



# Full wwPDB NMR Structure Validation Report ⓘ

Feb 12, 2017 – 10:42 pm GMT

PDB ID : 2K4T  
Title : Solution structure of human VDAC-1 in LDAO micelles  
Authors : Hiller, S.; Garces, R.G.; Malia, T.J.; Orekhov, V.Y.; Colombini, M.; Wagner, G.  
Deposited on : 2008-06-17

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

<http://wwpdb.org/validation/2016/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

Cyrange : Kirchner and Güntert (2011)  
NmrClust : Kelley et al. (1996)  
MolProbity : 4.02b-467  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
RCI : v\_1n\_11\_5\_13\_A (Berjanski et al., 2005)  
PANAV : Wang et al. (2010)  
ShiftChecker : trunk28760  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

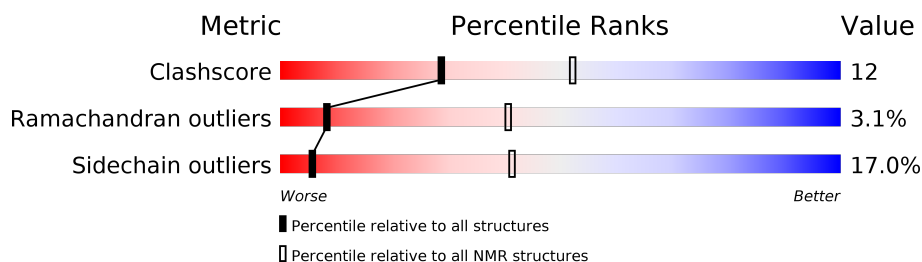
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 34%.

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	125131	11601
Ramachandran outliers	121729	10391
Sidechain outliers	121581	10367

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	291	 68% 23% 7% •

## 2 Ensemble composition and analysis

This entry contains 20 models. Model 1 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:5-A:15, A:24-A:249, A:254-A:281 (265)	2.04	1

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 4 clusters and 2 single-model clusters were found.

Cluster number	Models
1	1, 2, 3, 5, 6, 7, 8, 11, 16
2	9, 14, 17
3	10, 13, 19
4	12, 18, 20
Single-model clusters	4; 15

### 3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 4347 atoms, of which 2160 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Voltage-dependent anion-selective channel protein 1.

Mol	Chain	Residues	Atoms						Trace
1	A	285	Total	C	H	N	O	S	0
			4347	1383	2160	368	431	5	

There are 8 discrepancies between the modelled and reference sequences:

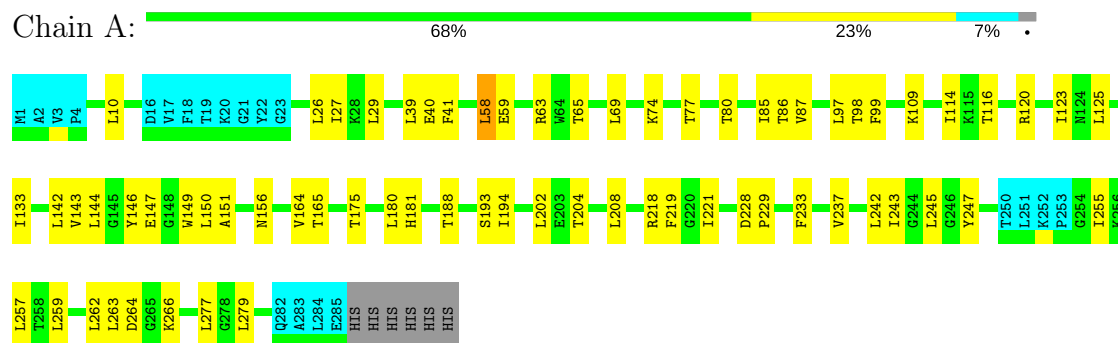
Chain	Residue	Modelled	Actual	Comment	Reference
A	284	LEU	-	EXPRESSION TAG	UNP P21796
A	285	GLU	-	EXPRESSION TAG	UNP P21796
A	286	HIS	-	EXPRESSION TAG	UNP P21796
A	287	HIS	-	EXPRESSION TAG	UNP P21796
A	288	HIS	-	EXPRESSION TAG	UNP P21796
A	289	HIS	-	EXPRESSION TAG	UNP P21796
A	290	HIS	-	EXPRESSION TAG	UNP P21796
A	291	HIS	-	EXPRESSION TAG	UNP P21796

## 4 Residue-property plots [i](#)

### 4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA and DNA 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: Voltage-dependent anion-selective channel protein 1

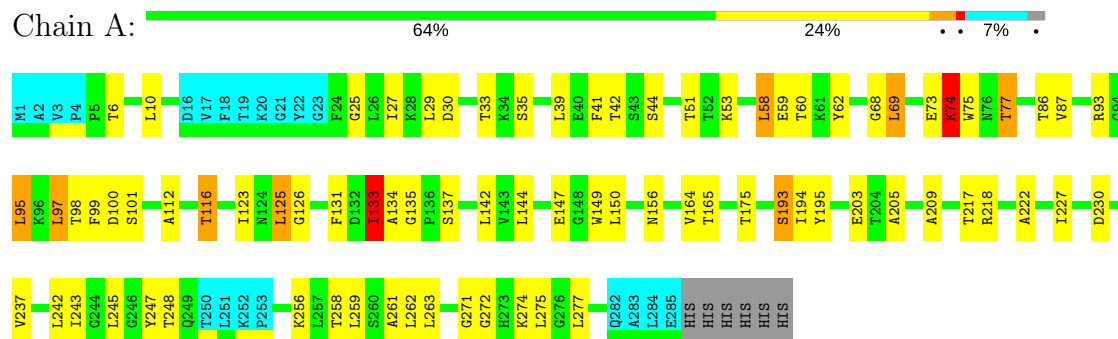


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

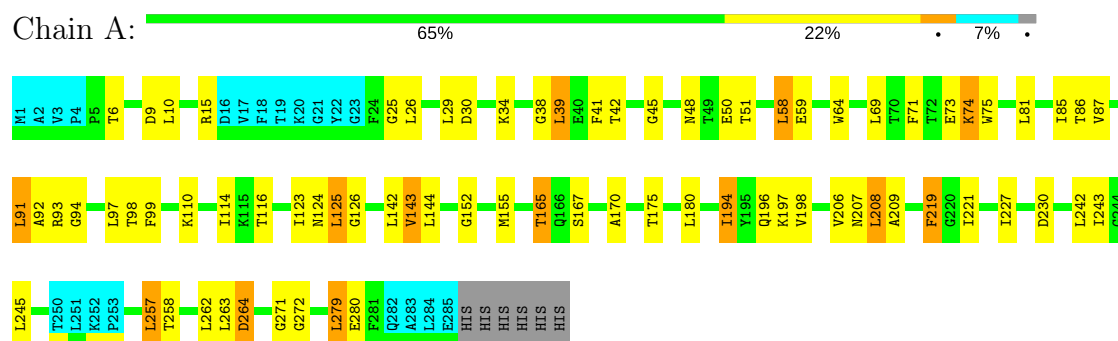
#### 4.2.1 Score per residue for model 1 (medoid)

- Molecule 1: Voltage-dependent anion-selective channel protein 1

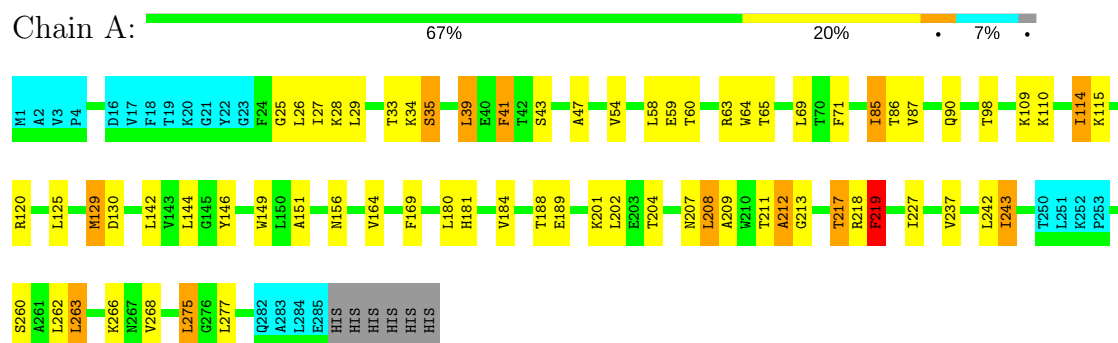


## 4.2.2 Score per residue for model 2

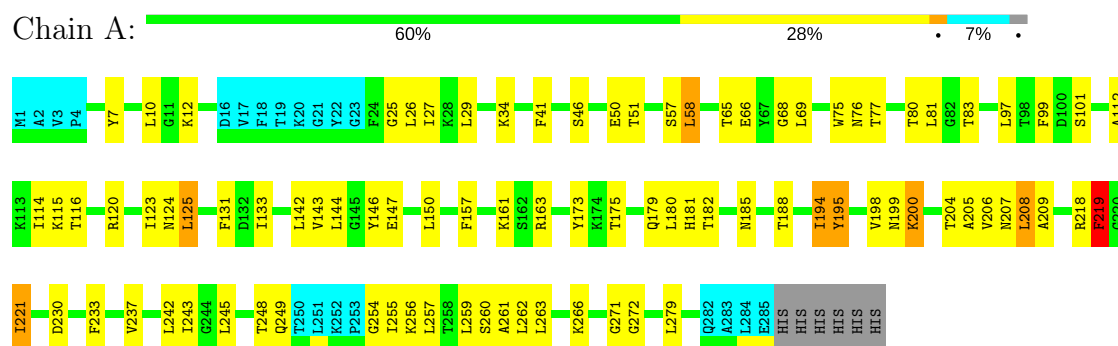
- Molecule 1: Voltage-dependent anion-selective channel protein 1



- Molecule 1: Voltage-dependent anion-selective channel protein 1

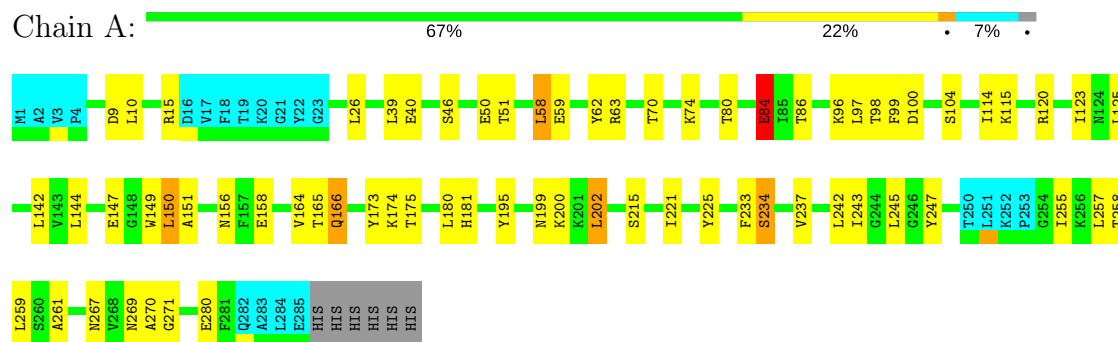


- Molecule 1: Voltage-dependent anion-selective channel protein 1



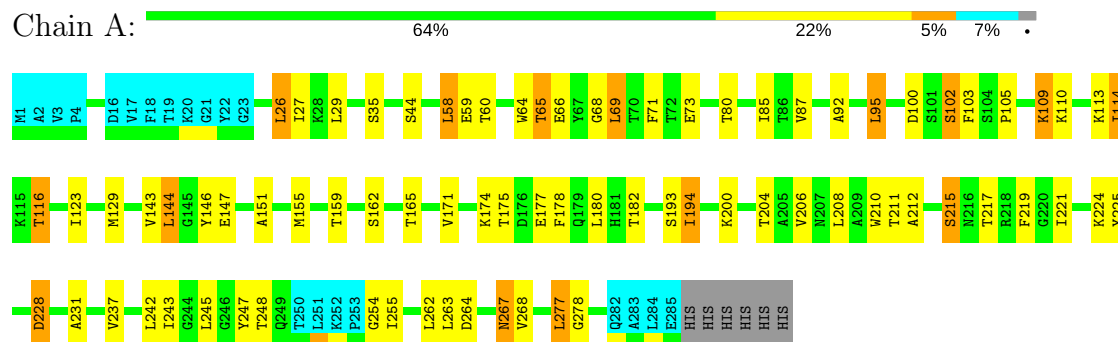
### 4.2.5 Score per residue for model 5

- Molecule 1: Voltage-dependent anion-selective channel protein 1



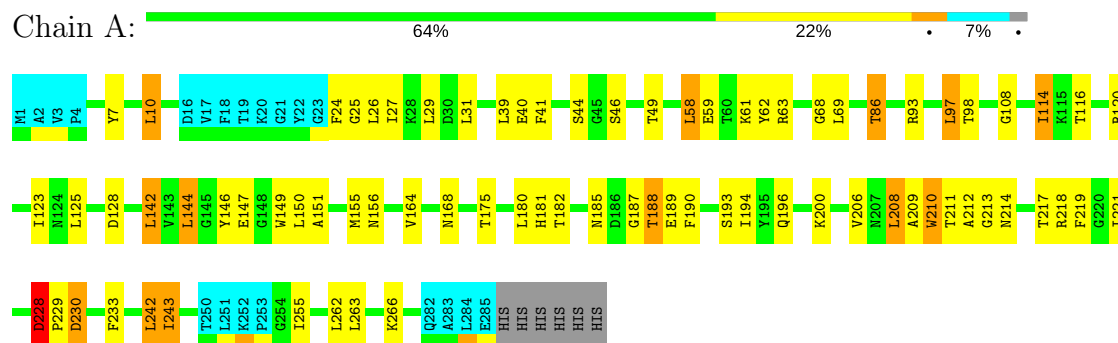
### 4.2.6 Score per residue for model 6

- Molecule 1: Voltage-dependent anion-selective channel protein 1



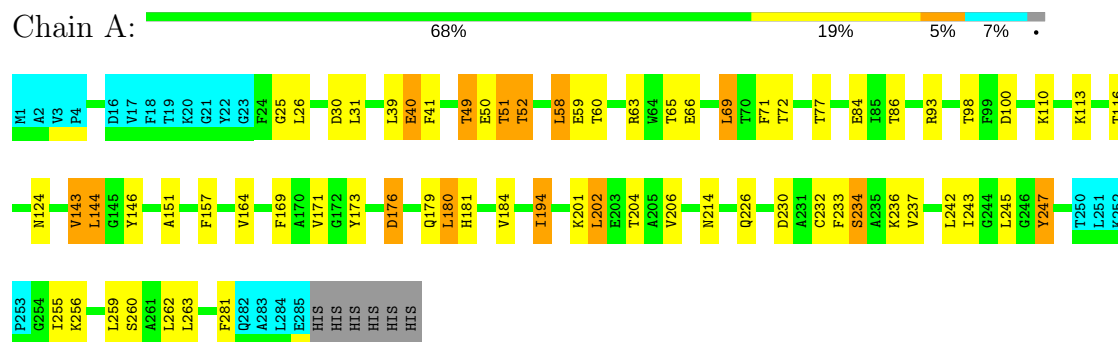
### 4.2.7 Score per residue for model 7

- Molecule 1: Voltage-dependent anion-selective channel protein 1



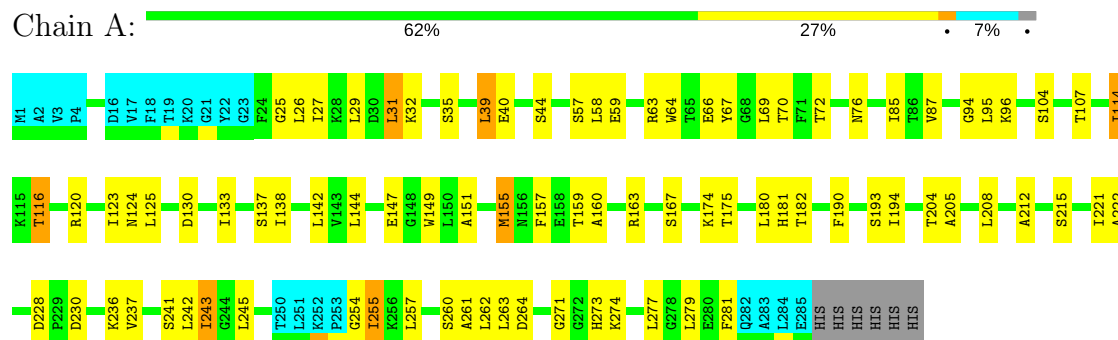
## 4.2.8 Score per residue for model 8

- Molecule 1: Voltage-dependent anion-selective channel protein 1



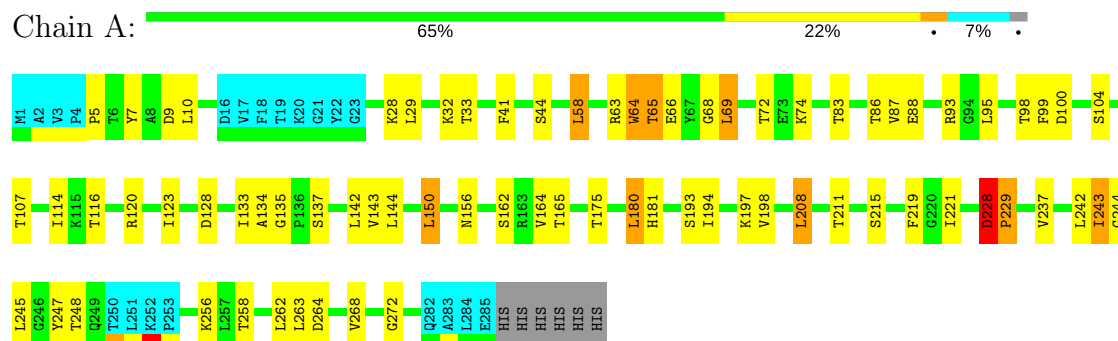
## 4.2.9 Score per residue for model 9

- Molecule 1: Voltage-dependent anion-selective channel protein 1



## 4.2.10 Score per residue for model 10

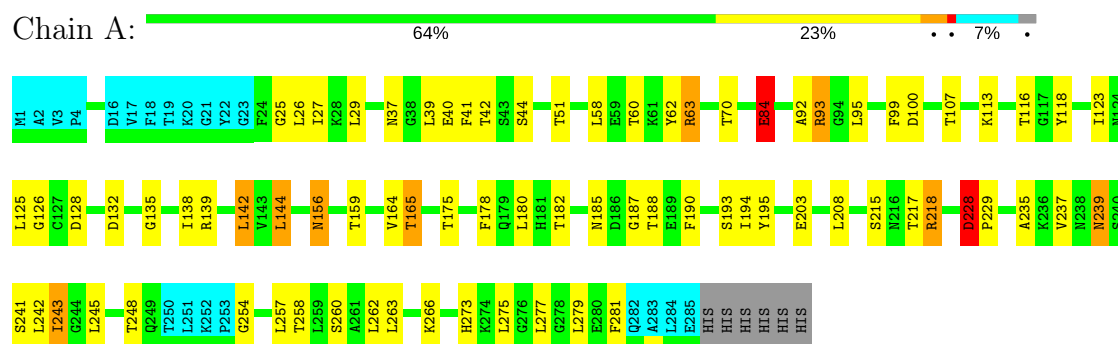
- Molecule 1: Voltage-dependent anion-selective channel protein 1





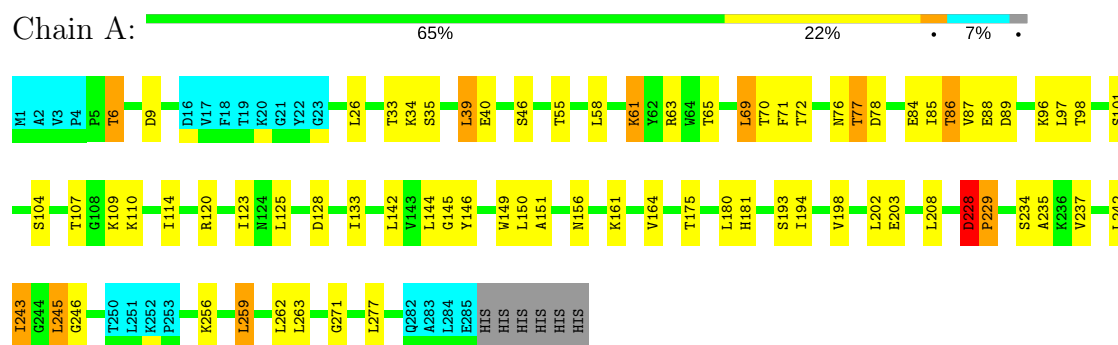
### 4.2.11 Score per residue for model 11

- Molecule 1: Voltage-dependent anion-selective channel protein 1



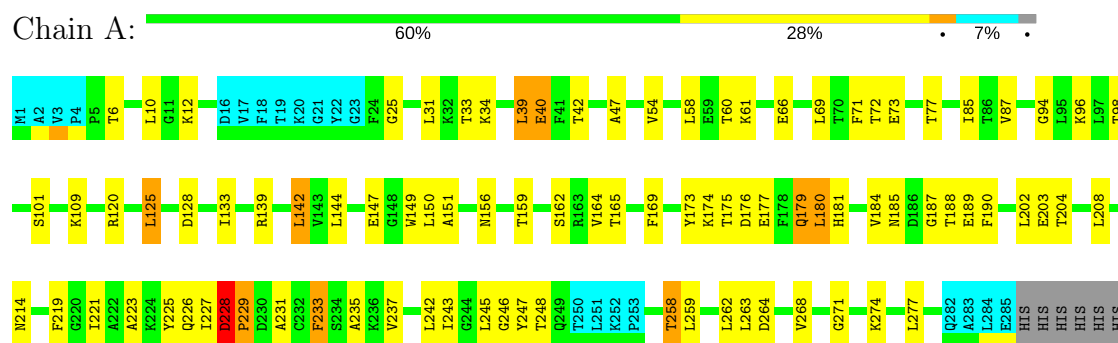
### 4.2.12 Score per residue for model 12

- Molecule 1: Voltage-dependent anion-selective channel protein 1



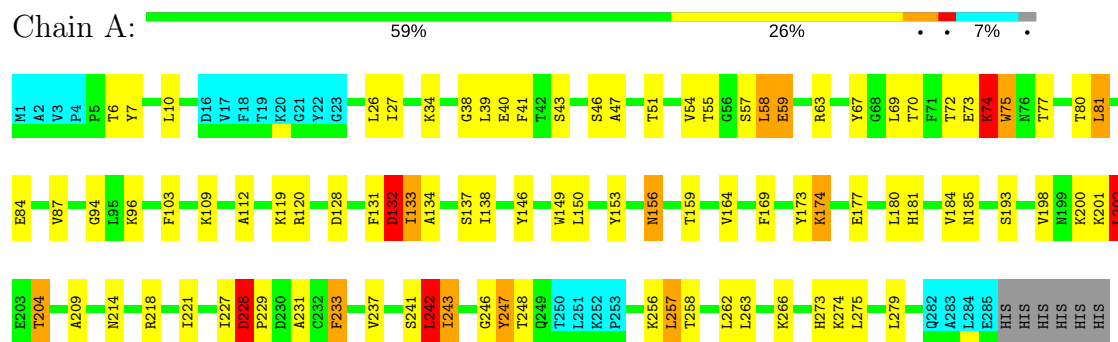
### 4.2.13 Score per residue for model 13

- Molecule 1: Voltage-dependent anion-selective channel protein 1



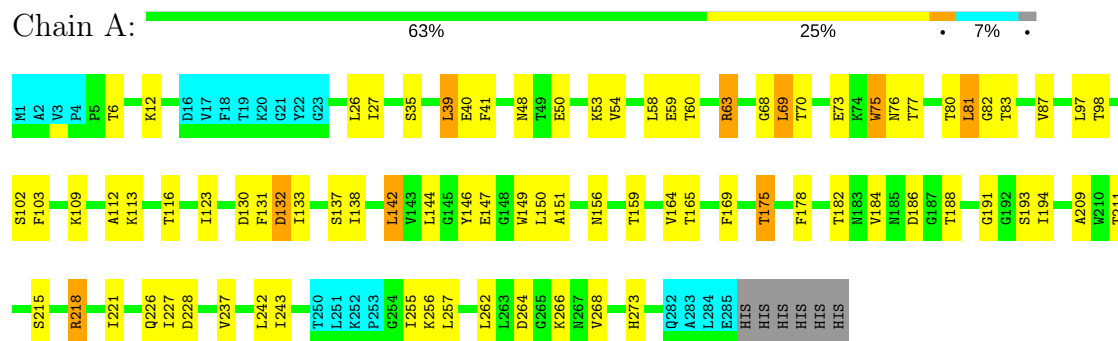
#### 4.2.14 Score per residue for model 14

- Molecule 1: Voltage-dependent anion-selective channel protein 1



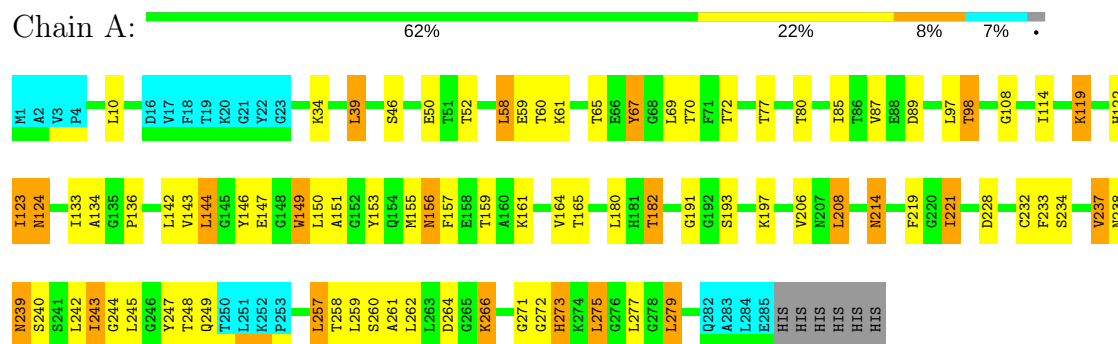
#### 4.2.15 Score per residue for model 15

- Molecule 1: Voltage-dependent anion-selective channel protein 1



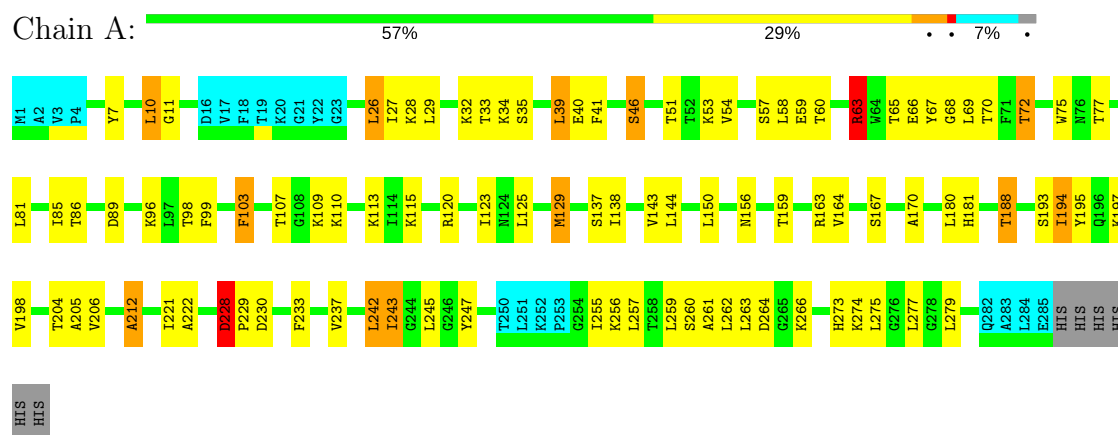
#### 4.2.16 Score per residue for model 16

- Molecule 1: Voltage-dependent anion-selective channel protein 1



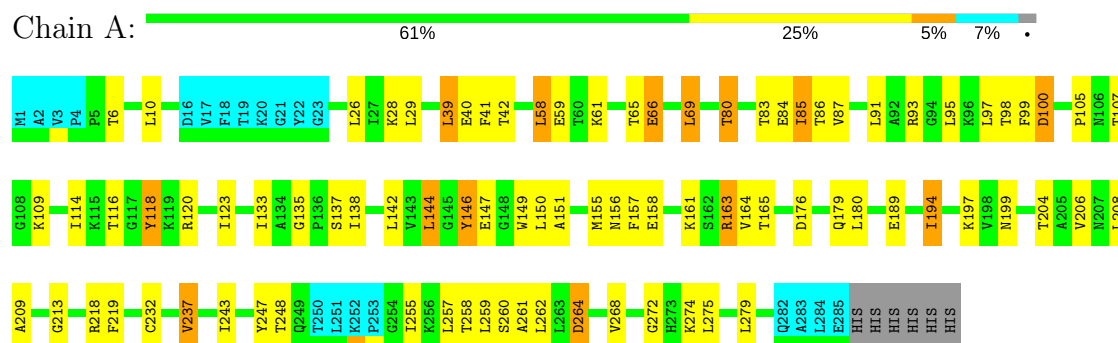
### 4.2.17 Score per residue for model 17

- Molecule 1: Voltage-dependent anion-selective channel protein 1



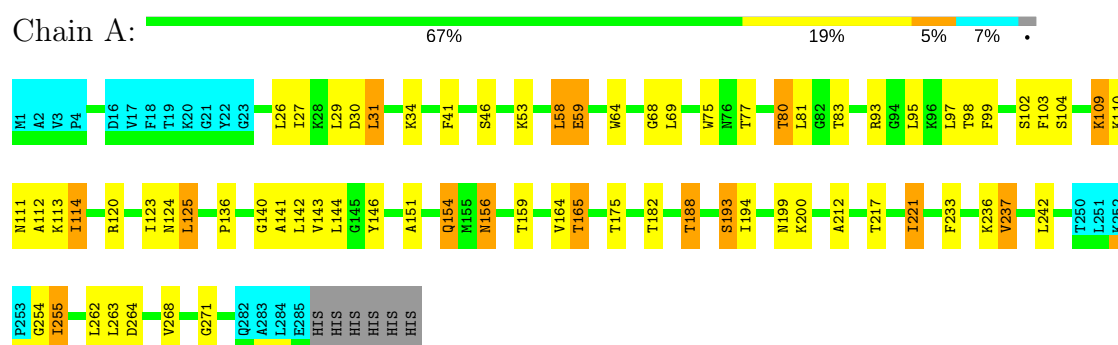
### 4.2.18 Score per residue for model 18

- Molecule 1: Voltage-dependent anion-selective channel protein 1



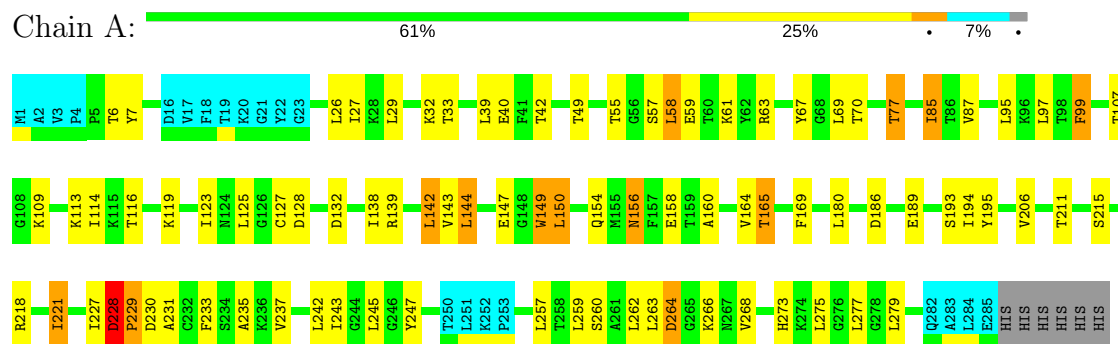
### 4.2.19 Score per residue for model 19

- Molecule 1: Voltage-dependent anion-selective channel protein 1



## 4.2.20 Score per residue for model 20

- Molecule 1: Voltage-dependent anion-selective channel protein 1



## 5 Refinement protocol and experimental data overview

The models were refined using the following method: *TORSION ANGLE DYNAMICS*.

Of the 500 calculated structures, 20 were deposited, based on the following criterion: *target function*.

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

Software name	Classification	Version
CYANA	structure solution	2.1
CYANA	refinement	2.1

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	BMRB entry 16381
Number of chemical shift lists	1
Total number of shifts	1224
Number of shifts mapped to atoms	1224
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	34%

No validations of the models with respect to experimental NMR restraints is performed at this time.

## 6 Model quality

### 6.1 Standard geometry

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

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	2036	2005	2005	48±10
All	All	40720	40100	40100	950

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 12.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:86:THR:HG23	1:A:98:THR:HG22	0.98	1.35	7	3
1:A:123:ILE:HD11	1:A:142:LEU:HD11	0.95	1.35	5	3
1:A:95:LEU:HD22	1:A:116:THR:HG22	0.94	1.37	20	1
1:A:263:LEU:HD12	1:A:268:VAL:HG21	0.91	1.40	3	2
1:A:242:LEU:HD11	1:A:262:LEU:HD21	0.89	1.45	13	3
1:A:248:THR:HG22	1:A:258:THR:HG23	0.87	1.46	18	1
1:A:237:VAL:HG22	1:A:243:ILE:HG23	0.86	1.48	13	8
1:A:81:LEU:HD13	1:A:81:LEU:N	0.83	1.87	15	2
1:A:205:ALA:HB3	1:A:222:ALA:HB3	0.83	1.49	9	3
1:A:242:LEU:HD21	1:A:262:LEU:HD21	0.82	1.49	2	9
1:A:233:PHE:HB3	1:A:246:GLY:O	0.81	1.75	13	2
1:A:69:LEU:HD11	1:A:87:VAL:HG23	0.80	1.54	2	1
1:A:206:VAL:HG23	1:A:221:ILE:HG22	0.79	1.54	4	4
1:A:190:PHE:HB2	1:A:209:ALA:HB1	0.79	1.54	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:85:ILE:O	1:A:99:PHE:HA	0.78	1.79	20	1
1:A:85:ILE:HD12	1:A:114:ILE:HG22	0.76	1.54	20	1
1:A:242:LEU:HD21	1:A:262:LEU:HD11	0.75	1.58	20	3
1:A:237:VAL:HG22	1:A:243:ILE:HG22	0.74	1.58	17	1
1:A:142:LEU:HD22	1:A:142:LEU:C	0.74	2.02	11	1
1:A:85:ILE:O	1:A:85:ILE:HD13	0.74	1.82	20	1
1:A:232:CYS:O	1:A:247:TYR:HB3	0.74	1.81	8	1
1:A:156:ASN:O	1:A:164:VAL:HG23	0.73	1.82	16	2
1:A:137:SER:O	1:A:138:ILE:HD13	0.73	1.83	17	2
1:A:95:LEU:HD22	1:A:95:LEU:C	0.73	2.03	1	1
1:A:247:TYR:HA	1:A:259:LEU:O	0.73	1.84	5	2
1:A:75:TRP:HB3	1:A:80:THR:O	0.73	1.82	15	1
1:A:69:LEU:HD23	1:A:87:VAL:HG22	0.72	1.60	18	1
1:A:237:VAL:HG13	1:A:243:ILE:HG22	0.72	1.62	12	3
1:A:69:LEU:N	1:A:69:LEU:HD13	0.72	2.00	1	1
1:A:29:LEU:HD23	1:A:279:LEU:HD11	0.72	1.61	2	1
1:A:142:LEU:HD21	1:A:144:LEU:HD21	0.71	1.60	10	1
1:A:69:LEU:HD13	1:A:69:LEU:N	0.71	2.01	6	1
1:A:245:LEU:CB	1:A:261:ALA:HB3	0.70	2.17	5	1
1:A:202:LEU:HD11	1:A:227:ILE:HD11	0.70	1.61	14	1
1:A:235:ALA:HB1	1:A:245:LEU:HD23	0.69	1.63	13	2
1:A:97:LEU:HD22	1:A:114:ILE:HD13	0.69	1.65	20	1
1:A:257:LEU:HD11	1:A:277:LEU:HD11	0.69	1.63	11	1
1:A:208:LEU:HD22	1:A:208:LEU:C	0.69	2.07	7	3
1:A:242:LEU:HD11	1:A:262:LEU:HD11	0.68	1.65	17	2
1:A:245:LEU:HD21	1:A:261:ALA:HB3	0.68	1.66	4	1
1:A:143:VAL:C	1:A:144:LEU:HD13	0.68	2.09	20	3
1:A:41:PHE:CZ	1:A:58:LEU:HD21	0.68	2.24	8	4
1:A:259:LEU:HD12	1:A:277:LEU:HD13	0.67	1.65	17	1
1:A:69:LEU:HD22	1:A:69:LEU:H	0.67	1.50	6	2
1:A:234:SER:O	1:A:245:LEU:HB3	0.67	1.89	12	1
1:A:87:VAL:HG21	1:A:97:LEU:HD12	0.67	1.65	20	1
1:A:247:TYR:CA	1:A:259:LEU:O	0.67	2.43	5	2
1:A:39:LEU:HD22	1:A:39:LEU:C	0.66	2.10	13	1
1:A:156:ASN:O	1:A:164:VAL:HG22	0.66	1.90	18	2
1:A:39:LEU:C	1:A:39:LEU:HD22	0.66	2.11	18	3
1:A:151:ALA:HB2	1:A:171:VAL:HG23	0.66	1.66	8	1
1:A:227:ILE:HD12	1:A:231:ALA:HB3	0.66	1.67	20	1
1:A:206:VAL:CG2	1:A:221:ILE:HG22	0.66	2.21	4	1
1:A:29:LEU:HD22	1:A:279:LEU:HD12	0.65	1.68	20	1
1:A:142:LEU:N	1:A:142:LEU:HD13	0.65	2.06	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:188:THR:HG22	1:A:212:ALA:HB3	0.65	1.66	19	2
1:A:248:THR:CG2	1:A:258:THR:HG22	0.65	2.22	14	1
1:A:69:LEU:HD23	1:A:87:VAL:CG2	0.65	2.22	18	1
1:A:69:LEU:HD12	1:A:87:VAL:HG22	0.65	1.66	15	1
1:A:257:LEU:HD22	1:A:279:LEU:HD13	0.65	1.67	18	1
1:A:208:LEU:HD13	1:A:208:LEU:N	0.64	2.07	2	1
1:A:208:LEU:C	1:A:208:LEU:HD22	0.64	2.13	4	1
1:A:208:LEU:HD22	1:A:208:LEU:O	0.64	1.92	4	1
1:A:68:GLY:C	1:A:69:LEU:HD13	0.64	2.11	6	3
1:A:248:THR:HG23	1:A:258:THR:HG22	0.64	1.68	14	1
1:A:194:ILE:HG12	1:A:206:VAL:HG13	0.64	1.67	17	6
1:A:26:LEU:C	1:A:26:LEU:HD22	0.63	2.14	17	1
1:A:35:SER:CB	1:A:39:LEU:HD11	0.63	2.24	3	1
1:A:86:THR:HB	1:A:98:THR:HG23	0.63	1.69	5	2
1:A:97:LEU:HD23	1:A:116:THR:HG23	0.63	1.68	2	1
1:A:69:LEU:HD23	1:A:86:THR:HG22	0.63	1.70	12	1
1:A:85:ILE:O	1:A:99:PHE:CA	0.63	2.47	20	1
1:A:217:THR:O	1:A:218:ARG:C	0.63	2.35	11	1
1:A:255:ILE:HD13	1:A:281:PHE:CD1	0.63	2.29	9	1
1:A:242:LEU:HD12	1:A:264:ASP:HA	0.63	1.70	2	3
1:A:210:TRP:O	1:A:210:TRP:CD1	0.63	2.52	7	1
1:A:241:SER:O	1:A:242:LEU:C	0.62	2.37	14	1
1:A:41:PHE:CE2	1:A:58:LEU:HD21	0.62	2.28	4	3
1:A:237:VAL:CG2	1:A:243:ILE:HG23	0.62	2.24	15	7
1:A:247:TYR:CZ	1:A:259:LEU:HD22	0.62	2.30	17	2
1:A:125:LEU:HD12	1:A:142:LEU:HD12	0.62	1.71	4	1
1:A:273:HIS:CD2	1:A:275:LEU:HD12	0.62	2.30	20	1
1:A:209:ALA:HB2	1:A:219:PHE:CD2	0.62	2.29	3	2
1:A:95:LEU:HD13	1:A:118:TYR:CE1	0.62	2.30	11	1
1:A:97:LEU:CD2	1:A:116:THR:HG22	0.62	2.25	7	1
1:A:124:ASN:HB2	1:A:143:VAL:HG23	0.62	1.72	2	4
1:A:190:PHE:HB3	1:A:210:TRP:O	0.61	1.95	7	1
1:A:209:ALA:HB3	1:A:218:ARG:HB2	0.61	1.72	1	3
1:A:247:TYR:HB3	1:A:259:LEU:C	0.61	2.16	16	2
1:A:84:GLU:HA	1:A:100:ASP:CB	0.61	2.25	18	1
1:A:194:ILE:HB	1:A:206:VAL:HG13	0.61	1.71	7	1
1:A:227:ILE:HD12	1:A:231:ALA:CB	0.61	2.24	20	1
1:A:26:LEU:N	1:A:26:LEU:HD13	0.61	2.11	6	1
1:A:249:GLN:NE2	1:A:257:LEU:HD13	0.61	2.11	16	1
1:A:138:ILE:O	1:A:157:PHE:CA	0.61	2.49	18	2
1:A:157:PHE:CA	1:A:164:VAL:HG12	0.61	2.26	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:149:TRP:C	1:A:150:LEU:HD22	0.61	2.16	7	2
1:A:33:THR:O	1:A:41:PHE:HA	0.61	1.95	3	1
1:A:242:LEU:HD21	1:A:262:LEU:CD2	0.61	2.26	16	3
1:A:129:MET:HB3	1:A:137:SER:O	0.60	1.96	17	1
1:A:85:ILE:C	1:A:85:ILE:HD13	0.60	2.15	20	1
1:A:231:ALA:HB3	1:A:247:TYR:CD1	0.60	2.31	14	1
1:A:140:GLY:O	1:A:154:GLN:HB3	0.60	1.95	19	1
1:A:195:TYR:CB	1:A:205:ALA:HA	0.60	2.27	4	1
1:A:26:LEU:O	1:A:27:ILE:HD13	0.60	1.97	11	2
1:A:180:LEU:HD11	1:A:182:THR:HG23	0.60	1.73	7	1
1:A:138:ILE:O	1:A:156:ASN:HB3	0.59	1.96	20	2
1:A:80:THR:HG23	1:A:105:PRO:HD3	0.59	1.74	18	1
1:A:69:LEU:CB	1:A:86:THR:O	0.59	2.50	10	2
1:A:143:VAL:O	1:A:144:LEU:HD13	0.59	1.98	8	2
1:A:58:LEU:HD13	1:A:59:GLU:N	0.59	2.12	3	13
1:A:33:THR:HG21	1:A:58:LEU:HD11	0.59	1.72	3	1
1:A:47:ALA:HB2	1:A:54:VAL:HG13	0.59	1.73	13	2
1:A:208:LEU:HD13	1:A:217:THR:OG1	0.59	1.97	6	1
1:A:39:LEU:HD13	1:A:61:LYS:O	0.59	1.98	20	1
1:A:274:LYS:O	1:A:275:LEU:HD22	0.59	1.97	18	1
1:A:144:LEU:N	1:A:144:LEU:HD22	0.59	2.12	20	5
1:A:138:ILE:O	1:A:157:PHE:HA	0.59	1.97	18	2
1:A:242:LEU:HD22	1:A:243:ILE:N	0.59	2.13	7	4
1:A:103:PHE:HB3	1:A:109:LYS:O	0.59	1.96	17	1
1:A:173:TYR:CE2	1:A:180:LEU:HD12	0.59	2.32	5	1
1:A:195:TYR:HB3	1:A:204:THR:O	0.58	1.97	4	1
1:A:244:GLY:O	1:A:245:LEU:HD22	0.58	1.98	10	1
1:A:26:LEU:C	1:A:27:ILE:HD12	0.58	2.19	14	6
1:A:235:ALA:HB2	1:A:245:LEU:HD13	0.58	1.75	20	1
1:A:256:LYS:CE	1:A:257:LEU:HD12	0.58	2.27	17	1
1:A:205:ALA:CB	1:A:222:ALA:HB3	0.58	2.27	9	1
1:A:35:SER:HB2	1:A:39:LEU:HD22	0.58	1.75	15	1
1:A:47:ALA:CB	1:A:54:VAL:HG22	0.58	2.28	3	2
1:A:237:VAL:HG13	1:A:243:ILE:CG2	0.58	2.28	12	1
1:A:69:LEU:HG	1:A:87:VAL:HG13	0.58	1.75	20	1
1:A:97:LEU:HD13	1:A:98:THR:N	0.58	2.13	2	3
1:A:256:LYS:O	1:A:257:LEU:HD22	0.58	1.97	15	1
1:A:138:ILE:C	1:A:157:PHE:HB3	0.58	2.19	9	1
1:A:27:ILE:HG23	1:A:277:LEU:HD12	0.58	1.73	9	1
1:A:7:TYR:CD1	1:A:150:LEU:HD23	0.58	2.34	14	1
1:A:156:ASN:O	1:A:164:VAL:HG13	0.58	1.98	11	11

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:180:LEU:HD13	1:A:181:HIS:N	0.58	2.14	9	7
1:A:158:GLU:CD	1:A:160:ALA:HB3	0.58	2.19	20	1
1:A:138:ILE:HD11	1:A:161:LYS:CG	0.58	2.28	18	1
1:A:80:THR:HG23	1:A:105:PRO:CD	0.58	2.29	18	1
1:A:69:LEU:CD1	1:A:87:VAL:HG13	0.58	2.29	16	3
1:A:75:TRP:NE1	1:A:81:LEU:HD12	0.58	2.13	14	1
1:A:97:LEU:HD12	1:A:116:THR:OG1	0.57	1.99	4	1
1:A:208:LEU:HD12	1:A:208:LEU:O	0.57	1.99	6	1
1:A:86:THR:CG2	1:A:98:THR:HG23	0.57	2.29	3	1
1:A:81:LEU:O	1:A:103:PHE:CA	0.57	2.52	19	1
1:A:242:LEU:HD13	1:A:243:ILE:N	0.57	2.14	5	3
1:A:97:LEU:HD21	1:A:114:ILE:HD11	0.57	1.74	2	2
1:A:69:LEU:HD11	1:A:87:VAL:HG13	0.57	1.76	16	2
1:A:257:LEU:HD22	1:A:279:LEU:CD1	0.57	2.28	18	1
1:A:202:LEU:HD11	1:A:227:ILE:CD1	0.57	2.30	14	1
1:A:257:LEU:HD12	1:A:257:LEU:O	0.57	2.00	4	1
1:A:69:LEU:CD2	1:A:87:VAL:HG13	0.57	2.29	9	1
1:A:132:ASP:C	1:A:133:ILE:HD12	0.57	2.20	14	1
1:A:233:PHE:CE2	1:A:259:LEU:HD22	0.57	2.35	5	1
1:A:233:PHE:CZ	1:A:245:LEU:HD12	0.57	2.34	20	1
1:A:144:LEU:HB2	1:A:151:ALA:HB3	0.57	1.77	19	8
1:A:69:LEU:HD12	1:A:71:PHE:CZ	0.57	2.35	8	1
1:A:248:THR:HG23	1:A:258:THR:OG1	0.56	2.00	11	2
1:A:33:THR:CG2	1:A:58:LEU:HD11	0.56	2.30	3	1
1:A:64:TRP:CD1	1:A:69:LEU:HD12	0.56	2.35	9	1
1:A:149:TRP:O	1:A:150:LEU:HD13	0.56	2.00	15	2
1:A:39:LEU:HD21	1:A:41:PHE:CD2	0.56	2.35	15	1
1:A:180:LEU:HD12	1:A:194:ILE:HG23	0.56	1.76	2	1
1:A:233:PHE:CE2	1:A:259:LEU:HD13	0.56	2.35	5	1
1:A:125:LEU:HD12	1:A:126:GLY:N	0.56	2.15	11	1
1:A:245:LEU:CD2	1:A:261:ALA:HB3	0.56	2.29	4	1
1:A:262:LEU:HD13	1:A:263:LEU:N	0.56	2.16	7	5
1:A:81:LEU:N	1:A:81:LEU:CD1	0.56	2.61	15	1
1:A:143:VAL:C	1:A:144:LEU:HD12	0.56	2.21	17	1
1:A:10:LEU:HD11	1:A:150:LEU:HB3	0.56	1.77	1	2
1:A:138:ILE:HD11	1:A:161:LYS:HG2	0.56	1.76	18	1
1:A:29:LEU:HD12	1:A:279:LEU:HB3	0.56	1.77	18	1
1:A:86:THR:HG22	1:A:98:THR:HG23	0.56	1.77	10	2
1:A:189:GLU:HG2	1:A:211:THR:HG23	0.56	1.78	20	1
1:A:238:ASN:O	1:A:239:ASN:C	0.56	2.43	16	1
1:A:233:PHE:CD2	1:A:259:LEU:HD13	0.56	2.36	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:138:ILE:N	1:A:157:PHE:CB	0.56	2.69	18	2
1:A:69:LEU:N	1:A:87:VAL:HA	0.56	2.16	10	1
1:A:232:CYS:O	1:A:248:THR:O	0.56	2.24	16	1
1:A:243:ILE:HD11	1:A:266:LYS:N	0.56	2.16	11	2
1:A:275:LEU:HD12	1:A:277:LEU:HD13	0.56	1.78	3	1
1:A:27:ILE:HG23	1:A:277:LEU:HB3	0.56	1.76	17	2
1:A:97:LEU:HD22	1:A:114:ILE:CD1	0.56	2.30	20	1
1:A:243:ILE:HD13	1:A:266:LYS:HG2	0.56	1.78	15	1
1:A:80:THR:HG23	1:A:103:PHE:C	0.56	2.21	14	1
1:A:257:LEU:HD11	1:A:277:LEU:CD1	0.56	2.31	11	1
1:A:202:LEU:HD11	1:A:226:GLN:CD	0.55	2.21	8	1
1:A:247:TYR:CE2	1:A:259:LEU:HD13	0.55	2.37	17	1
1:A:99:PHE:CZ	1:A:112:ALA:HB1	0.55	2.36	19	1
1:A:69:LEU:HD13	1:A:88:GLU:CB	0.55	2.32	12	2
1:A:237:VAL:HB	1:A:243:ILE:HG22	0.55	1.77	16	1
1:A:124:ASN:CB	1:A:143:VAL:HG23	0.55	2.32	8	1
1:A:39:LEU:HD23	1:A:40:GLU:N	0.55	2.16	5	1
1:A:81:LEU:N	1:A:103:PHE:CB	0.55	2.70	19	1
1:A:75:TRP:CE2	1:A:81:LEU:HD22	0.55	2.35	2	1
1:A:97:LEU:HD23	1:A:98:THR:N	0.55	2.16	19	2
1:A:136:PRO:O	1:A:159:THR:HG22	0.55	2.01	19	1
1:A:41:PHE:CE2	1:A:58:LEU:HD11	0.55	2.37	8	3
1:A:61:LYS:HG2	1:A:72:THR:HG22	0.55	1.77	12	1
1:A:208:LEU:HD23	1:A:217:THR:HB	0.55	1.78	7	1
1:A:241:SER:O	1:A:243:ILE:HG23	0.55	2.02	9	1
1:A:123:ILE:HB	1:A:144:LEU:HD23	0.55	1.77	18	1
1:A:10:LEU:HD23	1:A:11:GLY:N	0.55	2.17	17	1
1:A:71:PHE:CD1	1:A:85:ILE:HG22	0.55	2.37	2	2
1:A:245:LEU:HB2	1:A:261:ALA:HB3	0.55	1.79	5	1
1:A:39:LEU:HD12	1:A:40:GLU:N	0.55	2.16	8	1
1:A:125:LEU:HD12	1:A:142:LEU:CD1	0.54	2.32	4	2
1:A:41:PHE:CE1	1:A:58:LEU:HD21	0.54	2.36	19	3
1:A:233:PHE:CZ	1:A:245:LEU:HD11	0.54	2.37	17	1
1:A:26:LEU:HD12	1:A:48:ASN:OD1	0.54	2.02	2	1
1:A:142:LEU:HD23	1:A:144:LEU:HD21	0.54	1.79	20	1
1:A:264:ASP:O	1:A:268:VAL:HG22	0.54	2.02	19	3
1:A:245:LEU:HB3	1:A:261:ALA:HB3	0.54	1.78	5	1
1:A:81:LEU:O	1:A:103:PHE:HA	0.54	2.02	19	1
1:A:85:ILE:HD12	1:A:114:ILE:CG2	0.54	2.28	20	1
1:A:10:LEU:O	1:A:170:ALA:HB3	0.54	2.01	17	2
1:A:248:THR:OG1	1:A:258:THR:HG22	0.54	2.02	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:255:ILE:HG23	1:A:280:GLU:O	0.54	2.01	5	1
1:A:180:LEU:HD12	1:A:181:HIS:N	0.54	2.17	4	1
1:A:95:LEU:HD22	1:A:95:LEU:O	0.54	2.03	1	1
1:A:188:THR:HA	1:A:212:ALA:HB2	0.54	1.79	7	1
1:A:99:PHE:CE1	1:A:112:ALA:HB1	0.54	2.38	4	1
1:A:97:LEU:HD11	1:A:114:ILE:HD11	0.54	1.78	4	1
1:A:142:LEU:CD2	1:A:142:LEU:C	0.54	2.75	11	1
1:A:68:GLY:C	1:A:69:LEU:HD22	0.54	2.23	17	4
1:A:157:PHE:HA	1:A:164:VAL:HG12	0.54	1.79	8	1
1:A:64:TRP:CG	1:A:69:LEU:HD12	0.54	2.37	9	1
1:A:95:LEU:CD2	1:A:116:THR:HG22	0.54	2.25	20	1
1:A:137:SER:C	1:A:138:ILE:HD13	0.54	2.23	14	2
1:A:69:LEU:CD1	1:A:87:VAL:HG23	0.54	2.31	2	1
1:A:95:LEU:CD2	1:A:95:LEU:C	0.54	2.76	1	1
1:A:262:LEU:C	1:A:263:LEU:HD23	0.54	2.23	12	1
1:A:97:LEU:CD1	1:A:114:ILE:HD11	0.54	2.33	4	1
1:A:123:ILE:CG2	1:A:144:LEU:HD12	0.54	2.33	6	2
1:A:259:LEU:HD23	1:A:260:SER:N	0.54	2.18	8	2
1:A:26:LEU:HD23	1:A:46:SER:CB	0.54	2.33	17	1
1:A:138:ILE:HG22	1:A:155:MET:SD	0.54	2.42	9	1
1:A:141:ALA:HA	1:A:154:GLN:CB	0.54	2.33	19	1
1:A:149:TRP:C	1:A:150:LEU:HD13	0.54	2.23	20	2
1:A:39:LEU:H	1:A:39:LEU:HD13	0.54	1.63	16	3
1:A:42:THR:HG23	1:A:59:GLU:HG3	0.54	1.78	18	1
1:A:62:TYR:O	1:A:63:ARG:CB	0.54	2.55	11	1
1:A:195:TYR:CE2	1:A:205:ALA:HB2	0.53	2.39	17	1
1:A:81:LEU:C	1:A:103:PHE:HB3	0.53	2.24	19	1
1:A:242:LEU:HD13	1:A:242:LEU:C	0.53	2.24	12	6
1:A:193:SER:C	1:A:194:ILE:HD13	0.53	2.22	6	4
1:A:125:LEU:HD23	1:A:142:LEU:HD12	0.53	1.80	1	1
1:A:195:TYR:CD1	1:A:205:ALA:HB2	0.53	2.38	1	1
1:A:86:THR:OG1	1:A:98:THR:HG23	0.53	2.03	1	1
1:A:190:PHE:HA	1:A:210:TRP:O	0.53	2.03	7	1
1:A:77:THR:O	1:A:78:ASP:C	0.53	2.47	12	1
1:A:242:LEU:HD11	1:A:262:LEU:CD2	0.53	2.34	3	2
1:A:123:ILE:HD13	1:A:142:LEU:HD21	0.53	1.80	15	1
1:A:155:MET:HB3	1:A:164:VAL:HG21	0.53	1.79	18	1
1:A:112:ALA:HB3	1:A:131:PHE:O	0.53	2.04	1	2
1:A:69:LEU:HB2	1:A:87:VAL:HA	0.53	1.79	10	2
1:A:99:PHE:O	1:A:99:PHE:CD1	0.53	2.62	20	1
1:A:84:GLU:HB3	1:A:99:PHE:O	0.53	2.03	11	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:264:ASP:O	1:A:268:VAL:HG13	0.53	2.03	15	2
1:A:249:GLN:HB3	1:A:257:LEU:HD11	0.53	1.80	4	1
1:A:144:LEU:H	1:A:144:LEU:HD22	0.53	1.63	20	1
1:A:10:LEU:CD1	1:A:150:LEU:HD13	0.52	2.34	4	1
1:A:210:TRP:HB3	1:A:217:THR:HG22	0.52	1.81	6	1
1:A:97:LEU:HD12	1:A:116:THR:HG23	0.52	1.81	15	1
1:A:237:VAL:CG2	1:A:243:ILE:HG22	0.52	2.35	3	2
1:A:273:HIS:CD2	1:A:275:LEU:HD23	0.52	2.39	11	1
1:A:99:PHE:CD1	1:A:99:PHE:N	0.52	2.75	20	1
1:A:27:ILE:CD1	1:A:277:LEU:HD12	0.52	2.34	1	2
1:A:228:ASP:OD1	1:A:231:ALA:HB3	0.52	2.04	6	1
1:A:10:LEU:HG	1:A:150:LEU:HD12	0.52	1.80	5	1
1:A:262:LEU:O	1:A:263:LEU:HD13	0.52	2.04	3	1
1:A:233:PHE:CZ	1:A:245:LEU:HD13	0.52	2.38	4	1
1:A:189:GLU:CG	1:A:211:THR:HG23	0.52	2.33	20	1
1:A:87:VAL:CG2	1:A:97:LEU:HD12	0.52	2.35	20	1
1:A:114:ILE:HD12	1:A:115:LYS:N	0.52	2.20	3	2
1:A:180:LEU:HD12	1:A:194:ILE:CG1	0.52	2.35	11	1
1:A:29:LEU:CD2	1:A:279:LEU:HD11	0.52	2.34	2	1
1:A:6:THR:O	1:A:10:LEU:HD12	0.52	2.05	13	2
1:A:112:ALA:HB3	1:A:131:PHE:HB3	0.52	1.81	14	1
1:A:263:LEU:CD1	1:A:268:VAL:HG21	0.52	2.34	19	1
1:A:228:ASP:CB	1:A:229:PRO:CD	0.52	2.88	14	8
1:A:85:ILE:N	1:A:99:PHE:CB	0.52	2.73	20	1
1:A:81:LEU:O	1:A:81:LEU:HD22	0.52	2.05	15	2
1:A:69:LEU:HD22	1:A:69:LEU:N	0.52	2.19	6	1
1:A:257:LEU:HD13	1:A:258:THR:N	0.52	2.19	2	1
1:A:39:LEU:HD22	1:A:40:GLU:N	0.52	2.19	14	6
1:A:69:LEU:N	1:A:69:LEU:HD22	0.51	2.21	1	1
1:A:165:THR:HG22	1:A:166:GLN:NE2	0.51	2.20	5	1
1:A:6:THR:O	1:A:10:LEU:HD23	0.51	2.05	14	1
1:A:60:THR:HG22	1:A:73:GLU:HG2	0.51	1.82	13	1
1:A:209:ALA:HB3	1:A:218:ARG:O	0.51	2.04	4	1
1:A:233:PHE:CE1	1:A:245:LEU:HD12	0.51	2.41	20	1
1:A:29:LEU:CD2	1:A:279:LEU:HD12	0.51	2.34	20	1
1:A:39:LEU:HD22	1:A:62:TYR:HA	0.51	1.80	1	1
1:A:189:GLU:OE1	1:A:211:THR:HG22	0.51	2.05	3	1
1:A:61:LYS:HA	1:A:72:THR:HG22	0.51	1.82	13	1
1:A:6:THR:CB	1:A:150:LEU:HD12	0.51	2.36	20	1
1:A:35:SER:HB3	1:A:39:LEU:HD11	0.51	1.81	3	1
1:A:26:LEU:HD11	1:A:48:ASN:ND2	0.51	2.20	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:75:TRP:CG	1:A:80:THR:OG1	0.51	2.61	15	1
1:A:33:THR:O	1:A:41:PHE:CA	0.51	2.58	3	1
1:A:39:LEU:N	1:A:39:LEU:HD13	0.51	2.21	16	3
1:A:125:LEU:HD13	1:A:126:GLY:N	0.51	2.21	2	2
1:A:43:SER:HA	1:A:58:LEU:HD22	0.51	1.83	14	1
1:A:169:PHE:CZ	1:A:184:VAL:HG11	0.51	2.41	8	3
1:A:173:TYR:CB	1:A:180:LEU:HD23	0.50	2.35	4	1
1:A:63:ARG:HB2	1:A:70:THR:HG23	0.50	1.82	15	1
1:A:7:TYR:HA	1:A:10:LEU:HD22	0.50	1.81	17	1
1:A:6:THR:HG21	1:A:174:LYS:O	0.50	2.06	14	1
1:A:184:VAL:HG13	1:A:190:PHE:CD1	0.50	2.41	13	1
1:A:69:LEU:HB3	1:A:86:THR:O	0.50	2.06	12	1
1:A:144:LEU:HG	1:A:151:ALA:HB3	0.50	1.83	7	1
1:A:190:PHE:CA	1:A:210:TRP:O	0.50	2.59	7	1
1:A:244:GLY:C	1:A:245:LEU:HD22	0.50	2.27	10	2
1:A:210:TRP:CB	1:A:217:THR:HG22	0.50	2.36	6	1
1:A:206:VAL:HG23	1:A:221:ILE:CG2	0.50	2.33	2	1
1:A:144:LEU:CB	1:A:151:ALA:HB3	0.50	2.37	15	1
1:A:188:THR:HG22	1:A:212:ALA:CB	0.50	2.36	17	2
1:A:26:LEU:HD22	1:A:27:ILE:N	0.50	2.22	17	1
1:A:227:ILE:CG2	1:A:231:ALA:HB3	0.50	2.37	13	1
1:A:234:SER:C	1:A:245:LEU:HD12	0.50	2.26	12	1
1:A:234:SER:N	1:A:247:TYR:HB2	0.50	2.21	8	1
1:A:123:ILE:CD1	1:A:142:LEU:HD11	0.50	2.37	9	3
1:A:237:VAL:CG1	1:A:243:ILE:HG23	0.50	2.36	18	1
1:A:209:ALA:HB3	1:A:218:ARG:HB3	0.50	1.83	18	1
1:A:202:LEU:HD22	1:A:225:TYR:HA	0.50	1.83	13	1
1:A:49:THR:HG23	1:A:50:GLU:CG	0.50	2.37	8	1
1:A:279:LEU:HD13	1:A:279:LEU:N	0.50	2.21	16	1
1:A:70:THR:OG1	1:A:86:THR:HG23	0.50	2.07	5	1
1:A:242:LEU:C	1:A:242:LEU:HD22	0.50	2.27	7	1
1:A:242:LEU:C	1:A:242:LEU:HD13	0.49	2.28	10	7
1:A:69:LEU:CD1	1:A:69:LEU:N	0.49	2.70	1	2
1:A:73:GLU:O	1:A:74:LYS:HB2	0.49	2.08	1	2
1:A:63:ARG:HA	1:A:70:THR:HG22	0.49	1.85	5	1
1:A:150:LEU:HD21	1:A:174:LYS:HD3	0.49	1.82	13	1
1:A:6:THR:HG22	1:A:9:ASP:HB2	0.49	1.83	12	1
1:A:58:LEU:O	1:A:74:LYS:HB3	0.49	2.07	14	3
1:A:237:VAL:HG22	1:A:243:ILE:HA	0.49	1.83	9	3
1:A:26:LEU:HD23	1:A:28:LYS:CE	0.49	2.37	18	1
1:A:81:LEU:HD13	1:A:81:LEU:H	0.49	1.67	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:41:PHE:CZ	1:A:58:LEU:HD11	0.49	2.42	4	1
1:A:180:LEU:HD12	1:A:194:ILE:CG2	0.49	2.37	2	1
1:A:86:THR:CB	1:A:98:THR:HG23	0.49	2.38	5	1
1:A:209:ALA:HB3	1:A:218:ARG:CB	0.49	2.37	14	1
1:A:247:TYR:CB	1:A:259:LEU:N	0.49	2.75	16	2
1:A:227:ILE:HG23	1:A:229:PRO:HD2	0.49	1.85	13	1
1:A:243:ILE:O	1:A:243:ILE:HG12	0.49	2.07	12	1
1:A:144:LEU:HD13	1:A:144:LEU:N	0.49	2.22	20	1
1:A:85:ILE:C	1:A:99:PHE:HB3	0.49	2.28	20	1
1:A:119:LYS:HB3	1:A:123:ILE:O	0.49	2.07	16	1
1:A:262:LEU:O	1:A:263:LEU:HD23	0.49	2.07	12	1
1:A:99:PHE:HB2	1:A:114:ILE:HD13	0.49	1.83	4	1
1:A:180:LEU:HD13	1:A:194:ILE:CG2	0.49	2.38	4	1
1:A:217:THR:HG23	1:A:217:THR:O	0.49	2.07	11	1
1:A:76:ASN:O	1:A:77:THR:C	0.49	2.50	12	1
1:A:50:GLU:HG3	1:A:52:THR:HG23	0.48	1.83	16	1
1:A:193:SER:C	1:A:194:ILE:HD12	0.48	2.29	19	5
1:A:144:LEU:HD12	1:A:151:ALA:O	0.48	2.08	18	1
1:A:248:THR:HG22	1:A:258:THR:CG2	0.48	2.32	18	1
1:A:69:LEU:HD22	1:A:87:VAL:HG13	0.48	1.84	13	2
1:A:86:THR:CG2	1:A:98:THR:HG22	0.48	2.35	18	2
1:A:198:VAL:HG12	1:A:202:LEU:O	0.48	2.08	12	1
1:A:256:LYS:HE3	1:A:257:LEU:HD12	0.48	1.85	17	1
1:A:133:ILE:HD11	1:A:135:GLY:O	0.48	2.07	1	1
1:A:49:THR:HG23	1:A:50:GLU:HG2	0.48	1.85	8	1
1:A:195:TYR:CE1	1:A:205:ALA:HB2	0.48	2.44	1	1
1:A:259:LEU:HD23	1:A:277:LEU:CB	0.48	2.39	12	1
1:A:139:ARG:HA	1:A:156:ASN:CB	0.48	2.39	11	2
1:A:86:THR:HG23	1:A:98:THR:CG2	0.48	2.37	8	1
1:A:73:GLU:O	1:A:74:LYS:CB	0.48	2.61	14	1
1:A:145:GLY:HA2	1:A:150:LEU:HD23	0.48	1.85	12	1
1:A:95:LEU:HD13	1:A:118:TYR:CZ	0.48	2.44	11	1
1:A:85:ILE:HD11	1:A:87:VAL:CG2	0.48	2.38	20	1
1:A:75:TRP:CE3	1:A:75:TRP:HA	0.48	2.44	15	1
1:A:245:LEU:HD13	1:A:246:GLY:H	0.48	1.68	12	1
1:A:234:SER:O	1:A:245:LEU:HA	0.48	2.09	5	1
1:A:29:LEU:HD12	1:A:279:LEU:CB	0.48	2.39	18	1
1:A:68:GLY:O	1:A:69:LEU:HD22	0.48	2.09	19	1
1:A:55:THR:OG1	1:A:77:THR:HG21	0.48	2.08	20	1
1:A:60:THR:HG22	1:A:73:GLU:HB2	0.48	1.86	15	1
1:A:24:PHE:O	1:A:49:THR:HG22	0.48	2.09	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:85:ILE:N	1:A:99:PHE:HB2	0.47	2.23	20	1
1:A:233:PHE:HB2	1:A:247:TYR:HA	0.47	1.84	14	2
1:A:39:LEU:CD2	1:A:39:LEU:C	0.47	2.83	13	4
1:A:133:ILE:HD13	1:A:133:ILE:N	0.47	2.24	1	1
1:A:245:LEU:O	1:A:261:ALA:HB3	0.47	2.09	9	1
1:A:180:LEU:O	1:A:180:LEU:HD13	0.47	2.10	5	1
1:A:175:THR:HG22	1:A:178:PHE:O	0.47	2.09	11	1
1:A:151:ALA:HB1	1:A:171:VAL:HG22	0.47	1.86	6	1
1:A:6:THR:CG2	1:A:150:LEU:HD12	0.47	2.39	20	1
1:A:258:THR:C	1:A:259:LEU:HD22	0.47	2.30	13	1
1:A:245:LEU:HD12	1:A:245:LEU:O	0.47	2.09	1	1
1:A:124:ASN:O	1:A:142:LEU:HD12	0.47	2.10	9	1
1:A:257:LEU:HD13	1:A:259:LEU:CD1	0.47	2.40	4	1
1:A:211:THR:O	1:A:212:ALA:HB3	0.47	2.10	6	1
1:A:125:LEU:CD2	1:A:142:LEU:HD12	0.47	2.40	1	3
1:A:248:THR:CB	1:A:258:THR:HG22	0.47	2.39	1	1
1:A:31:LEU:HD13	1:A:32:LYS:N	0.47	2.24	9	1
1:A:33:THR:N	1:A:41:PHE:CB	0.47	2.78	3	1
1:A:203:GLU:O	1:A:223:ALA:HB1	0.47	2.10	13	1
1:A:234:SER:CB	1:A:245:LEU:HD12	0.47	2.40	12	1
1:A:39:LEU:HD23	1:A:62:TYR:CE2	0.47	2.45	7	1
1:A:69:LEU:HB2	1:A:87:VAL:CA	0.47	2.40	12	2
1:A:6:THR:HB	1:A:150:LEU:HD12	0.47	1.87	20	1
1:A:85:ILE:C	1:A:85:ILE:CD1	0.47	2.83	20	1
1:A:63:ARG:HB3	1:A:70:THR:HG23	0.47	1.85	17	1
1:A:97:LEU:HD22	1:A:116:THR:CG2	0.47	2.39	1	1
1:A:237:VAL:CB	1:A:243:ILE:HG22	0.47	2.40	16	1
1:A:217:THR:HG22	1:A:241:SER:HB2	0.47	1.86	11	1
1:A:262:LEU:C	1:A:262:LEU:HD13	0.47	2.30	14	9
1:A:103:PHE:CB	1:A:110:LYS:HA	0.47	2.40	17	1
1:A:279:LEU:H	1:A:279:LEU:HD13	0.47	1.69	16	1
1:A:97:LEU:HD21	1:A:114:ILE:CG1	0.47	2.40	19	1
1:A:86:THR:HG23	1:A:98:THR:OG1	0.47	2.10	12	1
1:A:187:GLY:O	1:A:188:THR:HG23	0.47	2.10	7	1
1:A:194:ILE:CG1	1:A:206:VAL:HG13	0.46	2.38	17	1
1:A:262:LEU:HD13	1:A:262:LEU:C	0.46	2.31	12	4
1:A:142:LEU:HD22	1:A:142:LEU:O	0.46	2.10	20	1
1:A:175:THR:HG23	1:A:178:PHE:CB	0.46	2.40	15	1
1:A:75:TRP:CD1	1:A:80:THR:HB	0.46	2.45	15	1
1:A:180:LEU:HD22	1:A:181:HIS:N	0.46	2.25	14	2
1:A:237:VAL:CG1	1:A:243:ILE:HG22	0.46	2.37	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:190:PHE:CB	1:A:210:TRP:O	0.46	2.62	7	1
1:A:142:LEU:CD1	1:A:142:LEU:N	0.46	2.77	20	1
1:A:6:THR:HG22	1:A:150:LEU:HD12	0.46	1.86	20	1
1:A:256:LYS:C	1:A:257:LEU:HD22	0.46	2.31	15	1
1:A:269:ASN:O	1:A:270:ALA:HB3	0.46	2.09	5	1
1:A:198:VAL:HG13	1:A:204:THR:OG1	0.46	2.11	14	1
1:A:97:LEU:CG	1:A:114:ILE:HD11	0.46	2.41	4	1
1:A:123:ILE:HD13	1:A:142:LEU:HD11	0.46	1.86	10	1
1:A:102:SER:O	1:A:110:LYS:HB3	0.46	2.10	6	1
1:A:26:LEU:HD23	1:A:46:SER:HB2	0.46	1.86	17	1
1:A:97:LEU:HD22	1:A:98:THR:N	0.46	2.25	12	1
1:A:123:ILE:HD11	1:A:142:LEU:HD21	0.46	1.87	7	1
1:A:142:LEU:HD23	1:A:143:VAL:N	0.46	2.25	4	1
1:A:208:LEU:N	1:A:208:LEU:CD1	0.46	2.78	2	2
1:A:86:THR:HB	1:A:98:THR:HG22	0.46	1.87	2	1
1:A:237:VAL:HG22	1:A:243:ILE:CG2	0.46	2.35	17	1
1:A:28:LYS:O	1:A:29:LEU:HD22	0.46	2.10	10	1
1:A:69:LEU:CG	1:A:87:VAL:HG13	0.46	2.40	20	2
1:A:85:ILE:HD11	1:A:87:VAL:HG23	0.46	1.87	20	1
1:A:242:LEU:CD2	1:A:262:LEU:HD21	0.46	2.33	2	1
1:A:195:TYR:HB3	1:A:205:ALA:HA	0.46	1.87	4	1
1:A:75:TRP:HB2	1:A:81:LEU:HA	0.46	1.87	15	1
1:A:256:LYS:CD	1:A:257:LEU:HD12	0.46	2.41	17	1
1:A:257:LEU:HD13	1:A:259:LEU:HD13	0.46	1.87	4	1
1:A:10:LEU:HD13	1:A:150:LEU:CD1	0.46	2.41	10	1
1:A:142:LEU:HD21	1:A:144:LEU:HD11	0.46	1.88	11	2
1:A:262:LEU:C	1:A:263:LEU:HD22	0.45	2.32	17	10
1:A:182:THR:HG22	1:A:191:GLY:O	0.45	2.11	16	1
1:A:132:ASP:O	1:A:133:ILE:HD12	0.45	2.12	14	1
1:A:180:LEU:HD13	1:A:180:LEU:C	0.45	2.31	14	4
1:A:151:ALA:HB2	1:A:171:VAL:CG2	0.45	2.39	8	1
1:A:190:PHE:HB3	1:A:210:TRP:C	0.45	2.32	7	1
1:A:92:ALA:HB1	1:A:95:LEU:HD21	0.45	1.88	6	1
1:A:182:THR:HG23	1:A:191:GLY:O	0.45	2.12	15	1
1:A:221:ILE:O	1:A:221:ILE:HD12	0.45	2.11	15	1
1:A:70:THR:HB	1:A:86:THR:HG23	0.45	1.87	17	1
1:A:237:VAL:HG11	1:A:243:ILE:HG23	0.45	1.88	18	1
1:A:81:LEU:H	1:A:103:PHE:CA	0.45	2.25	19	1
1:A:208:LEU:C	1:A:208:LEU:CD2	0.45	2.85	4	2
1:A:76:ASN:O	1:A:80:THR:OG1	0.45	2.34	15	1
1:A:273:HIS:NE2	1:A:275:LEU:HD12	0.45	2.26	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:259:LEU:HD23	1:A:277:LEU:HB2	0.45	1.88	12	1
1:A:60:THR:HG22	1:A:73:GLU:HB3	0.45	1.89	6	1
1:A:29:LEU:HD13	1:A:279:LEU:CB	0.45	2.41	17	1
1:A:138:ILE:N	1:A:138:ILE:HD12	0.45	2.27	9	1
1:A:261:ALA:HB2	1:A:275:LEU:HD13	0.45	1.88	18	1
1:A:26:LEU:HD23	1:A:28:LYS:HE2	0.45	1.87	18	1
1:A:120:ARG:HD3	1:A:123:ILE:HD11	0.45	1.89	17	1
1:A:247:TYR:CE1	1:A:259:LEU:HD22	0.45	2.47	18	1
1:A:210:TRP:CG	1:A:210:TRP:O	0.45	2.70	7	1
1:A:180:LEU:HD12	1:A:181:HIS:H	0.45	1.71	4	1
1:A:218:ARG:O	1:A:219:PHE:HB2	0.45	2.10	4	1
1:A:83:THR:O	1:A:100:ASP:HB3	0.45	2.10	18	1
1:A:68:GLY:O	1:A:69:LEU:HD12	0.45	2.12	10	1
1:A:257:LEU:CD2	1:A:279:LEU:HD23	0.45	2.41	14	1
1:A:208:LEU:HA	1:A:219:PHE:CB	0.45	2.42	4	1
1:A:7:TYR:HB2	1:A:143:VAL:HG21	0.45	1.88	20	1
1:A:75:TRP:CD1	1:A:81:LEU:N	0.45	2.85	15	1
1:A:91:LEU:HD13	1:A:92:ALA:N	0.45	2.27	2	1
1:A:144:LEU:HD12	1:A:151:ALA:HB3	0.45	1.88	3	1
1:A:58:LEU:HD13	1:A:59:GLU:H	0.44	1.71	20	2
1:A:231:ALA:HB1	1:A:247:TYR:OH	0.44	2.12	6	2
1:A:97:LEU:HD21	1:A:114:ILE:HG12	0.44	1.87	19	1
1:A:35:SER:HB2	1:A:39:LEU:HD11	0.44	1.89	3	1
1:A:274:LYS:O	1:A:275:LEU:HD12	0.44	2.12	14	1
1:A:180:LEU:HD21	1:A:182:THR:OG1	0.44	2.12	11	1
1:A:29:LEU:HD13	1:A:279:LEU:HB3	0.44	1.88	17	1
1:A:81:LEU:CD2	1:A:81:LEU:O	0.44	2.65	15	1
1:A:119:LYS:CB	1:A:124:ASN:HA	0.44	2.42	16	1
1:A:136:PRO:HD2	1:A:159:THR:HG21	0.44	1.89	16	1
1:A:39:LEU:C	1:A:39:LEU:HD13	0.44	2.33	14	1
1:A:124:ASN:HB3	1:A:143:VAL:HG23	0.44	1.90	4	1
1:A:180:LEU:HD23	1:A:194:ILE:HD12	0.44	1.90	6	1
1:A:67:TYR:HB2	1:A:69:LEU:HD13	0.44	1.90	14	2
1:A:235:ALA:HA	1:A:245:LEU:CB	0.44	2.42	12	1
1:A:7:TYR:O	1:A:10:LEU:HD23	0.44	2.11	7	1
1:A:150:LEU:N	1:A:150:LEU:HD22	0.44	2.28	20	2
1:A:68:GLY:O	1:A:69:LEU:HD13	0.44	2.12	15	1
1:A:84:GLU:CB	1:A:100:ASP:HA	0.44	2.43	11	2
1:A:221:ILE:HG23	1:A:237:VAL:HG13	0.44	1.90	19	1
1:A:63:ARG:HB3	1:A:70:THR:HG22	0.44	1.89	12	1
1:A:175:THR:HG23	1:A:178:PHE:HB3	0.44	1.89	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:75:TRP:CZ2	1:A:81:LEU:HD22	0.44	2.47	2	1
1:A:233:PHE:CB	1:A:247:TYR:HA	0.44	2.43	13	1
1:A:144:LEU:CD1	1:A:151:ALA:HB3	0.44	2.42	7	1
1:A:202:LEU:HD12	1:A:226:GLN:N	0.44	2.28	8	1
1:A:60:THR:O	1:A:72:THR:HG22	0.44	2.12	17	1
1:A:39:LEU:C	1:A:39:LEU:CD2	0.44	2.83	9	1
1:A:187:GLY:C	1:A:188:THR:HG23	0.44	2.33	13	1
1:A:243:ILE:O	1:A:262:LEU:HD22	0.44	2.13	13	1
1:A:129:MET:CB	1:A:138:ILE:HA	0.44	2.43	17	1
1:A:41:PHE:CD2	1:A:58:LEU:HD11	0.44	2.48	17	1
1:A:133:ILE:H	1:A:133:ILE:HD13	0.44	1.73	1	1
1:A:217:THR:HG22	1:A:241:SER:CB	0.44	2.43	11	1
1:A:217:THR:HG21	1:A:239:ASN:HB3	0.44	1.89	11	1
1:A:64:TRP:O	1:A:65:THR:HG23	0.43	2.13	10	2
1:A:208:LEU:CD2	1:A:208:LEU:C	0.43	2.82	16	2
1:A:103:PHE:HA	1:A:110:LYS:HB2	0.43	1.89	6	1
1:A:58:LEU:CD1	1:A:60:THR:HG23	0.43	2.43	8	1
1:A:184:VAL:HG13	1:A:190:PHE:CE1	0.43	2.47	13	1
1:A:277:LEU:HD13	1:A:278:GLY:N	0.43	2.27	6	1
1:A:245:LEU:HD22	1:A:245:LEU:N	0.43	2.29	16	1
1:A:142:LEU:HD22	1:A:144:LEU:HD22	0.43	1.91	4	1
1:A:208:LEU:H	1:A:208:LEU:HD13	0.43	1.73	4	1
1:A:114:ILE:HG23	1:A:129:MET:HG3	0.43	1.89	3	1
1:A:211:THR:HG21	1:A:215:SER:O	0.43	2.13	10	1
1:A:68:GLY:O	1:A:69:LEU:CD1	0.43	2.66	10	1
1:A:138:ILE:CD1	1:A:159:THR:HG23	0.43	2.43	15	1
1:A:58:LEU:C	1:A:58:LEU:HD13	0.43	2.34	15	1
1:A:29:LEU:HD12	1:A:45:GLY:O	0.43	2.14	2	1
1:A:60:THR:O	1:A:72:THR:HG23	0.43	2.13	16	1
1:A:47:ALA:HB1	1:A:54:VAL:HG22	0.43	1.89	3	2
1:A:85:ILE:HG22	1:A:99:PHE:O	0.43	2.12	18	1
1:A:69:LEU:HD13	1:A:88:GLU:HB3	0.43	1.91	12	1
1:A:133:ILE:HD12	1:A:134:ALA:N	0.43	2.29	16	1
1:A:33:THR:O	1:A:41:PHE:HB3	0.43	2.13	3	1
1:A:97:LEU:C	1:A:97:LEU:HD23	0.43	2.33	18	1
1:A:180:LEU:HD11	1:A:182:THR:CG2	0.43	2.41	7	1
1:A:103:PHE:CA	1:A:110:LYS:HB2	0.43	2.42	6	1
1:A:243:ILE:HD13	1:A:243:ILE:N	0.43	2.29	16	1
1:A:245:LEU:HD23	1:A:261:ALA:HB3	0.43	1.89	16	1
1:A:69:LEU:HG	1:A:87:VAL:HG22	0.43	1.90	14	1
1:A:228:ASP:N	1:A:229:PRO:HD2	0.43	2.28	7	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:47:ALA:HB2	1:A:54:VAL:HG22	0.43	1.91	3	1
1:A:125:LEU:CD1	1:A:142:LEU:HD12	0.43	2.44	20	1
1:A:262:LEU:HD12	1:A:264:ASP:OD1	0.43	2.13	6	1
1:A:51:THR:O	1:A:52:THR:C	0.43	2.56	8	1
1:A:188:THR:O	1:A:212:ALA:HB2	0.43	2.13	3	1
1:A:173:TYR:HB3	1:A:180:LEU:HD23	0.43	1.88	4	1
1:A:39:LEU:O	1:A:39:LEU:HD22	0.43	2.14	17	2
1:A:10:LEU:HD22	1:A:150:LEU:HD12	0.43	1.90	7	1
1:A:75:TRP:CD1	1:A:81:LEU:C	0.42	2.92	15	1
1:A:75:TRP:HD1	1:A:81:LEU:C	0.42	2.17	15	1
1:A:233:PHE:HA	1:A:247:TYR:CB	0.42	2.44	8	1
1:A:59:GLU:HA	1:A:74:LYS:CB	0.42	2.43	2	1
1:A:262:LEU:C	1:A:263:LEU:HD13	0.42	2.33	3	1
1:A:227:ILE:O	1:A:228:ASP:CB	0.42	2.67	14	1
1:A:175:THR:HG23	1:A:179:GLN:NE2	0.42	2.30	13	1
1:A:125:LEU:HD13	1:A:142:LEU:HB3	0.42	1.91	11	1
1:A:7:TYR:CE1	1:A:143:VAL:HG11	0.42	2.49	10	1
1:A:41:PHE:CE1	1:A:60:THR:HG23	0.42	2.49	1	1
1:A:95:LEU:HD23	1:A:95:LEU:H	0.42	1.75	19	1
1:A:75:TRP:HB2	1:A:81:LEU:CA	0.42	2.44	15	1
1:A:142:LEU:HD13	1:A:142:LEU:O	0.42	2.14	11	1
1:A:125:LEU:HD21	1:A:127:CYS:SG	0.42	2.55	20	1
1:A:114:ILE:HD11	1:A:116:THR:HG23	0.42	1.90	9	2
1:A:80:THR:HG22	1:A:103:PHE:CD1	0.42	2.49	19	1
1:A:69:LEU:HB2	1:A:86:THR:O	0.42	2.14	10	1
1:A:40:GLU:O	1:A:60:THR:HG23	0.42	2.13	11	1
1:A:39:LEU:HD13	1:A:39:LEU:C	0.42	2.35	7	1
1:A:243:ILE:HD13	1:A:266:LYS:N	0.42	2.30	4	1
1:A:26:LEU:C	1:A:26:LEU:CD2	0.42	2.85	17	1
1:A:75:TRP:CD1	1:A:81:LEU:HD13	0.42	2.50	17	1
1:A:208:LEU:HD12	1:A:217:THR:CG2	0.42	2.44	3	1
1:A:146:TYR:O	1:A:149:TRP:CD1	0.42	2.73	18	1
1:A:10:LEU:HD22	1:A:150:LEU:HB3	0.42	1.92	7	1
1:A:174:LYS:HB3	1:A:178:PHE:O	0.42	2.15	6	1
1:A:75:TRP:HB3	1:A:80:THR:C	0.42	2.35	15	1
1:A:155:MET:HB2	1:A:164:VAL:HG21	0.42	1.92	16	1
1:A:95:LEU:HD21	1:A:118:TYR:CE2	0.42	2.50	18	1
1:A:279:LEU:C	1:A:279:LEU:HD13	0.42	2.34	14	1
1:A:180:LEU:HD12	1:A:194:ILE:HG13	0.42	1.92	11	1
1:A:123:ILE:HD13	1:A:142:LEU:CD1	0.42	2.45	10	1
1:A:102:SER:O	1:A:110:LYS:CB	0.42	2.67	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:72:THR:HG23	1:A:84:GLU:HB3	0.42	1.92	14	1
1:A:97:LEU:C	1:A:97:LEU:HD13	0.42	2.35	12	1
1:A:180:LEU:CD1	1:A:182:THR:HG23	0.42	2.43	7	1
1:A:257:LEU:HD23	1:A:279:LEU:HD22	0.42	1.92	20	1
1:A:273:HIS:CE1	1:A:275:LEU:HD22	0.42	2.49	16	1
1:A:156:ASN:O	1:A:164:VAL:HB	0.42	2.14	20	1
1:A:151:ALA:HB2	1:A:171:VAL:HG13	0.42	1.92	6	1
1:A:26:LEU:CD1	1:A:26:LEU:N	0.42	2.81	6	1
1:A:242:LEU:HD21	1:A:262:LEU:CD1	0.42	2.39	8	1
1:A:205:ALA:HB3	1:A:222:ALA:CB	0.42	2.33	9	1
1:A:133:ILE:O	1:A:134:ALA:HB3	0.41	2.14	1	1
1:A:206:VAL:HG23	1:A:219:PHE:CZ	0.41	2.50	18	1
1:A:259:LEU:HD23	1:A:277:LEU:HA	0.41	1.92	12	1
1:A:259:LEU:HD22	1:A:277:LEU:HB3	0.41	1.92	20	1
1:A:71:PHE:HA	1:A:85:ILE:HG22	0.41	1.91	6	1
1:A:112:ALA:HB3	1:A:131:PHE:HB2	0.41	1.92	15	1
1:A:129:MET:CB	1:A:137:SER:O	0.41	2.68	17	1
1:A:242:LEU:HD22	1:A:243:ILE:H	0.41	1.74	12	1
1:A:58:LEU:HD13	1:A:58:LEU:C	0.41	2.36	17	1
1:A:69:LEU:HD23	1:A:87:VAL:HG12	0.41	1.92	3	1
1:A:75:TRP:HB2	1:A:82:GLY:N	0.41	2.30	15	1
1:A:233:PHE:CZ	1:A:245:LEU:HD21	0.41	2.50	17	1
1:A:247:TYR:HE2	1:A:259:LEU:HD13	0.41	1.75	17	1
1:A:227:ILE:HG22	1:A:229:PRO:HD2	0.41	1.92	14	1
1:A:264:ASP:HB3	1:A:268:VAL:HG13	0.41	1.91	10	1
1:A:138:ILE:O	1:A:156:ASN:CB	0.41	2.68	11	2
1:A:149:TRP:O	1:A:150:LEU:HD22	0.41	2.16	16	1
1:A:279:LEU:CD2	1:A:279:LEU:C	0.41	2.88	16	1
1:A:242:LEU:HD22	1:A:263:LEU:O	0.41	2.15	3	1
1:A:10:LEU:HD13	1:A:150:LEU:HD13	0.41	1.92	18	1
1:A:7:TYR:O	1:A:143:VAL:HG21	0.41	2.15	4	1
1:A:169:PHE:HB3	1:A:184:VAL:HG22	0.41	1.93	15	1
1:A:261:ALA:HB2	1:A:275:LEU:HD23	0.41	1.91	17	1
1:A:142:LEU:C	1:A:142:LEU:HD13	0.41	2.36	18	1
1:A:39:LEU:HD11	1:A:41:PHE:CE2	0.41	2.50	2	1
1:A:133:ILE:CD1	1:A:133:ILE:N	0.41	2.84	1	1
1:A:247:TYR:HB2	1:A:259:LEU:N	0.41	2.31	5	1
1:A:242:LEU:HD23	1:A:264:ASP:OD2	0.41	2.15	20	1
1:A:138:ILE:H	1:A:157:PHE:CA	0.41	2.29	18	2
1:A:180:LEU:C	1:A:180:LEU:HD13	0.41	2.36	5	2
1:A:185:ASN:C	1:A:187:GLY:N	0.41	2.74	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:143:VAL:HG23	1:A:143:VAL:O	0.41	2.16	4	1
1:A:75:TRP:CD2	1:A:81:LEU:HD11	0.41	2.51	4	1
1:A:180:LEU:HD22	1:A:194:ILE:HG13	0.41	1.92	10	1
1:A:221:ILE:H	1:A:221:ILE:HD13	0.41	1.75	20	1
1:A:75:TRP:CB	1:A:80:THR:O	0.41	2.63	15	1
1:A:208:LEU:O	1:A:208:LEU:HD22	0.41	2.15	2	1
1:A:29:LEU:HD13	1:A:279:LEU:HD13	0.41	1.92	9	1
1:A:242:LEU:CD1	1:A:242:LEU:N	0.41	2.84	7	1
1:A:143:VAL:HG12	1:A:152:GLY:CA	0.40	2.45	2	1
1:A:64:TRP:O	1:A:65:THR:C	0.40	2.59	3	1
1:A:123:ILE:CG2	1:A:144:LEU:HD23	0.40	2.46	11	1
1:A:194:ILE:O	1:A:206:VAL:CG1	0.40	2.69	4	1
1:A:255:ILE:HD12	1:A:281:PHE:CD2	0.40	2.51	8	1
1:A:233:PHE:CE2	1:A:245:LEU:HD11	0.40	2.50	17	1
1:A:209:ALA:HB2	1:A:219:PHE:HD2	0.40	1.73	2	1
1:A:188:THR:CG2	1:A:212:ALA:HB3	0.40	2.41	19	1
1:A:142:LEU:HD22	1:A:144:LEU:CD2	0.40	2.46	7	1
1:A:98:THR:HG22	1:A:100:ASP:OD1	0.40	2.17	10	1
1:A:80:THR:C	1:A:81:LEU:HD13	0.40	2.35	15	1
1:A:138:ILE:HG12	1:A:159:THR:HG22	0.40	1.92	14	1
1:A:123:ILE:HD11	1:A:142:LEU:CD1	0.40	2.37	12	1
1:A:69:LEU:HD13	1:A:88:GLU:HB2	0.40	1.92	12	1
1:A:103:PHE:O	1:A:105:PRO:HD3	0.40	2.17	6	1
1:A:123:ILE:HG22	1:A:144:LEU:HG	0.40	1.93	17	1
1:A:39:LEU:HD22	1:A:39:LEU:O	0.40	2.16	16	1
1:A:202:LEU:HD12	1:A:225:TYR:HA	0.40	1.92	5	1
1:A:123:ILE:HG22	1:A:144:LEU:HD12	0.40	1.92	19	1
1:A:180:LEU:HD23	1:A:180:LEU:C	0.40	2.37	11	1
1:A:97:LEU:HB2	1:A:116:THR:HG23	0.40	1.93	4	1
1:A:123:ILE:HG22	1:A:144:LEU:HB2	0.40	1.92	4	1
1:A:207:ASN:O	1:A:219:PHE:HB3	0.40	2.16	4	1
1:A:261:ALA:HB2	1:A:275:LEU:HD12	0.40	1.93	1	1
1:A:159:THR:HG23	1:A:160:ALA:N	0.40	2.32	9	1
1:A:125:LEU:HG	1:A:142:LEU:HD12	0.40	1.93	19	1
1:A:92:ALA:O	1:A:93:ARG:C	0.40	2.59	11	1

## 6.3 Torsion angles

### 6.3.1 Protein backbone

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	265/291 (91%)	224±6 (85±2%)	33±6 (12±2%)	8±2 (3±1%)	8	41
All	All	5300/5820 (91%)	4482 (85%)	654 (12%)	164 (3%)	8	41

All 54 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	25	GLY	9
1	A	165	THR	9
1	A	147	GLU	9
1	A	271	GLY	9
1	A	66	GLU	8
1	A	228	ASP	8
1	A	77	THR	7
1	A	255	ILE	7
1	A	272	GLY	6
1	A	214	ASN	5
1	A	229	PRO	4
1	A	254	GLY	4
1	A	219	PHE	4
1	A	94	GLY	4
1	A	67	TYR	3
1	A	213	GLY	3
1	A	133	ILE	3
1	A	50	GLU	3
1	A	212	ALA	3
1	A	135	GLY	3
1	A	215	SER	3
1	A	162	SER	3
1	A	74	LYS	3
1	A	63	ARG	2
1	A	38	GLY	2
1	A	132	ASP	2
1	A	200	LYS	2

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Mol	Chain	Res	Type	Models (Total)
1	A	176	ASP	2
1	A	84	GLU	2
1	A	108	GLY	2
1	A	51	THR	2
1	A	109	LYS	2
1	A	134	ALA	2
1	A	267	ASN	2
1	A	177	GLU	2
1	A	163	ARG	2
1	A	37	ASN	1
1	A	280	GLU	1
1	A	240	SER	1
1	A	242	LEU	1
1	A	230	ASP	1
1	A	49	THR	1
1	A	122	HIS	1
1	A	239	ASN	1
1	A	64	TRP	1
1	A	93	ARG	1
1	A	107	THR	1
1	A	218	ARG	1
1	A	83	THR	1
1	A	53	LYS	1
1	A	198	VAL	1
1	A	199	ASN	1
1	A	202	LEU	1
1	A	52	THR	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	216/238 (91%)	179±4 (83±2%)	37±4 (17±2%)	6	41
All	All	4320/4760 (91%)	3587 (83%)	733 (17%)	6	41

All 179 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	58	LEU	16
1	A	228	ASP	12
1	A	221	ILE	11
1	A	175	THR	11
1	A	208	LEU	11
1	A	120	ARG	11
1	A	146	TYR	11
1	A	243	ILE	10
1	A	125	LEU	10
1	A	39	LEU	10
1	A	114	ILE	10
1	A	63	ARG	9
1	A	34	LYS	9
1	A	109	LYS	9
1	A	149	TRP	9
1	A	85	ILE	8
1	A	204	THR	8
1	A	65	THR	8
1	A	144	LEU	8
1	A	46	SER	8
1	A	260	SER	7
1	A	93	ARG	7
1	A	133	ILE	7
1	A	116	THR	7
1	A	113	LYS	7
1	A	128	ASP	7
1	A	29	LEU	7
1	A	69	LEU	7
1	A	194	ILE	6
1	A	193	SER	6
1	A	266	LYS	6
1	A	26	LEU	6
1	A	96	LYS	6
1	A	264	ASP	6
1	A	80	THR	6
1	A	165	THR	6
1	A	51	THR	6
1	A	219	PHE	6
1	A	35	SER	6
1	A	142	LEU	6
1	A	107	THR	6
1	A	188	THR	6
1	A	44	SER	6

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Mol	Chain	Res	Type	Models (Total)
1	A	230	ASP	5
1	A	42	THR	5
1	A	156	ASN	5
1	A	31	LEU	5
1	A	200	LYS	5
1	A	99	PHE	5
1	A	182	THR	5
1	A	137	SER	5
1	A	77	THR	5
1	A	197	LYS	5
1	A	104	SER	5
1	A	70	THR	5
1	A	110	LYS	5
1	A	256	LYS	5
1	A	40	GLU	5
1	A	57	SER	5
1	A	33	THR	5
1	A	233	PHE	5
1	A	95	LEU	4
1	A	84	GLU	4
1	A	257	LEU	4
1	A	273	HIS	4
1	A	72	THR	4
1	A	101	SER	4
1	A	185	ASN	4
1	A	155	MET	4
1	A	247	TYR	4
1	A	6	THR	4
1	A	75	TRP	4
1	A	202	LEU	4
1	A	61	LYS	4
1	A	215	SER	4
1	A	150	LEU	4
1	A	242	LEU	4
1	A	180	LEU	4
1	A	227	ILE	4
1	A	245	LEU	4
1	A	100	ASP	4
1	A	195	TYR	4
1	A	132	ASP	4
1	A	159	THR	4
1	A	218	ARG	4

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Mol	Chain	Res	Type	Models (Total)
1	A	279	LEU	4
1	A	274	LYS	4
1	A	74	LYS	4
1	A	30	ASP	4
1	A	179	GLN	4
1	A	167	SER	3
1	A	12	LYS	3
1	A	248	THR	3
1	A	277	LEU	3
1	A	173	TYR	3
1	A	199	ASN	3
1	A	203	GLU	3
1	A	258	THR	3
1	A	237	VAL	3
1	A	123	ILE	3
1	A	163	ARG	3
1	A	53	LYS	3
1	A	83	THR	3
1	A	9	ASP	3
1	A	174	LYS	3
1	A	89	ASP	3
1	A	217	THR	3
1	A	102	SER	3
1	A	119	LYS	3
1	A	201	LYS	3
1	A	130	ASP	3
1	A	161	LYS	3
1	A	129	MET	3
1	A	236	LYS	3
1	A	234	SER	3
1	A	98	THR	3
1	A	198	VAL	3
1	A	97	LEU	3
1	A	189	GLU	3
1	A	157	PHE	2
1	A	190	PHE	2
1	A	207	ASN	2
1	A	186	ASP	2
1	A	15	ARG	2
1	A	158	GLU	2
1	A	196	GLN	2
1	A	87	VAL	2

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Mol	Chain	Res	Type	Models (Total)
1	A	115	LYS	2
1	A	55	THR	2
1	A	91	LEU	2
1	A	103	PHE	2
1	A	54	VAL	2
1	A	275	LEU	2
1	A	147	GLU	2
1	A	259	LEU	2
1	A	32	LYS	2
1	A	76	ASN	2
1	A	226	GLN	2
1	A	59	GLU	2
1	A	81	LEU	2
1	A	71	PHE	2
1	A	211	THR	2
1	A	10	LEU	2
1	A	86	THR	2
1	A	153	TYR	2
1	A	41	PHE	2
1	A	154	GLN	2
1	A	143	VAL	2
1	A	64	TRP	2
1	A	28	LYS	2
1	A	263	LEU	2
1	A	176	ASP	2
1	A	255	ILE	2
1	A	169	PHE	2
1	A	60	THR	1
1	A	66	GLU	1
1	A	49	THR	1
1	A	239	ASN	1
1	A	43	SER	1
1	A	214	ASN	1
1	A	177	GLU	1
1	A	124	ASN	1
1	A	62	TYR	1
1	A	67	TYR	1
1	A	281	PHE	1
1	A	118	TYR	1
1	A	90	GLN	1
1	A	232	CYS	1
1	A	181	HIS	1

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Mol	Chain	Res	Type	Models (Total)
1	A	111	ASN	1
1	A	224	LYS	1
1	A	225	TYR	1
1	A	268	VAL	1
1	A	166	GLN	1
1	A	139	ARG	1
1	A	210	TRP	1
1	A	50	GLU	1
1	A	267	ASN	1
1	A	168	ASN	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 carbohydrates 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

The completeness of assignment taking into account all chemical shift lists is 34% for the well-defined parts and 32% for the entire structure.

### 7.1 Chemical shift list 1

File name: BMRB entry 16381

Chemical shift list name: *assigned\_chem\_shift\_list\_1*

#### 7.1.1 Bookkeeping

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	1224
Number of shifts mapped to atoms	1224
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

#### 7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	233	$0.53 \pm 0.05$	Should be applied
$^{13}\text{C}_\beta$	199	$0.19 \pm 0.12$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}'$	0	—	None (insufficient data)
$^{15}\text{N}$	229	$-1.23 \pm 0.32$	Should be applied

#### 7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 34%, i.e. 1046 atoms were assigned a chemical shift out of a possible 3122. 35 out of 37 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	681/1317 (52%)	226/526 (43%)	229/530 (43%)	226/261 (87%)
Sidechain	357/1539 (23%)	81/894 (9%)	276/575 (48%)	0/70 (0%)

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	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Aromatic	8/266 (3%)	4/141 (3%)	0/118 (0%)	4/7 (57%)
Overall	1046/3122 (34%)	311/1561 (20%)	505/1223 (41%)	230/338 (68%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 32%, i.e. 1060 atoms were assigned a chemical shift out of a possible 3356. 35 out of 41 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Backbone	691/1413 (49%)	229/564 (41%)	233/570 (41%)	229/279 (82%)
Sidechain	361/1660 (22%)	81/965 (8%)	280/622 (45%)	0/73 (0%)
Aromatic	8/283 (3%)	4/150 (3%)	0/126 (0%)	4/7 (57%)
Overall	1060/3356 (32%)	314/1679 (19%)	513/1318 (39%)	233/359 (65%)

#### 7.1.4 Statistically unusual chemical shifts ⓘ

There are no statistically unusual chemical shifts.

#### 7.1.5 Random Coil Index (RCI) plots ⓘ

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition.

Random coil index (RCI) for chain A:

