



# Full wwPDB NMR Structure Validation Report ⓘ

May 29, 2020 – 11:34 am BST

PDB ID : 6TIQ  
Title : Refined solution NMR structure of hVDAC-1 in detergent micelles  
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Deposited on : 2019-11-22

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.

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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 : 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 : 2.11  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

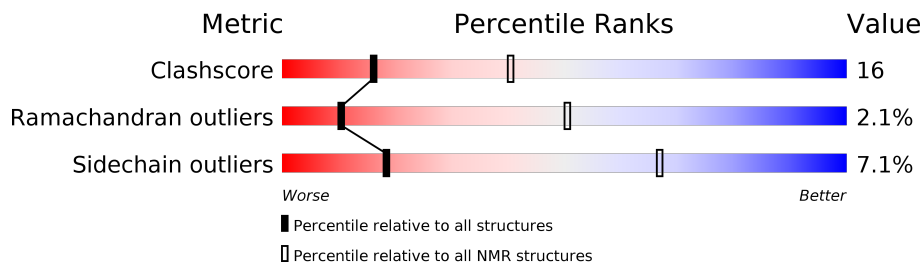
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 40%.

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	291	

## 2 Ensemble composition and analysis

This entry contains 20 models. Model 20 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *closest to the average*.

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:2-A:285 (284)	1.13	20

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 3 clusters and 1 single-model cluster was found.

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

### 3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 4352 atoms, of which 2165 are hydrogens and 0 are deuteriums.

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

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	285	4352	1383	2165	368	431	5	0

There are 8 discrepancies between the modelled and reference sequences:

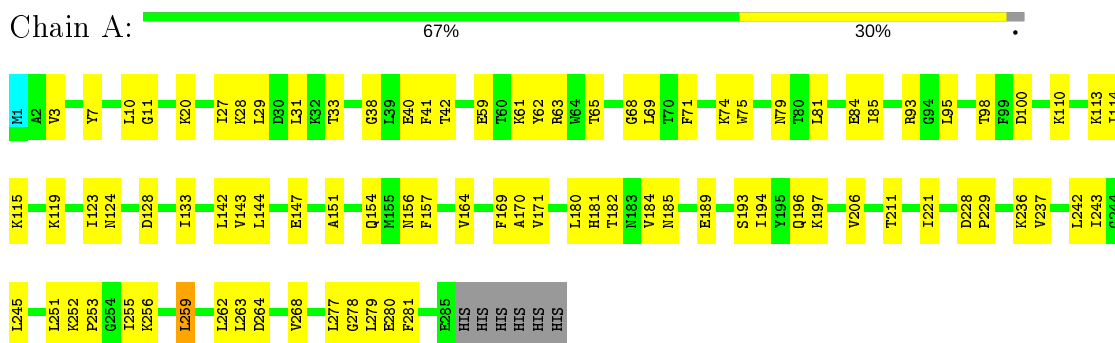
Chain	Residue	Modelled	Actual	Comment	Reference
A	284	LEU	-	expression tag	UNP P21796
A	285	GLU	-	expression tag	UNP P21796
A	286	HIS	-	expression tag	UNP P21796
A	287	HIS	-	expression tag	UNP P21796
A	288	HIS	-	expression tag	UNP P21796
A	289	HIS	-	expression tag	UNP P21796
A	290	HIS	-	expression tag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

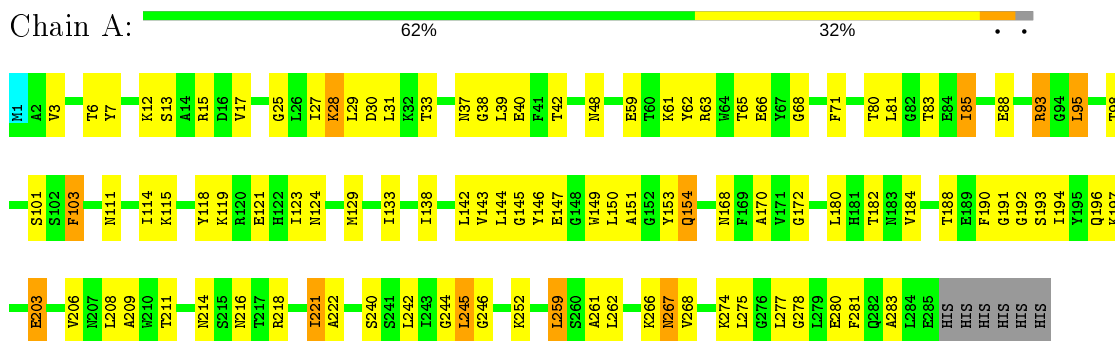


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

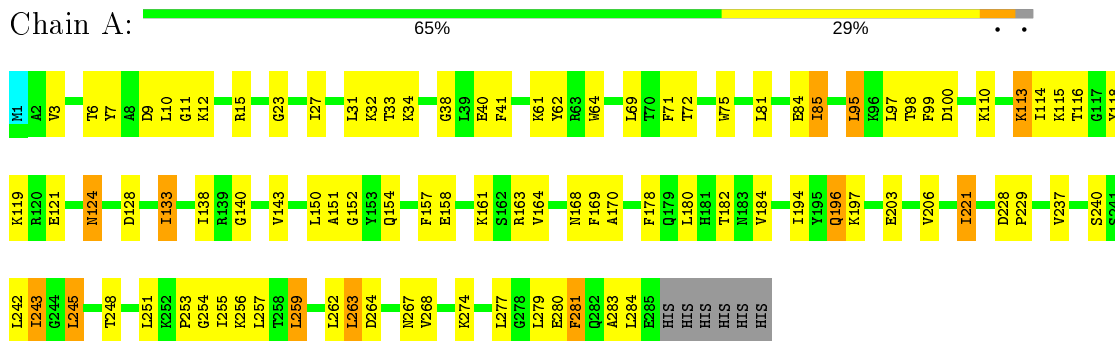
#### 4.2.1 Score per residue for model 1

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

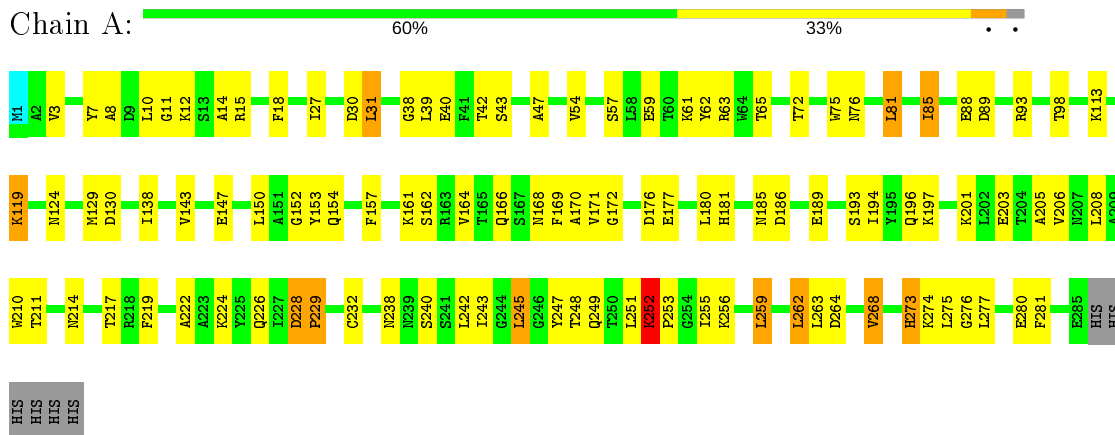


### 4.2.2 Score per residue for model 2

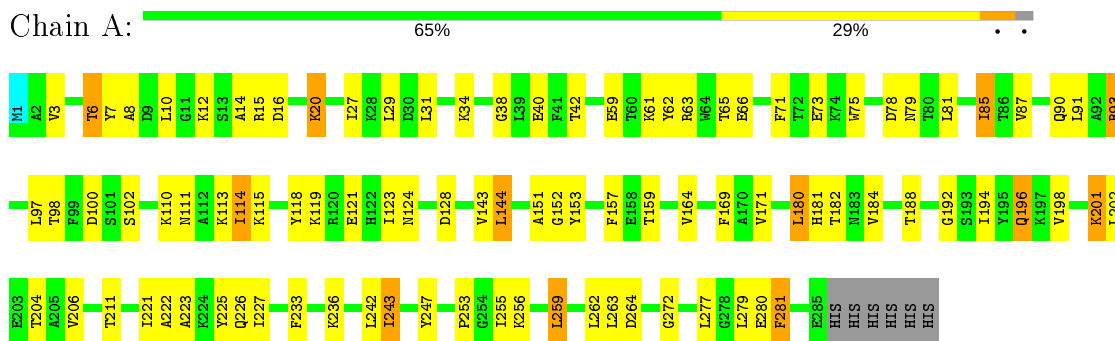
- Molecule 1: Voltage-dependent anion-selective channel protein 1



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

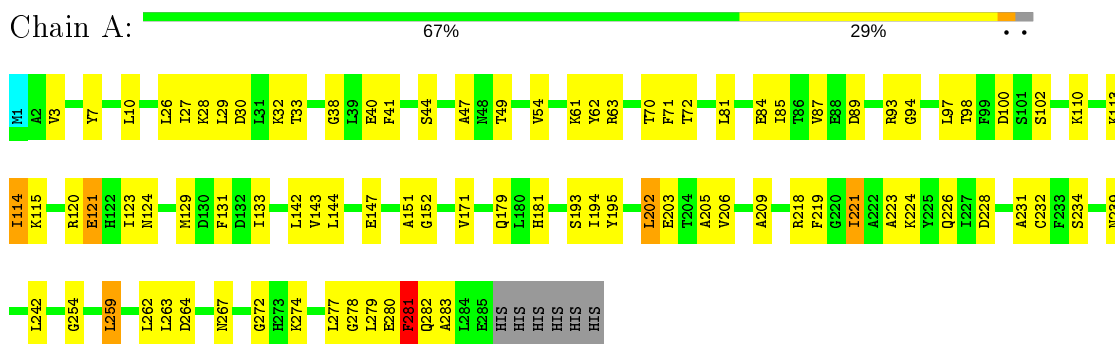


- Molecule 1: Voltage-dependent anion-selective channel protein 1



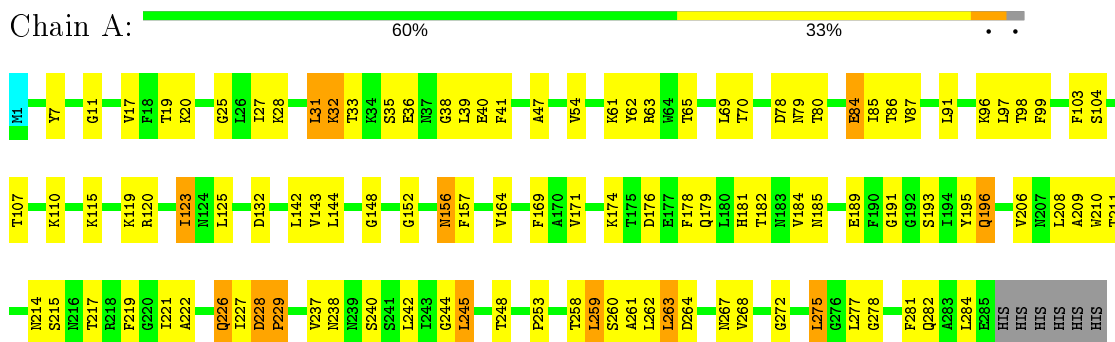
### 4.2.5 Score per residue for model 5

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



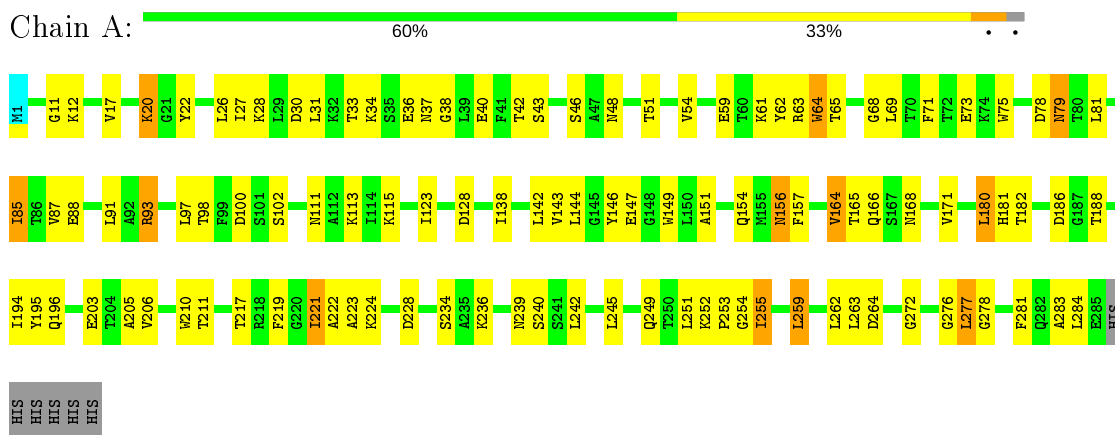
### 4.2.6 Score per residue for model 6

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



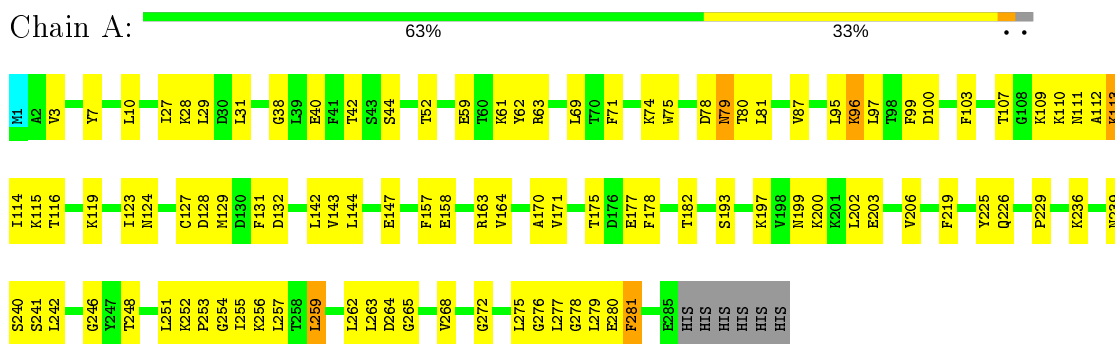
### 4.2.7 Score per residue for model 7

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



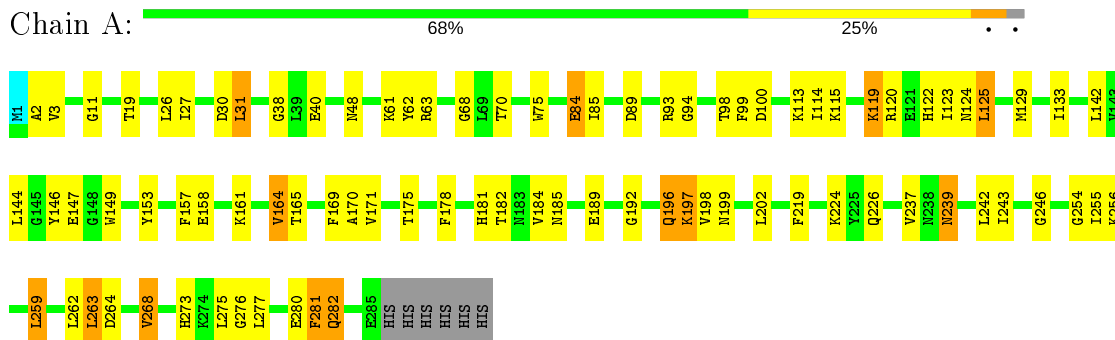
### 4.2.8 Score per residue for model 8

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



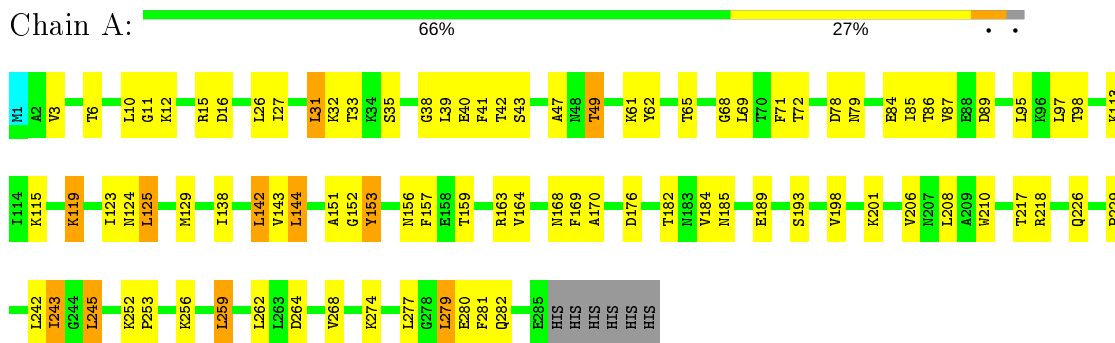
### 4.2.9 Score per residue for model 9

- 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



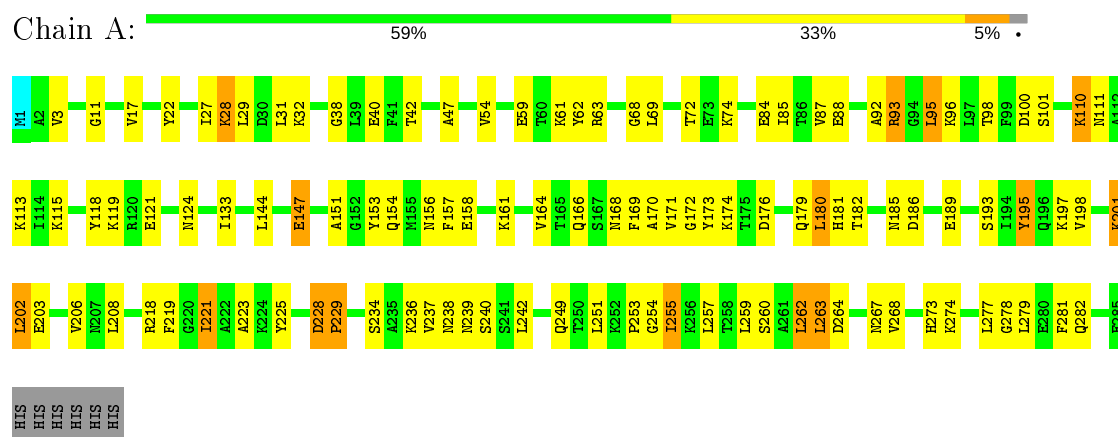






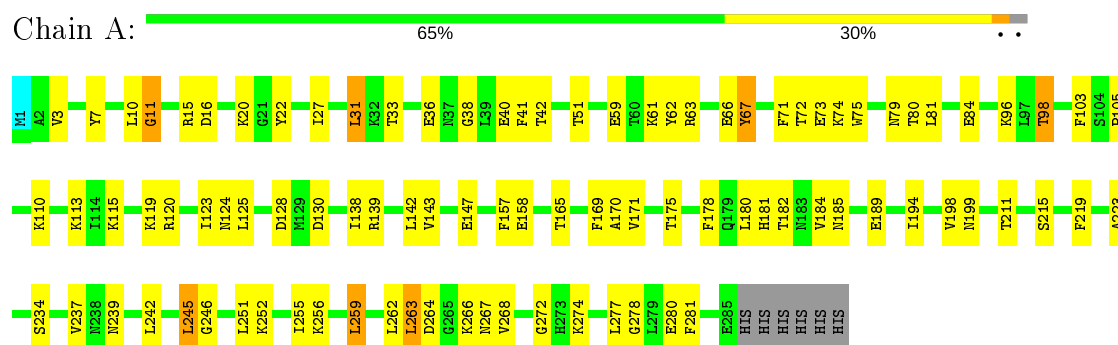
### 4.2.17 Score per residue for model 17

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



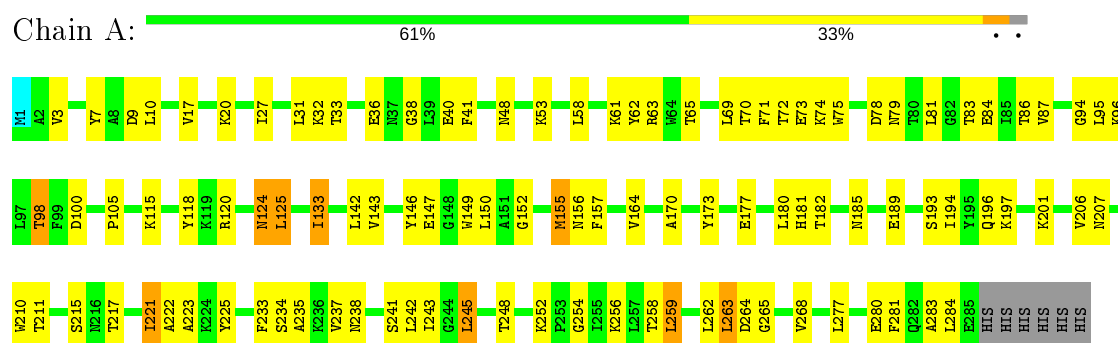
### 4.2.18 Score per residue for model 18

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



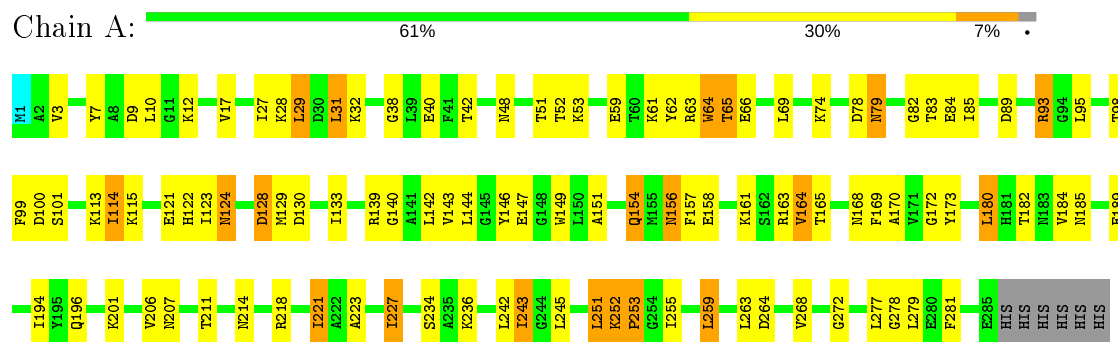
### 4.2.19 Score per residue for model 19

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



### 4.2.20 Score per residue for model 20 (medoid)

- 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 1000 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	refinement	
CYANA	structure calculation	

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)	input_cs.cif
Number of chemical shift lists	1
Total number of shifts	1507
Number of shifts mapped to atoms	1507
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	40%

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

## 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	0.1±0.3
All	All	0	2

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	64	TRP	Mainchain	1
1	A	103	PHE	Mainchain	1

### 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	2179	2154	2151	69±10
All	All	43580	43080	43020	1375

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 16.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:98:THR:HB	1:A:115:LYS:HG3	0.94	1.39	16	1
1:A:125:LEU:HG	1:A:142:LEU:HG	0.92	1.39	10	1
1:A:10:LEU:HD21	1:A:152:GLY:HA3	0.91	1.41	19	5
1:A:98:THR:HG23	1:A:115:LYS:HB2	0.90	1.43	18	2
1:A:194:ILE:HB	1:A:206:VAL:HB	0.90	1.41	4	8
1:A:3:VAL:HG22	1:A:119:LYS:HB3	0.89	1.40	13	1
1:A:153:TYR:CB	1:A:169:PHE:HA	0.89	1.98	10	1
1:A:15:ARG:HA	1:A:18:PHE:HB3	0.88	1.43	12	2
1:A:6:THR:HB	1:A:143:VAL:HG11	0.87	1.45	16	2
1:A:252:LYS:HB3	1:A:253:PRO:HD3	0.86	1.44	11	4
1:A:3:VAL:HG12	1:A:119:LYS:HB3	0.86	1.45	18	1
1:A:256:LYS:HB2	1:A:280:GLU:HB2	0.86	1.48	9	1
1:A:84:GLU:HA	1:A:100:ASP:HB3	0.86	1.46	13	1
1:A:242:LEU:HG	1:A:264:ASP:HA	0.85	1.48	4	10
1:A:119:LYS:HG3	1:A:124:ASN:HB2	0.85	1.46	9	1
1:A:196:GLN:HE21	1:A:196:GLN:HA	0.85	1.31	4	1
1:A:84:GLU:HA	1:A:100:ASP:CB	0.84	2.02	13	1
1:A:40:GLU:HB2	1:A:61:LYS:HB2	0.84	1.47	3	4
1:A:115:LYS:HB3	1:A:127:CYS:O	0.84	1.73	8	1
1:A:264:ASP:O	1:A:268:VAL:HB	0.83	1.73	9	3
1:A:242:LEU:HB3	1:A:262:LEU:HD11	0.83	1.50	11	12
1:A:146:TYR:HB2	1:A:149:TRP:HB2	0.83	1.50	7	7
1:A:40:GLU:HB3	1:A:61:LYS:HB3	0.83	1.51	18	6
1:A:31:LEU:HA	1:A:281:PHE:HA	0.82	1.50	9	1
1:A:221:ILE:O	1:A:236:LYS:HB3	0.82	1.75	4	1
1:A:153:TYR:HB3	1:A:168:ASN:O	0.81	1.74	10	1
1:A:259:LEU:HD22	1:A:277:LEU:HD23	0.81	1.49	12	14
1:A:196:GLN:HA	1:A:196:GLN:HE21	0.80	1.34	6	1
1:A:171:VAL:HB	1:A:182:THR:HB	0.80	1.53	4	7
1:A:268:VAL:HG22	1:A:273:HIS:HA	0.79	1.55	3	2
1:A:264:ASP:HB2	1:A:267:ASN:HB2	0.79	1.54	2	3
1:A:157:PHE:HA	1:A:164:VAL:HA	0.78	1.55	19	15
1:A:158:GLU:HB2	1:A:165:THR:HB	0.78	1.55	20	3
1:A:100:ASP:HB3	1:A:113:LYS:HB3	0.78	1.55	4	2
1:A:252:LYS:HB3	1:A:253:PRO:HD2	0.78	1.55	15	2
1:A:211:THR:HB	1:A:214:ASN:HB3	0.78	1.56	20	1
1:A:263:LEU:HD12	1:A:273:HIS:HB2	0.77	1.57	16	3
1:A:42:THR:HB	1:A:59:GLU:HB2	0.77	1.56	12	9
1:A:22:TYR:HB3	1:A:276:GLY:HA3	0.77	1.56	7	2
1:A:7:TYR:HA	1:A:10:LEU:HB3	0.77	1.57	4	1
1:A:252:LYS:HB2	1:A:255:ILE:HD11	0.77	1.55	16	1
1:A:75:TRP:HD1	1:A:81:LEU:HB3	0.77	1.40	14	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:124:ASN:HB2	1:A:143:VAL:HB	0.76	1.57	11	4
1:A:23:GLY:HA3	1:A:274:LYS:HB3	0.76	1.57	2	1
1:A:27:ILE:HG23	1:A:277:LEU:HD12	0.76	1.58	20	5
1:A:263:LEU:HB3	1:A:268:VAL:HG11	0.76	1.56	16	13
1:A:114:ILE:O	1:A:128:ASP:HB3	0.76	1.80	11	1
1:A:116:THR:H	1:A:128:ASP:HB2	0.76	1.41	11	1
1:A:264:ASP:H	1:A:268:VAL:HG21	0.75	1.41	9	2
1:A:42:THR:HB	1:A:59:GLU:HB3	0.75	1.55	11	2
1:A:40:GLU:HB3	1:A:61:LYS:HB2	0.75	1.59	20	7
1:A:125:LEU:CG	1:A:142:LEU:HG	0.75	2.10	10	1
1:A:202:LEU:HG	1:A:225:TYR:HB3	0.75	1.55	13	1
1:A:116:THR:N	1:A:128:ASP:HB2	0.75	1.97	11	1
1:A:203:GLU:HB2	1:A:224:LYS:HB3	0.74	1.57	3	2
1:A:86:THR:HG22	1:A:98:THR:HB	0.74	1.59	13	1
1:A:144:LEU:HB2	1:A:151:ALA:HB3	0.74	1.58	12	7
1:A:27:ILE:HG23	1:A:277:LEU:HD23	0.74	1.57	2	2
1:A:20:LYS:HD3	1:A:20:LYS:H	0.74	1.40	4	1
1:A:27:ILE:HG13	1:A:277:LEU:HB3	0.74	1.58	15	6
1:A:115:LYS:HA	1:A:128:ASP:HB3	0.74	1.59	11	1
1:A:180:LEU:HB3	1:A:194:ILE:HG13	0.74	1.57	20	1
1:A:31:LEU:HD22	1:A:281:PHE:HB2	0.74	1.58	14	4
1:A:83:THR:HB	1:A:101:SER:HB2	0.74	1.58	1	1
1:A:98:THR:HB	1:A:115:LYS:HB3	0.74	1.58	5	7
1:A:86:THR:HB	1:A:96:LYS:HE3	0.73	1.59	13	1
1:A:179:GLN:HB2	1:A:195:TYR:HB2	0.73	1.60	6	1
1:A:153:TYR:HB3	1:A:169:PHE:HA	0.73	1.58	10	1
1:A:197:LYS:HG3	1:A:203:GLU:HG2	0.73	1.60	2	1
1:A:123:ILE:HG13	1:A:142:LEU:HD21	0.73	1.58	10	1
1:A:206:VAL:HG22	1:A:221:ILE:HG22	0.73	1.58	1	10
1:A:248:THR:HG23	1:A:258:THR:HB	0.73	1.61	11	1
1:A:222:ALA:HA	1:A:236:LYS:HB2	0.73	1.61	4	1
1:A:123:ILE:HG22	1:A:145:GLY:H	0.72	1.44	1	2
1:A:31:LEU:HD22	1:A:281:PHE:HB3	0.72	1.61	10	3
1:A:113:LYS:HG3	1:A:130:ASP:HB3	0.72	1.60	11	1
1:A:35:SER:HB2	1:A:39:LEU:HB2	0.72	1.59	6	1
1:A:115:LYS:HB2	1:A:129:MET:N	0.72	2.00	8	1
1:A:125:LEU:HG	1:A:142:LEU:CG	0.71	2.15	10	1
1:A:96:LYS:HE3	1:A:119:LYS:HD2	0.71	1.60	6	1
1:A:83:THR:O	1:A:100:ASP:HB3	0.71	1.85	13	1
1:A:3:VAL:HB	1:A:119:LYS:HD3	0.71	1.61	3	1
1:A:7:TYR:HB3	1:A:143:VAL:HG21	0.71	1.63	5	9

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:59:GLU:HG2	1:A:74:LYS:HG2	0.71	1.60	17	1
1:A:154:GLN:HB2	1:A:168:ASN:HB2	0.71	1.62	12	5
1:A:64:TRP:HB3	1:A:69:LEU:HB2	0.71	1.62	11	4
1:A:3:VAL:HG11	1:A:121:GLU:HA	0.71	1.61	13	1
1:A:98:THR:HG23	1:A:115:LYS:HB3	0.71	1.62	1	2
1:A:33:THR:HB	1:A:41:PHE:HB3	0.70	1.61	18	2
1:A:40:GLU:HG3	1:A:63:ARG:HB2	0.70	1.63	12	1
1:A:29:LEU:HD12	1:A:279:LEU:HB2	0.70	1.62	17	5
1:A:153:TYR:HB2	1:A:169:PHE:HA	0.70	1.63	10	1
1:A:115:LYS:HB2	1:A:129:MET:H	0.70	1.47	8	1
1:A:120:ARG:HB3	1:A:123:ILE:HB	0.70	1.62	18	2
1:A:25:GLY:HA2	1:A:275:LEU:HB3	0.70	1.62	1	1
1:A:201:LYS:HB2	1:A:226:GLN:HB3	0.69	1.62	4	1
1:A:42:THR:HB	1:A:59:GLU:HG2	0.69	1.63	13	2
1:A:211:THR:HG23	1:A:214:ASN:HB3	0.69	1.65	3	1
1:A:133:ILE:HD12	1:A:133:ILE:H	0.69	1.47	12	1
1:A:115:LYS:CB	1:A:128:ASP:HA	0.69	2.17	8	1
1:A:9:ASP:HA	1:A:12:LYS:HB2	0.69	1.65	20	2
1:A:228:ASP:HB3	1:A:229:PRO:HD3	0.69	1.64	11	6
1:A:40:GLU:HB2	1:A:63:ARG:HG3	0.69	1.63	7	1
1:A:64:TRP:HA	1:A:69:LEU:O	0.69	1.88	7	1
1:A:138:ILE:HB	1:A:157:PHE:HB3	0.68	1.65	2	4
1:A:99:PHE:HD2	1:A:114:ILE:HB	0.68	1.47	13	1
1:A:114:ILE:HG22	1:A:129:MET:HB3	0.68	1.64	5	1
1:A:84:GLU:CA	1:A:100:ASP:HB3	0.68	2.19	13	1
1:A:185:ASN:HB3	1:A:189:GLU:HB3	0.68	1.66	15	5
1:A:62:TYR:HB2	1:A:71:PHE:HB2	0.68	1.66	1	1
1:A:22:TYR:HB3	1:A:274:LYS:HD2	0.68	1.66	18	1
1:A:256:LYS:HG2	1:A:280:GLU:HB2	0.67	1.65	4	1
1:A:38:GLY:O	1:A:62:TYR:HA	0.67	1.89	7	18
1:A:243:ILE:HG12	1:A:263:LEU:HB2	0.67	1.66	4	3
1:A:256:LYS:HG3	1:A:282:GLN:HG2	0.67	1.65	9	1
1:A:6:THR:HB	1:A:143:VAL:CG1	0.67	2.19	16	2
1:A:201:LYS:HG3	1:A:202:LEU:HD13	0.67	1.67	17	1
1:A:124:ASN:O	1:A:142:LEU:HD23	0.66	1.89	10	1
1:A:115:LYS:HA	1:A:128:ASP:CB	0.66	2.20	11	1
1:A:198:VAL:HB	1:A:202:LEU:HD12	0.66	1.66	4	1
1:A:3:VAL:HB	1:A:119:LYS:HB3	0.66	1.67	9	1
1:A:6:THR:HB	1:A:150:LEU:HD21	0.66	1.67	12	6
1:A:180:LEU:HD12	1:A:194:ILE:HG13	0.66	1.68	18	7
1:A:10:LEU:HD22	1:A:143:VAL:HG22	0.66	1.67	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:109:LYS:HE2	1:A:109:LYS:HA	0.66	1.67	13	1
1:A:128:ASP:HB2	1:A:139:ARG:HB2	0.66	1.66	20	2
1:A:222:ALA:HA	1:A:236:LYS:CB	0.65	2.22	4	1
1:A:264:ASP:OD1	1:A:266:LYS:HG2	0.65	1.92	18	1
1:A:98:THR:CG2	1:A:115:LYS:HB3	0.64	2.22	13	1
1:A:242:LEU:HD23	1:A:262:LEU:HD11	0.64	1.69	19	8
1:A:154:GLN:HG3	1:A:168:ASN:HB3	0.64	1.68	17	1
1:A:254:GLY:O	1:A:281:PHE:HB3	0.64	1.93	5	2
1:A:98:THR:HB	1:A:115:LYS:HB2	0.64	1.69	12	2
1:A:80:THR:HA	1:A:104:SER:HB2	0.64	1.68	6	1
1:A:153:TYR:HB2	1:A:170:ALA:N	0.64	2.08	10	1
1:A:185:ASN:HB2	1:A:189:GLU:HB2	0.64	1.69	10	1
1:A:3:VAL:HG22	1:A:121:GLU:HA	0.64	1.69	16	5
1:A:115:LYS:HD3	1:A:128:ASP:HB2	0.64	1.68	15	2
1:A:211:THR:HB	1:A:215:SER:HB2	0.64	1.68	6	1
1:A:133:ILE:H	1:A:133:ILE:HD13	0.63	1.52	19	3
1:A:144:LEU:N	1:A:144:LEU:HD23	0.63	2.08	10	1
1:A:48:ASN:HB3	1:A:53:LYS:HB3	0.63	1.68	19	1
1:A:227:ILE:HD13	1:A:227:ILE:H	0.63	1.53	20	1
1:A:62:TYR:HB2	1:A:71:PHE:HB3	0.63	1.70	18	5
1:A:95:LEU:HD22	1:A:118:TYR:HB3	0.63	1.69	16	2
1:A:203:GLU:HG3	1:A:224:LYS:HB3	0.63	1.68	5	1
1:A:115:LYS:HB3	1:A:128:ASP:HA	0.63	1.71	8	1
1:A:251:LEU:HB2	1:A:255:ILE:HB	0.63	1.69	12	2
1:A:3:VAL:HG11	1:A:119:LYS:HB3	0.63	1.70	12	3
1:A:70:THR:HG23	1:A:86:THR:HB	0.63	1.71	14	3
1:A:3:VAL:HB	1:A:121:GLU:HA	0.63	1.70	2	2
1:A:242:LEU:HD23	1:A:262:LEU:HD21	0.63	1.69	17	3
1:A:59:GLU:HA	1:A:73:GLU:O	0.63	1.94	18	4
1:A:66:GLU:HG3	1:A:67:TYR:H	0.63	1.53	12	1
1:A:233:PHE:HD1	1:A:247:TYR:HB3	0.63	1.54	16	1
1:A:38:GLY:HA3	1:A:63:ARG:O	0.63	1.93	16	2
1:A:256:LYS:HB3	1:A:280:GLU:HG3	0.63	1.71	12	2
1:A:115:LYS:CA	1:A:128:ASP:HB3	0.63	2.23	11	1
1:A:174:LYS:HB2	1:A:179:GLN:HG2	0.63	1.71	12	1
1:A:153:TYR:HB2	1:A:170:ALA:H	0.62	1.55	10	1
1:A:117:GLY:HA2	1:A:126:GLY:HA2	0.62	1.70	11	1
1:A:75:TRP:HD1	1:A:81:LEU:HG	0.62	1.52	2	3
1:A:123:ILE:HD11	1:A:142:LEU:HD11	0.62	1.71	8	7
1:A:199:ASN:HD22	1:A:200:LYS:HG3	0.62	1.53	12	1
1:A:181:HIS:HB2	1:A:193:SER:HB3	0.62	1.71	5	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:125:LEU:HB3	1:A:142:LEU:HD13	0.61	1.71	9	2
1:A:198:VAL:HB	1:A:201:LYS:HB3	0.61	1.72	17	1
1:A:238:ASN:HB2	1:A:242:LEU:HB2	0.61	1.72	16	3
1:A:62:TYR:O	1:A:70:THR:HA	0.61	1.96	14	6
1:A:128:ASP:HB2	1:A:139:ARG:HB3	0.61	1.73	16	2
1:A:201:LYS:HB3	1:A:226:GLN:HB3	0.61	1.72	3	1
1:A:154:GLN:HG3	1:A:168:ASN:HB2	0.61	1.71	11	1
1:A:173:TYR:CZ	1:A:180:LEU:HD21	0.61	2.31	20	2
1:A:86:THR:HG22	1:A:98:THR:CB	0.60	2.25	13	1
1:A:3:VAL:HB	1:A:119:LYS:HE3	0.60	1.73	16	1
1:A:81:LEU:O	1:A:103:PHE:HA	0.60	1.96	1	1
1:A:133:ILE:H	1:A:133:ILE:HD12	0.60	1.56	20	1
1:A:251:LEU:HG	1:A:253:PRO:HD2	0.60	1.73	2	1
1:A:93:ARG:HD3	1:A:93:ARG:H	0.60	1.56	1	2
1:A:193:SER:HA	1:A:206:VAL:O	0.60	1.97	19	10
1:A:264:ASP:N	1:A:268:VAL:HG21	0.60	2.12	3	3
1:A:195:TYR:HE2	1:A:203:GLU:HB3	0.60	1.57	17	2
1:A:166:GLN:HA	1:A:186:ASP:OD2	0.60	1.96	3	2
1:A:35:SER:HB3	1:A:39:LEU:HB2	0.60	1.74	10	1
1:A:30:ASP:HB3	1:A:280:GLU:HG2	0.60	1.73	1	1
1:A:27:ILE:HG13	1:A:277:LEU:HD23	0.60	1.74	3	1
1:A:180:LEU:HB2	1:A:194:ILE:HA	0.60	1.71	4	1
1:A:251:LEU:HD23	1:A:255:ILE:HG12	0.59	1.74	11	1
1:A:33:THR:HG22	1:A:41:PHE:HB3	0.59	1.74	19	1
1:A:83:THR:HB	1:A:101:SER:CB	0.59	2.28	1	1
1:A:10:LEU:HD12	1:A:150:LEU:HB3	0.59	1.75	3	2
1:A:251:LEU:HB3	1:A:255:ILE:HG23	0.59	1.74	17	2
1:A:113:LYS:HG2	1:A:130:ASP:HA	0.59	1.74	3	1
1:A:267:ASN:OD1	1:A:272:GLY:HA3	0.59	1.97	18	1
1:A:170:ALA:HA	1:A:182:THR:O	0.59	1.98	2	9
1:A:178:PHE:HD2	1:A:196:GLN:HE22	0.59	1.41	6	1
1:A:64:TRP:HB2	1:A:69:LEU:N	0.59	2.13	7	1
1:A:169:PHE:HB3	1:A:184:VAL:HB	0.58	1.74	11	1
1:A:20:LYS:H	1:A:20:LYS:HD2	0.58	1.58	12	1
1:A:124:ASN:HB3	1:A:143:VAL:HB	0.58	1.73	8	6
1:A:223:ALA:O	1:A:234:SER:HA	0.58	1.98	19	9
1:A:26:LEU:HB3	1:A:48:ASN:HA	0.58	1.75	11	1
1:A:17:VAL:HG13	1:A:222:ALA:HB3	0.58	1.72	13	1
1:A:33:THR:HG22	1:A:283:ALA:HB3	0.58	1.76	1	2
1:A:100:ASP:HB2	1:A:113:LYS:HB3	0.58	1.75	11	1
1:A:133:ILE:HD13	1:A:133:ILE:H	0.58	1.57	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:17:VAL:HB	1:A:207:ASN:HB2	0.58	1.74	19	1
1:A:191:GLY:HA3	1:A:209:ALA:HA	0.58	1.73	1	2
1:A:180:LEU:HB2	1:A:194:ILE:HG13	0.58	1.75	4	1
1:A:262:LEU:HB3	1:A:274:LYS:HB2	0.58	1.75	1	4
1:A:252:LYS:HB2	1:A:253:PRO:HD3	0.57	1.74	20	2
1:A:280:GLU:O	1:A:281:PHE:HB2	0.57	1.97	5	2
1:A:8:ALA:O	1:A:12:LYS:HB3	0.57	2.00	4	2
1:A:247:TYR:HD1	1:A:259:LEU:HB3	0.57	1.58	12	1
1:A:158:GLU:HG3	1:A:161:LYS:H	0.57	1.59	17	2
1:A:142:LEU:HD13	1:A:144:LEU:HD22	0.57	1.75	10	1
1:A:84:GLU:HA	1:A:99:PHE:O	0.57	1.99	20	2
1:A:28:LYS:O	1:A:278:GLY:HA2	0.57	2.00	20	10
1:A:210:TRP:HB2	1:A:217:THR:HG23	0.57	1.76	10	3
1:A:226:GLN:NE2	1:A:226:GLN:H	0.57	1.98	6	1
1:A:48:ASN:HB2	1:A:53:LYS:HB3	0.57	1.74	20	1
1:A:259:LEU:HD22	1:A:277:LEU:HG	0.57	1.75	7	1
1:A:100:ASP:HB3	1:A:113:LYS:HG2	0.56	1.77	15	3
1:A:196:GLN:CG	1:A:199:ASN:HB2	0.56	2.29	12	1
1:A:202:LEU:HB3	1:A:225:TYR:HD1	0.56	1.59	17	1
1:A:57:SER:HB2	1:A:77:THR:HG23	0.56	1.77	13	1
1:A:180:LEU:HD22	1:A:180:LEU:C	0.56	2.19	4	1
1:A:123:ILE:HD11	1:A:144:LEU:HG	0.56	1.77	6	1
1:A:27:ILE:HB	1:A:47:ALA:HB3	0.56	1.77	10	1
1:A:33:THR:HB	1:A:283:ALA:HB3	0.56	1.77	2	2
1:A:99:PHE:HD1	1:A:114:ILE:HB	0.56	1.60	8	1
1:A:252:LYS:HB3	1:A:253:PRO:CD	0.56	2.27	11	2
1:A:148:GLY:HA2	1:A:174:LYS:HB3	0.56	1.77	6	1
1:A:185:ASN:HB3	1:A:189:GLU:HB2	0.56	1.77	18	1
1:A:84:GLU:HB3	1:A:99:PHE:O	0.56	2.00	9	3
1:A:251:LEU:HB2	1:A:255:ILE:HG23	0.56	1.77	7	1
1:A:221:ILE:O	1:A:236:LYS:HA	0.56	2.01	16	5
1:A:72:THR:HB	1:A:84:GLU:HB3	0.56	1.78	2	3
1:A:253:PRO:HD2	1:A:255:ILE:CD1	0.56	2.31	11	1
1:A:102:SER:HB3	1:A:111:ASN:HB2	0.56	1.77	7	1
1:A:114:ILE:HG22	1:A:129:MET:HB2	0.56	1.77	20	1
1:A:14:ALA:HB2	1:A:181:HIS:HB2	0.56	1.77	4	1
1:A:196:GLN:HB3	1:A:199:ASN:HB2	0.56	1.77	9	1
1:A:202:LEU:HD12	1:A:226:GLN:H	0.56	1.61	9	1
1:A:30:ASP:O	1:A:280:GLU:HA	0.55	2.00	5	3
1:A:3:VAL:HB	1:A:119:LYS:HD2	0.55	1.77	4	1
1:A:184:VAL:HG22	1:A:190:PHE:HB2	0.55	1.76	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:40:GLU:CB	1:A:61:LYS:HB2	0.55	2.31	4	2
1:A:42:THR:HB	1:A:59:GLU:CG	0.55	2.31	4	2
1:A:40:GLU:HB3	1:A:61:LYS:CB	0.55	2.29	18	2
1:A:201:LYS:HG3	1:A:202:LEU:CD1	0.55	2.31	17	1
1:A:3:VAL:HB	1:A:119:LYS:HE2	0.55	1.77	14	2
1:A:33:THR:HB	1:A:41:PHE:HB2	0.55	1.77	10	3
1:A:37:ASN:HB3	1:A:39:LEU:HG	0.55	1.77	13	1
1:A:27:ILE:HG13	1:A:277:LEU:HD12	0.55	1.79	12	1
1:A:264:ASP:HB2	1:A:267:ASN:HB3	0.55	1.79	6	2
1:A:175:THR:HB	1:A:178:PHE:HB2	0.55	1.77	18	2
1:A:208:LEU:HD13	1:A:219:PHE:HB3	0.55	1.78	11	1
1:A:27:ILE:HD12	1:A:277:LEU:HD23	0.55	1.78	18	1
1:A:101:SER:HA	1:A:112:ALA:HA	0.55	1.78	13	1
1:A:209:ALA:HB3	1:A:218:ARG:HB2	0.55	1.78	5	1
1:A:282:GLN:HE21	1:A:284:LEU:HD21	0.55	1.62	6	1
1:A:59:GLU:HG2	1:A:74:LYS:HB3	0.55	1.78	8	1
1:A:40:GLU:HB2	1:A:61:LYS:CB	0.55	2.32	12	1
1:A:210:TRP:CZ2	1:A:215:SER:HA	0.55	2.37	13	1
1:A:32:LYS:HA	1:A:41:PHE:O	0.55	2.01	5	5
1:A:26:LEU:HG	1:A:48:ASN:HA	0.55	1.79	7	2
1:A:10:LEU:CD2	1:A:143:VAL:HG22	0.55	2.31	12	1
1:A:240:SER:HB2	1:A:242:LEU:CD1	0.54	2.32	2	3
1:A:107:THR:HB	1:A:109:LYS:HG2	0.54	1.77	8	1
1:A:238:ASN:HB3	1:A:242:LEU:HB2	0.54	1.78	14	2
1:A:260:SER:O	1:A:275:LEU:HB2	0.54	2.03	6	1
1:A:119:LYS:HG3	1:A:124:ASN:CB	0.54	2.29	9	1
1:A:123:ILE:CD1	1:A:144:LEU:HG	0.54	2.33	7	4
1:A:69:LEU:HD22	1:A:87:VAL:HA	0.54	1.78	10	1
1:A:100:ASP:HB3	1:A:113:LYS:HB2	0.54	1.78	5	1
1:A:15:ARG:HG3	1:A:16:ASP:N	0.54	2.17	10	1
1:A:168:ASN:HA	1:A:184:VAL:O	0.54	2.02	10	2
1:A:36:GLU:O	1:A:37:ASN:HB2	0.54	2.02	13	1
1:A:85:ILE:HG13	1:A:99:PHE:O	0.54	2.02	13	1
1:A:101:SER:HA	1:A:111:ASN:O	0.54	2.03	1	3
1:A:228:ASP:HB2	1:A:229:PRO:HD2	0.54	1.78	2	1
1:A:39:LEU:HD12	1:A:39:LEU:O	0.54	2.03	3	1
1:A:219:PHE:HB2	1:A:239:ASN:HB2	0.54	1.80	5	2
1:A:153:TYR:CB	1:A:169:PHE:CA	0.54	2.82	10	1
1:A:7:TYR:HA	1:A:10:LEU:CB	0.54	2.32	4	1
1:A:96:LYS:HD3	1:A:119:LYS:HD3	0.54	1.79	8	1
1:A:255:ILE:HA	1:A:281:PHE:HB3	0.54	1.80	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:123:ILE:HD12	1:A:142:LEU:HD11	0.54	1.80	1	1
1:A:214:ASN:HB2	1:A:216:ASN:HD21	0.54	1.63	1	1
1:A:196:GLN:HG2	1:A:199:ASN:HB2	0.54	1.78	12	1
1:A:256:LYS:HB3	1:A:280:GLU:CG	0.54	2.33	18	2
1:A:61:LYS:HA	1:A:71:PHE:O	0.54	2.02	19	11
1:A:256:LYS:CG	1:A:280:GLU:HB2	0.54	2.33	4	2
1:A:38:GLY:HA2	1:A:63:ARG:O	0.54	2.03	5	14
1:A:228:ASP:HB2	1:A:231:ALA:HB3	0.53	1.79	5	1
1:A:203:GLU:HB2	1:A:224:LYS:HG3	0.53	1.80	15	1
1:A:256:LYS:HB3	1:A:280:GLU:HB2	0.53	1.79	13	1
1:A:51:THR:HG23	1:A:52:THR:H	0.53	1.62	20	1
1:A:31:LEU:HB3	1:A:43:SER:HB3	0.53	1.79	10	2
1:A:31:LEU:HD13	1:A:281:PHE:HD1	0.53	1.62	17	1
1:A:155:MET:HB2	1:A:164:VAL:HG21	0.53	1.80	19	1
1:A:3:VAL:CG1	1:A:121:GLU:HA	0.53	2.32	13	1
1:A:97:LEU:HD12	1:A:116:THR:HG22	0.53	1.78	8	3
1:A:240:SER:HB2	1:A:242:LEU:HD13	0.53	1.81	13	5
1:A:263:LEU:HD12	1:A:273:HIS:CB	0.53	2.32	16	1
1:A:124:ASN:HD22	1:A:124:ASN:N	0.53	2.01	19	1
1:A:154:GLN:HG2	1:A:168:ASN:HB3	0.53	1.79	20	1
1:A:129:MET:HG3	1:A:138:ILE:HG13	0.53	1.80	1	1
1:A:248:THR:HA	1:A:257:LEU:O	0.53	2.03	2	3
1:A:87:VAL:HB	1:A:97:LEU:HB2	0.53	1.80	5	2
1:A:255:ILE:HG22	1:A:281:PHE:CD1	0.53	2.38	16	1
1:A:177:GLU:HA	1:A:197:LYS:HE3	0.53	1.80	19	1
1:A:31:LEU:HD13	1:A:281:PHE:HB3	0.53	1.79	1	3
1:A:259:LEU:CD2	1:A:277:LEU:HD13	0.53	2.34	18	2
1:A:256:LYS:HB3	1:A:280:GLU:HB3	0.53	1.80	19	1
1:A:196:GLN:NE2	1:A:196:GLN:HA	0.53	2.13	4	2
1:A:142:LEU:O	1:A:152:GLY:HA2	0.53	2.03	6	1
1:A:81:LEU:H	1:A:103:PHE:CA	0.52	2.17	1	1
1:A:3:VAL:CG1	1:A:119:LYS:HB3	0.52	2.34	8	2
1:A:179:GLN:HB2	1:A:195:TYR:HB3	0.52	1.79	11	2
1:A:40:GLU:HB2	1:A:63:ARG:HH12	0.52	1.64	16	1
1:A:121:GLU:HG3	1:A:122:HIS:HD2	0.52	1.64	20	1
1:A:178:PHE:HD1	1:A:196:GLN:HG2	0.52	1.64	2	1
1:A:171:VAL:O	1:A:181:HIS:HA	0.52	2.04	13	5
1:A:255:ILE:HA	1:A:281:PHE:CB	0.52	2.34	8	1
1:A:45:GLY:HA3	1:A:56:GLY:HA2	0.52	1.79	15	1
1:A:205:ALA:HB3	1:A:222:ALA:HB3	0.52	1.81	3	1
1:A:70:THR:CG2	1:A:86:THR:HB	0.52	2.33	12	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:75:TRP:CD1	1:A:81:LEU:HB3	0.52	2.35	11	4
1:A:10:LEU:HD12	1:A:143:VAL:HG13	0.52	1.79	4	1
1:A:27:ILE:HG23	1:A:277:LEU:HD22	0.52	1.79	8	1
1:A:61:LYS:HG2	1:A:72:THR:HB	0.52	1.82	3	1
1:A:3:VAL:HG11	1:A:119:LYS:HB2	0.52	1.81	10	3
1:A:259:LEU:CD2	1:A:277:LEU:HD12	0.52	2.35	8	1
1:A:171:VAL:HB	1:A:182:THR:CG2	0.52	2.34	9	1
1:A:34:LYS:CB	1:A:40:GLU:HG2	0.52	2.35	12	1
1:A:75:TRP:CD1	1:A:81:LEU:HD22	0.52	2.40	16	1
1:A:99:PHE:HD2	1:A:114:ILE:HG12	0.52	1.65	20	1
1:A:64:TRP:CA	1:A:69:LEU:O	0.52	2.58	7	1
1:A:173:TYR:HB3	1:A:180:LEU:CD2	0.52	2.35	15	1
1:A:236:LYS:NZ	1:A:236:LYS:HB2	0.52	2.18	13	1
1:A:81:LEU:C	1:A:103:PHE:HB3	0.52	2.24	1	1
1:A:85:ILE:O	1:A:98:THR:HA	0.52	2.05	17	5
1:A:121:GLU:HG3	1:A:122:HIS:CD2	0.52	2.40	20	1
1:A:266:LYS:O	1:A:267:ASN:HB2	0.52	2.05	1	1
1:A:29:LEU:HD23	1:A:279:LEU:HB2	0.52	1.80	5	2
1:A:81:LEU:N	1:A:103:PHE:CB	0.51	2.73	1	1
1:A:156:ASN:HB2	1:A:166:GLN:HB2	0.51	1.80	7	1
1:A:74:LYS:O	1:A:81:LEU:HA	0.51	2.05	18	1
1:A:245:LEU:H	1:A:245:LEU:HD23	0.51	1.65	7	1
1:A:17:VAL:HG21	1:A:205:ALA:CB	0.51	2.36	7	1
1:A:242:LEU:CG	1:A:264:ASP:HA	0.51	2.32	3	1
1:A:83:THR:HB	1:A:101:SER:HB3	0.51	1.83	11	1
1:A:26:LEU:CB	1:A:48:ASN:HA	0.51	2.36	11	1
1:A:62:TYR:HD2	1:A:71:PHE:HB2	0.51	1.65	19	1
1:A:95:LEU:HD23	1:A:118:TYR:HB3	0.51	1.80	19	1
1:A:99:PHE:HB2	1:A:114:ILE:HD13	0.51	1.81	13	1
1:A:143:VAL:HA	1:A:152:GLY:HA3	0.51	1.83	10	1
1:A:83:THR:C	1:A:100:ASP:HB3	0.51	2.26	13	1
1:A:123:ILE:CG1	1:A:142:LEU:HD21	0.51	2.33	10	1
1:A:125:LEU:HD13	1:A:142:LEU:HD13	0.51	1.82	6	2
1:A:115:LYS:CB	1:A:128:ASP:CA	0.51	2.88	8	1
1:A:40:GLU:HB2	1:A:61:LYS:HB3	0.51	1.81	12	1
1:A:174:LYS:HG2	1:A:179:GLN:HG2	0.51	1.80	17	1
1:A:158:GLU:HB2	1:A:165:THR:OG1	0.51	2.05	18	1
1:A:264:ASP:N	1:A:268:VAL:HG13	0.51	2.21	13	1
1:A:103:PHE:HB3	1:A:110:LYS:HG3	0.51	1.82	6	1
1:A:87:VAL:HG22	1:A:97:LEU:HB2	0.51	1.83	6	4
1:A:68:GLY:O	1:A:69:LEU:HD23	0.51	2.06	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:72:THR:HB	1:A:84:GLU:HB2	0.51	1.82	15	2
1:A:248:THR:HG22	1:A:258:THR:HB	0.51	1.83	16	1
1:A:197:LYS:O	1:A:198:VAL:HG22	0.51	2.05	12	2
1:A:70:THR:HB	1:A:86:THR:OG1	0.51	2.05	13	1
1:A:208:LEU:HA	1:A:218:ARG:O	0.50	2.06	1	2
1:A:143:VAL:HA	1:A:151:ALA:O	0.50	2.06	2	3
1:A:115:LYS:HA	1:A:127:CYS:O	0.50	2.06	16	1
1:A:242:LEU:HD23	1:A:262:LEU:CD1	0.50	2.37	19	4
1:A:2:ALA:HB1	1:A:94:GLY:HA2	0.50	1.81	9	1
1:A:7:TYR:HB3	1:A:143:VAL:CG2	0.50	2.35	13	1
1:A:26:LEU:HB2	1:A:47:ALA:O	0.50	2.06	5	2
1:A:156:ASN:O	1:A:164:VAL:HB	0.50	2.06	6	5
1:A:69:LEU:HG	1:A:87:VAL:HA	0.50	1.83	7	2
1:A:173:TYR:CE1	1:A:180:LEU:HD22	0.50	2.41	19	1
1:A:188:THR:O	1:A:211:THR:HA	0.50	2.07	7	4
1:A:115:LYS:HG2	1:A:128:ASP:OD1	0.50	2.07	7	1
1:A:100:ASP:HB2	1:A:113:LYS:HB2	0.50	1.84	9	2
1:A:142:LEU:HD23	1:A:143:VAL:N	0.50	2.21	10	1
1:A:39:LEU:HD23	1:A:62:TYR:HA	0.50	1.83	16	1
1:A:22:TYR:HA	1:A:260:SER:OG	0.50	2.06	17	1
1:A:274:LYS:HA	1:A:274:LYS:HE2	0.50	1.84	5	2
1:A:241:SER:O	1:A:265:GLY:HA3	0.50	2.07	8	2
1:A:34:LYS:HA	1:A:40:GLU:HG2	0.50	1.83	4	1
1:A:197:LYS:HD2	1:A:197:LYS:O	0.50	2.07	9	1
1:A:114:ILE:C	1:A:128:ASP:HB3	0.50	2.27	11	1
1:A:182:THR:HA	1:A:192:GLY:HA2	0.50	1.84	9	3
1:A:11:GLY:HA3	1:A:181:HIS:HB2	0.50	1.81	18	1
1:A:81:LEU:O	1:A:103:PHE:CA	0.49	2.59	1	1
1:A:99:PHE:CE2	1:A:114:ILE:HD13	0.49	2.41	2	1
1:A:180:LEU:CB	1:A:194:ILE:HG13	0.49	2.36	4	1
1:A:78:ASP:O	1:A:79:ASN:HB2	0.49	2.07	10	6
1:A:142:LEU:HD11	1:A:144:LEU:HD12	0.49	1.83	13	1
1:A:259:LEU:HD22	1:A:277:LEU:HD13	0.49	1.83	3	3
1:A:47:ALA:HB2	1:A:54:VAL:HG13	0.49	1.84	12	5
1:A:138:ILE:HB	1:A:157:PHE:HB2	0.49	1.84	7	3
1:A:171:VAL:HB	1:A:182:THR:HG22	0.49	1.84	17	1
1:A:12:LYS:HG3	1:A:13:SER:N	0.49	2.22	1	1
1:A:246:GLY:HA2	1:A:259:LEU:O	0.49	2.07	8	6
1:A:100:ASP:HB2	1:A:113:LYS:HD2	0.49	1.83	11	1
1:A:113:LYS:HG2	1:A:130:ASP:OD1	0.49	2.07	18	1
1:A:180:LEU:HD22	1:A:181:HIS:N	0.49	2.23	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:32:LYS:O	1:A:282:GLN:HA	0.49	2.07	10	3
1:A:115:LYS:HB3	1:A:128:ASP:CA	0.49	2.37	8	1
1:A:247:TYR:O	1:A:258:THR:HA	0.49	2.08	13	2
1:A:133:ILE:N	1:A:133:ILE:HD12	0.49	2.23	15	2
1:A:211:THR:HG23	1:A:215:SER:HB2	0.49	1.83	18	2
1:A:115:LYS:HB2	1:A:128:ASP:OD1	0.49	2.07	13	1
1:A:27:ILE:HD12	1:A:277:LEU:HD12	0.49	1.85	1	3
1:A:144:LEU:N	1:A:144:LEU:HD22	0.49	2.23	12	4
1:A:109:LYS:HE2	1:A:111:ASN:OD1	0.49	2.07	14	1
1:A:259:LEU:HB3	1:A:277:LEU:HD23	0.49	1.83	17	1
1:A:27:ILE:HG23	1:A:277:LEU:HD13	0.49	1.84	7	1
1:A:120:ARG:HB2	1:A:123:ILE:HG23	0.49	1.83	9	1
1:A:219:PHE:H	1:A:239:ASN:HB3	0.49	1.67	11	1
1:A:130:ASP:HB2	1:A:137:SER:HB3	0.49	1.84	12	1
1:A:95:LEU:HD23	1:A:118:TYR:HD1	0.49	1.66	1	2
1:A:275:LEU:HD13	1:A:276:GLY:N	0.49	2.23	16	6
1:A:156:ASN:N	1:A:156:ASN:HD22	0.49	2.05	20	2
1:A:81:LEU:N	1:A:103:PHE:HB2	0.48	2.23	1	1
1:A:140:GLY:O	1:A:154:GLN:HA	0.48	2.08	15	4
1:A:143:VAL:HA	1:A:152:GLY:CA	0.48	2.38	10	1
1:A:34:LYS:HB3	1:A:63:ARG:HH12	0.48	1.67	14	1
1:A:10:LEU:HD21	1:A:152:GLY:CA	0.48	2.28	19	1
1:A:194:ILE:O	1:A:205:ALA:HA	0.48	2.08	13	3
1:A:144:LEU:HG	1:A:151:ALA:O	0.48	2.08	10	1
1:A:86:THR:HG23	1:A:98:THR:HB	0.48	1.85	19	1
1:A:80:THR:HB	1:A:103:PHE:HB2	0.48	1.84	1	1
1:A:255:ILE:HD11	1:A:279:LEU:HB3	0.48	1.83	2	1
1:A:163:ARG:HG2	1:A:164:VAL:N	0.48	2.23	8	1
1:A:202:LEU:HD13	1:A:225:TYR:HD2	0.48	1.67	8	1
1:A:119:LYS:HB3	1:A:124:ASN:OD1	0.48	2.09	10	1
1:A:142:LEU:HD22	1:A:144:LEU:CD2	0.48	2.37	10	1
1:A:178:PHE:CD1	1:A:196:GLN:HG2	0.48	2.43	2	1
1:A:263:LEU:CD1	1:A:273:HIS:HB2	0.48	2.35	16	2
1:A:72:THR:O	1:A:83:THR:HA	0.48	2.08	19	1
1:A:268:VAL:HG22	1:A:273:HIS:CA	0.48	2.35	3	1
1:A:171:VAL:HB	1:A:182:THR:CB	0.48	2.37	8	2
1:A:115:LYS:CA	1:A:128:ASP:CB	0.48	2.91	11	1
1:A:75:TRP:HA	1:A:81:LEU:HA	0.48	1.85	3	1
1:A:202:LEU:HG	1:A:225:TYR:HB2	0.48	1.84	14	1
1:A:30:ASP:HA	1:A:43:SER:O	0.48	2.08	14	3
1:A:90:GLN:HG3	1:A:91:LEU:HG	0.48	1.85	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:115:LYS:HB3	1:A:127:CYS:C	0.48	2.27	8	1
1:A:115:LYS:HG2	1:A:128:ASP:HB2	0.48	1.84	18	1
1:A:264:ASP:O	1:A:268:VAL:HG22	0.48	2.08	13	4
1:A:158:GLU:HG2	1:A:161:LYS:H	0.48	1.67	13	1
1:A:169:PHE:HB2	1:A:184:VAL:HB	0.47	1.86	20	7
1:A:86:THR:CG2	1:A:96:LYS:HE3	0.47	2.39	16	1
1:A:144:LEU:HD22	1:A:144:LEU:N	0.47	2.23	17	4
1:A:237:VAL:HA	1:A:242:LEU:O	0.47	2.09	9	6
1:A:96:LYS:HG2	1:A:117:GLY:HA3	0.47	1.85	15	1
1:A:89:ASP:HA	1:A:93:ARG:HA	0.47	1.84	15	1
1:A:233:PHE:CD1	1:A:247:TYR:HB3	0.47	2.41	16	1
1:A:195:TYR:CE2	1:A:203:GLU:HB3	0.47	2.42	17	1
1:A:17:VAL:HG12	1:A:222:ALA:HB3	0.47	1.85	1	1
1:A:85:ILE:CG2	1:A:99:PHE:HB2	0.47	2.40	2	1
1:A:27:ILE:HA	1:A:277:LEU:O	0.47	2.09	16	3
1:A:3:VAL:HB	1:A:119:LYS:CE	0.47	2.40	16	1
1:A:64:TRP:HB3	1:A:69:LEU:C	0.47	2.29	7	1
1:A:157:PHE:CD2	1:A:164:VAL:HG12	0.47	2.43	11	2
1:A:153:TYR:HB2	1:A:169:PHE:CA	0.47	2.38	10	1
1:A:144:LEU:HD23	1:A:151:ALA:HB3	0.47	1.85	11	1
1:A:26:LEU:HD11	1:A:48:ASN:HA	0.47	1.85	15	1
1:A:3:VAL:HG11	1:A:121:GLU:CA	0.47	2.34	13	1
1:A:82:GLY:HA3	1:A:102:SER:HA	0.47	1.86	13	1
1:A:170:ALA:HB1	1:A:181:HIS:CE1	0.47	2.44	3	3
1:A:172:GLY:HA2	1:A:180:LEU:O	0.47	2.09	3	4
1:A:78:ASP:HB3	1:A:80:THR:HG22	0.47	1.85	8	1
1:A:79:ASN:O	1:A:105:PRO:HD2	0.47	2.10	11	3
1:A:29:LEU:HD13	1:A:29:LEU:O	0.47	2.09	20	1
1:A:245:LEU:N	1:A:245:LEU:HD13	0.47	2.25	18	4
1:A:47:ALA:HB1	1:A:54:VAL:HG22	0.47	1.87	3	1
1:A:233:PHE:HD2	1:A:247:TYR:HB3	0.47	1.69	4	1
1:A:261:ALA:HA	1:A:275:LEU:CB	0.47	2.40	6	1
1:A:129:MET:HG2	1:A:138:ILE:HG13	0.47	1.86	10	1
1:A:81:LEU:HG	1:A:103:PHE:HB2	0.47	1.86	14	1
1:A:180:LEU:HD13	1:A:180:LEU:N	0.47	2.25	20	2
1:A:39:LEU:CD2	1:A:62:TYR:HA	0.47	2.39	13	2
1:A:7:TYR:HA	1:A:143:VAL:HG21	0.47	1.87	18	1
1:A:16:ASP:O	1:A:20:LYS:HB2	0.47	2.09	13	2
1:A:83:THR:HB	1:A:101:SER:OG	0.47	2.10	20	1
1:A:243:ILE:H	1:A:243:ILE:HD13	0.47	1.70	10	4
1:A:268:VAL:CG2	1:A:273:HIS:HA	0.47	2.35	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:222:ALA:CA	1:A:236:LYS:HB2	0.47	2.37	4	1
1:A:69:LEU:CD1	1:A:87:VAL:HG12	0.47	2.40	6	1
1:A:10:LEU:HD23	1:A:10:LEU:O	0.47	2.09	4	1
1:A:268:VAL:HA	1:A:272:GLY:H	0.47	1.70	8	1
1:A:16:ASP:O	1:A:20:LYS:HD3	0.47	2.09	14	1
1:A:277:LEU:HD12	1:A:278:GLY:H	0.47	1.70	18	1
1:A:223:ALA:N	1:A:236:LYS:HB2	0.47	2.25	4	1
1:A:219:PHE:HB2	1:A:239:ASN:HB3	0.47	1.87	9	1
1:A:158:GLU:HB3	1:A:163:ARG:O	0.47	2.10	12	1
1:A:247:TYR:HB3	1:A:249:GLN:HE21	0.46	1.69	3	1
1:A:31:LEU:O	1:A:42:THR:HA	0.46	2.10	16	5
1:A:226:GLN:HA	1:A:232:CYS:HA	0.46	1.86	5	1
1:A:99:PHE:CD1	1:A:114:ILE:HB	0.46	2.44	8	1
1:A:94:GLY:HA2	1:A:119:LYS:HG3	0.46	1.85	11	1
1:A:81:LEU:HD21	1:A:103:PHE:HD1	0.46	1.69	11	1
1:A:168:ASN:ND2	1:A:185:ASN:HA	0.46	2.24	15	2
1:A:225:TYR:HD1	1:A:227:ILE:HD13	0.46	1.71	4	1
1:A:196:GLN:CA	1:A:196:GLN:HE21	0.46	2.15	6	2
1:A:208:LEU:HD13	1:A:219:PHE:HD2	0.46	1.71	6	1
1:A:81:LEU:HD23	1:A:81:LEU:H	0.46	1.70	8	1
1:A:71:PHE:CD1	1:A:85:ILE:HB	0.46	2.46	4	1
1:A:252:LYS:HB2	1:A:255:ILE:HG12	0.46	1.87	15	1
1:A:7:TYR:CB	1:A:143:VAL:HG21	0.46	2.37	5	1
1:A:40:GLU:HB2	1:A:63:ARG:CG	0.46	2.40	7	1
1:A:144:LEU:N	1:A:144:LEU:CD2	0.46	2.76	10	1
1:A:34:LYS:HB2	1:A:40:GLU:HG2	0.46	1.87	12	1
1:A:85:ILE:N	1:A:100:ASP:HB2	0.46	2.25	13	1
1:A:144:LEU:HD13	1:A:144:LEU:N	0.46	2.26	13	1
1:A:29:LEU:O	1:A:44:SER:HA	0.46	2.10	5	2
1:A:189:GLU:HA	1:A:210:TRP:O	0.46	2.10	19	1
1:A:29:LEU:HB2	1:A:279:LEU:HB2	0.46	1.86	20	1
1:A:48:ASN:HB3	1:A:51:THR:O	0.46	2.11	11	2
1:A:114:ILE:HG23	1:A:129:MET:HB3	0.46	1.87	9	1
1:A:142:LEU:HD22	1:A:144:LEU:HD22	0.46	1.85	10	1
1:A:31:LEU:CB	1:A:43:SER:HB3	0.46	2.40	10	1
1:A:84:GLU:HB2	1:A:100:ASP:HA	0.46	1.85	14	1
1:A:249:GLN:HB3	1:A:257:LEU:HB3	0.46	1.88	17	1
1:A:84:GLU:HA	1:A:100:ASP:HA	0.46	1.88	19	1
1:A:153:TYR:HD2	1:A:169:PHE:HD2	0.46	1.54	3	1
1:A:242:LEU:HD21	1:A:264:ASP:OD1	0.46	2.10	3	1
1:A:225:TYR:CD1	1:A:227:ILE:HD13	0.46	2.46	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:144:LEU:O	1:A:150:LEU:HD22	0.46	2.11	15	1
1:A:247:TYR:HD2	1:A:259:LEU:HB3	0.46	1.70	13	1
1:A:86:THR:HB	1:A:98:THR:HG23	0.45	1.87	10	2
1:A:175:THR:OG1	1:A:178:PHE:HB2	0.45	2.12	9	1
1:A:86:THR:HA	1:A:97:LEU:O	0.45	2.10	10	2
1:A:259:LEU:CD2	1:A:277:LEU:HD23	0.45	2.39	6	2
1:A:68:GLY:O	1:A:69:LEU:HD12	0.45	2.12	7	1
1:A:31:LEU:HD12	1:A:32:LYS:N	0.45	2.26	12	1
1:A:31:LEU:HD13	1:A:281:PHE:CG	0.45	2.46	12	1
1:A:154:GLN:CG	1:A:168:ASN:HB3	0.45	2.38	17	1
1:A:31:LEU:HA	1:A:281:PHE:O	0.45	2.11	19	6
1:A:11:GLY:O	1:A:15:ARG:HG3	0.45	2.11	2	1
1:A:245:LEU:HD13	1:A:245:LEU:N	0.45	2.27	6	5
1:A:142:LEU:HD12	1:A:143:VAL:N	0.45	2.25	20	2
1:A:264:ASP:HB3	1:A:268:VAL:HG23	0.45	1.88	9	1
1:A:94:GLY:HA2	1:A:119:LYS:HB2	0.45	1.89	15	1
1:A:31:LEU:HD13	1:A:281:PHE:CD2	0.45	2.46	2	2
1:A:103:PHE:HD2	1:A:110:LYS:HB3	0.45	1.72	11	2
1:A:158:GLU:N	1:A:163:ARG:O	0.45	2.50	2	2
1:A:221:ILE:HG12	1:A:237:VAL:HG12	0.45	1.88	14	2
1:A:57:SER:HB2	1:A:76:ASN:HA	0.45	1.89	15	1
1:A:88:GLU:HA	1:A:95:LEU:O	0.45	2.12	17	1
1:A:214:ASN:HB2	1:A:216:ASN:ND2	0.45	2.26	1	1
1:A:40:GLU:OE2	1:A:63:ARG:HD2	0.45	2.11	1	1
1:A:208:LEU:HD13	1:A:219:PHE:HD1	0.45	1.71	3	2
1:A:283:ALA:C	1:A:284:LEU:HD22	0.45	2.32	7	1
1:A:144:LEU:HD23	1:A:151:ALA:CB	0.45	2.42	11	1
1:A:238:ASN:ND2	1:A:242:LEU:HB2	0.45	2.27	3	1
1:A:196:GLN:HB2	1:A:204:THR:HB	0.45	1.89	4	1
1:A:17:VAL:HG11	1:A:222:ALA:HB2	0.45	1.89	6	1
1:A:226:GLN:HE21	1:A:229:PRO:HA	0.45	1.72	8	1
1:A:251:LEU:HG	1:A:252:LYS:H	0.45	1.72	8	1
1:A:58:LEU:HD12	1:A:74:LYS:HG3	0.45	1.89	13	1
1:A:161:LYS:HG3	1:A:162:SER:H	0.44	1.71	3	1
1:A:223:ALA:H	1:A:236:LYS:HB2	0.44	1.72	4	1
1:A:163:ARG:HA	1:A:163:ARG:NE	0.44	2.26	16	1
1:A:81:LEU:O	1:A:102:SER:HA	0.44	2.12	5	1
1:A:119:LYS:HD2	1:A:119:LYS:N	0.44	2.26	8	2
1:A:248:THR:CG2	1:A:256:LYS:HE2	0.44	2.41	8	1
1:A:40:GLU:OE1	1:A:61:LYS:HD3	0.44	2.13	1	1
1:A:237:VAL:HG22	1:A:242:LEU:O	0.44	2.12	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:256:LYS:HB2	1:A:280:GLU:CG	0.44	2.43	10	1
1:A:69:LEU:HD22	1:A:87:VAL:CA	0.44	2.43	10	1
1:A:222:ALA:HA	1:A:235:ALA:O	0.44	2.12	19	2
1:A:65:THR:HG22	1:A:67:TYR:H	0.44	1.72	16	1
1:A:92:ALA:O	1:A:95:LEU:HB2	0.44	2.12	17	1
1:A:93:ARG:HD3	1:A:93:ARG:N	0.44	2.27	17	1
1:A:72:THR:OG1	1:A:84:GLU:HB2	0.44	2.12	5	1
1:A:120:ARG:HB2	1:A:123:ILE:HG22	0.44	1.88	6	1
1:A:25:GLY:HA2	1:A:275:LEU:H	0.44	1.72	6	1
1:A:100:ASP:CB	1:A:113:LYS:HD2	0.44	2.43	11	1
1:A:163:ARG:HE	1:A:163:ARG:HA	0.44	1.73	16	1
1:A:211:THR:HB	1:A:214:ASN:CB	0.44	2.37	20	1
1:A:33:THR:HA	1:A:283:ALA:O	0.44	2.13	13	1
1:A:232:CYS:HB2	1:A:248:THR:HG23	0.44	1.90	3	1
1:A:210:TRP:CE3	1:A:217:THR:HB	0.44	2.47	6	2
1:A:219:PHE:H	1:A:239:ASN:HB2	0.44	1.72	7	2
1:A:197:LYS:HG2	1:A:203:GLU:HG2	0.44	1.89	8	1
1:A:74:LYS:NZ	1:A:74:LYS:HB2	0.44	2.27	14	1
1:A:208:LEU:HD12	1:A:218:ARG:O	0.44	2.12	17	1
1:A:93:ARG:HD3	1:A:93:ARG:O	0.44	2.13	20	1
1:A:7:TYR:HB2	1:A:143:VAL:HG21	0.44	1.89	2	2
1:A:115:LYS:HA	1:A:128:ASP:HA	0.44	1.89	13	2
1:A:64:TRP:CB	1:A:69:LEU:N	0.44	2.80	7	1
1:A:93:ARG:HD2	1:A:93:ARG:N	0.44	2.28	9	1
1:A:57:SER:CB	1:A:76:ASN:HA	0.44	2.42	15	1
1:A:10:LEU:HD23	1:A:170:ALA:HB3	0.44	1.90	13	1
1:A:156:ASN:HD21	1:A:166:GLN:HB3	0.44	1.71	13	1
1:A:17:VAL:HA	1:A:236:LYS:CE	0.44	2.43	17	1
1:A:125:LEU:CB	1:A:142:LEU:HD13	0.44	2.42	19	1
1:A:221:ILE:HB	1:A:237:VAL:HG12	0.44	1.89	11	1
1:A:150:LEU:HD13	1:A:151:ALA:N	0.44	2.28	12	2
1:A:18:PHE:HE2	1:A:220:GLY:HA3	0.44	1.72	16	1
1:A:39:LEU:HA	1:A:61:LYS:O	0.44	2.13	13	1
1:A:14:ALA:HB1	1:A:193:SER:HB2	0.43	1.89	3	1
1:A:57:SER:HB3	1:A:76:ASN:OD1	0.43	2.13	3	1
1:A:168:ASN:ND2	1:A:186:ASP:H	0.43	2.11	7	1
1:A:75:TRP:HD1	1:A:81:LEU:HD13	0.43	1.73	12	1
1:A:252:LYS:HZ3	1:A:252:LYS:HB2	0.43	1.72	3	1
1:A:248:THR:HG22	1:A:258:THR:HG23	0.43	1.90	6	1
1:A:157:PHE:CD1	1:A:164:VAL:HG12	0.43	2.48	9	1
1:A:10:LEU:HD11	1:A:143:VAL:HG22	0.43	1.90	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:251:LEU:HD23	1:A:255:ILE:HD12	0.43	1.90	3	1
1:A:35:SER:H	1:A:39:LEU:HD11	0.43	1.72	11	1
1:A:10:LEU:HD21	1:A:152:GLY:N	0.43	2.28	13	1
1:A:172:GLY:HA3	1:A:180:LEU:O	0.43	2.12	1	1
1:A:66:GLU:CD	1:A:66:GLU:H	0.43	2.16	1	1
1:A:10:LEU:HB3	1:A:170:ALA:CB	0.43	2.44	8	1
1:A:219:PHE:H	1:A:239:ASN:ND2	0.43	2.11	17	1
1:A:128:ASP:CB	1:A:139:ARG:HB2	0.43	2.41	20	1
1:A:111:ASN:ND2	1:A:132:ASP:HA	0.43	2.28	8	1
1:A:133:ILE:H	1:A:133:ILE:CD1	0.43	2.24	12	1
1:A:26:LEU:HD21	1:A:46:SER:HB3	0.43	1.89	14	1
1:A:26:LEU:HG	1:A:47:ALA:O	0.43	2.13	15	1
1:A:211:THR:CB	1:A:214:ASN:HB3	0.43	2.37	20	1
1:A:65:THR:HG22	1:A:66:GLU:H	0.43	1.73	20	1
1:A:113:LYS:CB	1:A:130:ASP:HA	0.43	2.44	15	1
1:A:194:ILE:HG22	1:A:196:GLN:HG2	0.43	1.90	4	1
1:A:46:SER:O	1:A:54:VAL:HA	0.43	2.14	7	1
1:A:80:THR:HA	1:A:103:PHE:O	0.43	2.13	8	1
1:A:153:TYR:CD1	1:A:169:PHE:HD1	0.43	2.32	17	1
1:A:175:THR:HB	1:A:178:PHE:O	0.43	2.12	13	1
1:A:28:LYS:HD3	1:A:29:LEU:N	0.43	2.29	1	1
1:A:39:LEU:C	1:A:39:LEU:HD13	0.43	2.33	1	1
1:A:123:ILE:HB	1:A:143:VAL:O	0.43	2.13	12	2
1:A:185:ASN:HB2	1:A:189:GLU:HB3	0.43	1.90	20	3
1:A:114:ILE:HD13	1:A:115:LYS:N	0.43	2.28	4	1
1:A:86:THR:HG22	1:A:96:LYS:HE3	0.43	1.90	16	1
1:A:198:VAL:HG12	1:A:199:ASN:N	0.43	2.29	18	2
1:A:31:LEU:HD13	1:A:281:PHE:HD2	0.43	1.73	19	1
1:A:198:VAL:HG12	1:A:199:ASN:H	0.43	1.74	13	1
1:A:227:ILE:O	1:A:228:ASP:HB2	0.43	2.14	6	1
1:A:78:ASP:HB3	1:A:107:THR:HG23	0.43	1.91	6	1
1:A:222:ALA:HB2	1:A:236:LYS:HG3	0.43	1.89	15	1
1:A:156:ASN:HB3	1:A:166:GLN:HB3	0.43	1.89	17	1
1:A:248:THR:HG22	1:A:258:THR:HG22	0.43	1.90	19	1
1:A:99:PHE:CD2	1:A:114:ILE:HB	0.43	2.39	13	1
1:A:66:GLU:H	1:A:66:GLU:CD	0.43	2.16	4	1
1:A:259:LEU:HD22	1:A:277:LEU:HD12	0.43	1.89	8	1
1:A:38:GLY:HA2	1:A:63:ARG:C	0.42	2.35	6	1
1:A:201:LYS:HG2	1:A:226:GLN:O	0.42	2.14	10	1
1:A:197:LYS:HG2	1:A:203:GLU:HG3	0.42	1.90	17	2
1:A:180:LEU:HA	1:A:193:SER:O	0.42	2.14	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:264:ASP:HB3	1:A:267:ASN:HB3	0.42	1.92	17	1
1:A:12:LYS:O	1:A:15:ARG:HG2	0.42	2.14	10	1
1:A:102:SER:O	1:A:110:LYS:HA	0.42	2.14	15	1
1:A:17:VAL:HA	1:A:236:LYS:HE2	0.42	1.91	17	1
1:A:146:TYR:HB3	1:A:149:TRP:HB2	0.42	1.90	19	1
1:A:84:GLU:CA	1:A:100:ASP:CB	0.42	2.85	13	1
1:A:181:HIS:O	1:A:193:SER:N	0.42	2.52	13	1
1:A:194:ILE:HB	1:A:206:VAL:CB	0.42	2.29	4	1
1:A:112:ALA:O	1:A:131:PHE:HB3	0.42	2.14	8	1
1:A:251:LEU:HD21	1:A:257:LEU:HB2	0.42	1.90	11	1
1:A:62:TYR:HB3	1:A:71:PHE:HB2	0.42	1.89	14	1
1:A:83:THR:O	1:A:84:GLU:HG2	0.42	2.14	14	1
1:A:120:ARG:HB3	1:A:123:ILE:HG22	0.42	1.91	5	1
1:A:208:LEU:HD13	1:A:219:PHE:CB	0.42	2.43	11	1
1:A:224:LYS:HG2	1:A:232:CYS:SG	0.42	2.55	12	1
1:A:38:GLY:HA3	1:A:63:ARG:HB2	0.42	1.91	13	1
1:A:243:ILE:N	1:A:243:ILE:HD13	0.42	2.30	15	2
1:A:253:PRO:HG2	1:A:255:ILE:HG12	0.42	1.91	12	1
1:A:267:ASN:HB3	1:A:272:GLY:HA3	0.42	1.92	15	1
1:A:31:LEU:CD2	1:A:281:PHE:HB2	0.42	2.42	16	1
1:A:2:ALA:CA	1:A:94:GLY:HA2	0.42	2.44	13	1
1:A:240:SER:HB2	1:A:242:LEU:HG	0.42	1.92	1	1
1:A:240:SER:HB2	1:A:242:LEU:HD11	0.42	1.91	2	1
1:A:244:GLY:HA2	1:A:261:ALA:O	0.42	2.15	6	2
1:A:18:PHE:CE2	1:A:209:ALA:HB2	0.42	2.48	12	1
1:A:94:GLY:O	1:A:119:LYS:HG2	0.42	2.15	14	1
1:A:120:ARG:CB	1:A:123:ILE:HB	0.42	2.39	18	1
1:A:27:ILE:CG2	1:A:277:LEU:HD12	0.42	2.39	20	1
1:A:153:TYR:HD1	1:A:169:PHE:HD2	0.42	1.56	4	1
1:A:93:ARG:HD2	1:A:93:ARG:H	0.42	1.75	4	1
1:A:64:TRP:O	1:A:68:GLY:HA2	0.42	2.15	7	1
1:A:10:LEU:HD21	1:A:143:VAL:HG13	0.42	1.92	10	2
1:A:3:VAL:HG21	1:A:120:ARG:O	0.42	2.15	19	1
1:A:71:PHE:CD1	1:A:85:ILE:HG13	0.42	2.50	1	1
1:A:283:ALA:O	1:A:284:LEU:HD22	0.42	2.15	2	2
1:A:85:ILE:CG2	1:A:99:PHE:HB3	0.42	2.45	15	1
1:A:85:ILE:HG22	1:A:99:PHE:HB3	0.42	1.91	15	1
1:A:18:PHE:CE2	1:A:220:GLY:HA3	0.42	2.49	16	1
1:A:110:LYS:HD3	1:A:110:LYS:O	0.42	2.15	17	1
1:A:3:VAL:HG11	1:A:120:ARG:O	0.42	2.14	18	1
1:A:124:ASN:HD22	1:A:124:ASN:H	0.42	1.58	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:124:ASN:ND2	1:A:124:ASN:N	0.42	2.68	19	1
1:A:74:LYS:HG2	1:A:82:GLY:O	0.42	2.15	20	1
1:A:89:ASP:O	1:A:93:ARG:HD2	0.41	2.15	3	1
1:A:40:GLU:OE1	1:A:61:LYS:HG2	0.41	2.14	11	1
1:A:33:THR:HG22	1:A:41:PHE:HB2	0.41	1.92	14	1
1:A:191:GLY:HA2	1:A:208:LEU:O	0.41	2.15	16	1
1:A:48:ASN:HB3	1:A:51:THR:HB	0.41	1.90	16	1
1:A:60:THR:HB	1:A:73:GLU:HB3	0.41	1.92	16	1
1:A:156:ASN:O	1:A:164:VAL:HG23	0.41	2.14	19	1
1:A:142:LEU:HD23	1:A:143:VAL:H	0.41	1.75	10	1
1:A:95:LEU:HD22	1:A:118:TYR:HD1	0.41	1.75	17	1
1:A:41:PHE:CZ	1:A:58:LEU:HD21	0.41	2.50	19	1
1:A:231:ALA:HB2	1:A:249:GLN:HG2	0.41	1.93	12	1
1:A:21:GLY:HA2	1:A:236:LYS:HE3	0.41	1.93	14	1
1:A:113:LYS:HA	1:A:129:MET:O	0.41	2.15	3	1
1:A:177:GLU:HB2	1:A:197:LYS:O	0.41	2.15	3	1
1:A:37:ASN:HB2	1:A:65:THR:HB	0.41	1.90	7	1
1:A:199:ASN:ND2	1:A:200:LYS:HG3	0.41	2.26	12	1
1:A:9:ASP:HB3	1:A:181:HIS:HE1	0.41	1.76	19	2
1:A:251:LEU:O	1:A:255:ILE:HB	0.41	2.15	15	1
1:A:142:LEU:HD23	1:A:153:TYR:OH	0.41	2.16	1	1
1:A:10:LEU:HD11	1:A:152:GLY:HA3	0.41	1.92	4	1
1:A:222:ALA:CB	1:A:236:LYS:HG2	0.41	2.44	7	1
1:A:132:ASP:OD2	1:A:133:ILE:HG13	0.41	2.16	11	1
1:A:93:ARG:CD	1:A:93:ARG:H	0.41	2.25	1	1
1:A:202:LEU:HD23	1:A:225:TYR:CD2	0.41	2.51	4	1
1:A:10:LEU:CD1	1:A:152:GLY:HA3	0.41	2.45	5	1
1:A:279:LEU:N	1:A:279:LEU:CD2	0.41	2.84	10	1
1:A:180:LEU:H	1:A:180:LEU:HD22	0.41	1.76	15	1
1:A:225:TYR:CE2	1:A:233:PHE:HB2	0.41	2.50	19	1
1:A:146:TYR:CE1	1:A:149:TRP:HB2	0.41	2.50	1	1
1:A:113:LYS:HB3	1:A:113:LYS:NZ	0.41	2.30	9	2
1:A:153:TYR:HD2	1:A:169:PHE:CD1	0.41	2.33	9	1
1:A:202:LEU:HB3	1:A:224:LYS:O	0.41	2.15	9	1
1:A:39:LEU:C	1:A:39:LEU:HD12	0.41	2.36	11	1
1:A:68:GLY:O	1:A:88:GLU:HG3	0.41	2.15	16	1
1:A:158:GLU:OE2	1:A:161:LYS:HD3	0.41	2.16	2	1
1:A:89:ASP:CG	1:A:94:GLY:H	0.41	2.19	5	1
1:A:17:VAL:HB	1:A:207:ASN:ND2	0.41	2.30	12	1
1:A:22:TYR:HE2	1:A:278:GLY:HA3	0.41	1.76	15	1
1:A:94:GLY:O	1:A:118:TYR:HA	0.41	2.15	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:184:VAL:HG22	1:A:190:PHE:CB	0.41	2.46	1	1
1:A:153:TYR:CD2	1:A:169:PHE:HD2	0.41	2.33	3	1
1:A:263:LEU:HA	1:A:268:VAL:HG21	0.41	1.91	3	1
1:A:27:ILE:HG23	1:A:277:LEU:CD2	0.41	2.46	8	1
1:A:142:LEU:CD2	1:A:143:VAL:N	0.41	2.84	10	1
1:A:167:SER:HB2	1:A:169:PHE:CZ	0.41	2.51	16	1
1:A:221:ILE:HD13	1:A:221:ILE:N	0.41	2.31	17	1
1:A:33:THR:CG2	1:A:41:PHE:HB3	0.41	2.45	19	1
1:A:15:ARG:HD2	1:A:15:ARG:O	0.41	2.16	4	1
1:A:231:ALA:CB	1:A:249:GLN:HG2	0.41	2.46	12	1
1:A:100:ASP:OD1	1:A:113:LYS:HD2	0.41	2.16	17	1
1:A:28:LYS:NZ	1:A:28:LYS:HB2	0.41	2.31	17	1
1:A:85:ILE:H	1:A:100:ASP:HB2	0.41	1.76	13	1
1:A:240:SER:HB3	1:A:242:LEU:HD13	0.40	1.92	3	1
1:A:69:LEU:CD1	1:A:87:VAL:HB	0.40	2.46	19	1
1:A:114:ILE:HB	1:A:131:PHE:HE2	0.40	1.75	5	1
1:A:181:HIS:HB3	1:A:193:SER:HB2	0.40	1.91	6	1
1:A:30:ASP:O	1:A:281:PHE:N	0.40	2.53	9	1
1:A:114:ILE:CG2	1:A:129:MET:HB2	0.40	2.46	12	1
1:A:186:ASP:CG	1:A:187:GLY:H	0.40	2.19	12	1
1:A:144:LEU:HB3	1:A:146:TYR:CE1	0.40	2.51	14	1
1:A:242:LEU:HD22	1:A:264:ASP:HA	0.40	1.93	20	1
1:A:19:THR:HG22	1:A:20:LYS:H	0.40	1.76	6	1
1:A:219:PHE:CE1	1:A:221:ILE:HD11	0.40	2.51	6	1
1:A:22:TYR:HB3	1:A:276:GLY:CA	0.40	2.40	7	1
1:A:72:THR:HB	1:A:84:GLU:O	0.40	2.16	12	1
1:A:57:SER:HB2	1:A:75:TRP:O	0.40	2.16	15	1
1:A:88:GLU:HG2	1:A:96:LYS:HG2	0.40	1.93	17	1
1:A:146:TYR:CB	1:A:149:TRP:HB2	0.40	2.43	20	1
1:A:251:LEU:HB2	1:A:255:ILE:HD11	0.40	1.94	11	1
1:A:87:VAL:CG1	1:A:97:LEU:HB2	0.40	2.46	11	1
1:A:88:GLU:HG2	1:A:96:LYS:HB2	0.40	1.93	15	1
1:A:211:THR:HB	1:A:216:ASN:OD1	0.40	2.17	16	1
1:A:48:ASN:CB	1:A:53:LYS:HB3	0.40	2.44	19	1
1:A:102:SER:HB2	1:A:111:ASN:HB2	0.40	1.93	4	1
1:A:6:THR:CB	1:A:143:VAL:HG11	0.40	2.47	4	1
1:A:228:ASP:N	1:A:229:PRO:HD2	0.40	2.32	6	1
1:A:23:GLY:O	1:A:274:LYS:HB3	0.40	2.15	14	1
1:A:281:PHE:HE1	1:A:283:ALA:HB2	0.40	1.77	15	1
1:A:31:LEU:HD13	1:A:281:PHE:CD1	0.40	2.50	17	1
1:A:66:GLU:O	1:A:67:TYR:HB2	0.40	2.16	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:78:ASP:O	1:A:79:ASN:HB3	0.40	2.15	19	1
1:A:17:VAL:CG1	1:A:207:ASN:HB2	0.40	2.47	20	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	283/291 (97%)	257±4 (91±1%)	20±3 (7±1%)	6±3 (2±1%)	10	50
All	All	5660/5820 (97%)	5146 (91%)	396 (7%)	118 (2%)	10	50

All 35 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	147	GLU	12
1	A	11	GLY	11
1	A	229	PRO	8
1	A	65	THR	8
1	A	68	GLY	8
1	A	228	ASP	7
1	A	176	ASP	6
1	A	253	PRO	6
1	A	272	GLY	6
1	A	254	GLY	6
1	A	252	LYS	4
1	A	36	GLU	3
1	A	84	GLU	3
1	A	49	THR	3
1	A	281	PHE	3
1	A	74	LYS	2
1	A	79	ASN	2
1	A	90	GLN	2
1	A	201	LYS	2
1	A	89	ASP	1

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Mol	Chain	Res	Type	Models (Total)
1	A	3	VAL	1
1	A	66	GLU	1
1	A	91	LEU	1
1	A	267	ASN	1
1	A	37	ASN	1
1	A	202	LEU	1
1	A	20	LYS	1
1	A	198	VAL	1
1	A	67	TYR	1
1	A	132	ASP	1
1	A	5	PRO	1
1	A	52	THR	1
1	A	251	LEU	1
1	A	214	ASN	1
1	A	105	PRO	1

### 6.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the sidechain conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	231/238 (97%)	215±4 (93±2%)	16±4 (7±2%)	18 67
All	All	4620/4760 (97%)	4291 (93%)	329 (7%)	18 67

All 116 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	259	LEU	19
1	A	85	ILE	14
1	A	263	LEU	11
1	A	245	LEU	11
1	A	243	ILE	10
1	A	95	LEU	10
1	A	221	ILE	9
1	A	133	ILE	9
1	A	196	GLN	9
1	A	124	ASN	8

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Mol	Chain	Res	Type	Models (Total)
1	A	31	LEU	8
1	A	255	ILE	7
1	A	114	ILE	6
1	A	180	LEU	6
1	A	110	LYS	6
1	A	93	ARG	6
1	A	119	LYS	5
1	A	252	LYS	5
1	A	144	LEU	4
1	A	113	LYS	4
1	A	268	VAL	4
1	A	81	LEU	4
1	A	281	PHE	4
1	A	20	LYS	4
1	A	164	VAL	4
1	A	28	LYS	3
1	A	156	ASN	3
1	A	262	LEU	3
1	A	96	LYS	3
1	A	125	LEU	3
1	A	88	GLU	3
1	A	128	ASP	3
1	A	236	LYS	3
1	A	123	ILE	3
1	A	34	LYS	3
1	A	32	LYS	3
1	A	98	THR	3
1	A	280	GLU	2
1	A	177	GLU	2
1	A	74	LYS	2
1	A	89	ASP	2
1	A	12	LYS	2
1	A	163	ARG	2
1	A	147	GLU	2
1	A	247	TYR	2
1	A	69	LEU	2
1	A	159	THR	2
1	A	150	LEU	2
1	A	197	LYS	2
1	A	195	TYR	2
1	A	15	ARG	2
1	A	202	LEU	2

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Mol	Chain	Res	Type	Models (Total)
1	A	226	GLN	2
1	A	121	GLU	2
1	A	65	THR	2
1	A	48	ASN	2
1	A	174	LYS	2
1	A	218	ARG	2
1	A	154	GLN	2
1	A	109	LYS	2
1	A	79	ASN	2
1	A	161	LYS	2
1	A	238	ASN	2
1	A	201	LYS	2
1	A	130	ASP	1
1	A	75	TRP	1
1	A	37	ASN	1
1	A	29	LEU	1
1	A	185	ASN	1
1	A	122	HIS	1
1	A	6	THR	1
1	A	277	LEU	1
1	A	211	THR	1
1	A	203	GLU	1
1	A	266	LYS	1
1	A	279	LEU	1
1	A	256	LYS	1
1	A	186	ASP	1
1	A	51	THR	1
1	A	198	VAL	1
1	A	91	LEU	1
1	A	10	LEU	1
1	A	237	VAL	1
1	A	249	GLN	1
1	A	139	ARG	1
1	A	64	TRP	1
1	A	158	GLU	1
1	A	78	ASP	1
1	A	227	ILE	1
1	A	49	THR	1
1	A	142	LEU	1
1	A	282	GLN	1
1	A	273	HIS	1
1	A	153	TYR	1

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Mol	Chain	Res	Type	Models (Total)
1	A	232	CYS	1
1	A	179	GLN	1
1	A	200	LYS	1
1	A	80	THR	1
1	A	239	ASN	1
1	A	90	GLN	1
1	A	73	GLU	1
1	A	165	THR	1
1	A	36	GLU	1
1	A	16	ASP	1
1	A	19	THR	1
1	A	274	LYS	1
1	A	251	LEU	1
1	A	228	ASP	1
1	A	199	ASN	1
1	A	275	LEU	1
1	A	118	TYR	1
1	A	115	LYS	1
1	A	267	ASN	1
1	A	26	LEU	1
1	A	155	MET	1
1	A	176	ASP	1

### 6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

### 6.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.5 Carbohydrates [i](#)

There are no 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 [i](#)

The completeness of assignment taking into account all chemical shift lists is 40% for the well-defined parts and 40% for the entire structure.

### 7.1 Chemical shift list 1

File name: input\_cs.cif

Chemical shift list name: *VDAC\_WT\_NMRStar.str*

#### 7.1.1 Bookkeeping [i](#)

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	1507
Number of shifts mapped to atoms	1507
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 [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	254	$0.14 \pm 0.09$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}_\beta$	210	$-0.16 \pm 0.07$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}'$	180	$0.86 \pm 0.09$	Should be applied
$^{15}\text{N}$	250	$-0.94 \pm 0.26$	Should be applied

#### 7.1.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 40%, i.e. 1339 atoms were assigned a chemical shift out of a possible 3346. 0 out of 41 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	931/1408 (66%)	249/562 (44%)	433/568 (76%)	249/278 (90%)
Sidechain	400/1652 (24%)	85/960 (9%)	313/619 (51%)	2/73 (3%)

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	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Aromatic	8/286 (3%)	4/150 (3%)	0/126 (0%)	4/10 (40%)
Overall	1339/3346 (40%)	338/1672 (20%)	746/1313 (57%)	255/361 (71%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 40%, i.e. 1339 atoms were assigned a chemical shift out of a possible 3359. 0 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	931/1413 (66%)	249/564 (44%)	433/570 (76%)	249/279 (89%)
Sidechain	400/1660 (24%)	85/965 (9%)	313/622 (50%)	2/73 (3%)
Aromatic	8/286 (3%)	4/150 (3%)	0/126 (0%)	4/10 (40%)
Overall	1339/3359 (40%)	338/1679 (20%)	746/1318 (57%)	255/362 (70%)

### 7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

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

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:

