



Full wwPDB NMR Structure Validation Report ⓘ

Mar 8, 2026 – 08:01 AM UTC

PDB ID : 6TIR / pdb_00006tir
BMRB ID : 34458
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
wwPDB-ShiftChecker : v1.2
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

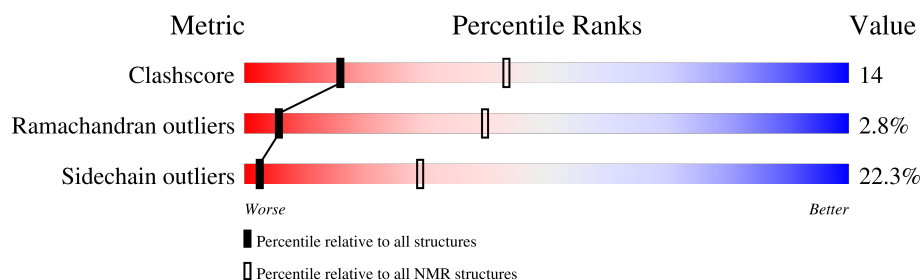
1 Overall quality at a glance

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	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

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	 69% 25% . .

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)	1.95	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.

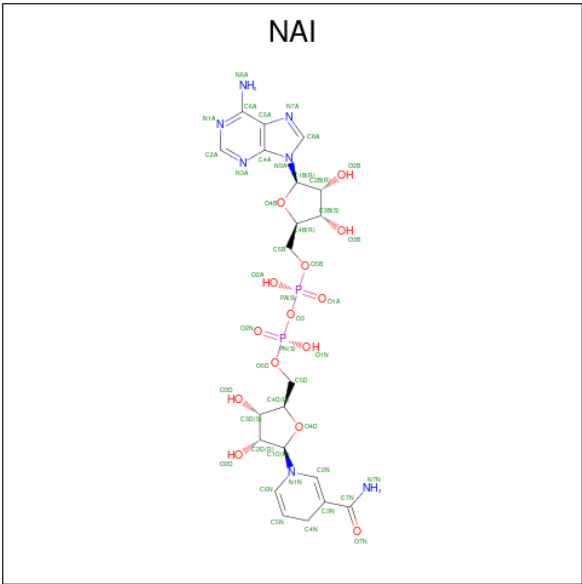
- Molecule 1 is a protein called Voltage-dependent anion-selective channel protein 1.

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 (CCD ID: NAI) (formula: C₂₁H₂₉N₇O₁₄P₂) (labeled as "Ligand of Interest" by depositor).

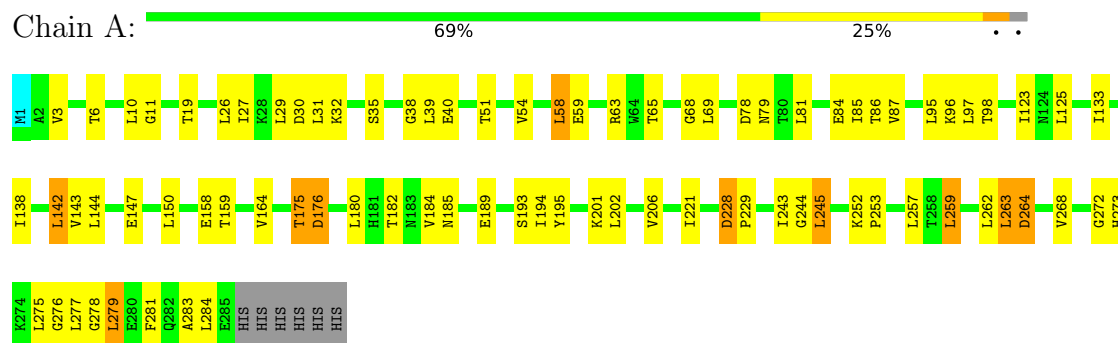


4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

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

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

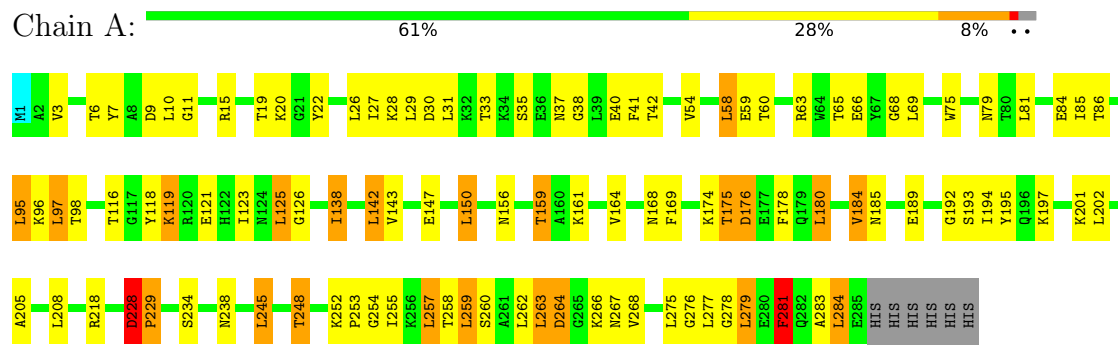


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

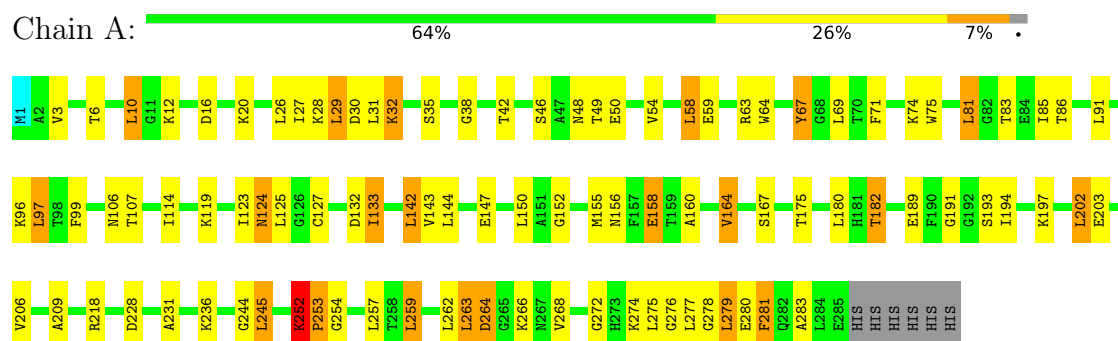
4.2.1 Score per residue for model 1 (medoid)

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



4.2.2 Score per residue for model 2

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



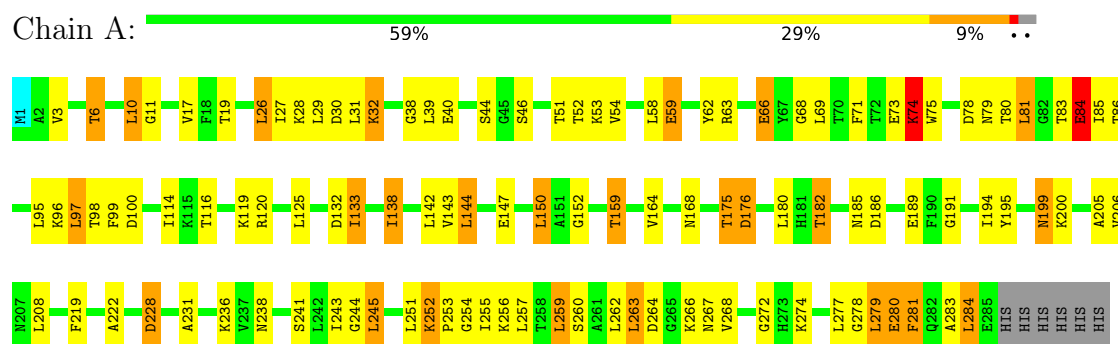
4.2.3 Score per residue for model 3

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



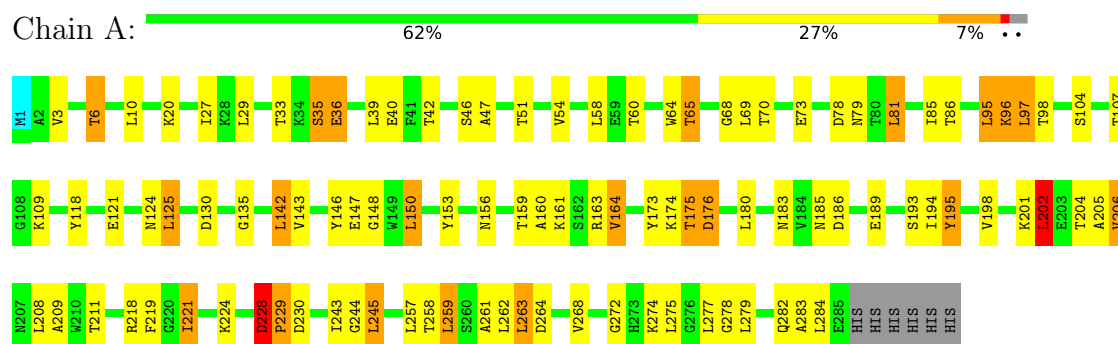
4.2.4 Score per residue for model 4

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



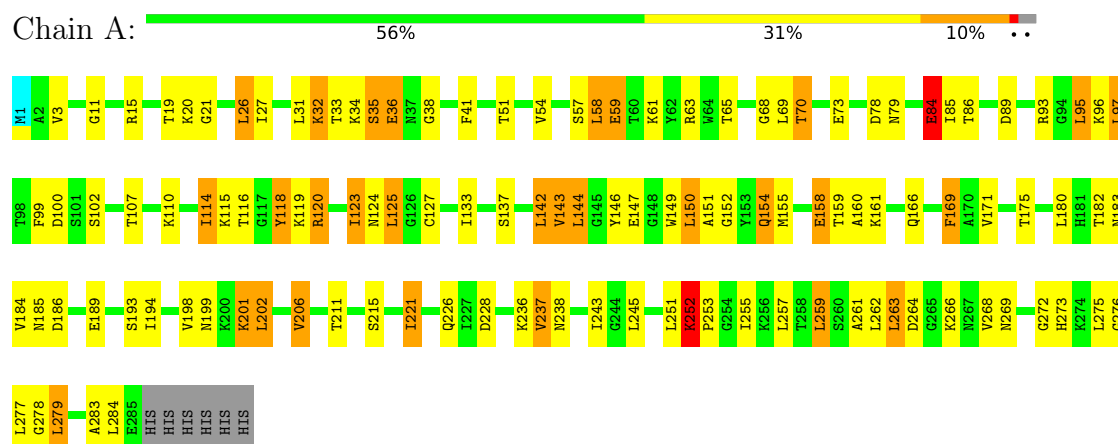
4.2.8 Score per residue for model 8

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



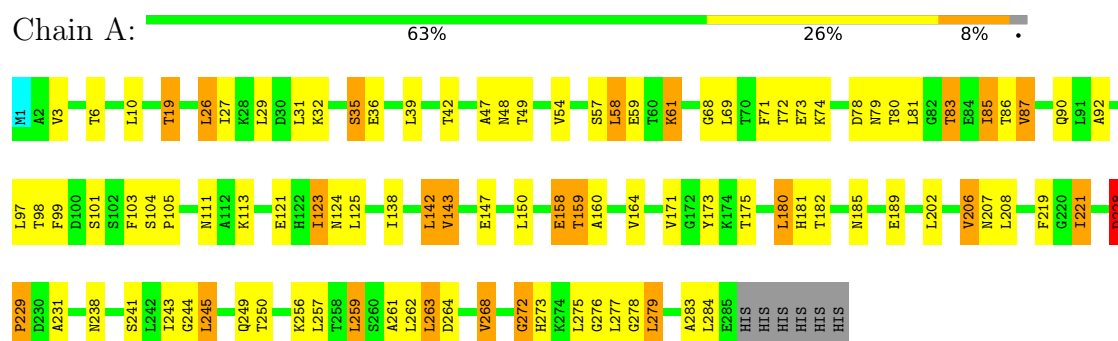
4.2.9 Score per residue for model 9

- 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



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)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	1507
Number of shifts mapped to atoms	1504
Number of unparsed shifts	0
Number of shifts with mapping errors	3
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	40%

6 Model quality

6.1 Standard geometry

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

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	64±8
2	A	44	29	27	0±1
All	All	22230	21800	21780	638

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:O	1:A:29:LEU:HD13	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:C	1:A:125:LEU:HD22	0.87	1.94	1	1
1:A:29:LEU:HD22	1:A:29:LEU:C	0.81	2.00	6	1
1:A:123:ILE:HD13	1:A:144:LEU:HD13	0.77	1.54	2	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:262:LEU:C	1:A:263:LEU:HD13	0.75	2.06	9	10

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:180:LEU:C	1:A:180:LEU:HD12	0.74	2.07	10	1
1:A:158:GLU:O	1:A:161:LYS:O	0.74	2.05	9	1
1:A:143:VAL:C	1:A:144:LEU:HD23	0.73	2.07	3	2
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:86:THR:HG23	1:A:98:THR:HG22	0.70	1.62	7	1
1:A:175:THR:O	1:A:176:ASP:C	0.70	2.34	3	7
1:A:27:ILE:HG23	1:A:277:LEU:CD1	0.70	2.17	4	2
1:A:206:VAL:HG22	1:A:221:ILE:HG22	0.69	1.64	6	1
1:A:123:ILE:HD11	1:A:142:LEU:CD2	0.68	2.19	2	1
1:A:26:LEU:HD13	1:A:26:LEU:N	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:278:GLY:C	1:A:279:LEU:HD13	0.67	2.15	2	4
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: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:31:LEU:HD11	1:A:283:ALA:HB3	0.64	1.70	2	2
1:A:123:ILE:HD13	1:A:144:LEU:CD1	0.64	2.22	2	1
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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:259:LEU:HD22	1:A:277:LEU:CD2	0.62	2.21	5	3
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: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:29:LEU:C	1:A:29:LEU:CD2	0.62	2.72	6	1
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:263:LEU:HD22	1:A:263:LEU:N	0.61	2.11	9	9
1:A:150:LEU:N	1:A:173:TYR:HB2	0.61	2.11	3	1
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:125:LEU:C	1:A:125:LEU:CD2	0.60	2.68	1	1
1:A:264:ASP:O	1:A:268:VAL:HG22	0.60	1.96	7	8
1:A:244:GLY:C	1:A:245:LEU:HD12	0.60	2.21	3	1
1:A:219:PHE:CE1	1:A:221:ILE:HD11	0.60	2.31	5	1
1:A:245:LEU:HD13	1:A:245:LEU:N	0.60	2.11	8	6
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:142:LEU:C	1:A:142:LEU:HD13	0.60	2.22	9	1
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:201:LYS:C	1:A:202:LEU:HD12	0.59	2.22	3	1
1:A:86:THR:OG1	1:A:98:THR:HG23	0.59	1.96	4	1
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:HD12	1:A:251:LEU:O	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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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
1:A:279:LEU:HD22	1:A:279:LEU:N	0.58	2.14	4	3
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:283:ALA:C	1:A:284:LEU:HD22	0.58	2.22	10	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:201:LYS:C	1:A:202:LEU:HD22	0.57	2.24	9	2
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:35:SER:O	1:A:36:GLU:C	0.56	2.47	9	3
1:A:84:GLU:HB3	1:A:99:PHE:O	0.56	2.00	4	2
1:A:3:VAL:HG22	1:A:121:GLU:HA	0.56	1.75	10	2
1:A:58:LEU:HD13	1:A:59:GLU:N	0.56	2.16	7	7
1:A:144:LEU:HD23	1:A:144:LEU:N	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:68:GLY:C	1:A:69:LEU:HD22	0.56	2.25	8	4
1:A:61:LYS:CB	1:A:72:THR:HA	0.56	2.30	10	1
1:A:96:LYS:C	1:A:97:LEU:HD13	0.56	2.25	9	5
1:A:142:LEU:HD22	1:A:144:LEU:CD2	0.56	2.30	3	1
1:A:283:ALA:C	1:A:284:LEU:HD23	0.55	2.26	9	2
1:A:61:LYS:HB3	1:A:71:PHE:O	0.55	2.00	10	1
1:A:180:LEU:C	1:A:180:LEU:HD13	0.55	2.26	8	6
1:A:26:LEU:C	1:A:26:LEU:HD22	0.55	2.25	4	1
1:A:26:LEU:C	1:A:27:ILE:HD12	0.55	2.26	6	5
1:A:180:LEU:HD12	1:A:194:ILE:HG23	0.55	1.77	7	1
1:A:257:LEU:HD11	1:A:277:LEU:HD21	0.55	1.78	5	1
1:A:3:VAL:HG11	1:A:119:LYS:C	0.55	2.26	2	2
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:125:LEU:HD22	1:A:142:LEU:HD23	0.55	1.79	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:178:PHE:CZ	1:A:194:ILE:HG23	0.55	2.37	1	1
1:A:277:LEU:C	1:A:277:LEU:HD13	0.55	2.27	5	5
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:193:SER:C	1:A:194:ILE:HD12	0.54	2.27	2	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:29:LEU:HD13	1:A:29:LEU:C	0.54	2.28	6	4
1:A:237:VAL:HG12	1:A:242:LEU:O	0.54	2.02	5	1
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:137:SER:C	1:A:138:ILE:HD12	0.53	2.28	7	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:142:LEU:HD13	1:A:142:LEU:O	0.53	2.03	9	1
1:A:180:LEU:C	1:A:180:LEU:CD1	0.53	2.78	10	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:242:LEU:HD22	1:A:264:ASP:HB3	0.52	1.81	6	1
1:A:3:VAL:HG13	1:A:121:GLU:HA	0.52	1.81	7	1
1:A:16:ASP:O	1:A:19:THR:HG23	0.52	2.03	7	1
1:A:68:GLY:C	1:A:69:LEU:HD23	0.52	2.28	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: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:30:ASP:C	1:A:281:PHE:HB3	0.52	2.29	5	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:73:GLU:CD	1:A:81:LEU:HD23	0.52	2.30	8	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:O	1:A:158:GLU:CG	0.51	2.58	6	1
1:A:195:TYR:HB3	1:A:205:ALA:HA	0.51	1.80	8	1
1:A:29:LEU:HD12	1:A:279:LEU:CB	0.51	2.36	7	1
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:26:LEU:C	1:A:26:LEU:CD2	0.51	2.84	4	1
1:A:26:LEU:HD12	1:A:27:ILE:N	0.51	2.21	5	4
1:A:251:LEU:HD23	1:A:253:PRO:HD2	0.51	1.81	6	1
1:A:245:LEU:HD21	1:A:263:LEU:HD21	0.50	1.83	1	1
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: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:251:LEU:HD23	1:A:253:PRO:CD	0.49	2.36	6	1
1:A:244:GLY:C	1:A:245:LEU:HD13	0.49	2.32	5	6
1:A:10:LEU:HD23	1:A:150:LEU:CD2	0.49	2.37	10	1
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:195:TYR:CD2	1:A:206:VAL:CG1	0.49	2.96	8	1
1:A:277:LEU:HD13	1:A:277:LEU:C	0.49	2.32	1	3
1:A:78:ASP:O	1:A:79:ASN:CB	0.49	2.59	9	7
1:A:231:ALA:HB2	1:A:249:GLN:HG3	0.49	1.84	10	2
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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:34:LYS:O	1:A:284:LEU:HD21	0.49	2.08	7	1
1:A:259:LEU:CD2	1:A:275:LEU:HD21	0.49	2.38	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:27:ILE:HG23	1:A:277:LEU:HB3	0.48	1.85	7	1
1:A:257:LEU:HD13	1:A:257:LEU:C	0.48	2.33	8	1
1:A:68:GLY:O	1:A:69:LEU:HD23	0.48	2.08	7	1
1:A:64:TRP:CD1	1:A:65:THR:HG1	0.48	2.26	8	1
1:A:209:ALA:HB3	1:A:218:ARG:CG	0.48	2.39	8	1
1:A:142:LEU:HD12	1:A:142:LEU:C	0.48	2.34	1	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:29:LEU:C	1:A:29:LEU:HD13	0.48	2.32	8	2
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:3:VAL:HG11	1:A:119:LYS:CG	0.48	2.39	1	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:283:ALA:C	1:A:284:LEU:HD12	0.47	2.34	5	2
1:A:249:GLN:HB2	1:A:257:LEU:HD23	0.47	1.86	5	1
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:31:LEU:C	1:A:31:LEU:HD13	0.46	2.35	1	1
1:A:26:LEU:C	1:A:27:ILE:HD13	0.46	2.35	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:28:LYS:O	1:A:279:LEU:HD22	0.46	2.11	2	3
1:A:95:LEU:HD12	1:A:97:LEU:HD11	0.46	1.88	1	2
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:67:TYR:CD1	1:A:69:LEU:HD23	0.46	2.45	6	1
1:A:242:LEU:HD12	2:A:301:NAI:O2D	0.46	2.11	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:199:ASN:O	1:A:200:LYS:C	0.45	2.59	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:HD12	1:A:133:ILE:O	0.45	2.12	2	2
1:A:257:LEU:HD23	1:A:258:THR:N	0.45	2.26	3	1
1:A:51:THR:O	1:A:52:THR:C	0.45	2.59	4	1
1:A:250:THR:O	1:A:251:LEU:CB	0.45	2.65	5	1
1:A:66:GLU:O	1:A:67:TYR:C	0.45	2.59	3	1
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:262:LEU:C	1:A:262:LEU:HD13	0.45	2.35	8	5
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: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: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	3
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:31:LEU:HD13	1:A:32:LYS:N	0.43	2.28	4	2
1:A:237:VAL:HG23	1:A:242:LEU:O	0.43	2.13	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:264:ASP:C	1:A:268:VAL:HG22	0.43	2.38	10	1
1:A:124:ASN:HB3	1:A:143:VAL:HG13	0.43	1.89	9	1
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:275:LEU:C	1:A:275:LEU:HD13	0.43	2.39	9	1
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:275:LEU:HD13	1:A:275:LEU:C	0.43	2.39	7	2
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:49:THR:O	1:A:50:GLU:C	0.42	2.62	2	1
1:A:38:GLY:O	1:A:62:TYR:HA	0.42	2.14	3	2
1:A:159:THR:HG23	1:A:160:ALA:N	0.42	2.29	3	2
1:A:279:LEU:HD22	1:A:279:LEU:H	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: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:264:ASP:C	1:A:266:LYS:N	0.42	2.78	1	2
1:A:31:LEU:HD13	1:A:31:LEU:C	0.42	2.39	4	2
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:26:LEU:HD12	1:A:27:ILE:C	0.42	2.40	2	1
1:A:242:LEU:HG	1:A:262:LEU:HD11	0.42	1.90	3	1
1:A:243:ILE:HG22	1:A:245:LEU:CD1	0.42	2.45	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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:193:SER:HA	1:A:206:VAL:O	0.42	2.15	8	1
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:263:LEU:HD13	1:A:263:LEU:N	0.42	2.29	9	1
1:A:27:ILE:N	1:A:27:ILE:CD1	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
1:A:193:SER:C	1:A:194:ILE:HD13	0.41	2.40	7	1
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:279:LEU:HD13	1:A:279:LEU:N	0.41	2.30	4	2
1:A:146:TYR:CB	1:A:149:TRP:O	0.41	2.68	3	1
1:A:59:GLU:HA	1:A:74:LYS:CB	0.41	2.45	4	1
1:A:195:TYR:CD2	1:A:205:ALA:HB2	0.41	2.51	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:HD12	1:A:227:ILE:O	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:29:LEU:C	1:A:29:LEU:CD1	0.41	2.93	6	1
1:A:263:LEU:N	1:A:263:LEU:CD2	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: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:142:LEU:HD22	1:A:142:LEU:C	0.40	2.40	9	1
1:A:75:TRP:CD1	1:A:75:TRP:C	0.40	3.00	1	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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:31:LEU:HD23	1:A:31:LEU:C	0.40	2.42	10	1
1:A:185:ASN:C	1:A:187:GLY:N	0.40	2.77	6	1

6.3 Torsion angles

6.3.1 Protein backbone

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	283/291 (97%)	250±2 (88±1%)	25±3 (9±1%)	8±2 (3±1%)	6	40
All	All	2830/2910 (97%)	2500 (88%)	250 (9%)	80 (3%)	6	40

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	65	THR	4
1	A	228	ASP	4
1	A	229	PRO	4
1	A	252	LYS	4
1	A	68	GLY	3
1	A	281	PHE	3
1	A	267	ASN	2
1	A	106	ASN	2
1	A	253	PRO	2
1	A	89	ASP	2
1	A	214	ASN	2
1	A	84	GLU	2
1	A	199	ASN	2
1	A	254	GLY	2

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Mol	Chain	Res	Type	Models (Total)
1	A	21	GLY	2
1	A	36	GLU	2
1	A	22	TYR	1
1	A	67	TYR	1
1	A	66	GLU	1
1	A	74	LYS	1
1	A	51	THR	1
1	A	91	LEU	1
1	A	202	LEU	1
1	A	169	PHE	1
1	A	198	VAL	1
1	A	201	LYS	1
1	A	19	THR	1
1	A	92	ALA	1

6.3.2 Protein sidechains ⓘ

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	231/238 (97%)	179±7 (78±3%)	52±7 (22±3%)	2	29
All	All	2310/2380 (97%)	1794 (78%)	516 (22%)	2	29

All 174 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	58	LEU	10
1	A	175	THR	10
1	A	259	LEU	10
1	A	263	LEU	10
1	A	189	GLU	9
1	A	245	LEU	9
1	A	142	LEU	8
1	A	164	VAL	8
1	A	279	LEU	8
1	A	206	VAL	8
1	A	40	GLU	7

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Mol	Chain	Res	Type	Models (Total)
1	A	85	ILE	7
1	A	150	LEU	7
1	A	185	ASN	7
1	A	182	THR	7
1	A	54	VAL	6
1	A	97	LEU	6
1	A	228	ASP	6
1	A	243	ILE	6
1	A	35	SER	5
1	A	42	THR	5
1	A	95	LEU	5
1	A	125	LEU	5
1	A	159	THR	5
1	A	257	LEU	5
1	A	264	ASP	5
1	A	6	THR	5
1	A	10	LEU	5
1	A	81	LEU	5
1	A	133	ILE	5
1	A	143	VAL	5
1	A	236	LYS	5
1	A	186	ASP	5
1	A	221	ILE	5
1	A	39	LEU	5
1	A	20	LYS	4
1	A	84	GLU	4
1	A	180	LEU	4
1	A	184	VAL	4
1	A	238	ASN	4
1	A	107	THR	4
1	A	158	GLU	4
1	A	202	LEU	4
1	A	51	THR	4
1	A	87	VAL	4
1	A	144	LEU	4
1	A	241	SER	4
1	A	19	THR	4
1	A	26	LEU	4
1	A	57	SER	4
1	A	104	SER	4
1	A	41	PHE	3
1	A	60	THR	3

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Mol	Chain	Res	Type	Models (Total)
1	A	69	LEU	3
1	A	123	ILE	3
1	A	161	LYS	3
1	A	168	ASN	3
1	A	174	LYS	3
1	A	248	THR	3
1	A	29	LEU	3
1	A	32	LYS	3
1	A	46	SER	3
1	A	74	LYS	3
1	A	83	THR	3
1	A	124	ASN	3
1	A	127	CYS	3
1	A	252	LYS	3
1	A	274	LYS	3
1	A	50	GLU	3
1	A	128	ASP	3
1	A	137	SER	3
1	A	163	ARG	3
1	A	171	VAL	3
1	A	224	LYS	3
1	A	49	THR	3
1	A	70	THR	3
1	A	102	SER	3
1	A	109	LYS	3
1	A	195	TYR	3
1	A	66	GLU	2
1	A	118	TYR	2
1	A	119	LYS	2
1	A	138	ILE	2
1	A	156	ASN	2
1	A	193	SER	2
1	A	197	LYS	2
1	A	281	PHE	2
1	A	284	LEU	2
1	A	64	TRP	2
1	A	86	THR	2
1	A	132	ASP	2
1	A	155	MET	2
1	A	167	SER	2
1	A	266	LYS	2
1	A	24	PHE	2

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Mol	Chain	Res	Type	Models (Total)
1	A	31	LEU	2
1	A	34	LYS	2
1	A	43	SER	2
1	A	53	LYS	2
1	A	72	THR	2
1	A	154	GLN	2
1	A	203	GLU	2
1	A	211	THR	2
1	A	242	LEU	2
1	A	59	GLU	2
1	A	80	THR	2
1	A	120	ARG	2
1	A	256	LYS	2
1	A	28	LYS	2
1	A	30	ASP	2
1	A	176	ASP	2
1	A	201	LYS	2
1	A	255	ILE	2
1	A	15	ARG	2
1	A	89	ASP	2
1	A	3	VAL	2
1	A	113	LYS	2
1	A	114	ILE	2
1	A	194	ILE	2
1	A	237	VAL	2
1	A	173	TYR	2
1	A	183	ASN	2
1	A	61	LYS	2
1	A	9	ASP	1
1	A	33	THR	1
1	A	37	ASN	1
1	A	79	ASN	1
1	A	218	ARG	1
1	A	234	SER	1
1	A	12	LYS	1
1	A	16	ASP	1
1	A	48	ASN	1
1	A	67	TYR	1
1	A	91	LEU	1
1	A	65	THR	1
1	A	146	TYR	1
1	A	157	PHE	1

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Mol	Chain	Res	Type	Models (Total)
1	A	181	HIS	1
1	A	200	LYS	1
1	A	227	ILE	1
1	A	277	LEU	1
1	A	285	GLU	1
1	A	44	SER	1
1	A	280	GLU	1
1	A	76	ASN	1
1	A	249	GLN	1
1	A	251	LEU	1
1	A	267	ASN	1
1	A	275	LEU	1
1	A	13	SER	1
1	A	165	THR	1
1	A	217	THR	1
1	A	262	LEU	1
1	A	90	GLN	1
1	A	100	ASP	1
1	A	106	ASN	1
1	A	116	THR	1
1	A	153	TYR	1
1	A	96	LYS	1
1	A	130	ASP	1
1	A	230	ASP	1
1	A	73	GLU	1
1	A	93	ARG	1
1	A	110	LYS	1
1	A	147	GLU	1
1	A	166	GLN	1
1	A	199	ASN	1
1	A	226	GLN	1
1	A	269	ASN	1
1	A	98	THR	1
1	A	103	PHE	1
1	A	207	ASN	1
1	A	208	LEU	1
1	A	268	VAL	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds for which Mogul statistics could be retrieved, the number of bonds that are observed in the model and the number of bonds that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length is the number of standard deviations the observed value is removed from the expected value. A bond length with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
2	NAI	A	301	-	47,48,48	1.05±0.00	2±0 (4±0%)

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of angles that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond angle is the number of standard deviations the observed value is removed from the expected value. A bond angle with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
2	NAI	A	301	-	64,73,73	1.62±0.00	9±0 (14±0%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAI	A	301	-	-	0±0,29,72,72	0±0,5,5,5

All unique bond outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	A	301	NAI	C7N-C3N	3.20	1.41	1.48	7	10
2	A	301	NAI	PN-O2N	3.11	1.61	1.50	4	10

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

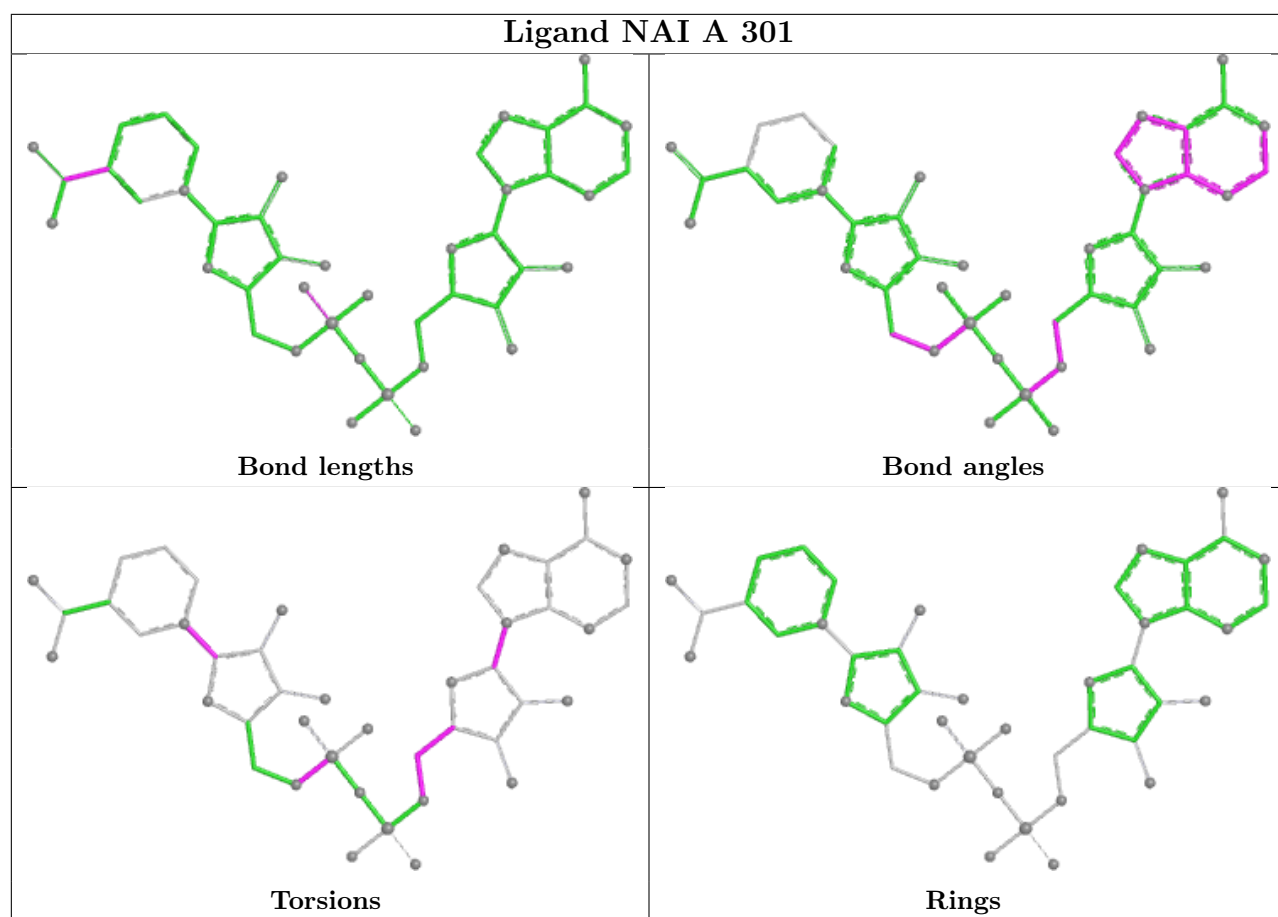
Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
2	A	301	NAI	C5A-C4A-N3A	5.58	119.04	126.72	6	10
2	A	301	NAI	N3A-C4A-N9A	4.58	134.95	127.17	2	10
2	A	301	NAI	N3A-C2A-N1A	4.03	122.47	128.58	8	10
2	A	301	NAI	C5A-N7A-C8A	3.86	109.51	103.45	5	10
2	A	301	NAI	C2A-N3A-C4A	3.60	120.62	111.83	2	10
2	A	301	NAI	C4A-C5A-N7A	3.02	107.13	110.58	9	10
2	A	301	NAI	N9A-C8A-N7A	2.83	109.92	113.94	1	10
2	A	301	NAI	PA-O5B-C5B	2.55	106.75	121.35	9	10
2	A	301	NAI	PN-O5D-C5D	2.54	106.78	121.35	3	10

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

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

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *VDAC_WT_NMRStar.str*

7.1.1 Bookkeeping

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

Total number of shifts	1507
Number of shifts mapped to atoms	1504
Number of unparsed shifts	0
Number of shifts with mapping errors	3
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	2

The following assigned chemical shifts were not mapped to the molecules present in the coordinate file.

- No matching atom found in the structure. All 3 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	287	HIS	H	7.821	0.020	1
1	A	287	HIS	CA	57.177	0.300	1
1	A	287	HIS	N	125.884	0.300	1

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	254	0.14 ± 0.07	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	210	-0.17 ± 0.09	None needed (< 0.5 ppm)
$^{13}\text{C}'$	180	0.86 ± 0.11	Should be applied
^{15}N	250	-0.93 ± 0.37	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. 1501 atoms were assigned a chemical shift out of a possible 3714. 0 out of 41 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	931/1440 (65%)	249/594 (42%)	433/568 (76%)	249/278 (90%)
Sidechain	562/1966 (29%)	255/1274 (20%)	305/619 (49%)	2/73 (3%)
Aromatic	8/308 (3%)	4/150 (3%)	0/151 (0%)	4/7 (57%)
Overall	1501/3714 (40%)	508/2018 (25%)	738/1338 (55%)	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. 1501 atoms were assigned a chemical shift out of a possible 3729. 0 out of 41 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	931/1445 (64%)	249/596 (42%)	433/570 (76%)	249/279 (89%)
Sidechain	562/1976 (28%)	255/1281 (20%)	305/622 (49%)	2/73 (3%)
Aromatic	8/308 (3%)	4/150 (3%)	0/151 (0%)	4/7 (57%)
Overall	1501/3729 (40%)	508/2027 (25%)	738/1343 (55%)	255/359 (71%)

7.1.4 Statistically unusual chemical shifts [i](#)

The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	116	THR	HG1	4.25	0.08 – 2.19	14.8
1	A	182	THR	HG1	3.58	0.08 – 2.19	11.6

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. If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A:

