:VAL:CG1	1:A:30:ILE:CD1	0.58	2.81	17	1
1:A:16:GLN:NE2	1:A:30:ILE:CG2	0.58	2.66	31	2
1:A:58:PHE:CG	1:A:58:PHE:O	0.58	2.55	1	1
1:A:44:ILE:HG22	1:A:45:ASN:H	0.58	1.57	7	5
1:A:44:ILE:CG2	1:A:45:ASN:N	0.58	2.67	21	1
1:A:14:PHE:O	1:A:15:GLY:C	0.58	2.41	28	1
1:A:52:ALA:HB3	1:A:58:PHE:O	0.58	1.99	13	9
1:A:42:LEU:N	1:A:42:LEU:CD1	0.58	2.66	27	11
1:A:10:TYR:CZ	1:A:44:ILE:HD11	0.58	2.33	11	5
1:A:10:TYR:CE1	1:A:44:ILE:HD11	0.58	2.34	28	1
1:A:39:LYS:O	1:A:41:PHE:CE2	0.57	2.57	20	4
1:A:8:LYS:HB2	1:A:34:ILE:HG23	0.57	1.76	19	3
1:A:30:ILE:CG2	1:A:31:ASN:N	0.57	2.67	11	13
1:A:45:ASN:ND2	1:A:45:ASN:N	0.57	2.52	5	3
1:A:7:LEU:HD23	1:A:34:ILE:HG13	0.57	1.76	21	1
1:A:55:VAL:HG22	1:A:56(D):VAL:HG12	0.57	1.76	26	3
1:A:7:LEU:HD21	1:A:34:ILE:HG13	0.57	1.77	14	2
1:A:10:TYR:O	1:A:14:PHE:CE2	0.57	2.58	15	1
1:A:8:LYS:CG	1:A:34:ILE:CG2	0.57	2.82	25	4
1:A:34:ILE:O	1:A:38:ARG:CD	0.57	2.53	14	8
1:A:33:ALA:CB	1:A:58:PHE:CE1	0.57	2.88	7	2
1:A:30:ILE:HD12	1:A:30:ILE:N	0.57	2.14	29	2
1:A:7:LEU:CD1	1:A:42:LEU:CD2	0.57	2.83	10	4

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:38:ARG:HG3	1:A:40:ILE:HD11	0.57	1.77	11	2
1:A:36:ALA:O	1:A:38:ARG:N	0.57	2.38	23	1
1:A:23:LEU:HD22	1:A:42:LEU:HD23	0.57	1.76	6	1
1:A:22:ASP:OD1	1:A:50:VAL:CG1	0.57	2.52	21	1
1:A:7:LEU:CD1	1:A:23:LEU:CD1	0.57	2.83	22	1
1:A:23:LEU:CD2	1:A:42:LEU:CD2	0.56	2.83	6	2
1:A:8:LYS:HG2	1:A:34:ILE:HG21	0.56	1.77	16	2
1:A:40:ILE:HG23	1:A:53:GLU:O	0.56	2.00	20	1
1:A:7:LEU:HD11	1:A:34:ILE:HG12	0.56	1.78	32	2
1:A:45:ASN:N	1:A:45:ASN:OD1	0.56	2.38	9	5
1:A:6:THR:O	1:A:10:TYR:HB2	0.56	2.00	24	28
1:A:49:SER:O	1:A:50:VAL:CG2	0.56	2.52	15	4
1:A:38:ARG:O	1:A:39:LYS:C	0.56	2.44	26	3
1:A:7:LEU:HD11	1:A:42:LEU:CD2	0.56	2.31	18	2
1:A:23:LEU:O	1:A:23:LEU:CG	0.56	2.53	22	1
1:A:40:ILE:HD13	1:A:54:GLU:HB2	0.56	1.75	32	1
1:A:46:ALA:HB3	1:A:49:SER:HB3	0.56	1.78	13	4
1:A:41:PHE:C	1:A:42:LEU:HD12	0.56	2.20	31	3
1:A:25:VAL:HG11	1:A:29:ALA:CB	0.56	2.29	29	1
1:A:46:ALA:O	1:A:47:ASP:HB3	0.56	2.01	13	10
1:A:36:ALA:O	1:A:37:GLY:C	0.56	2.44	23	2
1:A:25:VAL:CG1	1:A:29:ALA:CB	0.56	2.84	29	2
1:A:7:LEU:H	1:A:7:LEU:HD22	0.56	1.59	10	1
1:A:7:LEU:HD11	1:A:23:LEU:HD11	0.56	1.75	31	1
1:A:56:LYS:O	1:A:56(A):ASP:C	0.56	2.43	1	16
1:A:10:TYR:CE1	1:A:14:PHE:CE1	0.56	2.93	12	1
1:A:23:LEU:C	1:A:58:PHE:CZ	0.56	2.80	22	1
1:A:23:LEU:HD21	1:A:42:LEU:HD21	0.56	1.77	26	1
1:A:7:LEU:CD2	1:A:34:ILE:CG1	0.55	2.84	7	4
1:A:55:VAL:HG22	1:A:56(D):VAL:CG2	0.55	2.31	32	1
1:A:58:PHE:CD2	1:A:58:PHE:O	0.55	2.60	21	2
1:A:23:LEU:CB	1:A:42:LEU:HD21	0.55	2.31	22	1
1:A:25:VAL:HG22	1:A:59:PRO:HG3	0.55	1.77	22	1
1:A:7:LEU:CB	1:A:40:ILE:HG21	0.55	2.31	3	2
1:A:7:LEU:HB3	1:A:40:ILE:HG21	0.55	1.78	14	3
1:A:40:ILE:C	1:A:41:PHE:CD1	0.55	2.80	22	4
1:A:56:LYS:O	1:A:56(B):GLY:N	0.55	2.39	7	18
1:A:33:ALA:O	1:A:40:ILE:CD1	0.55	2.54	23	1
1:A:52:ALA:CB	1:A:58:PHE:O	0.55	2.55	31	8
1:A:33:ALA:O	1:A:38:ARG:CB	0.55	2.55	19	1
1:A:11:ALA:HB2	1:A:19:THR:CB	0.54	2.32	12	1

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:43:THR:O	1:A:49:SER:O	0.54	2.25	21	1
1:A:7:LEU:CD1	1:A:42:LEU:CD1	0.54	2.79	4	5
1:A:8:LYS:HG2	1:A:34:ILE:HG23	0.54	1.78	10	2
1:A:20:ALA:CB	1:A:30:ILE:HD13	0.54	2.32	10	1
1:A:30:ILE:CG2	1:A:34:ILE:CD1	0.54	2.86	10	3
1:A:22:ASP:OD1	1:A:50:VAL:CG2	0.54	2.56	27	1
1:A:6:THR:OG1	1:A:9:ASP:CB	0.54	2.56	21	9
1:A:4:ARG:O	1:A:4:ARG:CD	0.54	2.56	5	3
1:A:26:TYR:O	1:A:28:SER:N	0.54	2.41	6	3
1:A:44:ILE:O	1:A:45:ASN:CB	0.54	2.56	7	1
1:A:43:THR:HG22	1:A:48:GLY:O	0.54	2.03	21	1
1:A:44:ILE:CG1	1:A:50:VAL:HG22	0.54	2.32	22	1
1:A:40:ILE:C	1:A:41:PHE:CD2	0.54	2.80	14	13
1:A:40:ILE:HG22	1:A:41:PHE:N	0.54	2.18	16	4
1:A:10:TYR:CD1	1:A:14:PHE:CE1	0.54	2.96	12	1
1:A:40:ILE:CG2	1:A:53:GLU:O	0.54	2.55	20	1
1:A:7:LEU:CD2	1:A:42:LEU:HD11	0.54	2.33	31	1
1:A:43:THR:CG2	1:A:48:GLY:O	0.54	2.56	21	1
1:A:11:ALA:O	1:A:15:GLY:N	0.53	2.42	27	8
1:A:43:THR:OG1	1:A:51:TYR:CB	0.53	2.56	2	1
1:A:4:ARG:HA	1:A:42:LEU:O	0.53	2.04	4	13
1:A:20:ALA:CA	1:A:24:GLY:O	0.53	2.56	22	1
1:A:38:ARG:O	1:A:39:LYS:CB	0.53	2.55	14	4
1:A:7:LEU:HD11	1:A:30:ILE:HD12	0.53	1.80	25	1
1:A:14:PHE:CE1	1:A:18:LYS:HB3	0.53	2.37	25	1
1:A:54:GLU:OE1	1:A:56(C):GLU:CB	0.53	2.57	25	1
1:A:34:ILE:HA	1:A:38:ARG:CD	0.53	2.33	27	1
1:A:7:LEU:CD2	1:A:34:ILE:HG12	0.53	2.33	7	8
1:A:10:TYR:CE2	1:A:14:PHE:CZ	0.53	2.96	15	1
1:A:43:THR:O	1:A:43:THR:CG2	0.53	2.56	17	2
1:A:7:LEU:HB3	1:A:34:ILE:HD12	0.53	1.79	2	1
1:A:19:THR:O	1:A:23:LEU:CD2	0.53	2.57	17	2
1:A:38:ARG:HD3	1:A:38:ARG:O	0.53	2.03	28	1
1:A:44:ILE:CG2	1:A:49:SER:O	0.53	2.56	15	6
1:A:5:ILE:HB	1:A:10:TYR:CD1	0.53	2.38	31	1
1:A:26:TYR:O	1:A:30:ILE:CD1	0.53	2.57	32	1
1:A:53:GLU:CG	1:A:56(E):LYS:O	0.53	2.57	2	1
1:A:4:ARG:O	1:A:4:ARG:HD3	0.53	2.04	5	4
1:A:5:ILE:HG22	1:A:6:THR:H	0.53	1.64	32	2
1:A:54:GLU:C	1:A:55:VAL:CG2	0.53	2.77	19	7
1:A:5:ILE:CG2	1:A:10:TYR:CG	0.53	2.92	13	1

Continued on next page...

*Continued from previous page...*

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:41:PHE:O	1:A:53:GLU:CB	0.53	2.57	29	2
1:A:42:LEU:HD23	1:A:50:VAL:HG13	0.53	1.81	27	1
1:A:55:VAL:HG13	1:A:56(D):VAL:CG1	0.53	2.33	30	1
1:A:54:GLU:OE2	1:A:58:PHE:CD1	0.53	2.62	4	1
1:A:19:THR:O	1:A:23:LEU:HD21	0.52	2.03	17	1
1:A:7:LEU:HD22	1:A:40:ILE:HG13	0.52	1.81	32	1
1:A:23:LEU:HD21	1:A:42:LEU:CD2	0.52	2.34	1	2
1:A:43:THR:O	1:A:43:THR:HG23	0.52	2.03	8	1
1:A:16:GLN:OE1	1:A:30:ILE:HG21	0.52	2.04	7	1
1:A:19:THR:HG23	1:A:23:LEU:HD21	0.52	1.80	22	1
1:A:16:GLN:CG	1:A:17:THR:N	0.52	2.72	28	1
1:A:7:LEU:HD12	1:A:42:LEU:HD21	0.52	1.81	21	2
1:A:39:LYS:CG	1:A:39:LYS:O	0.52	2.57	6	2
1:A:38:ARG:O	1:A:38:ARG:HD3	0.52	2.05	8	1
1:A:38:ARG:CG	1:A:40:ILE:HD11	0.52	2.34	19	2
1:A:38:ARG:NE	1:A:40:ILE:HD11	0.52	2.19	8	2
1:A:33:ALA:HB1	1:A:58:PHE:CZ	0.52	2.39	15	1
1:A:20:ALA:CB	1:A:24:GLY:O	0.52	2.57	22	1
1:A:44:ILE:O	1:A:45:ASN:OD1	0.52	2.27	7	3
1:A:4:ARG:CZ	1:A:41:PHE:CB	0.52	2.88	29	1
1:A:7:LEU:CA	1:A:42:LEU:CD1	0.52	2.88	7	5
1:A:5:ILE:HG23	1:A:10:TYR:HB2	0.52	1.82	11	1
1:A:10:TYR:CZ	1:A:14:PHE:CE2	0.52	2.98	25	1
1:A:45:ASN:CG	1:A:46:ALA:N	0.52	2.61	7	2
1:A:5:ILE:O	1:A:42:LEU:CD1	0.52	2.58	8	1
1:A:33:ALA:O	1:A:34:ILE:HD13	0.52	2.05	30	1
1:A:31:ASN:O	1:A:35:HIS:HB3	0.52	2.05	5	20
1:A:5:ILE:HD12	1:A:10:TYR:CD1	0.52	2.40	20	3
1:A:3:GLN:HB3	1:A:45:ASN:ND2	0.51	2.21	15	1
1:A:22:ASP:OD1	1:A:23:LEU:N	0.51	2.43	9	1
1:A:14:PHE:CD1	1:A:14:PHE:O	0.51	2.62	25	1
1:A:45:ASN:C	1:A:47:ASP:H	0.51	2.06	28	1
1:A:32:LYS:O	1:A:36:ALA:CB	0.51	2.58	1	5
1:A:6:THR:O	1:A:10:TYR:HB3	0.51	2.05	4	13
1:A:10:TYR:CD1	1:A:14:PHE:CZ	0.51	2.98	12	1
1:A:7:LEU:CD2	1:A:34:ILE:HG13	0.51	2.35	14	1
1:A:14:PHE:CD1	1:A:15:GLY:N	0.51	2.78	15	1
1:A:52:ALA:O	1:A:57:PRO:HA	0.51	2.06	20	1
1:A:56(D):VAL:O	1:A:56(D):VAL:CG2	0.51	2.56	2	2
1:A:42:LEU:HA	1:A:51:TYR:O	0.51	2.06	4	12
1:A:7:LEU:HB3	1:A:40:ILE:CG2	0.51	2.36	7	2

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:26:TYR:CD1	1:A:28:SER:HB2	0.51	2.41	4	1
1:A:22:ASP:OD2	1:A:50:VAL:CG2	0.51	2.58	5	1
1:A:53:GLU:OE1	1:A:56(D):VAL:CG2	0.51	2.59	32	1
1:A:8:LYS:CD	1:A:8:LYS:C	0.51	2.78	23	5
1:A:46:ALA:O	1:A:47:ASP:HB2	0.51	2.06	12	2
1:A:33:ALA:HB2	1:A:58:PHE:CE1	0.51	2.41	7	1
1:A:7:LEU:CG	1:A:30:ILE:HG23	0.51	2.36	2	1
1:A:34:ILE:HA	1:A:40:ILE:HD11	0.51	1.82	7	1
1:A:30:ILE:N	1:A:30:ILE:HD12	0.51	2.20	2	3
1:A:23:LEU:HD13	1:A:30:ILE:HD11	0.51	1.82	5	1
1:A:37:GLY:O	1:A:38:ARG:O	0.51	2.29	14	2
1:A:8:LYS:CD	1:A:34:ILE:HG22	0.51	2.36	22	1
1:A:16:GLN:HG3	1:A:17:THR:N	0.51	2.21	28	1
1:A:10:TYR:CZ	1:A:44:ILE:CD1	0.51	2.93	28	5
1:A:38:ARG:H	1:A:38:ARG:HD2	0.51	1.66	10	1
1:A:5:ILE:CD1	1:A:10:TYR:CE1	0.51	2.94	17	1
1:A:38:ARG:HG2	1:A:40:ILE:CG1	0.51	2.36	18	1
1:A:8:LYS:HG3	1:A:34:ILE:CG2	0.51	2.35	25	3
1:A:44:ILE:HD13	1:A:50:VAL:HG22	0.51	1.83	10	1
1:A:57:PRO:O	1:A:58:PHE:O	0.50	2.30	26	6
1:A:46:ALA:CB	1:A:49:SER:HB2	0.50	2.33	25	2
1:A:16:GLN:O	1:A:20:ALA:CB	0.50	2.59	6	2
1:A:24:GLY:C	1:A:25:VAL:CG2	0.50	2.79	8	2
1:A:10:TYR:O	1:A:14:PHE:CE1	0.50	2.64	12	1
1:A:43:THR:CG2	1:A:48:GLY:HA2	0.50	2.36	15	1
1:A:52:ALA:HB1	1:A:58:PHE:O	0.50	2.04	17	2
1:A:7:LEU:HD23	1:A:34:ILE:CD1	0.50	2.34	21	1
1:A:42:LEU:HD23	1:A:50:VAL:HG21	0.50	1.82	32	1
1:A:34:ILE:O	1:A:38:ARG:HD2	0.50	2.05	2	6
1:A:22:ASP:OD1	1:A:50:VAL:CB	0.50	2.60	27	1
1:A:53:GLU:HA	1:A:56(E):LYS:O	0.50	2.06	16	9
1:A:30:ILE:HG23	1:A:34:ILE:HD11	0.50	1.84	14	1
1:A:41:PHE:CD1	1:A:41:PHE:N	0.50	2.79	30	1
1:A:17:THR:O	1:A:21:LYS:CG	0.50	2.60	2	1
1:A:19:THR:O	1:A:23:LEU:CD1	0.50	2.59	9	1
1:A:7:LEU:HD11	1:A:30:ILE:HD11	0.50	1.84	15	2
1:A:50:VAL:O	1:A:50:VAL:CG1	0.50	2.57	15	2
1:A:6:THR:HG22	1:A:7:LEU:H	0.50	1.66	22	9
1:A:43:THR:CG2	1:A:45:ASN:ND2	0.50	2.74	4	1
1:A:20:ALA:HB2	1:A:27:GLN:HG3	0.50	1.83	21	1
1:A:25:VAL:CG2	1:A:59:PRO:HG3	0.50	2.37	22	1

Continued on next page...



Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:5:ILE:CG2	1:A:10:TYR:HB2	0.50	2.37	16	8
1:A:23:LEU:HD23	1:A:23:LEU:N	0.49	2.22	7	3
1:A:55:VAL:HG13	1:A:56(D):VAL:HG12	0.49	1.83	23	3
1:A:22:ASP:O	1:A:50:VAL:CG1	0.49	2.60	32	1
1:A:7:LEU:HD21	1:A:34:ILE:HD11	0.49	1.84	24	2
1:A:23:LEU:O	1:A:23:LEU:HD12	0.49	2.05	22	1
1:A:25:VAL:HG12	1:A:29:ALA:HB3	0.49	1.82	26	1
1:A:42:LEU:HB3	1:A:50:VAL:HG23	0.49	1.83	32	1
1:A:8:LYS:HG2	1:A:34:ILE:CG2	0.49	2.37	28	8
1:A:38:ARG:HD2	1:A:38:ARG:N	0.49	2.22	2	3
1:A:23:LEU:CD1	1:A:25:VAL:HG23	0.49	2.37	8	1
1:A:38:ARG:CD	1:A:40:ILE:CG1	0.49	2.90	8	1
1:A:38:ARG:HD3	1:A:40:ILE:CG1	0.49	2.37	8	1
1:A:7:LEU:CD2	1:A:40:ILE:HB	0.49	2.37	16	2
1:A:42:LEU:HD12	1:A:42:LEU:H	0.49	1.67	23	1
1:A:10:TYR:CZ	1:A:44:ILE:HD12	0.49	2.42	9	2
1:A:58:PHE:O	1:A:58:PHE:CG	0.49	2.66	20	2
1:A:44:ILE:HG23	1:A:45:ASN:N	0.49	2.23	21	1
1:A:40:ILE:HG23	1:A:54:GLU:N	0.49	2.22	30	1
1:A:33:ALA:O	1:A:37:GLY:O	0.49	2.30	25	3
1:A:11:ALA:CB	1:A:19:THR:OG1	0.49	2.60	27	3
1:A:3:GLN:O	1:A:3:GLN:HG2	0.49	2.06	18	1
1:A:55:VAL:C	1:A:56(D):VAL:HG12	0.49	2.27	25	1
1:A:38:ARG:CD	1:A:38:ARG:C	0.49	2.80	28	1
1:A:48:GLY:O	1:A:49:SER:O	0.49	2.30	21	3
1:A:40:ILE:CG2	1:A:41:PHE:N	0.49	2.76	16	2
1:A:30:ILE:HG23	1:A:34:ILE:CD1	0.49	2.37	12	5
1:A:45:ASN:C	1:A:47:ASP:N	0.49	2.66	28	3
1:A:42:LEU:HD23	1:A:52:ALA:HB2	0.49	1.84	16	2
1:A:6:THR:CB	1:A:9:ASP:HB2	0.49	2.38	20	7
1:A:7:LEU:HD13	1:A:7:LEU:N	0.49	2.23	10	3
1:A:11:ALA:HB1	1:A:16:GLN:HA	0.49	1.84	4	1
1:A:8:LYS:CG	1:A:34:ILE:HG21	0.49	2.37	29	3
1:A:56(E):LYS:HB3	1:A:57:PRO:CD	0.48	2.38	9	4
1:A:23:LEU:CD1	1:A:30:ILE:HD11	0.48	2.37	5	1
1:A:56(D):VAL:O	1:A:56(E):LYS:HG2	0.48	2.08	25	5
1:A:43:THR:HG1	1:A:51:TYR:HD2	0.48	1.48	14	1
1:A:54:GLU:O	1:A:56(D):VAL:CA	0.48	2.61	25	1
1:A:7:LEU:CD1	1:A:7:LEU:N	0.48	2.75	16	2
1:A:25:VAL:HG12	1:A:30:ILE:CD1	0.48	2.37	17	1
1:A:14:PHE:O	1:A:15:GLY:O	0.48	2.31	28	2

Continued on next page...



Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:43:THR:O	1:A:43:THR:OG1	0.48	2.31	3	3
1:A:59:PRO:O	1:A:60:SER:C	0.48	2.52	8	4
1:A:38:ARG:O	1:A:39:LYS:HB2	0.48	2.08	28	3
1:A:25:VAL:HG12	1:A:26:TYR:H	0.48	1.68	27	1
1:A:43:THR:OG1	1:A:51:TYR:HB2	0.48	2.08	2	3
1:A:7:LEU:HG	1:A:34:ILE:CD1	0.48	2.38	12	4
1:A:5:ILE:O	1:A:6:THR:O	0.48	2.31	14	8
1:A:38:ARG:HG2	1:A:40:ILE:HG13	0.48	1.85	18	1
1:A:22:ASP:OD2	1:A:50:VAL:HG21	0.48	2.09	20	2
1:A:8:LYS:HD3	1:A:34:ILE:CG2	0.48	2.38	32	2
1:A:20:ALA:O	1:A:24:GLY:C	0.48	2.52	22	2
1:A:39:LYS:CG	1:A:55:VAL:O	0.48	2.61	8	1
1:A:7:LEU:HD23	1:A:34:ILE:HD11	0.48	1.85	21	1
1:A:19:THR:O	1:A:23:LEU:HG	0.48	2.09	22	2
1:A:45:ASN:OD1	1:A:46:ALA:N	0.48	2.46	21	2
1:A:7:LEU:HB2	1:A:42:LEU:CD1	0.48	2.38	7	2
1:A:57:PRO:O	1:A:58:PHE:C	0.48	2.50	4	5
1:A:44:ILE:O	1:A:45:ASN:O	0.48	2.32	28	5
1:A:54:GLU:N	1:A:56(E):LYS:O	0.48	2.47	25	3
1:A:38:ARG:O	1:A:38:ARG:HG2	0.48	2.08	10	1
1:A:54:GLU:CD	1:A:58:PHE:CD2	0.48	2.87	14	1
1:A:55:VAL:HB	1:A:56(D):VAL:HG12	0.48	1.86	14	1
1:A:25:VAL:HG11	1:A:59:PRO:HG2	0.48	1.85	16	1
1:A:45:ASN:ND2	1:A:49:SER:CB	0.48	2.76	2	2
1:A:44:ILE:HA	1:A:49:SER:O	0.47	2.09	4	6
1:A:53:GLU:CA	1:A:56(E):LYS:O	0.47	2.61	4	1
1:A:38:ARG:C	1:A:38:ARG:HD3	0.47	2.29	10	2
1:A:13:ARG:HB3	1:A:14:PHE:CD1	0.47	2.44	12	1
1:A:40:ILE:CD1	1:A:54:GLU:HB2	0.47	2.40	32	1
1:A:23:LEU:CD1	1:A:25:VAL:HG21	0.47	2.35	17	1
1:A:38:ARG:CG	1:A:40:ILE:HG13	0.47	2.39	18	1
1:A:44:ILE:O	1:A:45:ASN:C	0.47	2.53	16	5
1:A:5:ILE:O	1:A:42:LEU:HD13	0.47	2.09	8	1
1:A:19:THR:O	1:A:22:ASP:OD2	0.47	2.32	29	2
1:A:10:TYR:CE2	1:A:44:ILE:CD1	0.47	2.98	21	2
1:A:54:GLU:C	1:A:55:VAL:HG23	0.47	2.30	7	5
1:A:14:PHE:CZ	1:A:19:THR:OG1	0.47	2.66	15	1
1:A:38:ARG:CG	1:A:40:ILE:CG1	0.47	2.93	18	1
1:A:23:LEU:HD22	1:A:58:PHE:CE1	0.47	2.45	5	1
1:A:20:ALA:HB2	1:A:30:ILE:HG13	0.47	1.86	11	2
1:A:56(E):LYS:HB2	1:A:57:PRO:CD	0.47	2.40	30	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:57:PRO:O	1:A:58:PHE:HB2	0.47	2.10	22	7
1:A:19:THR:O	1:A:22:ASP:OD1	0.47	2.32	9	1
1:A:20:ALA:HB1	1:A:30:ILE:HD13	0.47	1.87	10	1
1:A:3:GLN:HB2	1:A:45:ASN:ND2	0.47	2.25	15	1
1:A:28:SER:OG	1:A:29:ALA:N	0.47	2.46	17	1
1:A:33:ALA:O	1:A:38:ARG:HB3	0.47	2.10	19	1
1:A:23:LEU:HG	1:A:24:GLY:N	0.47	2.24	27	1
1:A:56(A):ASP:OD1	1:A:56(A):ASP:O	0.47	2.33	5	1
1:A:52:ALA:O	1:A:58:PHE:O	0.47	2.33	4	1
1:A:47:ASP:O	1:A:47:ASP:OD1	0.47	2.33	12	1
1:A:58:PHE:CD1	1:A:58:PHE:C	0.47	2.88	27	3
1:A:34:ILE:HA	1:A:38:ARG:HD2	0.47	1.86	27	1
1:A:7:LEU:CD2	1:A:40:ILE:HG13	0.47	2.39	32	1
1:A:7:LEU:CB	1:A:40:ILE:CG2	0.46	2.92	3	2
1:A:42:LEU:CA	1:A:51:TYR:O	0.46	2.63	4	2
1:A:44:ILE:HG22	1:A:45:ASN:N	0.46	2.25	7	1
1:A:59:PRO:O	1:A:60:SER:O	0.46	2.33	27	3
1:A:30:ILE:HG23	1:A:34:ILE:HG13	0.46	1.87	30	1
1:A:7:LEU:HD21	1:A:34:ILE:CG1	0.46	2.41	7	3
1:A:10:TYR:HH	1:A:14:PHE:HE2	0.46	1.53	25	1
1:A:43:THR:OG1	1:A:43:THR:O	0.46	2.34	2	1
1:A:48:GLY:C	1:A:49:SER:OG	0.46	2.53	9	1
1:A:31:ASN:O	1:A:35:HIS:CD2	0.46	2.69	8	1
1:A:30:ILE:CG2	1:A:34:ILE:HD12	0.46	2.40	27	4
1:A:23:LEU:HG	1:A:25:VAL:HG23	0.46	1.86	27	1
1:A:45:ASN:O	1:A:47:ASP:OD1	0.46	2.33	28	1
1:A:19:THR:O	1:A:23:LEU:HD23	0.46	2.10	27	1
1:A:19:THR:HA	1:A:22:ASP:OD2	0.46	2.11	29	2
1:A:7:LEU:HA	1:A:42:LEU:CD1	0.46	2.41	24	9
1:A:45:ASN:HB2	1:A:48:GLY:N	0.46	2.26	24	1
1:A:22:ASP:C	1:A:50:VAL:HG11	0.46	2.30	32	1
1:A:31:ASN:O	1:A:32:LYS:C	0.46	2.53	2	1
1:A:45:ASN:O	1:A:47:ASP:N	0.46	2.49	4	2
1:A:7:LEU:CD2	1:A:19:THR:HG21	0.46	2.40	23	1
1:A:37:GLY:O	1:A:38:ARG:C	0.46	2.54	27	1
1:A:44:ILE:O	1:A:48:GLY:C	0.46	2.54	21	1
1:A:6:THR:OG1	1:A:9:ASP:HB3	0.46	2.11	21	7
1:A:23:LEU:O	1:A:25:VAL:CG2	0.46	2.64	3	1
1:A:7:LEU:HD21	1:A:34:ILE:HA	0.46	1.88	5	1
1:A:5:ILE:CG2	1:A:10:TYR:CB	0.46	2.93	8	2
1:A:7:LEU:HD13	1:A:23:LEU:CD1	0.46	2.41	22	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:14:PHE:CD1	1:A:14:PHE:C	0.46	2.89	25	1
1:A:8:LYS:CB	1:A:34:ILE:HD13	0.46	2.42	27	1
1:A:34:ILE:O	1:A:38:ARG:HD3	0.46	2.10	27	1
1:A:55:VAL:HG22	1:A:56(D):VAL:HG23	0.46	1.87	32	1
1:A:6:THR:OG1	1:A:9:ASP:N	0.45	2.50	15	4
1:A:39:LYS:HG3	1:A:55:VAL:O	0.45	2.11	8	1
1:A:7:LEU:HD11	1:A:30:ILE:HG13	0.45	1.87	2	1
1:A:33:ALA:O	1:A:38:ARG:HB2	0.45	2.11	30	4
1:A:54:GLU:O	1:A:56(D):VAL:CB	0.45	2.64	10	2
1:A:39:LYS:O	1:A:55:VAL:CG2	0.45	2.65	4	1
1:A:22:ASP:OD1	1:A:50:VAL:HG13	0.45	2.11	21	1
1:A:40:ILE:HG23	1:A:54:GLU:CB	0.45	2.42	24	1
1:A:3:GLN:OE1	1:A:44:ILE:O	0.45	2.35	32	1
1:A:22:ASP:N	1:A:22:ASP:OD1	0.45	2.49	3	1
1:A:26:TYR:CD1	1:A:28:SER:CB	0.45	2.99	4	1
1:A:56:LYS:HG3	1:A:56(A):ASP:N	0.45	2.26	4	2
1:A:26:TYR:CD1	1:A:26:TYR:N	0.45	2.84	6	2
1:A:42:LEU:HD23	1:A:50:VAL:CG1	0.45	2.42	28	1
1:A:49:SER:O	1:A:49:SER:OG	0.45	2.35	7	1
1:A:36:ALA:O	1:A:38:ARG:HD2	0.45	2.11	23	1
1:A:56(D):VAL:C	1:A:56(E):LYS:CG	0.45	2.84	10	2
1:A:45:ASN:ND2	1:A:49:SER:HB3	0.45	2.27	2	1
1:A:26:TYR:O	1:A:27:GLN:C	0.45	2.54	6	6
1:A:57:PRO:O	1:A:58:PHE:CB	0.45	2.65	22	2
1:A:23:LEU:HD11	1:A:42:LEU:HD21	0.45	1.89	13	1
1:A:23:LEU:CD1	1:A:23:LEU:O	0.45	2.65	22	1
1:A:51:TYR:O	1:A:52:ALA:C	0.45	2.54	29	1
1:A:8:LYS:O	1:A:9:ASP:C	0.45	2.53	11	20
1:A:56:LYS:O	1:A:56(A):ASP:HB3	0.45	2.12	13	7
1:A:38:ARG:O	1:A:38:ARG:CG	0.45	2.65	10	1
1:A:52:ALA:O	1:A:57:PRO:O	0.45	2.34	20	1
1:A:23:LEU:HD23	1:A:50:VAL:HG11	0.45	1.88	1	1
1:A:39:LYS:O	1:A:55:VAL:HG23	0.45	2.12	4	1
1:A:25:VAL:O	1:A:26:TYR:O	0.45	2.35	18	2
1:A:54:GLU:OE1	1:A:58:PHE:HB2	0.45	2.12	19	1
1:A:30:ILE:O	1:A:34:ILE:HB	0.45	2.12	30	3
1:A:57:PRO:HD2	1:A:60:SER:CB	0.45	2.42	3	2
1:A:40:ILE:HG21	1:A:58:PHE:CD2	0.45	2.47	4	2
1:A:7:LEU:CG	1:A:34:ILE:HG12	0.45	2.42	32	2
1:A:7:LEU:O	1:A:11:ALA:HB2	0.45	2.12	8	1
1:A:34:ILE:O	1:A:35:HIS:C	0.45	2.54	8	2

Continued on next page...

*Continued from previous page...*

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:20:ALA:CB	1:A:27:GLN:HG3	0.45	2.42	9	1
1:A:54:GLU:HG2	1:A:55:VAL:N	0.45	2.26	26	1
1:A:14:PHE:O	1:A:18:LYS:HB2	0.45	2.11	30	1
1:A:45:ASN:O	1:A:46:ALA:C	0.44	2.54	4	4
1:A:50:VAL:O	1:A:50:VAL:HG12	0.44	2.12	8	1
1:A:39:LYS:HD3	1:A:55:VAL:O	0.44	2.12	11	1
1:A:53:GLU:OE1	1:A:55:VAL:CG2	0.44	2.65	23	1
1:A:17:THR:O	1:A:20:ALA:HB3	0.44	2.13	25	1
1:A:51:TYR:CZ	1:A:53:GLU:CG	0.44	3.00	26	1
1:A:39:LYS:CB	1:A:55:VAL:O	0.44	2.65	28	1
1:A:53:GLU:HG2	1:A:56(E):LYS:O	0.44	2.12	2	1
1:A:55:VAL:HG22	1:A:56(D):VAL:CG1	0.44	2.42	3	1
1:A:46:ALA:CB	1:A:49:SER:CB	0.44	2.90	4	1
1:A:44:ILE:O	1:A:45:ASN:CG	0.44	2.55	7	1
1:A:7:LEU:HD21	1:A:34:ILE:CD1	0.44	2.42	30	2
1:A:8:LYS:HG3	1:A:34:ILE:HG21	0.44	1.88	27	1
1:A:6:THR:O	1:A:42:LEU:HD13	0.44	2.13	2	4
1:A:7:LEU:HB3	1:A:34:ILE:CD1	0.44	2.41	10	3
1:A:49:SER:C	1:A:50:VAL:HG23	0.44	2.31	30	2
1:A:38:ARG:HG3	1:A:40:ILE:CG1	0.44	2.43	19	1
1:A:54:GLU:O	1:A:56(D):VAL:C	0.44	2.56	25	1
1:A:5:ILE:HG22	1:A:10:TYR:N	0.44	2.26	10	2
1:A:24:GLY:C	1:A:25:VAL:HG23	0.44	2.33	8	1
1:A:53:GLU:O	1:A:53:GLU:HG3	0.44	2.13	8	1
1:A:25:VAL:HG11	1:A:30:ILE:CD1	0.44	2.42	17	1
1:A:40:ILE:HD13	1:A:58:PHE:CD1	0.44	2.48	17	1
1:A:28:SER:O	1:A:29:ALA:C	0.44	2.55	5	6
1:A:10:TYR:C	1:A:10:TYR:CD1	0.44	2.90	2	2
1:A:45:ASN:OD1	1:A:45:ASN:C	0.44	2.56	7	2
1:A:9:ASP:O	1:A:12:MET:CB	0.44	2.66	11	3
1:A:39:LYS:N	1:A:39:LYS:HD2	0.44	2.27	25	1
1:A:7:LEU:HD22	1:A:40:ILE:HB	0.44	1.90	30	1
1:A:4:ARG:N	1:A:4:ARG:HD2	0.44	2.28	5	1
1:A:20:ALA:O	1:A:24:GLY:O	0.44	2.35	6	1
1:A:39:LYS:O	1:A:39:LYS:HG2	0.44	2.12	6	2
1:A:42:LEU:CB	1:A:51:TYR:O	0.44	2.65	30	2
1:A:10:TYR:CD2	1:A:14:PHE:CZ	0.44	3.06	15	1
1:A:48:GLY:O	1:A:49:SER:HB2	0.44	2.13	15	4
1:A:5:ILE:HG21	1:A:10:TYR:HA	0.44	1.89	31	2
1:A:42:LEU:HB3	1:A:50:VAL:CG1	0.44	2.42	24	1
1:A:44:ILE:C	1:A:45:ASN:OD1	0.44	2.56	28	4

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:3:GLN:O	1:A:43:THR:HA	0.44	2.13	10	2
1:A:38:ARG:NE	1:A:38:ARG:HA	0.44	2.28	23	1
1:A:8:LYS:HD2	1:A:9:ASP:N	0.43	2.28	3	2
1:A:59:PRO:C	1:A:60:SER:OG	0.43	2.56	16	1
1:A:23:LEU:O	1:A:23:LEU:HG	0.43	2.12	22	1
1:A:38:ARG:NH1	1:A:54:GLU:HB2	0.43	2.28	28	1
1:A:7:LEU:CD1	1:A:34:ILE:HG12	0.43	2.43	32	1
1:A:57:PRO:O	1:A:58:PHE:CD2	0.43	2.72	1	1
1:A:58:PHE:O	1:A:58:PHE:CD2	0.43	2.70	1	2
1:A:9:ASP:O	1:A:12:MET:HB3	0.43	2.14	19	4
1:A:38:ARG:HE	1:A:40:ILE:HD11	0.43	1.73	8	1
1:A:23:LEU:HD22	1:A:59:PRO:HD3	0.43	1.89	14	1
1:A:8:LYS:HB2	1:A:34:ILE:CG2	0.43	2.43	17	2
1:A:40:ILE:HG12	1:A:54:GLU:CG	0.43	2.43	21	1
1:A:26:TYR:N	1:A:26:TYR:CD1	0.43	2.82	31	1
1:A:22:ASP:CB	1:A:50:VAL:HG21	0.43	2.42	2	1
1:A:57:PRO:HB2	1:A:60:SER:CA	0.43	2.42	9	1
1:A:22:ASP:CA	1:A:50:VAL:HG11	0.43	2.43	32	1
1:A:55:VAL:HG23	1:A:56(D):VAL:HG12	0.43	1.90	2	1
1:A:57:PRO:O	1:A:58:PHE:HB3	0.43	2.13	28	5
1:A:58:PHE:CD2	1:A:59:PRO:HA	0.43	2.48	5	1
1:A:33:ALA:O	1:A:38:ARG:CD	0.43	2.66	18	1
1:A:5:ILE:CG2	1:A:10:TYR:HA	0.43	2.44	19	1
1:A:14:PHE:CZ	1:A:18:LYS:HB3	0.43	2.48	25	1
1:A:35:HIS:CD2	1:A:35:HIS:C	0.43	2.91	15	1
1:A:36:ALA:O	1:A:38:ARG:HG2	0.43	2.13	23	1
1:A:54:GLU:O	1:A:56(D):VAL:HB	0.43	2.13	31	1
1:A:39:LYS:CE	1:A:56:LYS:HB2	0.43	2.44	3	1
1:A:56(E):LYS:CB	1:A:57:PRO:CD	0.43	2.97	9	2
1:A:46:ALA:O	1:A:49:SER:OG	0.43	2.32	14	1
1:A:53:GLU:O	1:A:53:GLU:OE2	0.43	2.37	16	1
1:A:23:LEU:HB2	1:A:25:VAL:HG23	0.43	1.90	32	1
1:A:9:ASP:O	1:A:10:TYR:C	0.43	2.56	16	3
1:A:53:GLU:CB	1:A:56(E):LYS:O	0.43	2.67	4	1
1:A:39:LYS:HB3	1:A:55:VAL:O	0.43	2.14	7	1
1:A:34:ILE:O	1:A:38:ARG:NE	0.43	2.52	14	1
1:A:56(A):ASP:OD1	1:A:56(A):ASP:C	0.43	2.57	25	1
1:A:5:ILE:CG2	1:A:10:TYR:CA	0.43	2.96	31	2
1:A:22:ASP:C	1:A:22:ASP:OD1	0.43	2.57	10	1
1:A:10:TYR:HD2	1:A:42:LEU:HD22	0.43	1.73	20	1
1:A:34:ILE:HG13	1:A:40:ILE:HD12	0.43	1.91	2	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:6:THR:C	1:A:42:LEU:CD1	0.43	2.88	15	1
1:A:51:TYR:CD1	1:A:51:TYR:N	0.43	2.84	18	1
1:A:30:ILE:O	1:A:34:ILE:CB	0.43	2.66	30	1
1:A:28:SER:O	1:A:30:ILE:N	0.43	2.52	5	1
1:A:27:GLN:O	1:A:30:ILE:HB	0.43	2.14	15	4
1:A:42:LEU:CD1	1:A:42:LEU:N	0.43	2.81	21	1
1:A:27:GLN:HA	1:A:30:ILE:HG12	0.43	1.90	31	1
1:A:51:TYR:CD1	1:A:52:ALA:N	0.42	2.87	14	1
1:A:7:LEU:CB	1:A:34:ILE:HG12	0.42	2.44	8	1
1:A:56:LYS:CG	1:A:56(A):ASP:OD2	0.42	2.67	22	1
1:A:38:ARG:CZ	1:A:40:ILE:HG12	0.42	2.43	28	1
1:A:23:LEU:CB	1:A:52:ALA:HB2	0.42	2.44	6	1
1:A:56:LYS:HG3	1:A:56(A):ASP:OD2	0.42	2.14	22	1
1:A:14:PHE:CE1	1:A:18:LYS:CB	0.42	3.03	25	1
1:A:55:VAL:CA	1:A:56(D):VAL:HA	0.42	2.44	25	1
1:A:43:THR:O	1:A:43:THR:HG22	0.42	2.13	25	2
1:A:10:TYR:CE1	1:A:44:ILE:HD12	0.42	2.48	28	1
1:A:16:GLN:OE1	1:A:31:ASN:OD1	0.42	2.37	30	1
1:A:52:ALA:O	1:A:53:GLU:HG2	0.42	2.15	30	1
1:A:56(A):ASP:O	1:A:56(B):GLY:C	0.42	2.57	20	1
1:A:45:ASN:ND2	1:A:47:ASP:HB3	0.42	2.30	22	1
1:A:54:GLU:C	1:A:56(D):VAL:HA	0.42	2.35	25	1
1:A:38:ARG:HD3	1:A:38:ARG:C	0.42	2.34	28	1
1:A:22:ASP:OD1	1:A:50:VAL:HG11	0.42	2.13	29	1
1:A:39:LYS:O	1:A:39:LYS:HG3	0.42	2.14	1	3
1:A:7:LEU:HG	1:A:30:ILE:HG23	0.42	1.90	2	1
1:A:45:ASN:OD1	1:A:45:ASN:N	0.42	2.53	2	1
1:A:38:ARG:O	1:A:39:LYS:HB3	0.42	2.15	21	2
1:A:43:THR:HB	1:A:51:TYR:CB	0.42	2.44	10	2
1:A:34:ILE:HA	1:A:40:ILE:CD1	0.42	2.44	7	1
1:A:22:ASP:HB3	1:A:50:VAL:CG1	0.42	2.43	20	1
1:A:44:ILE:O	1:A:48:GLY:HA3	0.42	2.15	21	1
1:A:7:LEU:CD2	1:A:40:ILE:HG21	0.42	2.45	3	1
1:A:43:THR:CG2	1:A:51:TYR:HB3	0.42	2.44	17	1
1:A:7:LEU:HD22	1:A:58:PHE:CE2	0.42	2.49	24	1
1:A:40:ILE:HG23	1:A:54:GLU:HB3	0.42	1.91	24	1
1:A:14:PHE:CD1	1:A:14:PHE:N	0.42	2.87	25	1
1:A:22:ASP:OD1	1:A:22:ASP:C	0.42	2.57	25	1
1:A:45:ASN:OD1	1:A:49:SER:HB3	0.42	2.14	30	1
1:A:8:LYS:H	1:A:34:ILE:HD13	0.42	1.73	2	1
1:A:8:LYS:C	1:A:8:LYS:CD	0.42	2.87	6	1

Continued on next page...

*Continued from previous page...*

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:14:PHE:CD2	1:A:18:LYS:HE3	0.42	2.50	11	1
1:A:5:ILE:HG21	1:A:10:TYR:CD2	0.42	2.50	13	1
1:A:36:ALA:HB3	1:A:38:ARG:CZ	0.42	2.44	22	1
1:A:44:ILE:O	1:A:44:ILE:CG2	0.42	2.61	25	1
1:A:22:ASP:HB3	1:A:50:VAL:HG21	0.42	1.90	2	1
1:A:38:ARG:CD	1:A:40:ILE:HD11	0.42	2.45	10	1
1:A:7:LEU:HD11	1:A:42:LEU:CD1	0.42	2.45	18	1
1:A:30:ILE:O	1:A:34:ILE:CG1	0.42	2.67	27	1
1:A:5:ILE:HG13	1:A:44:ILE:CD1	0.42	2.44	8	1
1:A:58:PHE:HA	1:A:59:PRO:HA	0.42	1.77	24	5
1:A:43:THR:O	1:A:51:TYR:HB2	0.42	2.15	13	1
1:A:51:TYR:CD1	1:A:51:TYR:C	0.42	2.92	27	2
1:A:14:PHE:HB3	1:A:18:LYS:CB	0.42	2.44	23	1
1:A:8:LYS:CG	1:A:34:ILE:HG23	0.42	2.44	25	1
1:A:22:ASP:C	1:A:50:VAL:CG1	0.42	2.89	32	1
1:A:23:LEU:HB2	1:A:52:ALA:CB	0.41	2.44	6	1
1:A:57:PRO:HB2	1:A:60:SER:C	0.41	2.35	9	1
1:A:54:GLU:HB2	1:A:56(E):LYS:O	0.41	2.14	25	1
1:A:23:LEU:HB3	1:A:50:VAL:CG1	0.41	2.45	27	1
1:A:52:ALA:O	1:A:53:GLU:CG	0.41	2.68	30	1
1:A:8:LYS:HD3	1:A:34:ILE:HG23	0.41	1.92	32	1
1:A:44:ILE:HG23	1:A:50:VAL:HG22	0.41	1.91	4	1
1:A:26:TYR:HB2	1:A:29:ALA:HB3	0.41	1.92	6	1
1:A:23:LEU:N	1:A:23:LEU:CD2	0.41	2.83	7	1
1:A:8:LYS:CD	1:A:9:ASP:N	0.41	2.83	17	1
1:A:35:HIS:CD2	1:A:35:HIS:O	0.41	2.73	26	1
1:A:4:ARG:CZ	1:A:41:PHE:CG	0.41	3.03	29	1
1:A:54:GLU:O	1:A:55:VAL:CG2	0.41	2.68	3	1
1:A:16:GLN:NE2	1:A:27:GLN:HG2	0.41	2.31	4	1
1:A:6:THR:OG1	1:A:9:ASP:HB2	0.41	2.15	21	3
1:A:43:THR:HG22	1:A:45:ASN:ND2	0.41	2.29	11	1
1:A:7:LEU:HD13	1:A:40:ILE:CG2	0.41	2.38	21	1
1:A:42:LEU:HD23	1:A:50:VAL:HG12	0.41	1.92	24	1
1:A:33:ALA:HB1	1:A:40:ILE:HD11	0.41	1.86	31	1
1:A:42:LEU:HB3	1:A:50:VAL:CG2	0.41	2.46	32	1
1:A:56(E):LYS:HB2	1:A:60:SER:OG	0.41	2.15	32	1
1:A:8:LYS:HB2	1:A:34:ILE:CD1	0.41	2.39	2	2
1:A:20:ALA:HA	1:A:24:GLY:HA3	0.41	1.91	6	1
1:A:39:LYS:HD2	1:A:55:VAL:O	0.41	2.16	8	1
1:A:30:ILE:O	1:A:34:ILE:HG13	0.41	2.15	29	3
1:A:4:ARG:HG2	1:A:41:PHE:HB3	0.41	1.92	15	1

*Continued on next page...*



Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:14:PHE:CE1	1:A:18:LYS:HB2	0.41	2.51	15	1
1:A:45:ASN:CG	1:A:49:SER:HB3	0.41	2.36	1	1
1:A:48:GLY:O	1:A:49:SER:C	0.41	2.58	9	2
1:A:55:VAL:CB	1:A:56(D):VAL:HG12	0.41	2.46	14	1
1:A:22:ASP:OD1	1:A:50:VAL:HB	0.41	2.15	27	1
1:A:45:ASN:OD1	1:A:49:SER:CB	0.41	2.69	29	1
1:A:5:ILE:CB	1:A:10:TYR:CD1	0.41	3.03	31	1
1:A:3:GLN:HB2	1:A:44:ILE:O	0.41	2.15	32	1
1:A:30:ILE:HG22	1:A:31:ASN:H	0.41	1.74	13	2
1:A:54:GLU:O	1:A:55:VAL:HG22	0.41	2.16	19	1
1:A:52:ALA:O	1:A:57:PRO:HB3	0.41	2.15	25	1
1:A:54:GLU:OE1	1:A:56(C):GLU:HB2	0.41	2.15	25	1
1:A:30:ILE:O	1:A:32:LYS:N	0.41	2.54	5	1
1:A:23:LEU:CG	1:A:25:VAL:HG23	0.41	2.46	8	1
1:A:56(B):GLY:O	1:A:56(C):GLU:HB2	0.41	2.14	25	2
1:A:9:ASP:O	1:A:12:MET:HB2	0.41	2.15	27	1
1:A:14:PHE:CD2	1:A:18:LYS:HD3	0.41	2.50	31	1
1:A:41:PHE:O	1:A:53:GLU:O	0.41	2.39	31	1
1:A:22:ASP:HB3	1:A:50:VAL:CG2	0.41	2.46	2	1
1:A:55:VAL:HA	1:A:56(C):GLU:O	0.41	2.16	2	1
1:A:41:PHE:O	1:A:42:LEU:HG	0.41	2.16	9	1
1:A:7:LEU:CD2	1:A:33:ALA:O	0.41	2.68	19	1
1:A:42:LEU:HB3	1:A:51:TYR:O	0.41	2.15	21	2
1:A:44:ILE:O	1:A:48:GLY:CA	0.41	2.69	21	1
1:A:24:GLY:N	1:A:58:PHE:CZ	0.41	2.89	22	1
1:A:43:THR:OG1	1:A:51:TYR:HB3	0.41	2.16	26	1
1:A:46:ALA:C	1:A:47:ASP:CG	0.41	2.78	28	1
1:A:34:ILE:CG2	1:A:35:HIS:N	0.41	2.83	2	1
1:A:54:GLU:O	1:A:56(C):GLU:O	0.41	2.38	2	1
1:A:4:ARG:HD2	1:A:43:THR:HG22	0.41	1.92	19	1
1:A:40:ILE:HG12	1:A:54:GLU:CB	0.40	2.46	1	1
1:A:28:SER:C	1:A:30:ILE:N	0.40	2.74	7	1
1:A:7:LEU:HD11	1:A:42:LEU:HD11	0.40	1.92	8	1
1:A:6:THR:CB	1:A:9:ASP:HB3	0.40	2.46	9	1
1:A:4:ARG:HA	1:A:42:LEU:C	0.40	2.37	18	2
1:A:5:ILE:HG22	1:A:6:THR:N	0.40	2.30	21	1
1:A:23:LEU:CB	1:A:42:LEU:CD2	0.40	3.00	22	1
1:A:13:ARG:NH1	1:A:13:ARG:HG2	0.40	2.30	7	1
1:A:23:LEU:HB3	1:A:25:VAL:CG2	0.40	2.46	9	1
1:A:50:VAL:C	1:A:51:TYR:CD1	0.40	2.94	18	1
1:A:42:LEU:HD23	1:A:50:VAL:CG2	0.40	2.46	32	1

Continued on next page...



Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:7:LEU:CB	1:A:42:LEU:HD11	0.40	2.42	3	1
1:A:5:ILE:O	1:A:41:PHE:HA	0.40	2.16	4	1
1:A:23:LEU:HD22	1:A:58:PHE:CD1	0.40	2.51	5	1
1:A:26:TYR:C	1:A:28:SER:N	0.40	2.75	6	1
1:A:34:ILE:HG22	1:A:38:ARG:HE	0.40	1.76	14	1
1:A:5:ILE:CD1	1:A:10:TYR:CD1	0.40	3.04	17	1
1:A:56(A):ASP:O	1:A:56(A):ASP:CG	0.40	2.60	19	1
1:A:7:LEU:HD12	1:A:42:LEU:CD2	0.40	2.46	21	1
1:A:8:LYS:CD	1:A:34:ILE:CG2	0.40	2.99	22	1
1:A:36:ALA:CB	1:A:38:ARG:CZ	0.40	2.98	22	1
1:A:54:GLU:OE2	1:A:58:PHE:CB	0.40	2.69	27	1
1:A:4:ARG:NH2	1:A:53:GLU:OE1	0.40	2.55	31	1
1:A:57:PRO:HD2	1:A:60:SER:OG	0.40	2.16	32	1
1:A:7:LEU:HA	1:A:42:LEU:HD11	0.40	1.93	6	1
1:A:5:ILE:HG13	1:A:44:ILE:HD12	0.40	1.93	8	1
1:A:5:ILE:HG22	1:A:10:TYR:CA	0.40	2.46	10	1
1:A:56:LYS:HB3	1:A:56(C):GLU:CB	0.40	2.46	19	1
1:A:4:ARG:HD2	1:A:4:ARG:N	0.40	2.31	4	1
1:A:24:GLY:HA3	1:A:30:ILE:CG1	0.40	2.46	6	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	63/71 (89%)	45±4 (71±6%)	13±3 (21±5%)	5±2 (7±4%)	2	16
All	All	2016/2272 (89%)	1441 (71%)	428 (21%)	147 (7%)	2	16

All 20 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	56(A)	ASP	21
1	A	6	THR	14
1	A	49	SER	12

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type	Models (Total)
1	A	58	PHE	10
1	A	47	ASP	10
1	A	45	ASN	10
1	A	57	PRO	9
1	A	60	SER	9
1	A	44	ILE	8
1	A	36	ALA	6
1	A	37	GLY	6
1	A	39	LYS	6
1	A	50	VAL	5
1	A	59	PRO	4
1	A	26	TYR	4
1	A	38	ARG	4
1	A	48	GLY	3
1	A	15	GLY	3
1	A	27	GLN	2
1	A	55	VAL	1

### 6.3.2 Protein sidechains ⓘ

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	51/58 (88%)	36±3 (71±6%)	15±3 (29±6%)	1	17
All	All	1632/1856 (88%)	1155 (71%)	477 (29%)	1	17

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	8	LYS	23
1	A	6	THR	21
1	A	38	ARG	20
1	A	13	ARG	19
1	A	16	GLN	19
1	A	18	LYS	17
1	A	31	ASN	16
1	A	12	MET	16

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Models (Total)
1	A	32	LYS	16
1	A	53	GLU	15
1	A	39	LYS	15
1	A	49	SER	15
1	A	9	ASP	14
1	A	27	GLN	14
1	A	4	ARG	14
1	A	30	ILE	13
1	A	56(E)	LYS	13
1	A	25	VAL	13
1	A	56	LYS	13
1	A	21	LYS	12
1	A	54	GLU	12
1	A	58	PHE	11
1	A	56(C)	GLU	11
1	A	7	LEU	10
1	A	45	ASN	10
1	A	47	ASP	9
1	A	60	SER	9
1	A	19	THR	9
1	A	14	PHE	9
1	A	17	THR	8
1	A	28	SER	7
1	A	22	ASP	7
1	A	35	HIS	6
1	A	51	TYR	6
1	A	23	LEU	6
1	A	56(A)	ASP	5
1	A	43	THR	5
1	A	42	LEU	4
1	A	3	GLN	4
1	A	56(D)	VAL	3
1	A	26	TYR	2
1	A	44	ILE	2
1	A	34	ILE	1
1	A	59	PRO	1
1	A	5	ILE	1
1	A	55	VAL	1

### 6.3.3 RNA ⓘ

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

No chemical shift data were provided