



Full wwPDB NMR Structure Validation Report ⓘ

Apr 27, 2016 – 03:51 AM BST

PDB ID : 2MZZ
Title : NMR structure of APOBEC3G NTD variant, sNTD
Authors : Kouno, T.; Luengas, E.M.; Shigematu, M.; Shandilya, S.M.D.; Zhang, J.;
Chen, L.; Hara, M.; Schiffer, C.A.; Harris, R.S.; Matsuo, H.
Deposited on : 2015-02-28

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
<http://wwpdb.org/validation/2016/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 : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : rb-20027457
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027457

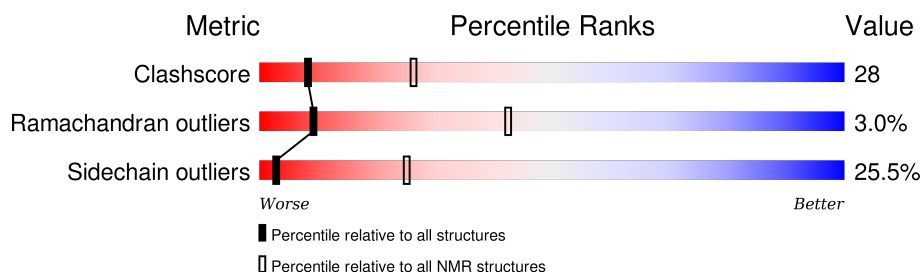
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 33%.

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	114402	11133
Ramachandran outliers	111179	9975
Sidechain outliers	111093	9958

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	180	

2 Ensemble composition and analysis

This entry contains 10 models. Model 2 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *minimized average structure*.

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:4-A:31, A:40-A:47, A:56-A:180 (161)	0.90	2

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 2 clusters and 1 single-model cluster was found.

Cluster number	Models
1	1, 2, 3, 4, 5, 8, 9
2	6, 7
Single-model clusters	10

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2938 atoms, of which 1432 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Apolipoprotein B mRNA-editing enzyme, catalytic polypeptide-like 3G variant.

Mol	Chain	Residues	Atoms						Trace
1	A	180	Total	C	H	N	O	S	0
			2937	965	1432	259	273	8	

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

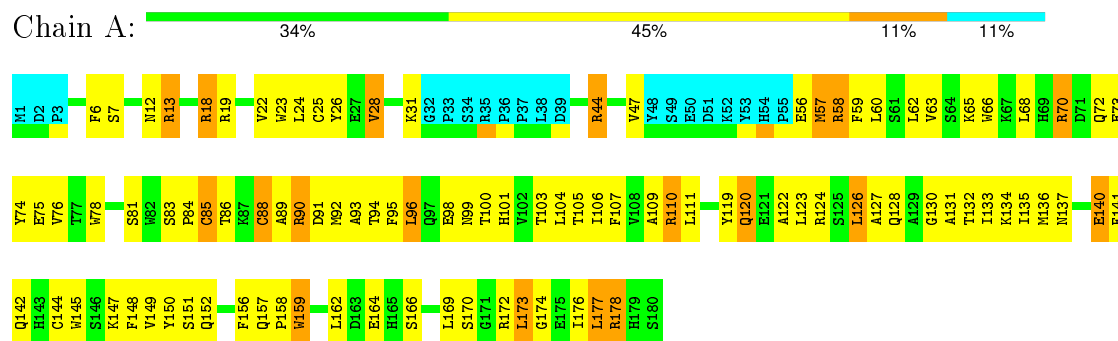
Mol	Chain	Residues	Atoms	
2	A	1	Total	Zn
			1	1

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: Apolipoprotein B mRNA-editing enzyme, catalytic polypeptide-like 3G variant

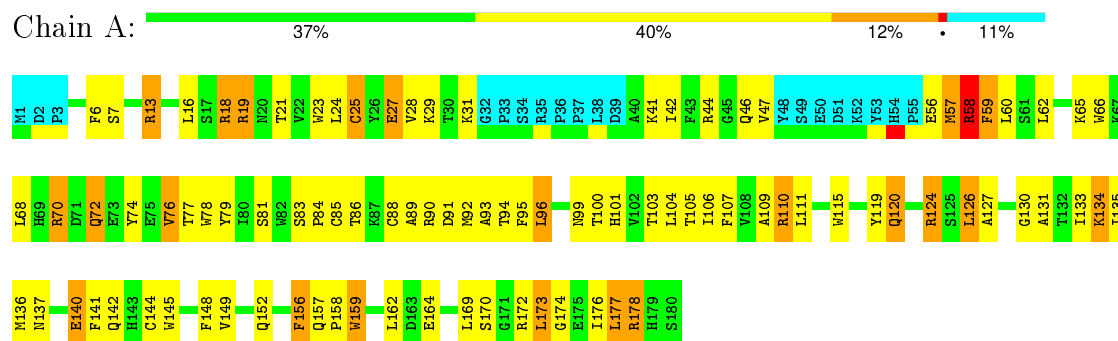


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

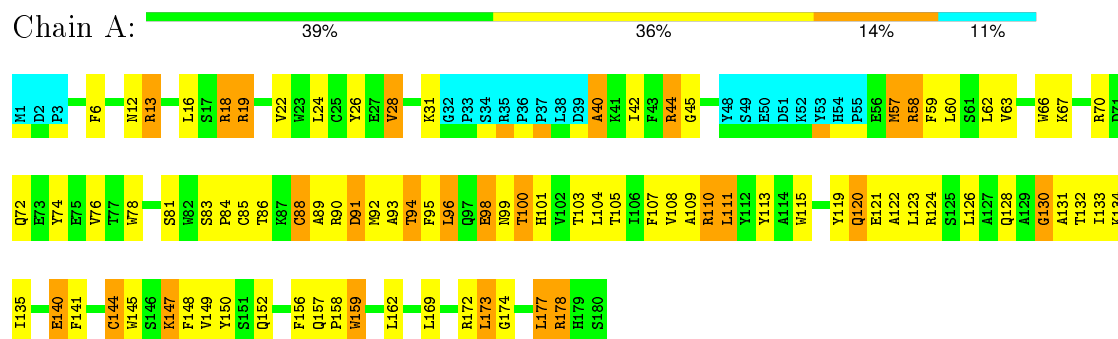
4.2.1 Score per residue for model 1

- Molecule 1: Apolipoprotein B mRNA-editing enzyme, catalytic polypeptide-like 3G variant



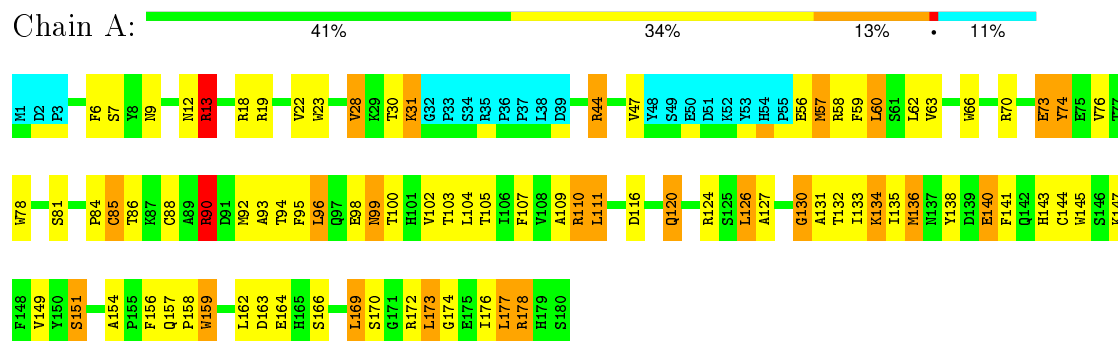
4.2.2 Score per residue for model 2 (medoid)

- Molecule 1: Apolipoprotein B mRNA-editing enzyme, catalytic polypeptide-like 3G variant



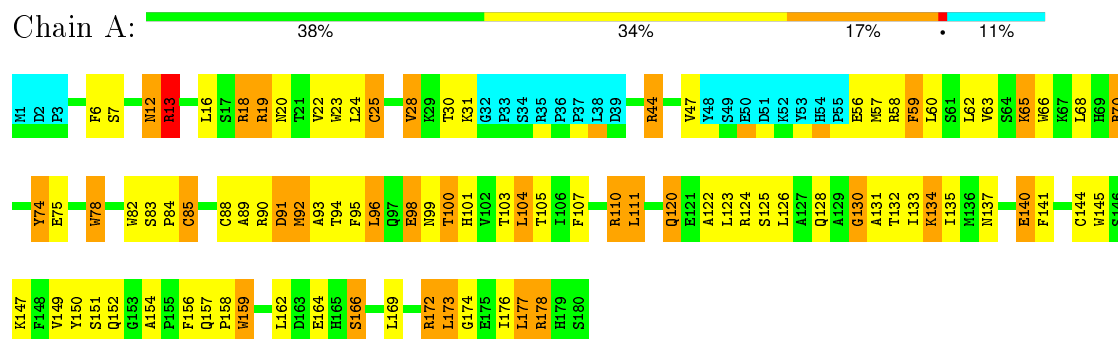
4.2.3 Score per residue for model 3

- Molecule 1: Apolipoprotein B mRNA-editing enzyme, catalytic polypeptide-like 3G variant



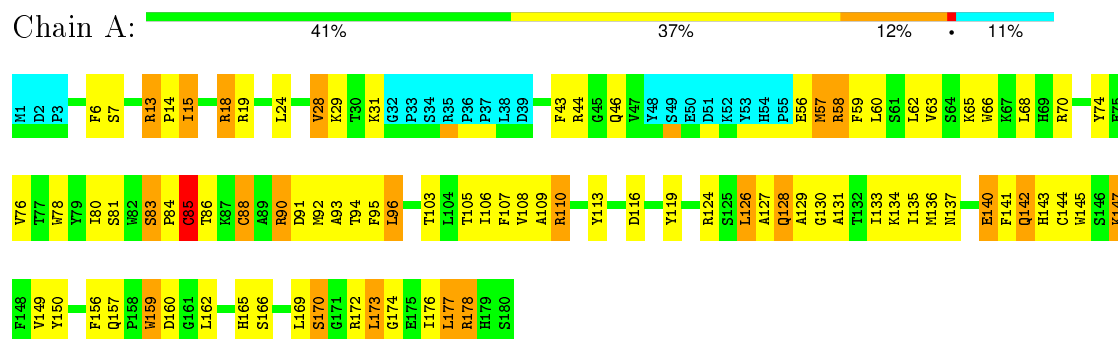
4.2.4 Score per residue for model 4

- Molecule 1: Apolipoprotein B mRNA-editing enzyme, catalytic polypeptide-like 3G variant



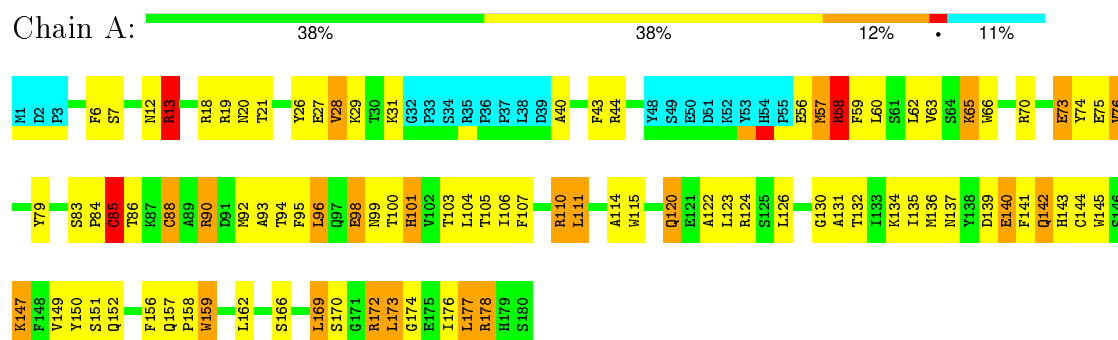
4.2.5 Score per residue for model 5

- Molecule 1: Apolipoprotein B mRNA-editing enzyme, catalytic polypeptide-like 3G variant



4.2.6 Score per residue for model 6

- Molecule 1: Apolipoprotein B mRNA-editing enzyme, catalytic polypeptide-like 3G variant



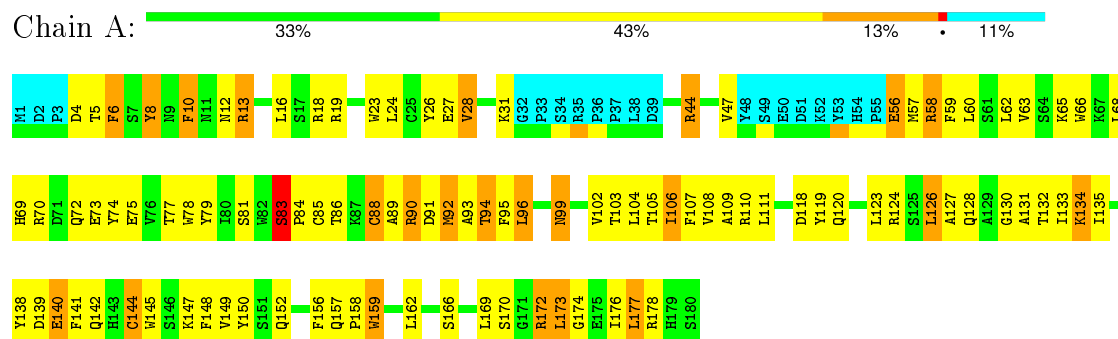
4.2.7 Score per residue for model 7

- Molecule 1: Apolipoprotein B mRNA-editing enzyme, catalytic polypeptide-like 3G variant



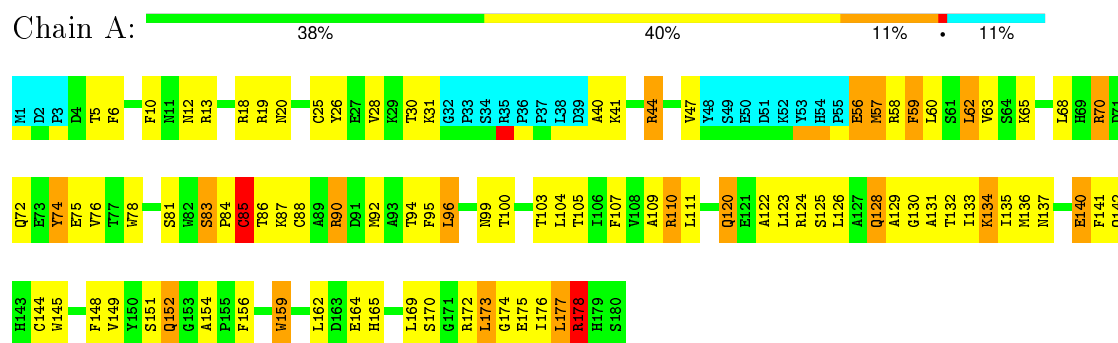
4.2.8 Score per residue for model 8

- Molecule 1: Apolipoprotein B mRNA-editing enzyme, catalytic polypeptide-like 3G variant



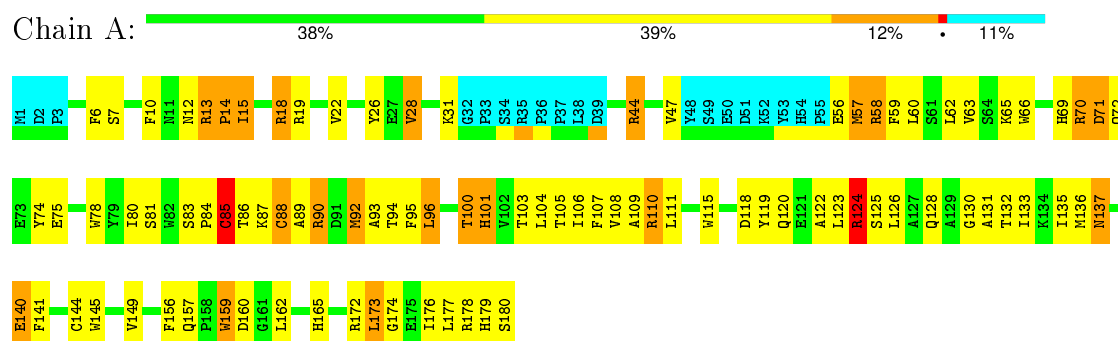
4.2.9 Score per residue for model 9

- Molecule 1: Apolipoprotein B mRNA-editing enzyme, catalytic polypeptide-like 3G variant



4.2.10 Score per residue for model 10

- Molecule 1: Apolipoprotein B mRNA-editing enzyme, catalytic polypeptide-like 3G variant



5 Refinement protocol and experimental data overview

The models were refined using the following method: *simulated annealing*.

Of the 100 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
X-PLOR NIH	structure solution	
X-PLOR NIH	refinement	

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)	2mzz_cs.str
Number of chemical shift lists	1
Total number of shifts	753
Number of shifts mapped to atoms	753
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	33%

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

6 Model quality

6.1 Standard geometry

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

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	11.0±0.0
All	All	0	110

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	44	ARG	Sidechain	10
1	A	19	ARG	Sidechain	10
1	A	178	ARG	Sidechain	10
1	A	172	ARG	Sidechain	10
1	A	18	ARG	Sidechain	10
1	A	70	ARG	Sidechain	10
1	A	110	ARG	Sidechain	10
1	A	90	ARG	Sidechain	10
1	A	58	ARG	Sidechain	10
1	A	13	ARG	Sidechain	10
1	A	124	ARG	Sidechain	10

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	1351	1294	1294	75±13
All	All	13520	12940	12940	750

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 28.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:60:LEU:HD13	1:A:95:PHE:CG	0.90	2.01	7	4
1:A:56:GLU:C	1:A:60:LEU:HD13	0.90	1.86	8	1
1:A:93:ALA:HB2	1:A:126:LEU:HG	0.85	1.47	6	4
1:A:111:LEU:HD22	1:A:169:LEU:HD13	0.84	1.45	6	1
1:A:57:MET:HA	1:A:60:LEU:HD12	0.83	1.47	5	4
1:A:60:LEU:HD22	1:A:95:PHE:CE1	0.83	2.08	2	4
1:A:92:MET:CE	1:A:104:LEU:HD21	0.82	2.04	4	1
1:A:62:LEU:HD22	1:A:63:VAL:N	0.82	1.89	9	1
1:A:22:VAL:HG13	1:A:83:SER:HB2	0.80	1.52	2	1
1:A:92:MET:SD	1:A:104:LEU:HD11	0.78	2.18	4	1
1:A:60:LEU:HD23	1:A:60:LEU:N	0.78	1.94	3	1
1:A:123:LEU:HA	1:A:126:LEU:HD13	0.76	1.57	4	5
1:A:127:ALA:HB2	1:A:133:ILE:HD13	0.76	1.54	5	4
1:A:126:LEU:CD1	1:A:133:ILE:HD11	0.76	2.10	3	5
1:A:109:ALA:HB2	1:A:136:MET:SD	0.76	2.20	3	1
1:A:145:TRP:CE3	1:A:149:VAL:HG21	0.76	2.16	7	9
1:A:93:ALA:HA	1:A:126:LEU:HD23	0.75	1.58	3	3
1:A:60:LEU:HD13	1:A:95:PHE:CB	0.75	2.11	10	4
1:A:92:MET:SD	1:A:106:ILE:HD11	0.75	2.21	10	2
1:A:85:CYS:HA	1:A:88:CYS:HB3	0.74	1.59	1	4
1:A:62:LEU:HD12	1:A:63:VAL:N	0.73	1.98	4	8
1:A:60:LEU:HD13	1:A:95:PHE:CD1	0.72	2.19	6	5
1:A:126:LEU:O	1:A:126:LEU:HD22	0.71	1.85	3	3
1:A:96:LEU:HD12	1:A:131:ALA:HB2	0.70	1.63	6	10
1:A:92:MET:SD	1:A:106:ILE:CD1	0.70	2.79	10	5
1:A:126:LEU:HD22	1:A:126:LEU:O	0.70	1.86	8	2
1:A:84:PRO:O	1:A:88:CYS:HB2	0.70	1.86	6	5
1:A:93:ALA:CA	1:A:126:LEU:HD23	0.69	2.17	8	5
1:A:60:LEU:CD2	1:A:95:PHE:CG	0.69	2.75	8	1
1:A:56:GLU:O	1:A:60:LEU:HD13	0.69	1.86	8	1
1:A:78:TRP:CZ3	1:A:92:MET:HG2	0.69	2.22	4	1
1:A:85:CYS:HA	1:A:88:CYS:SG	0.68	2.28	7	3
1:A:62:LEU:C	1:A:62:LEU:HD12	0.67	2.09	3	4
1:A:169:LEU:HD12	1:A:169:LEU:O	0.67	1.89	6	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:62:LEU:HD13	1:A:66:TRP:CE2	0.67	2.25	3	8
1:A:80:ILE:HD12	1:A:106:ILE:HG23	0.67	1.67	10	2
1:A:60:LEU:HD23	1:A:95:PHE:CD1	0.66	2.24	8	1
1:A:60:LEU:HD11	1:A:95:PHE:CD1	0.66	2.25	4	2
1:A:60:LEU:HD22	1:A:95:PHE:CG	0.66	2.25	8	1
1:A:92:MET:HE3	1:A:104:LEU:HD21	0.65	1.67	4	1
1:A:135:ILE:HG21	1:A:169:LEU:HG	0.65	1.67	6	2
1:A:92:MET:HE1	1:A:104:LEU:HD21	0.65	1.69	4	1
1:A:59:PHE:CZ	1:A:76:VAL:HG11	0.65	2.27	3	4
1:A:127:ALA:HB2	1:A:133:ILE:CD1	0.65	2.21	5	5
1:A:96:LEU:CD1	1:A:131:ALA:HB2	0.64	2.22	8	8
1:A:79:TYR:CE2	1:A:144:CYS:SG	0.64	2.91	8	1
1:A:26:TYR:CZ	1:A:45:GLY:HA3	0.64	2.27	2	1
1:A:173:LEU:HA	1:A:176:ILE:HD12	0.64	1.69	10	8
1:A:60:LEU:HD22	1:A:95:PHE:CD1	0.64	2.27	3	2
1:A:147:LYS:N	1:A:147:LYS:HD2	0.64	2.08	5	1
1:A:60:LEU:HD13	1:A:95:PHE:HB2	0.64	1.68	6	3
1:A:81:SER:HA	1:A:109:ALA:HB3	0.63	1.70	8	5
1:A:62:LEU:HD12	1:A:62:LEU:C	0.63	2.14	5	4
1:A:4:ASP:O	1:A:149:VAL:HG13	0.63	1.94	8	1
1:A:107:PHE:CZ	1:A:134:LYS:HD2	0.63	2.29	2	3
1:A:60:LEU:CD2	1:A:60:LEU:N	0.62	2.62	3	1
1:A:60:LEU:HD22	1:A:95:PHE:CZ	0.62	2.29	7	2
1:A:56:GLU:HG3	1:A:92:MET:HA	0.62	1.71	8	1
1:A:60:LEU:HB3	1:A:95:PHE:CE2	0.62	2.30	8	1
1:A:147:LYS:HD2	1:A:147:LYS:N	0.62	2.08	6	2
1:A:133:ILE:HD12	1:A:133:ILE:N	0.61	2.09	8	4
1:A:84:PRO:O	1:A:88:CYS:CB	0.61	2.48	10	5
1:A:126:LEU:HD13	1:A:126:LEU:C	0.61	2.15	7	3
1:A:62:LEU:C	1:A:62:LEU:HD22	0.60	2.15	9	1
1:A:133:ILE:N	1:A:133:ILE:HD12	0.60	2.12	1	5
1:A:117:PRO:HB2	1:A:176:ILE:HG23	0.60	1.72	7	1
1:A:22:VAL:HG21	1:A:81:SER:CB	0.60	2.27	3	1
1:A:85:CYS:HA	1:A:88:CYS:CB	0.60	2.27	1	4
1:A:122:ALA:O	1:A:126:LEU:HD12	0.60	1.96	6	5
1:A:85:CYS:HA	1:A:88:CYS:HB2	0.60	1.73	7	1
1:A:62:LEU:HB3	1:A:66:TRP:CZ2	0.60	2.32	1	1
1:A:60:LEU:HB3	1:A:95:PHE:CD1	0.59	2.32	7	3
1:A:60:LEU:CD2	1:A:95:PHE:CD1	0.59	2.85	3	2
1:A:126:LEU:C	1:A:126:LEU:HD13	0.59	2.18	1	2
1:A:173:LEU:HG	1:A:174:GLY:N	0.58	2.13	3	10

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:4:ASP:C	1:A:149:VAL:HG13	0.58	2.18	8	1
1:A:57:MET:HA	1:A:60:LEU:CD1	0.58	2.28	1	7
1:A:86:THR:HG23	1:A:119:TYR:CD2	0.58	2.34	7	1
1:A:60:LEU:N	1:A:60:LEU:HD12	0.58	2.12	8	1
1:A:111:LEU:HD12	1:A:135:ILE:HD11	0.58	1.74	10	1
1:A:177:LEU:HD23	1:A:178:ARG:HG3	0.58	1.76	5	3
1:A:159:TRP:CD1	1:A:162:LEU:HB2	0.58	2.34	7	10
1:A:96:LEU:HD11	1:A:130:GLY:C	0.57	2.20	7	10
1:A:111:LEU:HD21	1:A:169:LEU:HD22	0.57	1.76	2	1
1:A:62:LEU:HD13	1:A:66:TRP:CZ2	0.57	2.35	4	5
1:A:96:LEU:HG	1:A:104:LEU:HD12	0.57	1.75	4	3
1:A:60:LEU:HD23	1:A:95:PHE:CE1	0.57	2.34	8	1
1:A:56:GLU:HG2	1:A:95:PHE:CB	0.56	2.30	8	1
1:A:85:CYS:O	1:A:89:ALA:HB2	0.56	2.00	8	3
1:A:136:MET:HB2	1:A:141:PHE:CZ	0.56	2.36	5	5
1:A:96:LEU:HB2	1:A:104:LEU:HD12	0.56	1.75	4	1
1:A:93:ALA:CB	1:A:126:LEU:HG	0.56	2.31	4	2
1:A:142:GLN:HG3	1:A:143:HIS:N	0.56	2.15	6	2
1:A:26:TYR:CE1	1:A:45:GLY:HA3	0.56	2.36	2	1
1:A:26:TYR:CE2	1:A:45:GLY:HA3	0.56	2.36	2	1
1:A:137:ASN:HA	1:A:166:SER:HB2	0.55	1.77	7	2
1:A:60:LEU:HD13	1:A:95:PHE:HD1	0.55	1.62	2	1
1:A:135:ILE:CD1	1:A:169:LEU:HD11	0.55	2.32	3	2
1:A:83:SER:HB2	1:A:84:PRO:HD2	0.55	1.79	2	3
1:A:177:LEU:HD23	1:A:178:ARG:HG2	0.55	1.78	3	1
1:A:60:LEU:CD1	1:A:95:PHE:CD1	0.55	2.89	2	1
1:A:56:GLU:HG2	1:A:95:PHE:HB2	0.55	1.79	8	1
1:A:26:TYR:HB2	1:A:78:TRP:CD1	0.55	2.36	9	2
1:A:56:GLU:HG2	1:A:91:ASP:HB3	0.55	1.79	5	1
1:A:83:SER:N	1:A:84:PRO:HD3	0.55	2.17	6	1
1:A:60:LEU:HD12	1:A:60:LEU:H	0.54	1.62	8	1
1:A:145:TRP:CD1	1:A:156:PHE:HB2	0.54	2.37	5	5
1:A:62:LEU:HD13	1:A:62:LEU:N	0.54	2.18	9	1
1:A:107:PHE:CE2	1:A:140:GLU:CB	0.54	2.90	7	4
1:A:111:LEU:HD22	1:A:176:ILE:CD1	0.54	2.33	8	1
1:A:135:ILE:HG21	1:A:169:LEU:CB	0.54	2.32	1	6
1:A:126:LEU:HD13	1:A:127:ALA:N	0.54	2.18	3	4
1:A:96:LEU:HD12	1:A:104:LEU:HD12	0.54	1.80	9	3
1:A:137:ASN:HA	1:A:166:SER:CB	0.53	2.31	7	3
1:A:28:VAL:HG13	1:A:59:PHE:CZ	0.53	2.38	8	3
1:A:5:THR:HB	1:A:8:TYR:HB2	0.53	1.80	8	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:135:ILE:CG1	1:A:170:SER:HA	0.53	2.33	3	2
1:A:28:VAL:HG23	1:A:43:PHE:HB2	0.53	1.81	6	1
1:A:84:PRO:O	1:A:85:CYS:O	0.53	2.26	10	5
1:A:86:THR:HG23	1:A:119:TYR:CD1	0.53	2.39	1	1
1:A:78:TRP:CE3	1:A:92:MET:SD	0.53	3.02	10	1
1:A:145:TRP:CD1	1:A:156:PHE:CB	0.53	2.92	2	7
1:A:107:PHE:CE2	1:A:140:GLU:HB3	0.53	2.39	5	4
1:A:86:THR:HA	1:A:119:TYR:CE2	0.53	2.39	5	1
1:A:108:VAL:HB	1:A:135:ILE:HD13	0.52	1.80	5	3
1:A:56:GLU:CG	1:A:92:MET:HA	0.52	2.33	8	1
1:A:60:LEU:HB3	1:A:95:PHE:CE1	0.52	2.40	10	3
1:A:145:TRP:HA	1:A:149:VAL:HG23	0.52	1.82	8	1
1:A:60:LEU:HD11	1:A:95:PHE:HD1	0.52	1.65	4	1
1:A:151:SER:OG	1:A:154:ALA:HB2	0.52	2.04	7	2
1:A:22:VAL:HG13	1:A:83:SER:CB	0.52	2.29	2	1
1:A:147:LYS:CE	1:A:147:LYS:HA	0.52	2.35	5	2
1:A:28:VAL:HG12	1:A:74:TYR:CE2	0.52	2.38	4	2
1:A:92:MET:HB3	1:A:126:LEU:HD21	0.52	1.80	2	1
1:A:145:TRP:O	1:A:149:VAL:HB	0.52	2.05	1	8
1:A:56:GLU:O	1:A:56:GLU:HG2	0.52	2.03	8	1
1:A:92:MET:CE	1:A:104:LEU:HD13	0.52	2.35	10	1
1:A:56:GLU:HB3	1:A:78:TRP:CH2	0.52	2.40	3	1
1:A:157:GLN:HB2	1:A:158:PRO:HD2	0.51	1.81	2	6
1:A:6:PHE:CE2	1:A:141:PHE:HB3	0.51	2.39	3	8
1:A:111:LEU:HD22	1:A:176:ILE:HD11	0.51	1.82	8	1
1:A:58:ARG:HD3	1:A:59:PHE:N	0.51	2.20	1	1
1:A:169:LEU:HD12	1:A:169:LEU:C	0.51	2.24	6	1
1:A:86:THR:HA	1:A:119:TYR:CE1	0.51	2.40	2	3
1:A:119:TYR:CZ	1:A:123:LEU:HD11	0.51	2.41	2	2
1:A:85:CYS:HB2	1:A:88:CYS:HB2	0.51	1.82	3	2
1:A:56:GLU:CG	1:A:88:CYS:SG	0.51	2.99	6	2
1:A:62:LEU:CD1	1:A:62:LEU:N	0.51	2.74	9	1
1:A:111:LEU:HB3	1:A:169:LEU:HD13	0.51	1.82	3	1
1:A:30:THR:HG22	1:A:74:TYR:CE1	0.51	2.41	9	1
1:A:28:VAL:HG21	1:A:66:TRP:CH2	0.51	2.40	2	1
1:A:59:PHE:O	1:A:62:LEU:CD1	0.51	2.59	9	1
1:A:62:LEU:HA	1:A:65:LYS:HG2	0.51	1.83	4	3
1:A:22:VAL:O	1:A:22:VAL:HG13	0.51	2.06	4	2
1:A:83:SER:CB	1:A:84:PRO:CD	0.50	2.88	7	4
1:A:96:LEU:CG	1:A:104:LEU:HD12	0.50	2.35	7	4
1:A:169:LEU:C	1:A:169:LEU:HD12	0.50	2.27	3	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:145:TRP:CD1	1:A:156:PHE:HB3	0.50	2.41	1	3
1:A:13:ARG:HB2	1:A:14:PRO:HD3	0.50	1.83	10	1
1:A:140:GLU:HG3	1:A:141:PHE:N	0.50	2.21	1	10
1:A:95:PHE:CE1	1:A:102:VAL:HG11	0.50	2.41	8	1
1:A:138:TYR:O	1:A:142:GLN:HG3	0.50	2.07	8	1
1:A:135:ILE:HG13	1:A:170:SER:HA	0.50	1.84	5	6
1:A:85:CYS:CA	1:A:88:CYS:HB3	0.50	2.35	1	1
1:A:124:ARG:HG2	1:A:125:SER:N	0.50	2.21	10	1
1:A:99:ASN:HB3	1:A:102:VAL:HG12	0.50	1.83	8	2
1:A:29:LYS:HG3	1:A:42:ILE:HG23	0.50	1.84	7	1
1:A:139:ASP:HA	1:A:142:GLN:HG2	0.50	1.82	6	1
1:A:59:PHE:O	1:A:62:LEU:HD11	0.49	2.07	9	1
1:A:111:LEU:HD21	1:A:135:ILE:HD11	0.49	1.83	8	1
1:A:85:CYS:CA	1:A:88:CYS:HB2	0.49	2.36	7	1
1:A:92:MET:C	1:A:92:MET:SD	0.49	2.90	4	1
1:A:12:ASN:HB3	1:A:13:ARG:HD3	0.49	1.84	4	1
1:A:123:LEU:HB3	1:A:133:ILE:HG21	0.49	1.83	2	1
1:A:62:LEU:CD1	1:A:62:LEU:H	0.49	2.20	9	1
1:A:78:TRP:CZ3	1:A:92:MET:CG	0.49	2.96	1	3
1:A:6:PHE:HA	1:A:10:PHE:HB2	0.49	1.85	9	2
1:A:60:LEU:HD23	1:A:95:PHE:CG	0.49	2.43	8	1
1:A:60:LEU:HD22	1:A:95:PHE:CE2	0.49	2.43	5	3
1:A:107:PHE:CZ	1:A:134:LYS:HD3	0.49	2.43	1	5
1:A:162:LEU:C	1:A:162:LEU:HD23	0.48	2.28	6	5
1:A:126:LEU:HD22	1:A:126:LEU:C	0.48	2.26	3	2
1:A:56:GLU:O	1:A:60:LEU:HD11	0.48	2.09	4	1
1:A:126:LEU:C	1:A:126:LEU:HD22	0.48	2.29	5	3
1:A:6:PHE:CZ	1:A:141:PHE:HB3	0.48	2.43	5	4
1:A:80:ILE:HG21	1:A:84:PRO:HD3	0.48	1.85	10	1
1:A:123:LEU:HD22	1:A:133:ILE:HG12	0.48	1.83	4	1
1:A:83:SER:HB3	1:A:84:PRO:HD2	0.48	1.83	7	1
1:A:13:ARG:HD2	1:A:159:TRP:CE2	0.48	2.44	3	3
1:A:159:TRP:CE2	1:A:162:LEU:HD12	0.48	2.43	6	2
1:A:59:PHE:CD1	1:A:59:PHE:C	0.48	2.87	4	2
1:A:83:SER:HB3	1:A:84:PRO:CD	0.48	2.39	7	1
1:A:56:GLU:HA	1:A:78:TRP:CH2	0.48	2.44	7	1
1:A:145:TRP:HE1	1:A:154:ALA:HB3	0.48	1.69	4	3
1:A:56:GLU:O	1:A:60:LEU:CD1	0.48	2.61	4	1
1:A:81:SER:CA	1:A:109:ALA:HB3	0.47	2.39	5	2
1:A:60:LEU:HD21	1:A:95:PHE:HD1	0.47	1.69	9	1
1:A:120:GLN:HB3	1:A:177:LEU:HB2	0.47	1.86	9	6

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:78:TRP:CZ3	1:A:92:MET:HG3	0.47	2.44	1	1
1:A:60:LEU:CD1	1:A:95:PHE:HB2	0.47	2.36	6	2
1:A:93:ALA:CB	1:A:126:LEU:HD23	0.47	2.40	7	1
1:A:60:LEU:HD21	1:A:95:PHE:CD1	0.47	2.44	9	2
1:A:111:LEU:HB3	1:A:176:ILE:HD11	0.47	1.86	10	1
1:A:92:MET:HB3	1:A:126:LEU:CD2	0.47	2.39	2	1
1:A:104:LEU:O	1:A:132:THR:N	0.47	2.48	4	8
1:A:15:ILE:O	1:A:15:ILE:HG22	0.47	2.09	5	1
1:A:148:PHE:CD1	1:A:148:PHE:N	0.47	2.83	8	1
1:A:100:THR:O	1:A:101:HIS:HB2	0.47	2.10	10	2
1:A:99:ASN:O	1:A:101:HIS:N	0.47	2.46	7	1
1:A:177:LEU:HD23	1:A:178:ARG:N	0.47	2.25	9	3
1:A:26:TYR:CZ	1:A:45:GLY:CA	0.47	2.98	2	1
1:A:22:VAL:HG21	1:A:81:SER:HB3	0.47	1.87	3	1
1:A:93:ALA:N	1:A:126:LEU:HD23	0.47	2.24	5	2
1:A:96:LEU:CB	1:A:104:LEU:HD12	0.46	2.40	4	1
1:A:120:GLN:HG2	1:A:176:ILE:HG22	0.46	1.87	3	1
1:A:162:LEU:O	1:A:162:LEU:HD23	0.46	2.10	7	5
1:A:57:MET:O	1:A:60:LEU:HG	0.46	2.09	3	1
1:A:79:TYR:CE1	1:A:140:GLU:HB2	0.46	2.45	1	2
1:A:126:LEU:HD13	1:A:133:ILE:HD11	0.46	1.84	5	3
1:A:27:GLU:CG	1:A:77:THR:HB	0.46	2.40	1	1
1:A:141:PHE:CE2	1:A:162:LEU:HD21	0.46	2.45	5	2
1:A:123:LEU:HD13	1:A:133:ILE:HG21	0.46	1.85	7	2
1:A:59:PHE:O	1:A:63:VAL:HG23	0.46	2.10	3	1
1:A:62:LEU:C	1:A:62:LEU:CD1	0.46	2.83	3	2
1:A:147:LYS:HA	1:A:147:LYS:HE2	0.46	1.86	5	2
1:A:135:ILE:HG21	1:A:169:LEU:CG	0.46	2.39	6	2
1:A:28:VAL:HG23	1:A:43:PHE:HB3	0.46	1.88	5	1
1:A:157:GLN:HB2	1:A:158:PRO:CD	0.46	2.41	8	1
1:A:144:CYS:SG	1:A:148:PHE:CD2	0.46	3.09	7	1
1:A:92:MET:CE	1:A:106:ILE:HD11	0.46	2.40	10	1
1:A:15:ILE:HG22	1:A:15:ILE:O	0.46	2.11	10	1
1:A:92:MET:O	1:A:92:MET:SD	0.46	2.74	4	1
1:A:6:PHE:CD1	1:A:6:PHE:C	0.46	2.90	7	2
1:A:21:THR:O	1:A:21:THR:HG23	0.46	2.10	1	1
1:A:29:LYS:HG3	1:A:75:GLU:HB3	0.46	1.88	6	1
1:A:28:VAL:HG13	1:A:59:PHE:HZ	0.45	1.71	5	2
1:A:23:TRP:HB2	1:A:47:VAL:HB	0.45	1.88	8	2
1:A:111:LEU:HD23	1:A:172:ARG:CB	0.45	2.41	4	1
1:A:93:ALA:HB2	1:A:126:LEU:CG	0.45	2.41	4	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:86:THR:O	1:A:90:ARG:HG3	0.45	2.11	3	5
1:A:6:PHE:CE2	1:A:10:PHE:CE2	0.45	3.05	8	1
1:A:26:TYR:CE1	1:A:59:PHE:CE1	0.45	3.04	8	2
1:A:9:ASN:CG	1:A:22:VAL:HG23	0.45	2.32	3	1
1:A:83:SER:HB2	1:A:84:PRO:CD	0.45	2.42	1	2
1:A:147:LYS:N	1:A:147:LYS:CD	0.45	2.77	2	2
1:A:120:GLN:HB2	1:A:177:LEU:HB2	0.45	1.89	8	1
1:A:44:ARG:HD3	1:A:147:LYS:HB3	0.45	1.88	8	2
1:A:99:ASN:HB3	1:A:102:VAL:CG1	0.45	2.41	3	2
1:A:120:GLN:CG	1:A:177:LEU:HB2	0.45	2.42	7	1
1:A:106:ILE:CD1	1:A:126:LEU:HD11	0.45	2.42	1	1
1:A:60:LEU:CD1	1:A:95:PHE:CB	0.45	2.94	6	1
1:A:144:CYS:O	1:A:148:PHE:HB2	0.45	2.12	8	1
1:A:159:TRP:CD1	1:A:160:ASP:N	0.44	2.85	10	3
1:A:29:LYS:HD2	1:A:42:ILE:HG23	0.44	1.89	1	1
1:A:145:TRP:HA	1:A:149:VAL:CG2	0.44	2.42	3	2
1:A:78:TRP:CZ3	1:A:92:MET:SD	0.44	3.11	10	1
1:A:83:SER:CB	1:A:84:PRO:HD2	0.44	2.42	7	1
1:A:47:VAL:O	1:A:47:VAL:HG13	0.44	2.13	7	1
1:A:83:SER:N	1:A:84:PRO:CD	0.44	2.80	6	1
1:A:91:ASP:O	1:A:94:THR:HB	0.44	2.12	2	2
1:A:92:MET:HE1	1:A:104:LEU:HD13	0.44	1.89	10	1
1:A:136:MET:CG	1:A:136:MET:O	0.44	2.65	6	1
1:A:123:LEU:HA	1:A:126:LEU:CD1	0.44	2.39	6	1
1:A:62:LEU:HA	1:A:65:LYS:CG	0.44	2.43	4	1
1:A:6:PHE:CE2	1:A:144:CYS:HB3	0.44	2.47	8	1
1:A:95:PHE:C	1:A:95:PHE:CD1	0.44	2.91	8	1
1:A:31:LYS:HB3	1:A:73:GLU:CB	0.44	2.43	7	1
1:A:109:ALA:HA	1:A:136:MET:SD	0.44	2.53	10	1
1:A:99:ASN:C	1:A:100:THR:HG23	0.43	2.33	9	3
1:A:111:LEU:HD13	1:A:176:ILE:CD1	0.43	2.42	10	1
1:A:31:LYS:HG2	1:A:73:GLU:CB	0.43	2.43	3	1
1:A:145:TRP:CE2	1:A:149:VAL:HG11	0.43	2.48	2	1
1:A:22:VAL:HG23	1:A:22:VAL:O	0.43	2.13	7	1
1:A:89:ALA:HB2	1:A:119:TYR:OH	0.43	2.14	10	1
1:A:59:PHE:C	1:A:59:PHE:CD1	0.43	2.92	9	1
1:A:135:ILE:HD12	1:A:169:LEU:HD11	0.43	1.88	3	1
1:A:24:LEU:O	1:A:46:GLN:HA	0.43	2.14	5	1
1:A:133:ILE:N	1:A:133:ILE:CD1	0.43	2.79	8	2
1:A:10:PHE:CZ	1:A:79:TYR:HB3	0.43	2.49	8	1
1:A:27:GLU:HG2	1:A:77:THR:HB	0.43	1.91	8	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:111:LEU:CD2	1:A:169:LEU:HD13	0.43	2.31	6	1
1:A:85:CYS:O	1:A:89:ALA:CB	0.43	2.66	8	3
1:A:26:TYR:O	1:A:45:GLY:N	0.43	2.52	2	1
1:A:143:HIS:O	1:A:147:LYS:HG2	0.43	2.14	3	1
1:A:25:CYS:SG	1:A:148:PHE:CE2	0.43	3.11	1	1
1:A:71:ASP:O	1:A:72:GLN:CB	0.43	2.67	10	1
1:A:59:PHE:CZ	1:A:76:VAL:CG1	0.43	3.01	2	1
1:A:92:MET:CE	1:A:106:ILE:HD13	0.43	2.43	8	1
1:A:78:TRP:CZ2	1:A:92:MET:HE2	0.43	2.49	4	1
1:A:86:THR:O	1:A:89:ALA:HB3	0.43	2.13	1	1
1:A:137:ASN:O	1:A:141:PHE:CD2	0.43	2.72	10	3
1:A:59:PHE:O	1:A:62:LEU:HG	0.43	2.14	8	2
1:A:106:ILE:HD12	1:A:126:LEU:HD11	0.43	1.91	1	1
1:A:24:LEU:HD21	1:A:47:VAL:HG21	0.43	1.90	4	1
1:A:58:ARG:HG2	1:A:59:PHE:N	0.42	2.29	2	1
1:A:56:GLU:HB2	1:A:78:TRP:CH2	0.42	2.49	9	2
1:A:145:TRP:CE2	1:A:156:PHE:HB2	0.42	2.49	1	1
1:A:98:GLU:HG3	1:A:99:ASN:N	0.42	2.30	4	3
1:A:135:ILE:HG21	1:A:169:LEU:HB3	0.42	1.90	5	1
1:A:162:LEU:HD23	1:A:162:LEU:O	0.42	2.14	4	4
1:A:24:LEU:HG	1:A:47:VAL:HG23	0.42	1.90	8	1
1:A:139:ASP:HA	1:A:142:GLN:HG3	0.42	1.91	8	1
1:A:89:ALA:HB3	1:A:119:TYR:OH	0.42	2.14	7	1
1:A:138:TYR:HB2	1:A:163:ASP:HB3	0.42	1.91	3	1
1:A:135:ILE:HG12	1:A:173:LEU:HD22	0.42	1.90	5	1
1:A:81:SER:O	1:A:109:ALA:HB3	0.42	2.15	10	1
1:A:145:TRP:NE1	1:A:156:PHE:HB2	0.42	2.30	2	3
1:A:92:MET:HE3	1:A:106:ILE:HD13	0.42	1.91	8	1
1:A:56:GLU:O	1:A:56:GLU:CG	0.42	2.67	8	1
1:A:23:TRP:CB	1:A:47:VAL:HB	0.42	2.44	1	1
1:A:88:CYS:SG	1:A:92:MET:HE3	0.42	2.55	2	1
1:A:144:CYS:O	1:A:148:PHE:N	0.42	2.53	2	1
1:A:6:PHE:CE2	1:A:144:CYS:SG	0.42	3.13	8	1
1:A:23:TRP:CZ3	1:A:25:CYS:SG	0.42	3.13	4	1
1:A:69:HIS:HB3	1:A:101:HIS:NE2	0.42	2.30	10	1
1:A:13:ARG:HG3	1:A:159:TRP:NE1	0.42	2.30	5	1
1:A:92:MET:CE	1:A:104:LEU:HD11	0.42	2.45	4	1
1:A:107:PHE:CE2	1:A:140:GLU:HB2	0.42	2.50	7	1
1:A:108:VAL:HG11	1:A:111:LEU:HD11	0.42	1.92	10	1
1:A:73:GLU:HG3	1:A:101:HIS:CD2	0.42	2.49	6	1
1:A:60:LEU:HD22	1:A:95:PHE:CD2	0.41	2.50	5	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:26:TYR:CD1	1:A:26:TYR:C	0.41	2.93	8	2
1:A:110:ARG:CD	1:A:176:ILE:HD11	0.41	2.45	7	1
1:A:128:GLN:HG3	1:A:129:ALA:N	0.41	2.29	9	3
1:A:85:CYS:O	1:A:88:CYS:HB2	0.41	2.15	7	1
1:A:136:MET:HG3	1:A:141:PHE:CZ	0.41	2.50	3	1
1:A:157:GLN:CB	1:A:158:PRO:HD2	0.41	2.45	1	1
1:A:47:VAL:O	1:A:47:VAL:HG12	0.41	2.15	9	1
1:A:111:LEU:HD23	1:A:172:ARG:HB2	0.41	1.92	4	1
1:A:28:VAL:CG2	1:A:43:PHE:HB2	0.41	2.44	6	1
1:A:13:ARG:N	1:A:14:PRO:HD2	0.41	2.30	10	1
1:A:24:LEU:O	1:A:24:LEU:HD12	0.41	2.16	5	1
1:A:23:TRP:HA	1:A:47:VAL:HG11	0.41	1.91	7	1
1:A:28:VAL:HG23	1:A:43:PHE:O	0.41	2.15	7	1
1:A:145:TRP:CG	1:A:156:PHE:CB	0.41	3.04	2	1
1:A:62:LEU:C	1:A:62:LEU:CD2	0.41	2.88	9	1
1:A:60:LEU:N	1:A:60:LEU:CD1	0.41	2.80	8	1
1:A:10:PHE:HB3	1:A:141:PHE:CE1	0.41	2.51	8	1
1:A:26:TYR:CD1	1:A:59:PHE:CE1	0.41	3.09	6	1
1:A:81:SER:CB	1:A:109:ALA:HB3	0.41	2.45	5	1
1:A:162:LEU:HD23	1:A:162:LEU:C	0.41	2.36	5	1
1:A:107:PHE:CD2	1:A:136:MET:HA	0.41	2.50	3	1
1:A:25:CYS:HB2	1:A:148:PHE:CE2	0.41	2.50	9	1
1:A:162:LEU:C	1:A:162:LEU:CD2	0.41	2.89	3	3
1:A:13:ARG:N	1:A:14:PRO:CD	0.41	2.84	7	2
1:A:120:GLN:HG2	1:A:176:ILE:CG2	0.41	2.45	3	1
1:A:13:ARG:HB3	1:A:14:PRO:HD2	0.41	1.92	5	1
1:A:86:THR:HA	1:A:119:TYR:CZ	0.41	2.51	8	1
1:A:123:LEU:O	1:A:133:ILE:HD13	0.41	2.16	4	1
1:A:28:VAL:HG12	1:A:74:TYR:HE2	0.41	1.76	4	1
1:A:136:MET:HB2	1:A:140:GLU:HG2	0.41	1.91	3	1
1:A:27:GLU:HB3	1:A:44:ARG:HG2	0.40	1.92	8	1
1:A:22:VAL:HB	1:A:82:TRP:CZ2	0.40	2.51	4	1
1:A:92:MET:CE	1:A:104:LEU:CD1	0.40	2.99	10	1
1:A:88:CYS:SG	1:A:92:MET:CE	0.40	3.09	2	1
1:A:115:TRP:N	1:A:115:TRP:CD1	0.40	2.89	2	1
1:A:175:GLU:HG2	1:A:178:ARG:HD3	0.40	1.92	9	1
1:A:141:PHE:O	1:A:145:TRP:N	0.40	2.52	8	1
1:A:136:MET:O	1:A:136:MET:CG	0.40	2.70	7	1
1:A:127:ALA:HA	1:A:131:ALA:HB3	0.40	1.92	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	160/180 (89%)	132±5 (83±3%)	23±5 (14±3%)	5±2 (3±1%)	9	42
All	All	1600/1800 (89%)	1322 (83%)	230 (14%)	48 (3%)	9	42

All 21 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	83	SER	5
1	A	85	CYS	5
1	A	100	THR	5
1	A	72	GLN	4
1	A	130	GLY	4
1	A	31	LYS	3
1	A	110	ARG	3
1	A	15	ILE	2
1	A	152	GLN	2
1	A	114	ALA	2
1	A	40	ALA	2
1	A	116	ASP	2
1	A	101	HIS	1
1	A	21	THR	1
1	A	149	VAL	1
1	A	69	HIS	1
1	A	115	TRP	1
1	A	14	PRO	1
1	A	118	ASP	1
1	A	82	TRP	1
1	A	111	LEU	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	144/162 (89%)	107±5 (75±3%)	37±5 (25±3%)	3	25
All	All	1440/1620 (89%)	1073 (75%)	367 (25%)	3	25

All 90 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	159	TRP	10
1	A	177	LEU	10
1	A	173	LEU	10
1	A	105	THR	10
1	A	94	THR	10
1	A	74	TYR	10
1	A	140	GLU	10
1	A	144	CYS	10
1	A	57	MET	10
1	A	28	VAL	10
1	A	103	THR	10
1	A	96	LEU	10
1	A	65	LYS	7
1	A	13	ARG	7
1	A	128	GLN	7
1	A	12	ASN	7
1	A	120	GLN	7
1	A	31	LYS	7
1	A	110	ARG	6
1	A	18	ARG	6
1	A	111	LEU	6
1	A	85	CYS	5
1	A	152	GLN	5
1	A	88	CYS	5
1	A	150	TYR	5
1	A	151	SER	5
1	A	7	SER	5
1	A	68	LEU	5
1	A	92	MET	5
1	A	70	ARG	5
1	A	164	GLU	5
1	A	126	LEU	5
1	A	134	LYS	5
1	A	16	LEU	4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	75	GLU	4
1	A	44	ARG	4
1	A	76	VAL	4
1	A	142	GLN	4
1	A	166	SER	4
1	A	98	GLU	4
1	A	19	ARG	3
1	A	83	SER	3
1	A	101	HIS	3
1	A	147	LYS	3
1	A	165	HIS	3
1	A	91	ASP	3
1	A	137	ASN	3
1	A	56	GLU	3
1	A	78	TRP	3
1	A	178	ARG	3
1	A	20	ASN	3
1	A	73	GLU	3
1	A	59	PHE	3
1	A	87	LYS	3
1	A	172	ARG	2
1	A	27	GLU	2
1	A	113	TYR	2
1	A	169	LEU	2
1	A	179	HIS	2
1	A	41	LYS	2
1	A	90	ARG	2
1	A	156	PHE	2
1	A	157	GLN	2
1	A	30	THR	2
1	A	124	ARG	2
1	A	121	GLU	2
1	A	136	MET	2
1	A	115	TRP	2
1	A	6	PHE	2
1	A	72	GLN	2
1	A	125	SER	2
1	A	25	CYS	2
1	A	99	ASN	2
1	A	100	THR	2
1	A	58	ARG	2
1	A	8	TYR	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	10	PHE	1
1	A	71	ASP	1
1	A	118	ASP	1
1	A	104	LEU	1
1	A	62	LEU	1
1	A	180	SER	1
1	A	116	ASP	1
1	A	67	LYS	1
1	A	60	LEU	1
1	A	5	THR	1
1	A	170	SER	1
1	A	29	LYS	1
1	A	106	ILE	1
1	A	46	GLN	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](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

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 33% for the well-defined parts and 32% for the entire structure.

7.1 Chemical shift list 1

File name: 2mzz_cs.str

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping

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

Total number of shifts	753
Number of shifts mapped to atoms	753
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	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
$^{13}\text{C}_\alpha$	161	0.12 ± 0.14	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	0	—	—
$^{13}\text{C}'$	156	-0.05 ± 0.08	None needed (< 0.5 ppm)
^{15}N	147	-0.50 ± 0.31	None needed (imprecise)

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 33%, i.e. 684 atoms were assigned a chemical shift out of a possible 2102. 0 out of 22 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	684/795 (86%)	264/317 (83%)	285/322 (89%)	135/156 (87%)
Sidechain	0/1035 (0%)	0/612 (0%)	0/367 (0%)	0/56 (0%)

Continued on next page...

Continued from previous page...

	Total	¹ H	¹³ C	¹⁵ N
Aromatic	0/272 (0%)	0/143 (0%)	0/117 (0%)	0/12 (0%)
Overall	684/2102 (33%)	264/1072 (25%)	285/806 (35%)	135/224 (60%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 32%, i.e. 747 atoms were assigned a chemical shift out of a possible 2336. 0 out of 23 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	747/880 (85%)	283/350 (81%)	317/360 (88%)	147/170 (86%)
Sidechain	0/1162 (0%)	0/691 (0%)	0/411 (0%)	0/60 (0%)
Aromatic	0/294 (0%)	0/155 (0%)	0/127 (0%)	0/12 (0%)
Overall	747/2336 (32%)	283/1196 (24%)	317/898 (35%)	147/242 (61%)

7.1.4 Statistically unusual chemical shifts ⓘ

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.

Mol	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	80	ILE	CA	43.84	75.08 – 48.18	-6.6

7.1.5 Random Coil Index (RCI) plots ⓘ

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

Random coil index (RCI) for chain A:

