



Full wwPDB NMR Structure Validation Report ⓘ

May 29, 2020 – 12:17 pm BST

PDB ID : 6TIR
Title : NOE based model of hVDAC-1 bound to beta-NADH in detergent micelles
Authors : Boehm, R.; Hiller, S.; Wagner, G.
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

Cyrange : Kirchner and Güntert (2011)
NmrClust : Kelley et al. (1996)
MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
buster-report : 1.1.7 (2018)
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

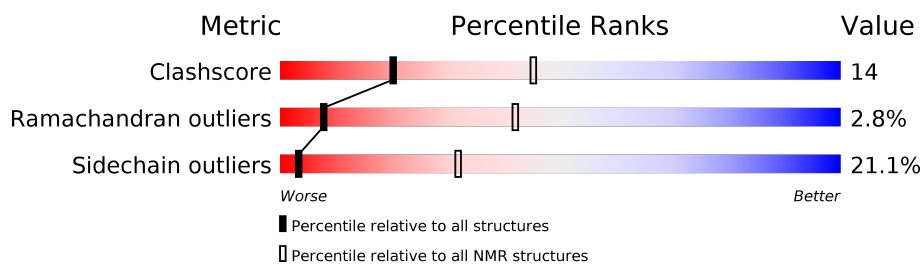
1 Overall quality at a glance

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 ≥ 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 10 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:2-A:285 (284)	1.13	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 2 clusters. No single-model clusters were found.

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

3 Entry composition i

There are 2 unique types of molecules in this entry. The entry contains 4420 atoms, of which 2189 are hydrogens and 0 are deuteriums.

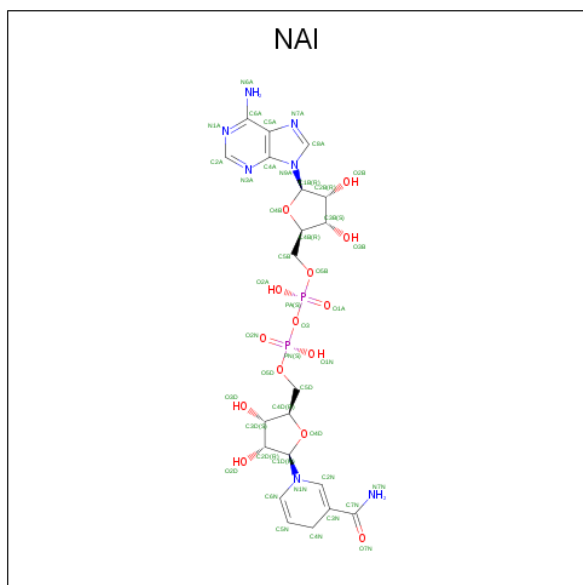
- Molecule 1 is a protein called Voltage-dependent anion-selective channel protein 1.

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

- Molecule 2 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (three-letter code: NAI) (formula: C₂₁H₂₉N₇O₁₄P₂) (labeled as "Ligand of Interest" by author).



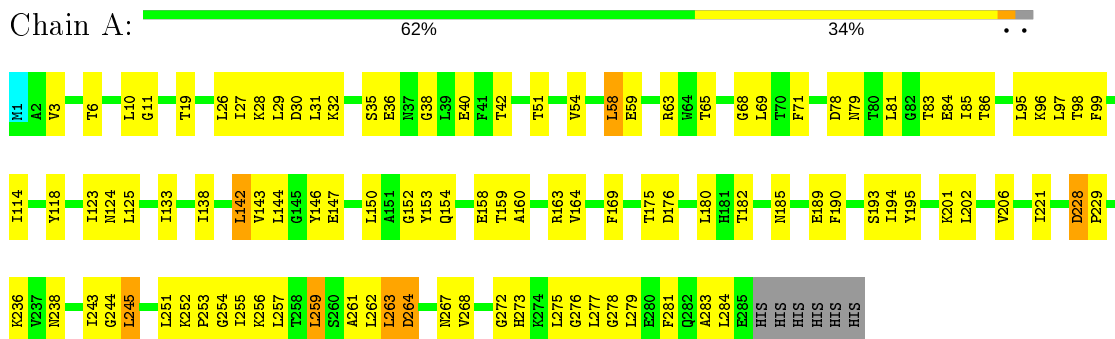
Mol	Chain	Residues	Atoms					
			Total	C	H	N	O	P
2	A	1	73	21	29	7	14	2

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

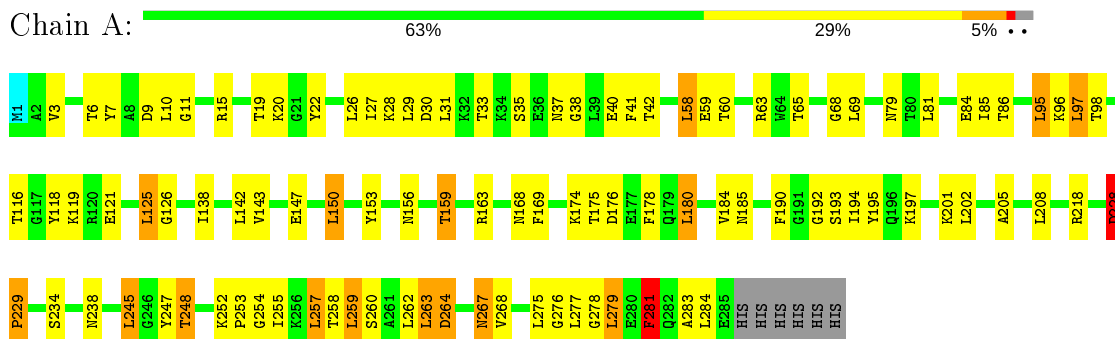


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

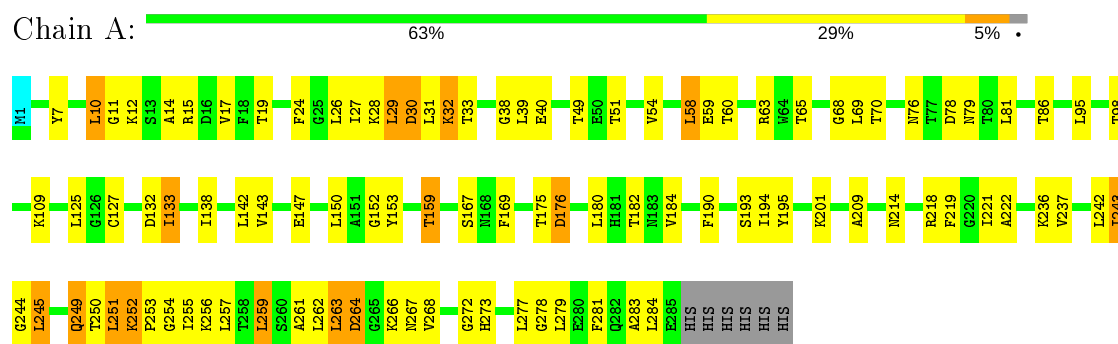
4.2.1 Score per residue for model 1 (medoid)

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



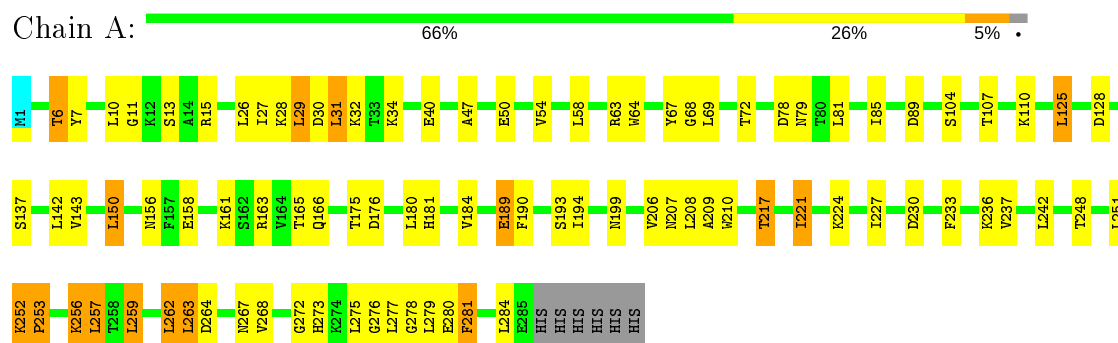
4.2.5 Score per residue for model 5

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



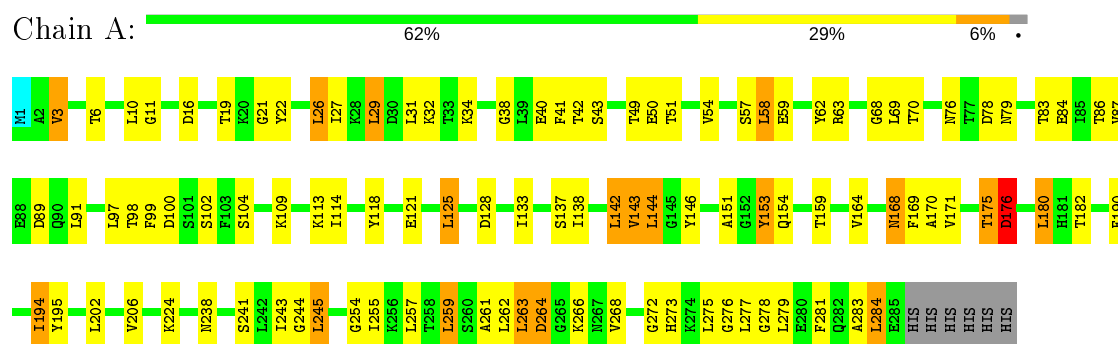
4.2.6 Score per residue for model 6

- 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



5 Refinement protocol and experimental data overview

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

Of the 500 calculated structures, 10 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
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

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

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts i

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	2179	2151	2151	60±7
2	A	44	29	27	0±1
All	All	22230	21800	21780	605

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 14.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:27:ILE:HG23	1:A:277:LEU:HD12	0.92	1.40	10	5
1:A:29:LEU:HD13	1:A:29:LEU:O	0.91	1.66	6	1
1:A:6:THR:HG22	1:A:150:LEU:HD21	0.90	1.41	6	2
1:A:259:LEU:HD22	1:A:277:LEU:HD23	0.89	1.40	5	7
1:A:125:LEU:HD22	1:A:125:LEU:C	0.82	1.94	1	1
1:A:123:ILE:HD13	1:A:144:LEU:HD13	0.77	1.54	2	1
1:A:29:LEU:HD22	1:A:29:LEU:C	0.76	2.00	6	1
1:A:125:LEU:HD13	1:A:125:LEU:O	0.76	1.78	1	1
1:A:47:ALA:HB2	1:A:54:VAL:HG13	0.76	1.54	10	2
1:A:33:THR:HG23	1:A:284:LEU:HD13	0.75	1.59	5	1
1:A:158:GLU:O	1:A:161:LYS:O	0.74	2.05	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:227:ILE:HG23	1:A:229:PRO:HD2	0.73	1.59	3	1
1:A:206:VAL:HG12	1:A:221:ILE:HG22	0.72	1.60	10	4
1:A:123:ILE:HD11	1:A:142:LEU:HD21	0.71	1.62	2	1
1:A:262:LEU:C	1:A:263:LEU:HD13	0.70	2.06	9	10
1:A:86:THR:HG23	1:A:98:THR:HG22	0.70	1.62	7	1
1:A:27:ILE:HG23	1:A:277:LEU:CD1	0.70	2.17	4	2
1:A:180:LEU:HD12	1:A:180:LEU:C	0.70	2.07	10	1
1:A:206:VAL:HG22	1:A:221:ILE:HG22	0.69	1.64	6	1
1:A:143:VAL:C	1:A:144:LEU:HD23	0.69	2.07	3	2
1:A:123:ILE:HD11	1:A:142:LEU:CD2	0.68	2.19	2	1
1:A:26:LEU:N	1:A:26:LEU:HD13	0.68	2.03	4	1
1:A:263:LEU:HB3	1:A:268:VAL:HG21	0.68	1.65	1	2
1:A:248:THR:HG23	1:A:258:THR:HG23	0.68	1.65	1	1
1:A:195:TYR:CB	1:A:205:ALA:HA	0.68	2.18	8	1
1:A:29:LEU:HD22	1:A:30:ASP:N	0.67	2.03	6	1
1:A:153:TYR:HB3	1:A:168:ASN:O	0.67	1.90	7	1
1:A:245:LEU:HD21	1:A:261:ALA:HB3	0.67	1.65	8	1
1:A:10:LEU:HD21	1:A:152:GLY:HA3	0.67	1.66	2	4
1:A:275:LEU:HD13	1:A:276:GLY:N	0.66	2.06	3	7
1:A:125:LEU:CB	1:A:142:LEU:HD13	0.65	2.21	1	2
1:A:153:TYR:CD1	1:A:170:ALA:HB3	0.65	2.26	7	1
1:A:175:THR:O	1:A:176:ASP:C	0.65	2.34	3	3
1:A:142:LEU:HD12	1:A:143:VAL:N	0.65	2.07	1	5
1:A:123:ILE:HD11	1:A:144:LEU:HD23	0.65	1.69	9	1
1:A:29:LEU:HB2	1:A:279:LEU:HD23	0.65	1.68	5	2
1:A:99:PHE:CD1	1:A:114:ILE:HD13	0.65	2.27	4	1
1:A:180:LEU:HD12	1:A:194:ILE:CG2	0.64	2.23	7	1
1:A:27:ILE:HD12	1:A:277:LEU:HD12	0.64	1.69	4	2
1:A:263:LEU:HB3	1:A:268:VAL:HG11	0.64	1.68	2	4
1:A:7:TYR:CB	1:A:143:VAL:HG21	0.64	2.22	3	2
1:A:123:ILE:HD13	1:A:144:LEU:CD1	0.64	2.22	2	1
1:A:31:LEU:HD11	1:A:283:ALA:HB3	0.64	1.70	2	2
1:A:152:GLY:O	1:A:169:PHE:HB3	0.63	1.92	9	1
1:A:201:LYS:O	1:A:202:LEU:HD22	0.63	1.94	1	1
1:A:34:LYS:HG2	1:A:284:LEU:HD21	0.63	1.71	6	1
1:A:96:LYS:O	1:A:97:LEU:HD13	0.62	1.94	9	5
1:A:68:GLY:O	1:A:69:LEU:HD22	0.62	1.94	10	5
1:A:29:LEU:HD12	1:A:279:LEU:HG	0.62	1.71	5	1
1:A:142:LEU:HD13	1:A:153:TYR:OH	0.62	1.93	8	1
1:A:125:LEU:HB3	1:A:142:LEU:HD13	0.62	1.70	1	2
1:A:259:LEU:HD22	1:A:277:LEU:CD2	0.62	2.21	5	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:142:LEU:HD22	1:A:143:VAL:N	0.62	2.09	9	1
1:A:245:LEU:CD2	1:A:261:ALA:HB3	0.62	2.24	5	2
1:A:3:VAL:HG11	1:A:119:LYS:O	0.62	1.95	2	1
1:A:278:GLY:C	1:A:279:LEU:HD13	0.62	2.15	2	2
1:A:31:LEU:HD11	1:A:283:ALA:CB	0.62	2.24	1	3
1:A:259:LEU:CD2	1:A:277:LEU:HD23	0.62	2.25	6	5
1:A:283:ALA:O	1:A:284:LEU:HD12	0.62	1.95	8	2
1:A:15:ARG:O	1:A:19:THR:HG22	0.62	1.95	5	1
1:A:123:ILE:CD1	1:A:144:LEU:HD23	0.62	2.25	9	1
1:A:99:PHE:CD2	1:A:114:ILE:HD13	0.61	2.31	2	1
1:A:138:ILE:HD12	1:A:159:THR:OG1	0.61	1.95	1	4
1:A:158:GLU:OE1	1:A:160:ALA:HB3	0.61	1.94	3	1
1:A:142:LEU:HD22	1:A:144:LEU:HD21	0.61	1.72	3	1
1:A:268:VAL:HG12	1:A:272:GLY:O	0.61	1.95	7	4
1:A:150:LEU:N	1:A:173:TYR:HB2	0.61	2.11	3	1
1:A:263:LEU:N	1:A:263:LEU:HD22	0.61	2.11	9	2
1:A:27:ILE:CG2	1:A:277:LEU:HD12	0.60	2.27	7	2
1:A:184:VAL:HG13	1:A:190:PHE:HB3	0.60	1.72	6	1
1:A:209:ALA:HB3	1:A:218:ARG:CD	0.60	2.26	8	1
1:A:264:ASP:O	1:A:268:VAL:HG22	0.60	1.96	7	8
1:A:219:PHE:CE1	1:A:221:ILE:HD11	0.60	2.31	5	1
1:A:245:LEU:N	1:A:245:LEU:HD13	0.60	2.11	8	4
1:A:257:LEU:CD1	1:A:277:LEU:HD21	0.60	2.26	5	2
1:A:158:GLU:OE2	1:A:160:ALA:HB3	0.60	1.96	10	2
1:A:33:THR:HG23	1:A:284:LEU:CD1	0.60	2.26	5	1
1:A:195:TYR:CD2	1:A:206:VAL:HG13	0.60	2.32	8	1
1:A:180:LEU:HD12	1:A:181:HIS:N	0.60	2.11	10	1
1:A:86:THR:OG1	1:A:98:THR:HG23	0.59	1.96	4	1
1:A:245:LEU:HD13	1:A:245:LEU:N	0.59	2.12	2	2
1:A:249:GLN:CB	1:A:257:LEU:HD23	0.59	2.26	5	1
1:A:277:LEU:HD13	1:A:278:GLY:N	0.59	2.12	7	6
1:A:251:LEU:O	1:A:251:LEU:HD12	0.59	1.98	5	1
1:A:262:LEU:HD21	2:A:301:NAI:H6N	0.59	1.75	6	1
1:A:262:LEU:HD21	2:A:301:NAI:C6N	0.59	2.28	6	1
1:A:95:LEU:HD22	1:A:118:TYR:HB3	0.58	1.75	8	2
1:A:262:LEU:O	1:A:263:LEU:HD13	0.58	1.98	1	9
1:A:31:LEU:HA	1:A:281:PHE:HA	0.58	1.75	5	2
1:A:123:ILE:CD1	1:A:144:LEU:HD22	0.58	2.29	3	1
1:A:257:LEU:HA	1:A:279:LEU:HD12	0.58	1.76	2	3
1:A:71:PHE:CD1	1:A:85:ILE:HG22	0.58	2.34	4	1
1:A:33:THR:HG23	1:A:283:ALA:HB3	0.58	1.74	9	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:279:LEU:HD22	1:A:279:LEU:N	0.58	2.14	4	2
1:A:29:LEU:HD13	1:A:30:ASP:N	0.58	2.14	3	4
1:A:86:THR:HG23	1:A:98:THR:OG1	0.58	1.98	3	3
1:A:251:LEU:HD12	1:A:255:ILE:HG21	0.58	1.75	9	1
1:A:3:VAL:HG22	1:A:121:GLU:CA	0.57	2.29	1	1
1:A:125:LEU:HD22	1:A:126:GLY:N	0.57	2.13	1	1
1:A:138:ILE:HD13	1:A:159:THR:HB	0.57	1.74	7	1
1:A:263:LEU:HD12	1:A:273:HIS:CG	0.57	2.33	9	1
1:A:86:THR:CG2	1:A:98:THR:HG22	0.57	2.28	7	1
1:A:29:LEU:CD2	1:A:29:LEU:C	0.57	2.72	6	1
1:A:31:LEU:HD12	1:A:32:LYS:N	0.57	2.14	7	1
1:A:97:LEU:CD1	1:A:116:THR:HG23	0.57	2.29	9	2
1:A:29:LEU:CB	1:A:279:LEU:HD23	0.56	2.30	6	1
1:A:84:GLU:HB3	1:A:99:PHE:O	0.56	2.00	4	2
1:A:58:LEU:HD13	1:A:59:GLU:N	0.56	2.16	7	7
1:A:3:VAL:HG22	1:A:121:GLU:HA	0.56	1.75	10	2
1:A:144:LEU:N	1:A:144:LEU:HD23	0.56	2.14	3	2
1:A:202:LEU:HD12	1:A:224:LYS:O	0.56	2.00	7	1
1:A:47:ALA:CB	1:A:54:VAL:HG13	0.56	2.30	10	2
1:A:283:ALA:O	1:A:284:LEU:HD22	0.56	2.01	1	1
1:A:61:LYS:CB	1:A:72:THR:HA	0.56	2.30	10	1
1:A:142:LEU:HD22	1:A:144:LEU:CD2	0.56	2.30	3	1
1:A:61:LYS:HB3	1:A:71:PHE:O	0.55	2.00	10	1
1:A:244:GLY:C	1:A:245:LEU:HD12	0.55	2.21	3	1
1:A:279:LEU:N	1:A:279:LEU:HD22	0.55	2.15	2	1
1:A:180:LEU:HD12	1:A:194:ILE:HG23	0.55	1.77	7	1
1:A:142:LEU:HD13	1:A:142:LEU:C	0.55	2.22	9	1
1:A:257:LEU:HD11	1:A:277:LEU:HD21	0.55	1.78	5	1
1:A:69:LEU:HD11	1:A:87:VAL:HG13	0.55	1.78	10	1
1:A:228:ASP:HB2	1:A:231:ALA:HB3	0.55	1.78	4	2
1:A:201:LYS:C	1:A:202:LEU:HD12	0.55	2.22	3	1
1:A:125:LEU:HD22	1:A:142:LEU:HD23	0.55	1.79	9	1
1:A:178:PHE:CZ	1:A:194:ILE:HG23	0.55	2.37	1	1
1:A:7:TYR:HB2	1:A:143:VAL:HG21	0.55	1.78	5	2
1:A:245:LEU:HD22	1:A:261:ALA:HB3	0.54	1.79	5	1
1:A:198:VAL:HG21	1:A:202:LEU:HD12	0.54	1.77	8	1
1:A:71:PHE:CD2	1:A:85:ILE:HG22	0.54	2.37	2	1
1:A:32:LYS:N	1:A:281:PHE:HB2	0.54	2.18	6	2
1:A:3:VAL:HG11	1:A:119:LYS:HG2	0.54	1.79	1	1
1:A:7:TYR:HB3	1:A:143:VAL:HG21	0.54	1.77	1	2
1:A:237:VAL:HG12	1:A:242:LEU:O	0.54	2.02	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:189:GLU:HG3	1:A:209:ALA:HB1	0.54	1.80	6	1
1:A:73:GLU:O	1:A:74:LYS:HB2	0.54	2.03	4	1
1:A:257:LEU:HD12	1:A:258:THR:N	0.53	2.18	1	1
1:A:31:LEU:HD22	1:A:281:PHE:HB3	0.53	1.78	3	1
1:A:10:LEU:HD21	1:A:143:VAL:HG13	0.53	1.80	6	1
1:A:3:VAL:HG22	1:A:121:GLU:N	0.53	2.18	8	1
1:A:169:PHE:HB3	1:A:184:VAL:HG22	0.53	1.80	5	2
1:A:17:VAL:HG21	1:A:222:ALA:HB2	0.53	1.79	4	1
1:A:31:LEU:HD11	1:A:283:ALA:HB2	0.53	1.79	1	1
1:A:70:THR:HG23	1:A:86:THR:OG1	0.53	2.04	9	1
1:A:283:ALA:C	1:A:284:LEU:HD22	0.53	2.22	10	1
1:A:142:LEU:HD13	1:A:142:LEU:O	0.53	2.03	9	1
1:A:125:LEU:CD2	1:A:142:LEU:HD13	0.53	2.34	5	2
1:A:263:LEU:HD12	1:A:273:HIS:CB	0.52	2.34	7	4
1:A:195:TYR:HB3	1:A:204:THR:O	0.52	2.04	8	1
1:A:211:THR:HG23	1:A:215:SER:CB	0.52	2.34	9	1
1:A:125:LEU:CD2	1:A:125:LEU:C	0.52	2.68	1	1
1:A:201:LYS:C	1:A:202:LEU:HD22	0.52	2.24	9	2
1:A:242:LEU:HD22	1:A:264:ASP:HB3	0.52	1.81	6	1
1:A:16:ASP:O	1:A:19:THR:HG23	0.52	2.03	7	1
1:A:3:VAL:HG13	1:A:121:GLU:HA	0.52	1.81	7	1
1:A:253:PRO:HG2	1:A:255:ILE:HD12	0.52	1.82	9	1
1:A:156:ASN:O	1:A:164:VAL:HG22	0.52	2.04	2	1
1:A:261:ALA:HB2	1:A:275:LEU:CD2	0.52	2.34	9	3
1:A:6:THR:OG1	1:A:150:LEU:HD21	0.52	2.04	1	1
1:A:254:GLY:O	1:A:281:PHE:HB3	0.52	2.04	1	3
1:A:35:SER:O	1:A:36:GLU:C	0.52	2.47	9	3
1:A:38:GLY:HA2	1:A:63:ARG:O	0.52	2.05	2	7
1:A:34:LYS:CG	1:A:284:LEU:HD21	0.52	2.35	6	1
1:A:245:LEU:HD21	1:A:263:LEU:CD2	0.51	2.35	1	1
1:A:29:LEU:HD12	1:A:279:LEU:CG	0.51	2.35	5	1
1:A:123:ILE:CG2	1:A:125:LEU:HD23	0.51	2.35	10	1
1:A:158:GLU:CG	1:A:158:GLU:O	0.51	2.58	6	1
1:A:195:TYR:HB3	1:A:205:ALA:HA	0.51	1.80	8	1
1:A:68:GLY:C	1:A:69:LEU:HD22	0.51	2.25	8	3
1:A:29:LEU:HD12	1:A:279:LEU:CB	0.51	2.36	7	1
1:A:96:LYS:C	1:A:97:LEU:HD13	0.51	2.25	9	4
1:A:283:ALA:C	1:A:284:LEU:HD23	0.51	2.26	9	2
1:A:282:GLN:HG2	1:A:284:LEU:HD13	0.51	1.81	8	1
1:A:180:LEU:HD12	1:A:194:ILE:HG13	0.51	1.81	1	1
1:A:3:VAL:HG11	1:A:119:LYS:C	0.51	2.26	2	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:26:LEU:HD12	1:A:27:ILE:N	0.51	2.21	5	4
1:A:26:LEU:C	1:A:26:LEU:HD22	0.51	2.25	4	1
1:A:251:LEU:HD23	1:A:253:PRO:HD2	0.51	1.81	6	1
1:A:180:LEU:C	1:A:180:LEU:HD13	0.51	2.26	8	1
1:A:245:LEU:HD21	1:A:263:LEU:HD21	0.50	1.83	1	1
1:A:26:LEU:C	1:A:27:ILE:HD12	0.50	2.26	6	5
1:A:207:ASN:O	1:A:208:LEU:HD22	0.50	2.06	6	1
1:A:27:ILE:HG13	1:A:277:LEU:HD12	0.50	1.82	1	1
1:A:202:LEU:HD23	1:A:225:TYR:CE1	0.50	2.41	3	1
1:A:26:LEU:N	1:A:26:LEU:CD1	0.50	2.73	4	1
1:A:31:LEU:HD13	1:A:281:PHE:HB3	0.50	1.84	7	1
1:A:95:LEU:HD12	1:A:96:LYS:N	0.50	2.22	3	1
1:A:209:ALA:HB3	1:A:218:ARG:HB2	0.50	1.83	5	1
1:A:125:LEU:CD2	1:A:142:LEU:HD23	0.50	2.36	9	1
1:A:277:LEU:HD13	1:A:277:LEU:C	0.50	2.27	5	6
1:A:66:GLU:O	1:A:69:LEU:HD23	0.50	2.06	4	1
1:A:259:LEU:CD1	1:A:277:LEU:HD23	0.50	2.36	10	1
1:A:228:ASP:N	1:A:229:PRO:HD2	0.50	2.22	10	4
1:A:278:GLY:O	1:A:279:LEU:HD13	0.49	2.07	3	2
1:A:184:VAL:HG22	1:A:190:PHE:HB2	0.49	1.82	6	1
1:A:263:LEU:HD22	1:A:263:LEU:N	0.49	2.22	7	7
1:A:251:LEU:HD23	1:A:253:PRO:CD	0.49	2.36	6	1
1:A:10:LEU:HD23	1:A:150:LEU:CD2	0.49	2.37	10	1
1:A:193:SER:C	1:A:194:ILE:HD12	0.49	2.27	2	2
1:A:198:VAL:CG2	1:A:202:LEU:HD12	0.49	2.37	8	1
1:A:261:ALA:HB2	1:A:275:LEU:HD12	0.49	1.84	8	1
1:A:29:LEU:HD13	1:A:29:LEU:C	0.49	2.28	6	2
1:A:195:TYR:CD2	1:A:206:VAL:CG1	0.49	2.96	8	1
1:A:231:ALA:HB2	1:A:249:GLN:HG3	0.49	1.84	10	2
1:A:78:ASP:O	1:A:79:ASN:CB	0.49	2.59	9	7
1:A:263:LEU:HD12	1:A:273:HIS:HB3	0.49	1.85	9	1
1:A:27:ILE:HD12	1:A:27:ILE:N	0.49	2.23	3	1
1:A:277:LEU:HD11	1:A:279:LEU:HD11	0.49	1.83	7	2
1:A:263:LEU:HD12	1:A:273:HIS:HB2	0.49	1.82	3	2
1:A:69:LEU:CD1	1:A:87:VAL:HG12	0.49	2.38	3	1
1:A:209:ALA:HB3	1:A:218:ARG:CB	0.49	2.38	5	1
1:A:259:LEU:CD2	1:A:275:LEU:HD21	0.49	2.38	7	1
1:A:34:LYS:O	1:A:284:LEU:HD21	0.49	2.08	7	1
1:A:101:SER:HA	1:A:111:ASN:O	0.49	2.07	10	1
1:A:208:LEU:HD11	1:A:219:PHE:CE1	0.48	2.42	4	1
1:A:137:SER:C	1:A:138:ILE:HD12	0.48	2.28	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:27:ILE:HG23	1:A:277:LEU:HB3	0.48	1.85	7	1
1:A:68:GLY:O	1:A:69:LEU:HD23	0.48	2.08	7	1
1:A:209:ALA:HB3	1:A:218:ARG:CG	0.48	2.39	8	1
1:A:86:THR:HG22	1:A:98:THR:HG23	0.48	1.85	5	1
1:A:259:LEU:HD21	1:A:275:LEU:HD11	0.48	1.84	7	1
1:A:62:TYR:O	1:A:70:THR:HG23	0.48	2.09	7	1
1:A:31:LEU:HD21	1:A:283:ALA:HB2	0.48	1.85	4	1
1:A:195:TYR:CE2	1:A:205:ALA:HB2	0.48	2.44	1	1
1:A:180:LEU:CD1	1:A:180:LEU:C	0.48	2.78	10	1
1:A:3:VAL:HG11	1:A:119:LYS:CG	0.48	2.39	1	1
1:A:68:GLY:C	1:A:69:LEU:HD23	0.48	2.28	7	1
1:A:35:SER:HB3	1:A:39:LEU:HD23	0.48	1.86	10	1
1:A:31:LEU:HD23	1:A:32:LYS:N	0.47	2.23	5	3
1:A:250:THR:HG23	1:A:256:LYS:HG2	0.47	1.84	10	1
1:A:252:LYS:CB	1:A:253:PRO:HD2	0.47	2.39	5	1
1:A:210:TRP:CE3	1:A:217:THR:HG23	0.47	2.44	6	1
1:A:252:LYS:CB	1:A:253:PRO:CD	0.47	2.93	4	4
1:A:81:LEU:HD23	1:A:105:PRO:CD	0.47	2.40	10	1
1:A:29:LEU:HD12	1:A:279:LEU:HB2	0.47	1.85	7	1
1:A:69:LEU:CD1	1:A:87:VAL:HG13	0.47	2.39	10	1
1:A:249:GLN:HB2	1:A:257:LEU:HD23	0.47	1.86	5	1
1:A:73:GLU:CD	1:A:81:LEU:HD23	0.47	2.30	8	1
1:A:30:ASP:C	1:A:281:PHE:HB3	0.47	2.29	5	2
1:A:264:ASP:O	1:A:268:VAL:HB	0.47	2.09	4	2
1:A:153:TYR:HB2	1:A:169:PHE:HA	0.47	1.87	7	1
1:A:280:GLU:O	1:A:281:PHE:HB2	0.46	2.10	4	2
1:A:30:ASP:O	1:A:281:PHE:CA	0.46	2.63	6	2
1:A:97:LEU:HD12	1:A:116:THR:HG23	0.46	1.87	1	1
1:A:84:GLU:CB	1:A:100:ASP:HA	0.46	2.40	4	2
1:A:256:LYS:O	1:A:279:LEU:HA	0.46	2.11	6	2
1:A:34:LYS:O	1:A:284:LEU:HD11	0.46	2.10	7	1
1:A:252:LYS:HG2	1:A:255:ILE:HD11	0.46	1.85	1	1
1:A:251:LEU:HD12	1:A:255:ILE:HD11	0.46	1.87	4	1
1:A:135:GLY:HA3	1:A:160:ALA:HB2	0.46	1.88	8	1
1:A:26:LEU:C	1:A:26:LEU:CD2	0.46	2.84	4	1
1:A:95:LEU:HD12	1:A:97:LEU:HD11	0.46	1.88	1	2
1:A:28:LYS:O	1:A:279:LEU:HD22	0.46	2.11	2	3
1:A:283:ALA:HB1	1:A:284:LEU:HD12	0.46	1.86	5	1
1:A:10:LEU:HD23	1:A:150:LEU:HD22	0.46	1.87	1	1
1:A:208:LEU:HD21	1:A:219:PHE:CD2	0.46	2.46	8	1
1:A:242:LEU:HD12	2:A:301:NAI:O2D	0.46	2.11	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:67:TYR:CD1	1:A:69:LEU:HD23	0.46	2.45	6	1
1:A:7:TYR:HA	1:A:10:LEU:HD13	0.46	1.87	3	1
1:A:228:ASP:CB	1:A:229:PRO:CD	0.46	2.93	3	1
1:A:125:LEU:HD22	1:A:142:LEU:HD13	0.45	1.88	5	1
1:A:90:GLN:CB	1:A:97:LEU:HD23	0.45	2.42	10	1
1:A:6:THR:HB	1:A:150:LEU:HD21	0.45	1.88	4	1
1:A:249:GLN:HB3	1:A:257:LEU:HD23	0.45	1.87	5	1
1:A:138:ILE:HD13	1:A:159:THR:CB	0.45	2.42	7	1
1:A:277:LEU:HD22	1:A:278:GLY:N	0.45	2.26	2	1
1:A:219:PHE:CZ	1:A:221:ILE:HD12	0.45	2.47	10	1
1:A:133:ILE:O	1:A:133:ILE:HD12	0.45	2.12	2	1
1:A:257:LEU:HD23	1:A:258:THR:N	0.45	2.26	3	1
1:A:133:ILE:HD12	1:A:133:ILE:O	0.45	2.10	4	1
1:A:250:THR:O	1:A:251:LEU:CB	0.45	2.65	5	1
1:A:180:LEU:HD13	1:A:180:LEU:C	0.45	2.32	3	4
1:A:184:VAL:HG13	1:A:190:PHE:CB	0.45	2.42	6	1
1:A:260:SER:O	1:A:275:LEU:HD22	0.45	2.12	1	1
1:A:83:THR:OG1	1:A:84:GLU:N	0.45	2.49	4	1
1:A:125:LEU:CD2	1:A:142:LEU:HD22	0.45	2.42	7	1
1:A:252:LYS:N	1:A:253:PRO:HD2	0.44	2.27	6	4
1:A:153:TYR:CE1	1:A:170:ALA:HB3	0.44	2.47	7	1
1:A:277:LEU:C	1:A:277:LEU:HD13	0.44	2.32	1	1
1:A:142:LEU:HD23	1:A:143:VAL:N	0.44	2.27	10	1
1:A:180:LEU:HD23	1:A:194:ILE:HG13	0.44	1.88	4	3
1:A:244:GLY:C	1:A:245:LEU:HD13	0.44	2.32	5	6
1:A:153:TYR:CB	1:A:169:PHE:HA	0.44	2.42	7	1
1:A:47:ALA:HB1	1:A:54:VAL:HG22	0.44	1.88	8	2
1:A:6:THR:HG22	1:A:150:LEU:CD2	0.44	2.30	6	1
1:A:69:LEU:HD22	1:A:87:VAL:HB	0.44	1.89	7	1
1:A:97:LEU:N	1:A:97:LEU:HD22	0.44	2.28	9	2
1:A:257:LEU:C	1:A:257:LEU:HD13	0.44	2.33	8	1
1:A:252:LYS:HB3	1:A:253:PRO:HD2	0.44	1.90	1	1
1:A:257:LEU:HD13	1:A:277:LEU:HD21	0.44	1.90	1	1
1:A:73:GLU:HG3	1:A:83:THR:HG23	0.44	1.90	10	1
1:A:142:LEU:HD12	1:A:142:LEU:C	0.43	2.34	1	1
1:A:31:LEU:HD13	1:A:32:LYS:N	0.43	2.28	4	2
1:A:29:LEU:C	1:A:29:LEU:HD13	0.43	2.32	8	3
1:A:237:VAL:HG23	1:A:242:LEU:O	0.43	2.13	6	1
1:A:146:TYR:O	1:A:149:TRP:CD1	0.43	2.71	9	1
1:A:252:LYS:CG	1:A:255:ILE:HD11	0.43	2.44	1	1
1:A:124:ASN:HB3	1:A:143:VAL:HG13	0.43	1.89	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:257:LEU:HD13	1:A:279:LEU:HD11	0.43	1.89	5	1
1:A:123:ILE:HD12	1:A:124:ASN:H	0.43	1.72	2	1
1:A:73:GLU:O	1:A:74:LYS:CB	0.43	2.66	4	1
1:A:10:LEU:CD2	1:A:150:LEU:HD22	0.43	2.42	1	1
1:A:148:GLY:O	1:A:173:TYR:HB3	0.43	2.13	3	1
1:A:243:ILE:O	1:A:262:LEU:HD22	0.43	2.13	3	1
1:A:259:LEU:HD13	1:A:260:SER:N	0.43	2.28	4	2
1:A:97:LEU:HD12	1:A:116:THR:HG22	0.43	1.91	4	1
1:A:192:GLY:O	1:A:208:LEU:HD23	0.43	2.14	1	1
1:A:86:THR:HG22	1:A:98:THR:HB	0.43	1.89	8	1
1:A:10:LEU:HD12	1:A:150:LEU:CD2	0.43	2.44	3	1
1:A:209:ALA:HB3	1:A:218:ARG:HB3	0.43	1.90	2	1
1:A:75:TRP:CD1	1:A:81:LEU:HD22	0.43	2.49	4	1
1:A:14:ALA:HB1	1:A:193:SER:CB	0.43	2.44	5	1
1:A:159:THR:HG23	1:A:160:ALA:N	0.42	2.29	3	2
1:A:38:GLY:O	1:A:62:TYR:HA	0.42	2.14	3	2
1:A:279:LEU:H	1:A:279:LEU:HD22	0.42	1.73	4	1
1:A:245:LEU:N	1:A:245:LEU:CD1	0.42	2.82	2	3
1:A:237:VAL:HG12	1:A:243:ILE:HA	0.42	1.91	5	1
1:A:257:LEU:CD2	1:A:277:LEU:HD21	0.42	2.44	6	1
1:A:283:ALA:C	1:A:284:LEU:HD12	0.42	2.34	5	1
1:A:144:LEU:HD12	1:A:151:ALA:O	0.42	2.14	7	1
1:A:209:ALA:HB3	1:A:218:ARG:HG2	0.42	1.90	8	1
1:A:123:ILE:HD12	1:A:124:ASN:N	0.42	2.29	2	1
1:A:221:ILE:HG12	1:A:237:VAL:HG12	0.42	1.89	9	1
1:A:75:TRP:CD1	1:A:81:LEU:CB	0.42	3.02	2	1
1:A:26:LEU:HD11	1:A:48:ASN:HD22	0.42	1.75	10	1
1:A:243:ILE:HG22	1:A:245:LEU:CD1	0.42	2.45	3	1
1:A:242:LEU:HG	1:A:262:LEU:HD11	0.42	1.90	3	1
1:A:227:ILE:HD12	1:A:233:PHE:CD2	0.42	2.50	6	1
1:A:202:LEU:HD12	1:A:203:GLU:O	0.42	2.15	2	1
1:A:17:VAL:HG13	1:A:222:ALA:CB	0.42	2.45	5	1
1:A:193:SER:HA	1:A:206:VAL:O	0.42	2.15	8	1
1:A:263:LEU:N	1:A:263:LEU:HD13	0.42	2.29	9	2
1:A:180:LEU:HD22	1:A:181:HIS:N	0.42	2.30	6	1
1:A:10:LEU:HD23	1:A:150:LEU:HD12	0.42	1.90	8	1
1:A:27:ILE:CD1	1:A:27:ILE:N	0.42	2.83	3	1
1:A:6:THR:HB	1:A:143:VAL:HG21	0.42	1.91	7	1
1:A:227:ILE:HG22	1:A:231:ALA:O	0.42	2.15	3	1
1:A:144:LEU:O	1:A:150:LEU:HD23	0.42	2.14	9	1
1:A:15:ARG:O	1:A:19:THR:HG23	0.41	2.15	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:114:ILE:HD13	1:A:115:LYS:H	0.41	1.75	9	1
1:A:120:ARG:N	1:A:123:ILE:O	0.41	2.48	9	1
1:A:146:TYR:CB	1:A:149:TRP:O	0.41	2.68	3	1
1:A:279:LEU:N	1:A:279:LEU:HD13	0.41	2.30	4	1
1:A:59:GLU:HA	1:A:74:LYS:CB	0.41	2.45	4	1
1:A:26:LEU:C	1:A:27:ILE:HD13	0.41	2.35	7	1
1:A:195:TYR:CD2	1:A:205:ALA:HB2	0.41	2.51	1	1
1:A:31:LEU:HD13	1:A:31:LEU:C	0.41	2.35	1	1
1:A:259:LEU:HD11	1:A:275:LEU:HD21	0.41	1.92	2	1
1:A:97:LEU:HD12	1:A:116:THR:CB	0.41	2.46	4	1
1:A:30:ASP:O	1:A:281:PHE:HA	0.41	2.15	5	1
1:A:227:ILE:O	1:A:227:ILE:HD12	0.41	2.15	3	1
1:A:258:THR:O	1:A:277:LEU:HD22	0.41	2.15	8	1
1:A:61:LYS:CG	1:A:71:PHE:O	0.41	2.69	10	1
1:A:182:THR:HG22	1:A:191:GLY:O	0.41	2.16	4	2
1:A:263:LEU:CD2	1:A:263:LEU:N	0.41	2.81	9	1
1:A:81:LEU:HD23	1:A:81:LEU:H	0.41	1.76	1	1
1:A:277:LEU:HD22	1:A:278:GLY:H	0.41	1.75	2	3
1:A:199:ASN:O	1:A:200:LYS:C	0.41	2.59	4	1
1:A:156:ASN:O	1:A:164:VAL:HB	0.41	2.16	8	1
1:A:151:ALA:CB	1:A:171:VAL:HG13	0.41	2.46	9	1
1:A:85:ILE:HG22	1:A:99:PHE:O	0.41	2.15	10	1
1:A:14:ALA:HB1	1:A:193:SER:OG	0.41	2.16	5	1
1:A:154:GLN:H	1:A:169:PHE:HB2	0.41	1.75	9	1
1:A:125:LEU:HB2	1:A:142:LEU:HG	0.40	1.92	8	1
1:A:282:GLN:CG	1:A:284:LEU:HD13	0.40	2.46	8	1
1:A:26:LEU:O	1:A:27:ILE:HD12	0.40	2.15	9	1
1:A:97:LEU:HD22	1:A:97:LEU:N	0.40	2.31	10	1
1:A:125:LEU:HB2	1:A:142:LEU:HD13	0.40	1.92	1	1
1:A:195:TYR:HD1	1:A:205:ALA:HB2	0.40	1.75	4	1
1:A:133:ILE:N	1:A:133:ILE:HD13	0.40	2.32	5	1
1:A:146:TYR:O	1:A:148:GLY:N	0.40	2.54	8	1
1:A:263:LEU:HD22	1:A:263:LEU:H	0.40	1.74	9	1
1:A:262:LEU:HD13	1:A:263:LEU:N	0.40	2.31	1	1
1:A:279:LEU:HD13	1:A:279:LEU:N	0.40	2.31	2	1
1:A:51:THR:O	1:A:52:THR:C	0.40	2.59	4	1
1:A:262:LEU:HD13	1:A:262:LEU:C	0.40	2.35	8	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%)	250±2 (88±1%)	25±3 (9±1%)	8±2 (3±1%)	8	42
All	All	2830/2910 (97%)	2500 (88%)	250 (9%)	80 (3%)	8	42

All 32 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	7
1	A	176	ASP	7
1	A	11	GLY	6
1	A	272	GLY	6
1	A	228	ASP	4
1	A	252	LYS	4
1	A	229	PRO	4
1	A	65	THR	4
1	A	281	PHE	3
1	A	68	GLY	3
1	A	21	GLY	2
1	A	267	ASN	2
1	A	84	GLU	2
1	A	214	ASN	2
1	A	89	ASP	2
1	A	254	GLY	2
1	A	106	ASN	2
1	A	253	PRO	2
1	A	36	GLU	2
1	A	199	ASN	2
1	A	22	TYR	1
1	A	74	LYS	1
1	A	201	LYS	1
1	A	51	THR	1
1	A	19	THR	1
1	A	169	PHE	1
1	A	202	LEU	1

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Mol	Chain	Res	Type	Models (Total)
1	A	92	ALA	1
1	A	91	LEU	1
1	A	67	TYR	1
1	A	198	VAL	1
1	A	66	GLU	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%)	182±5 (79±2%)	49±5 (21±2%)	3	32
All	All	2310/2380 (97%)	1822 (79%)	488 (21%)	3	32

All 172 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	263	LEU	10
1	A	259	LEU	10
1	A	58	LEU	9
1	A	175	THR	9
1	A	245	LEU	8
1	A	40	GLU	7
1	A	182	THR	7
1	A	228	ASP	6
1	A	243	ILE	6
1	A	238	ASN	6
1	A	264	ASP	6
1	A	150	LEU	6
1	A	236	LYS	6
1	A	142	LEU	6
1	A	190	PHE	6
1	A	42	THR	5
1	A	163	ARG	5
1	A	257	LEU	5
1	A	6	THR	5
1	A	97	LEU	5

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Mol	Chain	Res	Type	Models (Total)
1	A	85	ILE	5
1	A	125	LEU	5
1	A	35	SER	5
1	A	159	THR	5
1	A	164	VAL	5
1	A	221	ILE	5
1	A	81	LEU	5
1	A	185	ASN	5
1	A	95	LEU	5
1	A	127	CYS	4
1	A	10	LEU	4
1	A	84	GLU	4
1	A	51	THR	4
1	A	144	LEU	4
1	A	189	GLU	4
1	A	20	LYS	4
1	A	32	LYS	4
1	A	180	LEU	4
1	A	132	ASP	4
1	A	281	PHE	4
1	A	154	GLN	4
1	A	104	SER	4
1	A	241	SER	4
1	A	29	LEU	4
1	A	266	LYS	4
1	A	158	GLU	4
1	A	118	TYR	4
1	A	99	PHE	3
1	A	83	THR	3
1	A	79	ASN	3
1	A	284	LEU	3
1	A	57	SER	3
1	A	168	ASN	3
1	A	128	ASP	3
1	A	109	LYS	3
1	A	143	VAL	3
1	A	26	LEU	3
1	A	171	VAL	3
1	A	41	PHE	3
1	A	202	LEU	3
1	A	107	THR	3
1	A	49	THR	3

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Mol	Chain	Res	Type	Models (Total)
1	A	279	LEU	3
1	A	137	SER	3
1	A	248	THR	3
1	A	195	TYR	3
1	A	46	SER	3
1	A	124	ASN	3
1	A	274	LYS	3
1	A	64	TRP	3
1	A	133	ILE	3
1	A	50	GLU	3
1	A	267	ASN	3
1	A	54	VAL	3
1	A	153	TYR	3
1	A	60	THR	3
1	A	186	ASP	3
1	A	206	VAL	3
1	A	39	LEU	2
1	A	173	TYR	2
1	A	256	LYS	2
1	A	110	LYS	2
1	A	63	ARG	2
1	A	167	SER	2
1	A	3	VAL	2
1	A	183	ASN	2
1	A	100	ASP	2
1	A	31	LEU	2
1	A	262	LEU	2
1	A	30	ASP	2
1	A	123	ILE	2
1	A	193	SER	2
1	A	18	PHE	2
1	A	174	LYS	2
1	A	43	SER	2
1	A	146	TYR	2
1	A	194	ILE	2
1	A	61	LYS	2
1	A	102	SER	2
1	A	211	THR	2
1	A	76	ASN	2
1	A	155	MET	2
1	A	70	THR	2
1	A	230	ASP	2

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Mol	Chain	Res	Type	Models (Total)
1	A	114	ILE	2
1	A	24	PHE	2
1	A	176	ASP	2
1	A	15	ARG	2
1	A	166	GLN	2
1	A	72	THR	2
1	A	28	LYS	2
1	A	12	LYS	2
1	A	120	ARG	2
1	A	69	LEU	2
1	A	157	PHE	2
1	A	34	LYS	2
1	A	9	ASP	2
1	A	71	PHE	2
1	A	86	THR	2
1	A	22	TYR	2
1	A	74	LYS	2
1	A	252	LYS	2
1	A	280	GLU	2
1	A	16	ASP	2
1	A	255	ILE	2
1	A	19	THR	2
1	A	156	ASN	2
1	A	89	ASP	2
1	A	161	LYS	2
1	A	78	ASP	1
1	A	80	THR	1
1	A	48	ASN	1
1	A	98	THR	1
1	A	93	ARG	1
1	A	277	LEU	1
1	A	67	TYR	1
1	A	269	ASN	1
1	A	237	VAL	1
1	A	201	LYS	1
1	A	207	ASN	1
1	A	224	LYS	1
1	A	65	THR	1
1	A	178	PHE	1
1	A	234	SER	1
1	A	242	LEU	1
1	A	247	TYR	1

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Mol	Chain	Res	Type	Models (Total)
1	A	13	SER	1
1	A	59	GLU	1
1	A	33	THR	1
1	A	217	THR	1
1	A	169	PHE	1
1	A	285	GLU	1
1	A	226	GLN	1
1	A	197	LYS	1
1	A	165	THR	1
1	A	249	GLN	1
1	A	200	LYS	1
1	A	119	LYS	1
1	A	139	ARG	1
1	A	218	ARG	1
1	A	251	LEU	1
1	A	273	HIS	1
1	A	44	SER	1
1	A	113	LYS	1
1	A	103	PHE	1
1	A	147	GLU	1
1	A	87	VAL	1
1	A	90	GLN	1
1	A	181	HIS	1
1	A	73	GLU	1
1	A	37	ASN	1
1	A	53	LYS	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.

LIGAND-GEOMETRY INFOmissingINFO

6.6 Other polymers [i](#)

There are no such molecules in this entry.

6.7 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 ± 0.09	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	210	-0.16 ± 0.07	None needed (< 0.5 ppm)
$^{13}\text{C}'$	180	0.86 ± 0.09	Should be applied
^{15}N	250	-0.94 ± 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 3343. 0 out of 41 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}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	¹ H	¹³ C	¹⁵ N
Aromatic	8/283 (3%)	4/150 (3%)	0/126 (0%)	4/7 (57%)
Overall	1339/3343 (40%)	338/1672 (20%)	746/1313 (57%)	255/358 (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 3356. 0 out of 41 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ 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	8/283 (3%)	4/150 (3%)	0/126 (0%)	4/7 (57%)
Overall	1339/3356 (40%)	338/1679 (20%)	746/1318 (57%)	255/359 (71%)

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:

