



Full wwPDB NMR Structure Validation Report ⓘ

Feb 13, 2022 – 09:42 PM EST

PDB ID : 1IKU
Title : myristoylated recoverin in the calcium-free state, NMR, 22 structures
Authors : Tanaka, T.; Ames, J.B.; Harvey, T.S.; Stryer, L.; Ikura, M.
Deposited on : 1996-01-18

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:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
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 : 2.26
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.26

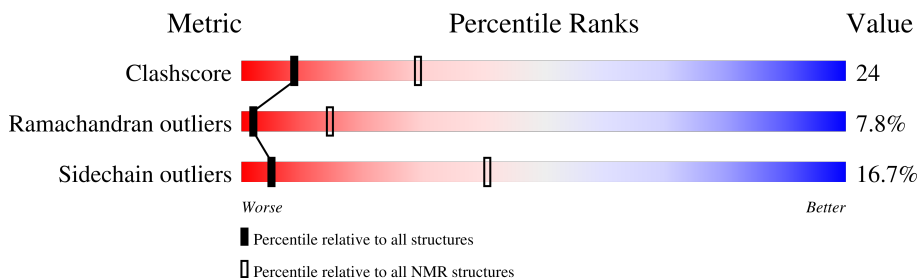
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment was not calculated.

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	201	

2 Ensemble composition and analysis

This entry contains 22 models. Model 14 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:74, A:80-A:189 (183)	0.70	14

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

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

The models can be grouped into 4 clusters and 3 single-model clusters were found.

Cluster number	Models
1	2, 3, 13, 15, 16, 19, 20
2	5, 9, 10, 11, 12, 14
3	6, 7, 17, 21
4	1, 22
Single-model clusters	4; 8; 18

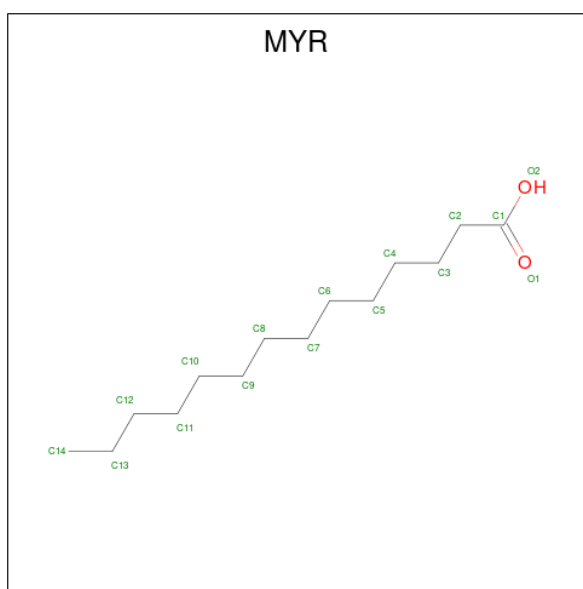
3 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 3053 atoms, of which 1511 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called RECOVERIN.

Mol	Chain	Residues	Atoms					Trace	
			Total	C	H	N	O		S
1	A	188	3011	975	1484	246	303	3	0

- Molecule 2 is MYRISTIC ACID (three-letter code: MYR) (formula: $C_{14}H_{28}O_2$).



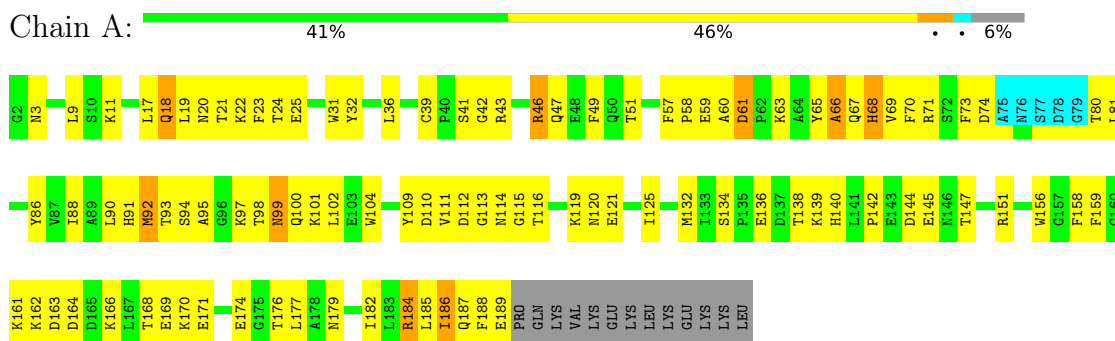
Mol	Chain	Residues	Atoms			
			Total	C	H	O
2	A	1	42	14	27	1

4 Residue-property plots [i](#)

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: RECOVERIN

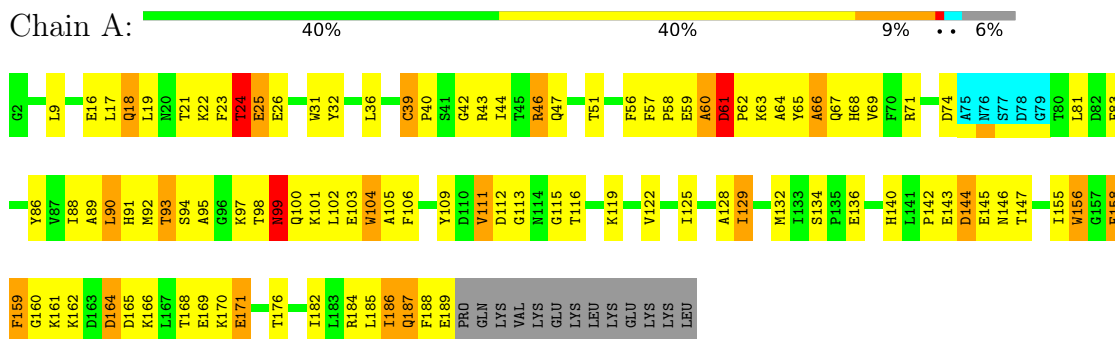


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

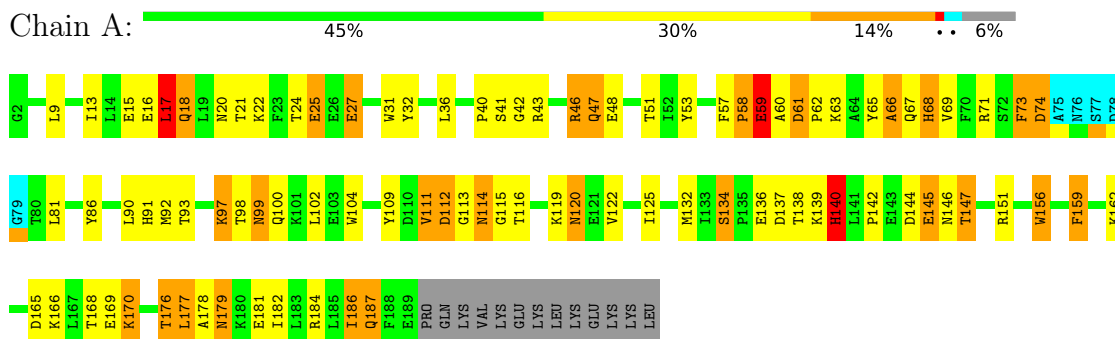
4.2.1 Score per residue for model 1

- Molecule 1: RECOVERIN



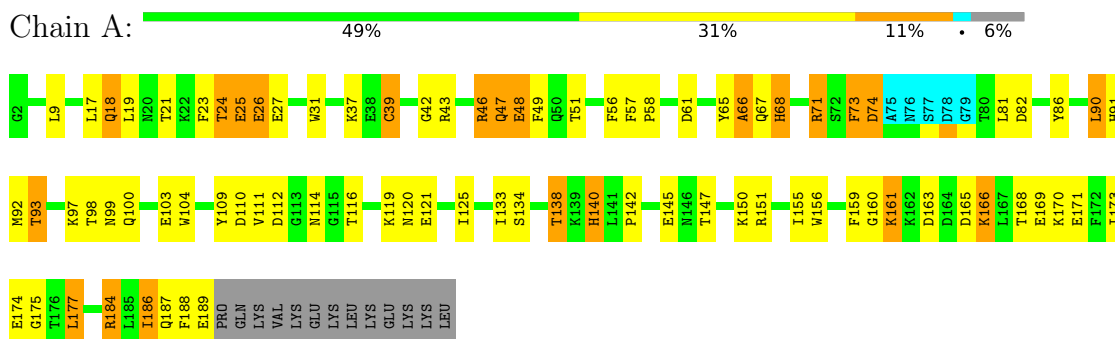
4.2.2 Score per residue for model 2

- Molecule 1: RECOVERIN



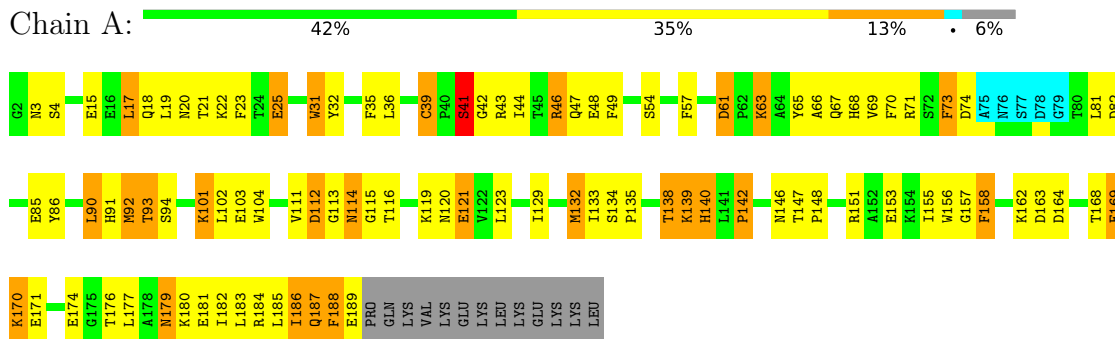
4.2.3 Score per residue for model 3

- Molecule 1: RECOVERIN



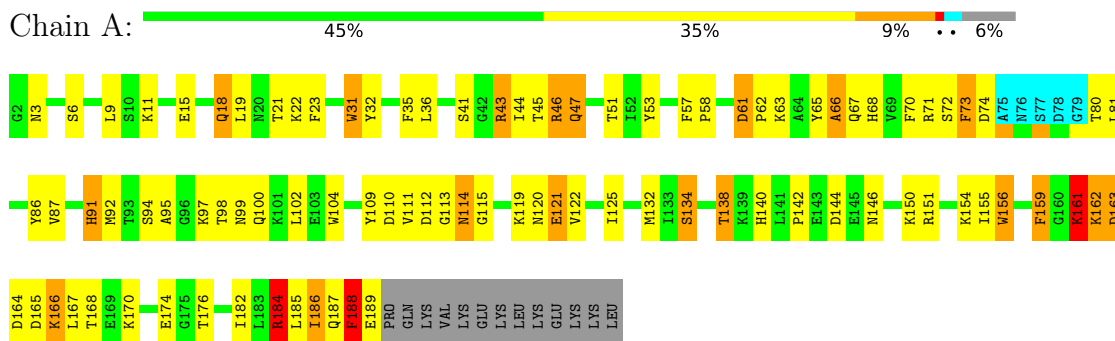
4.2.4 Score per residue for model 4

- Molecule 1: RECOVERIN



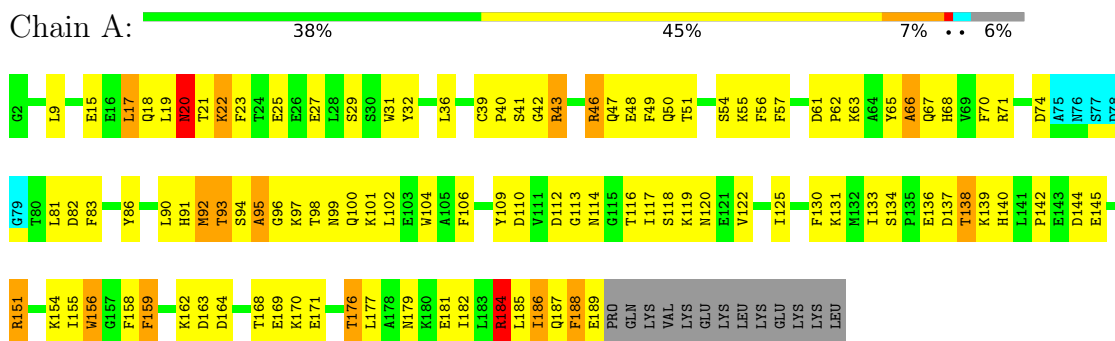
4.2.5 Score per residue for model 5

- Molecule 1: RECOVERIN



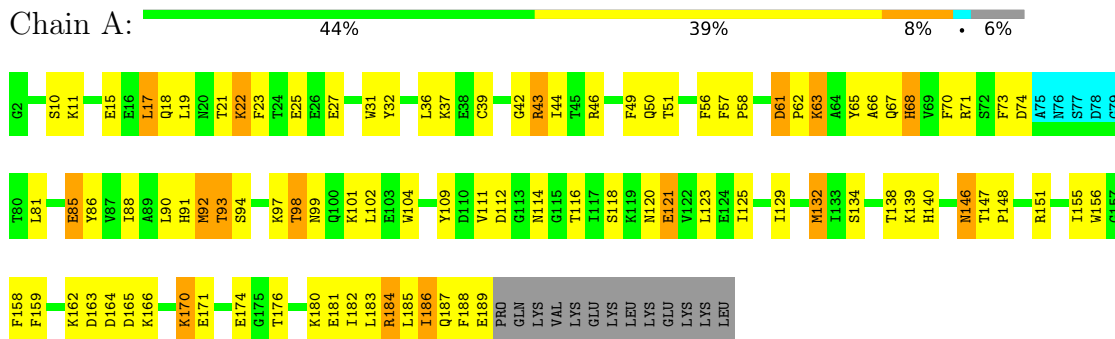
4.2.6 Score per residue for model 6

- Molecule 1: RECOVERIN



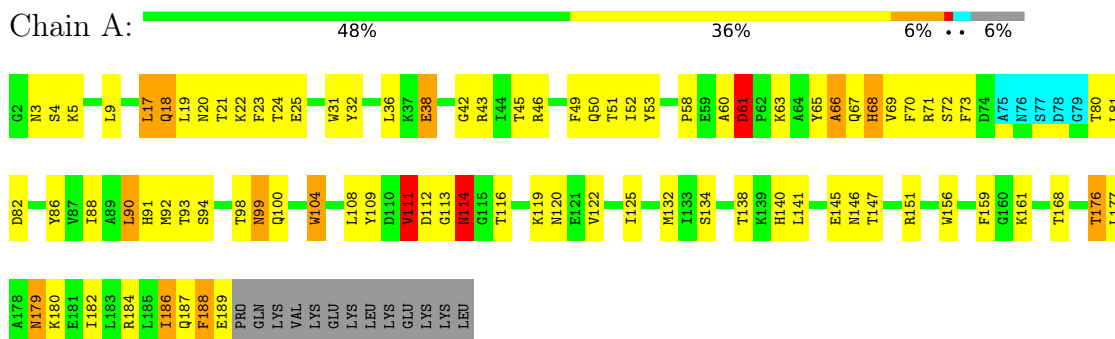
4.2.7 Score per residue for model 7

- Molecule 1: RECOVERIN



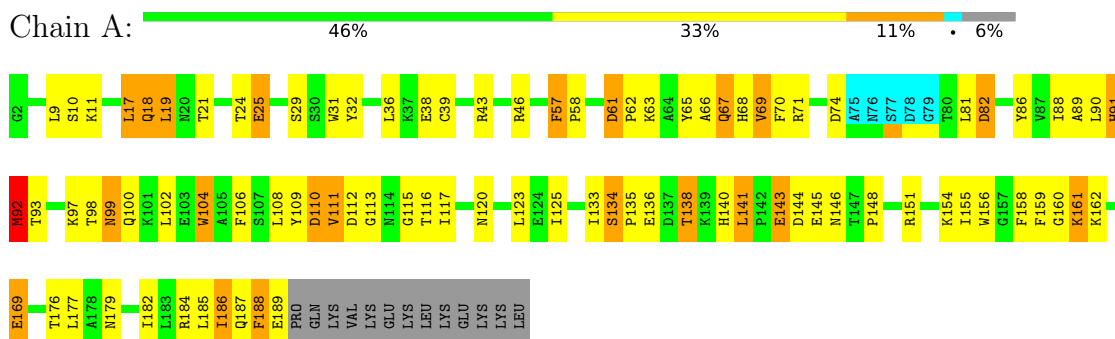
4.2.11 Score per residue for model 11

- Molecule 1: RECOVERIN



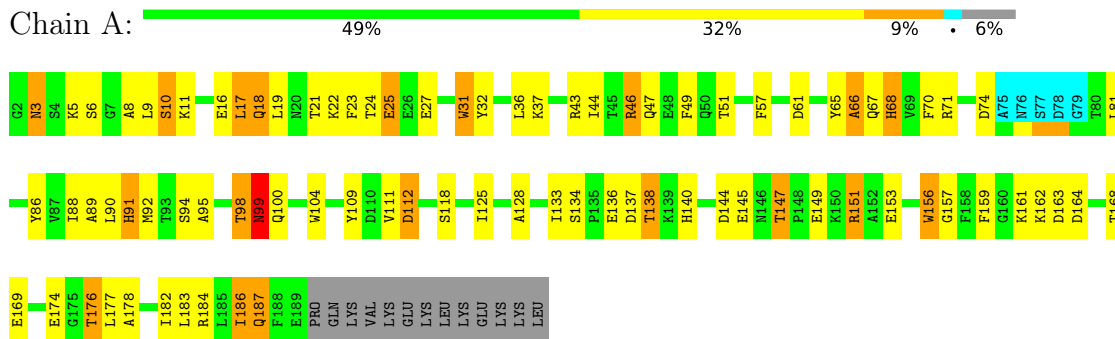
4.2.12 Score per residue for model 12

- Molecule 1: RECOVERIN



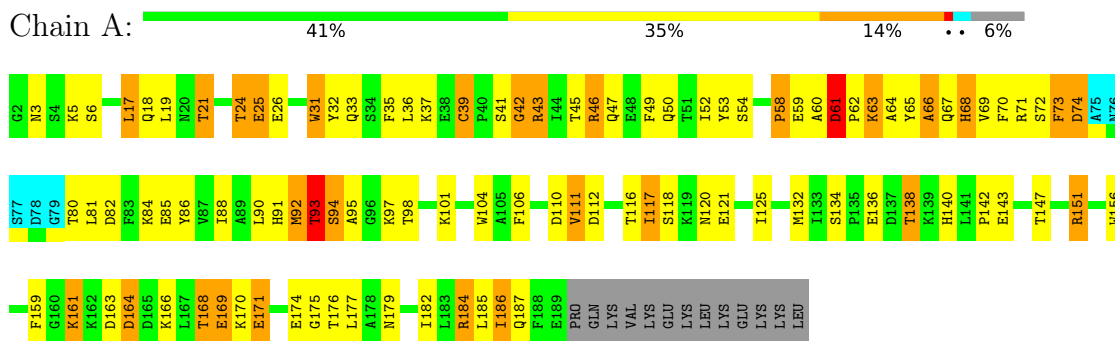
4.2.13 Score per residue for model 13

- Molecule 1: RECOVERIN



4.2.14 Score per residue for model 14 (medoid)

- Molecule 1: RECOVERIN



5 Refinement protocol and experimental data overview

Of the ? calculated structures, 22 were deposited, based on the following criterion: ?.

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

Software name	Classification	Version
X-PLOR	refinement	2.1

No chemical shift data was provided.

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: MYR

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the (average) root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	1.09±0.00	6±0/1529 (0.4± 0.0%)	1.28±0.00	17±0/2058 (0.8± 0.0%)
All	All	1.09	132/33638 (0.4%)	1.28	376/45276 (0.8%)

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	4.7±0.6
All	All	0	103

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
1	A	156	TRP	CG-CD2	-7.53	1.30	1.43	8	22
1	A	104	TRP	CG-CD2	-7.27	1.31	1.43	20	22
1	A	31	TRP	CG-CD2	-6.93	1.31	1.43	20	22
1	A	91	HIS	CG-ND1	-6.39	1.24	1.38	9	22
1	A	140	HIS	CG-ND1	-6.21	1.25	1.38	1	22
1	A	68	HIS	CG-ND1	-6.20	1.25	1.38	11	22

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
1	A	156	TRP	NE1-CE2-CZ2	9.10	140.41	130.40	8	22
1	A	104	TRP	NE1-CE2-CZ2	8.80	140.08	130.40	20	22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	31	TRP	NE1-CE2-CZ2	8.75	140.03	130.40	19	22
1	A	156	TRP	NE1-CE2-CD2	-7.66	99.64	107.30	9	22
1	A	104	TRP	NE1-CE2-CD2	-7.47	99.83	107.30	1	22
1	A	31	TRP	NE1-CE2-CD2	-7.44	99.86	107.30	1	22
1	A	156	TRP	CG-CD1-NE1	-6.59	103.51	110.10	7	22
1	A	31	TRP	CD1-CG-CD2	6.44	111.45	106.30	18	22
1	A	31	TRP	CG-CD1-NE1	-6.43	103.67	110.10	19	22
1	A	104	TRP	CD1-CG-CD2	6.30	111.34	106.30	20	22
1	A	104	TRP	CG-CD1-NE1	-6.28	103.82	110.10	16	22
1	A	156	TRP	CD1-CG-CD2	6.25	111.30	106.30	13	22
1	A	156	TRP	CG-CD2-CE3	-6.15	128.37	133.90	8	22
1	A	104	TRP	CD1-NE1-CE2	5.80	114.22	109.00	5	22
1	A	31	TRP	CD1-NE1-CE2	5.80	114.22	109.00	14	22
1	A	156	TRP	CD1-NE1-CE2	5.73	114.16	109.00	6	22
1	A	156	TRP	CE2-CD2-CG	5.38	111.60	107.30	9	21
1	A	104	TRP	CG-CD2-CE3	-5.15	129.26	133.90	20	3

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	43	ARG	Sidechain	22
1	A	184	ARG	Sidechain	22
1	A	46	ARG	Sidechain	21
1	A	71	ARG	Sidechain	20
1	A	151	ARG	Sidechain	18

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	1496	1461	1460	71±9
2	A	15	27	27	0±1
All	All	33242	32736	32714	1555

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 24.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:111:VAL:HG23	1:A:112:ASP:H	0.88	1.29	2	10
1:A:32:TYR:CE1	1:A:36:LEU:HD11	0.85	2.06	9	14
1:A:69:VAL:HG22	1:A:132:MET:SD	0.79	2.16	11	5
1:A:188:PHE:CD1	1:A:189:GLU:N	0.79	2.51	5	1
1:A:35:PHE:CE1	1:A:39:CYS:SG	0.78	2.77	9	1
1:A:90:LEU:O	1:A:90:LEU:HD13	0.77	1.79	9	5
1:A:111:VAL:HG23	1:A:112:ASP:N	0.77	1.95	15	13
1:A:39:CYS:SG	1:A:42:GLY:N	0.76	2.58	4	7
1:A:68:HIS:CD2	1:A:69:VAL:N	0.76	2.53	16	5
1:A:146:ASN:ND2	1:A:146:ASN:H	0.75	1.77	17	2
1:A:95:ALA:C	1:A:101:LYS:HZ1	0.74	1.85	14	1
1:A:86:TYR:CE1	1:A:90:LEU:CD1	0.74	2.70	16	2
1:A:19:LEU:HD11	1:A:53:TYR:OH	0.73	1.83	17	3
1:A:183:LEU:HD11	1:A:187:GLN:NE2	0.72	1.98	18	4
1:A:186:ILE:CG2	1:A:187:GLN:N	0.72	2.53	17	21
1:A:98:THR:HG23	1:A:99:ASN:H	0.72	1.44	7	2
1:A:17:LEU:HD11	1:A:65:TYR:CE2	0.72	2.19	2	1
1:A:109:TYR:O	1:A:111:VAL:HG13	0.72	1.85	21	1
1:A:188:PHE:CG	1:A:189:GLU:N	0.72	2.56	6	5
1:A:154:LYS:NZ	1:A:185:LEU:HD11	0.71	1.99	12	1
1:A:32:TYR:CZ	1:A:36:LEU:HD11	0.71	2.19	19	19
1:A:69:VAL:HG11	1:A:90:LEU:HD11	0.71	1.61	12	2
1:A:19:LEU:HD13	1:A:57:PHE:CG	0.70	2.22	19	14
1:A:65:TYR:CD2	1:A:66:ALA:N	0.69	2.60	20	11
1:A:170:LYS:H	1:A:170:LYS:CD	0.69	2.01	22	2
1:A:90:LEU:C	1:A:90:LEU:HD13	0.68	2.09	13	4
1:A:158:PHE:CD1	1:A:158:PHE:N	0.68	2.61	10	8
1:A:32:TYR:CE2	1:A:36:LEU:CD1	0.67	2.77	10	7
1:A:69:VAL:HG22	1:A:132:MET:CE	0.67	2.20	22	4
1:A:21:THR:O	1:A:21:THR:HG23	0.66	1.90	6	8
1:A:89:ALA:O	1:A:93:THR:HG22	0.66	1.90	12	5
1:A:106:PHE:CZ	1:A:169:GLU:N	0.66	2.63	10	4
1:A:93:THR:HG23	1:A:93:THR:O	0.66	1.91	9	5
1:A:49:PHE:CD2	1:A:70:PHE:CD2	0.66	2.84	7	3
1:A:86:TYR:CE1	1:A:90:LEU:HD12	0.66	2.26	14	2
1:A:109:TYR:CE2	1:A:125:ILE:HD11	0.65	2.26	18	17
1:A:49:PHE:CD2	1:A:70:PHE:CD1	0.65	2.84	10	4
1:A:53:TYR:CZ	1:A:66:ALA:HB3	0.65	2.27	14	4

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:179:ASN:HD22	1:A:180:LYS:N	0.65	1.89	4	2
1:A:155:ILE:HD11	1:A:185:LEU:O	0.64	1.92	5	2
1:A:68:HIS:CD2	1:A:68:HIS:C	0.64	2.71	16	8
1:A:19:LEU:HD13	1:A:57:PHE:CD2	0.63	2.27	19	8
1:A:145:GLU:N	1:A:145:GLU:OE1	0.63	2.32	10	1
1:A:86:TYR:CZ	1:A:90:LEU:HD11	0.63	2.28	16	2
1:A:161:LYS:CG	1:A:162:LYS:H	0.63	2.06	16	1
1:A:67:GLN:CG	1:A:68:HIS:N	0.63	2.61	9	1
1:A:165:ASP:CG	1:A:166:LYS:N	0.63	2.51	18	6
1:A:94:SER:O	1:A:95:ALA:HB3	0.63	1.94	22	5
1:A:155:ILE:CG2	1:A:159:PHE:CZ	0.63	2.82	1	2
1:A:153:GLU:N	1:A:153:GLU:OE1	0.63	2.32	21	1
1:A:99:ASN:HD22	1:A:100:GLN:N	0.63	1.92	22	2
1:A:25:GLU:OE2	1:A:26:GLU:N	0.62	2.32	17	3
1:A:163:ASP:CG	1:A:164:ASP:N	0.62	2.51	22	1
1:A:25:GLU:H	1:A:25:GLU:CD	0.62	1.98	13	4
1:A:68:HIS:NE2	1:A:69:VAL:HG23	0.62	2.10	15	3
1:A:144:ASP:CG	1:A:145:GLU:N	0.62	2.51	17	1
1:A:45:THR:HG22	1:A:80:THR:HG22	0.62	1.71	10	9
1:A:25:GLU:OE1	1:A:26:GLU:N	0.62	2.32	14	1
1:A:109:TYR:CE1	1:A:121:GLU:OE1	0.62	2.53	3	1
1:A:146:ASN:ND2	1:A:146:ASN:N	0.62	2.45	17	2
1:A:86:TYR:CZ	1:A:90:LEU:CD1	0.62	2.83	16	3
1:A:120:ASN:ND2	1:A:121:GLU:OE2	0.61	2.33	9	1
1:A:24:THR:CG2	1:A:25:GLU:N	0.61	2.64	10	1
1:A:27:GLU:N	1:A:27:GLU:OE1	0.61	2.32	2	1
1:A:32:TYR:CE1	1:A:36:LEU:CD1	0.61	2.83	20	2
1:A:28:LEU:CD2	1:A:56:PHE:CE2	0.61	2.83	15	2
1:A:25:GLU:OE1	1:A:25:GLU:N	0.61	2.34	16	2
1:A:151:ARG:NH1	1:A:185:LEU:HD22	0.61	2.10	18	1
1:A:3:ASN:ND2	1:A:6:SER:OG	0.61	2.32	13	1
1:A:120:ASN:N	1:A:120:ASN:ND2	0.61	2.47	15	1
1:A:164:ASP:N	1:A:164:ASP:OD1	0.61	2.33	1	1
1:A:9:LEU:HD22	1:A:100:GLN:O	0.61	1.95	13	13
1:A:86:TYR:C	1:A:86:TYR:CD1	0.61	2.74	12	10
1:A:12:GLU:OE1	1:A:100:GLN:NE2	0.61	2.34	20	1
1:A:111:VAL:CG2	1:A:112:ASP:H	0.60	2.07	14	7
1:A:97:LYS:N	1:A:97:LYS:CD	0.60	2.62	10	2
1:A:66:ALA:HB1	1:A:86:TYR:OH	0.60	1.95	8	4
1:A:102:LEU:CD1	1:A:176:THR:OG1	0.60	2.49	19	6
1:A:98:THR:HG21	1:A:183:LEU:HD11	0.60	1.74	15	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:86:TYR:CE2	1:A:90:LEU:HD12	0.60	2.32	3	2
1:A:186:ILE:HG22	1:A:187:GLN:N	0.60	2.11	15	15
1:A:61:ASP:HB2	1:A:64:ALA:HB2	0.60	1.74	16	1
1:A:120:ASN:ND2	1:A:120:ASN:H	0.60	1.95	15	1
1:A:46:ARG:CG	1:A:47:GLN:N	0.60	2.65	17	6
1:A:139:LYS:NZ	1:A:140:HIS:NE2	0.60	2.47	4	1
1:A:81:LEU:HD12	1:A:81:LEU:O	0.60	1.97	9	2
1:A:179:ASN:HD22	1:A:179:ASN:N	0.59	1.94	2	1
1:A:89:ALA:O	1:A:93:THR:HG23	0.59	1.97	8	1
1:A:24:THR:OG1	1:A:25:GLU:N	0.59	2.33	8	9
1:A:24:THR:CG2	1:A:27:GLU:OE1	0.59	2.51	2	1
1:A:23:PHE:N	1:A:23:PHE:CD1	0.59	2.65	6	3
1:A:100:GLN:CD	1:A:100:GLN:N	0.59	2.55	12	1
1:A:133:ILE:HD11	1:A:188:PHE:CZ	0.59	2.33	3	3
1:A:99:ASN:ND2	1:A:100:GLN:N	0.59	2.50	22	1
1:A:186:ILE:HG23	1:A:187:GLN:N	0.59	2.10	20	10
1:A:140:HIS:ND1	1:A:140:HIS:C	0.59	2.56	2	1
1:A:139:LYS:NZ	1:A:140:HIS:CD2	0.59	2.71	4	1
1:A:99:ASN:ND2	1:A:99:ASN:H	0.59	1.95	9	1
1:A:32:TYR:CZ	1:A:36:LEU:CD1	0.59	2.86	9	10
1:A:10:SER:OG	1:A:11:LYS:N	0.59	2.34	7	4
1:A:133:ILE:HD11	1:A:188:PHE:CE1	0.59	2.32	16	2
1:A:49:PHE:CD2	1:A:70:PHE:CE1	0.59	2.89	4	2
1:A:82:ASP:OD1	1:A:83:PHE:N	0.59	2.36	6	1
1:A:68:HIS:CG	1:A:69:VAL:N	0.59	2.71	16	3
1:A:133:ILE:CG2	1:A:138:THR:HG23	0.59	2.28	6	2
1:A:86:TYR:CE2	1:A:90:LEU:HD11	0.59	2.33	8	1
1:A:72:SER:OG	1:A:73:PHE:N	0.59	2.35	19	2
1:A:99:ASN:HD22	1:A:99:ASN:N	0.59	1.95	22	2
1:A:61:ASP:N	1:A:61:ASP:OD1	0.58	2.35	7	2
1:A:90:LEU:HD13	1:A:90:LEU:C	0.58	2.19	21	3
1:A:39:CYS:SG	1:A:42:GLY:CA	0.58	2.91	16	3
1:A:69:VAL:HG11	1:A:90:LEU:CD1	0.58	2.28	12	2
1:A:111:VAL:CG2	1:A:112:ASP:N	0.58	2.65	9	8
1:A:183:LEU:CD1	1:A:187:GLN:NE2	0.58	2.66	4	3
1:A:49:PHE:CG	1:A:70:PHE:CE1	0.58	2.91	4	1
1:A:133:ILE:HG22	1:A:138:THR:HG23	0.58	1.76	12	4
1:A:144:ASP:CG	1:A:145:GLU:H	0.58	2.01	17	1
1:A:155:ILE:HD11	1:A:185:LEU:HB3	0.58	1.75	4	3
1:A:98:THR:O	1:A:100:GLN:N	0.58	2.37	15	18
1:A:119:LYS:CG	1:A:120:ASN:N	0.58	2.67	4	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:39:CYS:SG	1:A:43:ARG:N	0.58	2.76	7	2
1:A:92:MET:SD	1:A:186:ILE:CD1	0.58	2.92	12	2
1:A:120:ASN:N	1:A:120:ASN:HD22	0.58	1.97	15	1
1:A:46:ARG:CG	1:A:47:GLN:H	0.57	2.12	13	3
1:A:32:TYR:CD2	1:A:36:LEU:CD1	0.57	2.87	10	4
1:A:161:LYS:CG	1:A:162:LYS:N	0.57	2.65	16	1
1:A:179:ASN:HD22	1:A:180:LYS:H	0.57	1.39	4	2
1:A:99:ASN:HD22	1:A:100:GLN:H	0.57	1.40	22	1
1:A:177:LEU:O	1:A:177:LEU:HD23	0.57	2.00	4	5
1:A:24:THR:HG22	1:A:25:GLU:N	0.57	2.13	10	3
1:A:60:ALA:O	1:A:64:ALA:HB2	0.57	2.00	1	2
1:A:118:SER:OG	1:A:120:ASN:ND2	0.56	2.38	14	1
1:A:146:ASN:H	1:A:146:ASN:HD22	0.56	1.43	7	2
1:A:94:SER:OG	1:A:95:ALA:N	0.56	2.36	17	3
1:A:121:GLU:N	1:A:121:GLU:OE1	0.56	2.39	4	1
1:A:97:LYS:CD	1:A:97:LYS:H	0.56	2.13	10	1
1:A:49:PHE:CG	1:A:70:PHE:CE2	0.56	2.93	11	1
1:A:10:SER:OG	1:A:91:HIS:NE2	0.56	2.33	13	1
1:A:65:TYR:O	1:A:67:GLN:N	0.56	2.39	11	21
1:A:130:PHE:CD1	1:A:151:ARG:NH1	0.56	2.73	6	1
1:A:170:LYS:NZ	1:A:174:GLU:OE2	0.56	2.39	8	1
1:A:109:TYR:C	1:A:111:VAL:H	0.56	2.04	8	4
1:A:112:ASP:N	1:A:112:ASP:OD1	0.56	2.39	14	1
1:A:86:TYR:CE2	1:A:90:LEU:CD1	0.56	2.89	8	2
1:A:61:ASP:C	1:A:63:LYS:H	0.56	2.04	12	11
1:A:187:GLN:O	1:A:189:GLU:N	0.56	2.39	20	3
1:A:88:ILE:HG21	1:A:125:ILE:HG23	0.56	1.76	7	4
1:A:90:LEU:C	1:A:90:LEU:CD1	0.56	2.74	10	7
1:A:99:ASN:C	1:A:99:ASN:ND2	0.56	2.59	10	3
1:A:109:TYR:O	1:A:111:VAL:N	0.55	2.39	12	8
1:A:156:TRP:O	1:A:161:LYS:N	0.55	2.39	13	1
1:A:162:LYS:C	1:A:164:ASP:H	0.55	2.04	13	2
1:A:53:TYR:CZ	1:A:66:ALA:CB	0.55	2.89	14	1
1:A:25:GLU:N	1:A:25:GLU:OE2	0.55	2.40	21	1
1:A:19:LEU:HD23	1:A:19:LEU:N	0.55	2.14	11	11
1:A:90:LEU:HD13	1:A:90:LEU:O	0.55	2.01	13	2
1:A:58:PRO:O	1:A:60:ALA:N	0.55	2.40	2	2
1:A:68:HIS:CD2	1:A:132:MET:SD	0.55	2.99	14	2
1:A:25:GLU:CD	1:A:25:GLU:N	0.55	2.60	7	3
1:A:145:GLU:OE1	1:A:145:GLU:CA	0.55	2.54	2	2
1:A:88:ILE:CD1	1:A:109:TYR:OH	0.55	2.55	10	6

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:3:ASN:ND2	1:A:4:SER:H	0.55	2.00	4	2
1:A:98:THR:OG1	1:A:99:ASN:N	0.55	2.33	18	1
1:A:21:THR:OG1	1:A:23:PHE:CG	0.55	2.60	3	1
1:A:53:TYR:CE1	1:A:66:ALA:HB3	0.55	2.36	20	1
1:A:69:VAL:HG22	1:A:132:MET:HE3	0.55	1.77	22	1
1:A:186:ILE:HG22	1:A:187:GLN:H	0.55	1.61	4	15
1:A:22:LYS:O	1:A:23:PHE:CG	0.54	2.61	20	1
1:A:92:MET:O	1:A:94:SER:N	0.54	2.39	15	8
1:A:47:GLN:H	1:A:47:GLN:CD	0.54	2.06	3	1
1:A:92:MET:O	1:A:93:THR:CB	0.54	2.54	1	1
1:A:165:ASP:OD1	1:A:166:LYS:N	0.54	2.38	9	2
1:A:55:LYS:NZ	1:A:56:PHE:CE1	0.54	2.76	6	1
1:A:117:ILE:CG1	1:A:118:SER:N	0.54	2.71	10	3
1:A:155:ILE:HG22	1:A:159:PHE:CE1	0.54	2.38	1	1
1:A:56:PHE:O	1:A:57:PHE:CD1	0.54	2.61	7	6
1:A:98:THR:HG23	1:A:187:GLN:NE2	0.54	2.17	12	2
1:A:3:ASN:HD22	1:A:4:SER:H	0.54	1.45	10	1
1:A:3:ASN:ND2	1:A:6:SER:H	0.54	2.00	14	1
1:A:61:ASP:CB	1:A:64:ALA:HB2	0.54	2.32	21	1
1:A:21:THR:O	1:A:23:PHE:CD1	0.54	2.61	3	2
1:A:136:GLU:C	1:A:138:THR:H	0.54	2.06	14	2
1:A:68:HIS:NE2	1:A:132:MET:CE	0.54	2.71	16	1
1:A:99:ASN:OD1	1:A:100:GLN:N	0.53	2.41	11	2
1:A:68:HIS:CD2	1:A:68:HIS:O	0.53	2.61	3	2
1:A:118:SER:OG	1:A:119:LYS:N	0.53	2.41	9	3
1:A:24:THR:HG22	1:A:25:GLU:H	0.53	1.63	12	2
1:A:25:GLU:N	1:A:25:GLU:CD	0.53	2.62	1	2
1:A:92:MET:O	1:A:93:THR:HG22	0.53	2.03	1	2
1:A:160:GLY:O	1:A:161:LYS:CB	0.53	2.56	12	2
1:A:176:THR:O	1:A:178:ALA:N	0.53	2.41	13	1
1:A:92:MET:C	1:A:94:SER:H	0.53	2.05	7	1
1:A:176:THR:HG22	1:A:182:ILE:HG22	0.53	1.80	18	6
1:A:25:GLU:N	1:A:25:GLU:OE1	0.53	2.41	9	1
1:A:46:ARG:O	1:A:48:GLU:N	0.53	2.41	3	6
1:A:113:GLY:C	1:A:115:GLY:H	0.53	2.06	5	3
1:A:41:SER:C	1:A:43:ARG:H	0.53	2.06	19	3
1:A:144:ASP:OD2	1:A:154:LYS:NZ	0.53	2.39	5	1
1:A:119:LYS:NZ	1:A:163:ASP:OD1	0.53	2.36	3	1
1:A:161:LYS:O	1:A:162:LYS:CB	0.53	2.56	5	1
1:A:111:VAL:HG13	1:A:112:ASP:N	0.53	2.19	20	1
1:A:165:ASP:OD2	1:A:166:LYS:N	0.53	2.41	1	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:137:ASP:O	1:A:140:HIS:CD2	0.53	2.62	22	2
1:A:187:GLN:NE2	1:A:188:PHE:O	0.53	2.42	10	1
1:A:143:GLU:O	1:A:145:GLU:N	0.53	2.41	12	1
1:A:40:PRO:O	1:A:42:GLY:N	0.53	2.42	2	8
1:A:63:LYS:O	1:A:67:GLN:NE2	0.53	2.42	9	1
1:A:120:ASN:ND2	1:A:121:GLU:OE1	0.53	2.42	7	1
1:A:109:TYR:O	1:A:110:ASP:C	0.53	2.48	21	2
1:A:58:PRO:C	1:A:60:ALA:H	0.52	2.08	2	5
1:A:31:TRP:O	1:A:35:PHE:N	0.52	2.42	4	5
1:A:113:GLY:O	1:A:115:GLY:N	0.52	2.43	4	5
1:A:68:HIS:NE2	1:A:69:VAL:CG2	0.52	2.72	18	2
1:A:165:ASP:CG	1:A:166:LYS:H	0.52	2.05	18	1
1:A:72:SER:O	1:A:74:ASP:N	0.52	2.42	8	3
1:A:17:LEU:C	1:A:19:LEU:H	0.52	2.08	6	2
1:A:99:ASN:HD22	1:A:99:ASN:C	0.52	2.07	8	1
1:A:168:THR:H	1:A:171:GLU:CB	0.52	2.17	21	1
1:A:19:LEU:O	1:A:20:ASN:ND2	0.52	2.42	22	3
1:A:65:TYR:C	1:A:67:GLN:N	0.52	2.63	2	22
1:A:49:PHE:CD1	1:A:49:PHE:C	0.52	2.83	21	2
1:A:134:SER:C	1:A:136:GLU:H	0.52	2.07	12	2
1:A:70:PHE:C	1:A:70:PHE:CD1	0.52	2.82	8	6
1:A:171:GLU:O	1:A:175:GLY:N	0.52	2.43	14	5
1:A:136:GLU:C	1:A:138:THR:N	0.52	2.62	6	3
1:A:95:ALA:O	1:A:101:LYS:NZ	0.52	2.43	18	2
1:A:102:LEU:HD23	1:A:102:LEU:N	0.52	2.20	22	4
1:A:16:GLU:C	1:A:18:GLN:H	0.52	2.09	2	2
1:A:21:THR:C	1:A:23:PHE:H	0.52	2.07	5	6
1:A:53:TYR:CE1	1:A:57:PHE:CD2	0.52	2.97	20	1
1:A:160:GLY:C	1:A:162:LYS:H	0.52	2.07	1	1
1:A:153:GLU:O	1:A:157:GLY:N	0.52	2.43	8	5
1:A:41:SER:C	1:A:43:ARG:N	0.52	2.62	19	2
1:A:132:MET:SD	1:A:132:MET:O	0.52	2.68	20	1
1:A:73:PHE:C	1:A:74:ASP:CG	0.52	2.68	22	4
1:A:17:LEU:O	1:A:19:LEU:N	0.52	2.43	14	2
1:A:114:ASN:HD22	1:A:114:ASN:N	0.52	2.01	7	1
1:A:154:LYS:HZ2	1:A:185:LEU:HD11	0.52	1.65	12	1
1:A:49:PHE:CE2	1:A:70:PHE:CD1	0.52	2.97	13	1
1:A:86:TYR:CE1	1:A:90:LEU:HD13	0.52	2.40	18	2
1:A:186:ILE:CG1	1:A:187:GLN:N	0.52	2.73	13	1
1:A:40:PRO:C	1:A:42:GLY:N	0.51	2.63	2	8
1:A:156:TRP:CZ3	1:A:167:LEU:HD11	0.51	2.40	5	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:163:ASP:O	1:A:164:ASP:CB	0.51	2.58	14	3
1:A:136:GLU:O	1:A:138:THR:N	0.51	2.43	6	3
1:A:170:LYS:CD	1:A:170:LYS:N	0.51	2.73	4	2
1:A:143:GLU:C	1:A:145:GLU:N	0.51	2.63	12	1
1:A:160:GLY:C	1:A:162:LYS:N	0.51	2.64	1	2
1:A:21:THR:O	1:A:23:PHE:N	0.51	2.43	11	5
1:A:181:GLU:H	1:A:181:GLU:CD	0.51	2.08	8	1
1:A:173:ILE:HG22	1:A:174:GLU:N	0.51	2.19	19	2
1:A:41:SER:O	1:A:43:ARG:N	0.51	2.44	19	2
1:A:38:GLU:CD	1:A:38:GLU:C	0.51	2.69	11	2
1:A:143:GLU:C	1:A:145:GLU:H	0.51	2.07	12	1
1:A:61:ASP:HB3	1:A:64:ALA:HB2	0.51	1.82	14	1
1:A:40:PRO:C	1:A:42:GLY:H	0.51	2.09	6	4
1:A:60:ALA:C	1:A:61:ASP:CG	0.51	2.69	1	2
1:A:50:GLN:NE2	1:A:62:PRO:O	0.51	2.43	7	1
1:A:32:TYR:CD2	1:A:36:LEU:HD12	0.51	2.41	10	1
1:A:59:GLU:C	1:A:61:ASP:H	0.51	2.08	10	1
1:A:98:THR:C	1:A:100:GLN:N	0.51	2.63	10	18
1:A:17:LEU:C	1:A:17:LEU:HD23	0.51	2.26	7	7
1:A:120:ASN:OD1	1:A:121:GLU:N	0.51	2.44	14	3
1:A:19:LEU:C	1:A:20:ASN:CG	0.51	2.69	17	3
1:A:113:GLY:C	1:A:115:GLY:N	0.51	2.64	5	4
1:A:163:ASP:C	1:A:165:ASP:H	0.51	2.09	5	3
1:A:21:THR:CG2	1:A:22:LYS:N	0.51	2.73	7	1
1:A:174:GLU:O	1:A:178:ALA:HB2	0.51	2.05	13	2
1:A:86:TYR:CZ	1:A:90:LEU:HD12	0.51	2.40	19	1
1:A:39:CYS:O	1:A:39:CYS:SG	0.50	2.69	10	2
1:A:186:ILE:HG13	1:A:187:GLN:N	0.50	2.21	13	1
1:A:106:PHE:CE2	1:A:110:ASP:OD2	0.50	2.64	20	1
1:A:145:GLU:OE1	1:A:147:THR:OG1	0.50	2.28	2	1
1:A:99:ASN:ND2	1:A:99:ASN:N	0.50	2.57	22	1
1:A:70:PHE:CE2	1:A:81:LEU:HD21	0.50	2.41	9	2
1:A:3:ASN:O	1:A:5:LYS:N	0.50	2.43	11	1
1:A:95:ALA:C	1:A:101:LYS:NZ	0.50	2.61	14	1
1:A:67:GLN:CD	1:A:67:GLN:C	0.50	2.69	4	3
1:A:110:ASP:C	1:A:110:ASP:OD1	0.50	2.50	15	2
1:A:163:ASP:N	1:A:163:ASP:OD1	0.50	2.40	20	2
1:A:113:GLY:O	1:A:114:ASN:C	0.50	2.50	15	1
1:A:19:LEU:CD1	1:A:57:PHE:CG	0.50	2.95	1	5
1:A:109:TYR:O	1:A:111:VAL:HG22	0.50	2.07	7	1
1:A:25:GLU:CD	1:A:26:GLU:N	0.50	2.65	14	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:11:LYS:CB	1:A:11:LYS:NZ	0.50	2.75	19	1
1:A:188:PHE:CD2	1:A:189:GLU:O	0.50	2.64	21	1
1:A:3:ASN:N	2:A:1:MYR:C1	0.50	2.74	4	2
1:A:99:ASN:O	1:A:99:ASN:ND2	0.50	2.45	12	1
1:A:61:ASP:C	1:A:63:LYS:N	0.49	2.65	7	11
1:A:21:THR:O	1:A:21:THR:CG2	0.49	2.59	9	12
1:A:72:SER:C	1:A:74:ASP:N	0.49	2.66	14	2
1:A:102:LEU:O	1:A:105:ALA:N	0.49	2.45	1	1
1:A:35:PHE:O	1:A:39:CYS:SG	0.49	2.69	9	1
1:A:89:ALA:O	1:A:93:THR:CG2	0.49	2.59	18	3
1:A:43:ARG:NE	1:A:80:THR:OG1	0.49	2.45	20	1
1:A:31:TRP:O	1:A:34:SER:N	0.49	2.45	22	1
1:A:133:ILE:HD11	1:A:188:PHE:CE2	0.49	2.41	3	1
1:A:114:ASN:N	1:A:114:ASN:OD1	0.49	2.45	5	1
1:A:65:TYR:C	1:A:67:GLN:H	0.49	2.11	5	14
1:A:123:LEU:CD1	1:A:148:PRO:O	0.49	2.61	7	4
1:A:99:ASN:N	1:A:99:ASN:ND2	0.49	2.59	1	2
1:A:13:ILE:O	1:A:15:GLU:N	0.49	2.46	2	1
1:A:58:PRO:C	1:A:60:ALA:N	0.49	2.66	22	3
1:A:183:LEU:HD11	1:A:187:GLN:CD	0.49	2.28	13	1
1:A:21:THR:C	1:A:23:PHE:N	0.49	2.66	4	6
1:A:183:LEU:HD11	1:A:187:GLN:HE22	0.49	1.64	4	1
1:A:49:PHE:CE2	1:A:70:PHE:CD2	0.49	3.01	11	2
1:A:99:ASN:C	1:A:99:ASN:HD22	0.49	2.11	10	1
1:A:159:PHE:CE1	1:A:182:ILE:HD13	0.49	2.43	13	1
1:A:106:PHE:CD1	1:A:169:GLU:OE1	0.49	2.65	19	1
1:A:179:ASN:N	1:A:179:ASN:ND2	0.48	2.61	2	2
1:A:114:ASN:O	1:A:116:THR:N	0.48	2.46	3	1
1:A:134:SER:O	1:A:136:GLU:N	0.48	2.46	1	2
1:A:13:ILE:C	1:A:15:GLU:N	0.48	2.64	2	1
1:A:17:LEU:O	1:A:18:GLN:CB	0.48	2.60	10	3
1:A:92:MET:C	1:A:94:SER:N	0.48	2.66	7	2
1:A:176:THR:C	1:A:178:ALA:N	0.48	2.65	13	1
1:A:160:GLY:O	1:A:162:LYS:N	0.48	2.46	1	2
1:A:3:ASN:H	2:A:1:MYR:C1	0.48	2.21	14	1
1:A:155:ILE:HD11	1:A:185:LEU:C	0.48	2.29	20	1
1:A:186:ILE:HG13	1:A:187:GLN:H	0.48	1.67	13	1
1:A:168:THR:O	1:A:170:LYS:N	0.48	2.47	20	1
1:A:181:GLU:OE1	1:A:181:GLU:N	0.48	2.47	21	1
1:A:125:ILE:O	1:A:129:ILE:HD12	0.48	2.08	10	1
1:A:53:TYR:CE1	1:A:66:ALA:CB	0.48	2.96	20	3

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:134:SER:C	1:A:136:GLU:N	0.48	2.66	1	6
1:A:104:TRP:CH2	1:A:108:LEU:HD22	0.48	2.44	22	3
1:A:19:LEU:CD1	1:A:57:PHE:CD2	0.48	2.96	21	3
1:A:69:VAL:HG12	1:A:86:TYR:CE2	0.48	2.44	14	3
1:A:3:ASN:C	1:A:5:LYS:N	0.48	2.67	11	1
1:A:25:GLU:OE1	1:A:25:GLU:C	0.48	2.51	20	4
1:A:186:ILE:CG2	1:A:187:GLN:H	0.48	2.20	20	1
1:A:61:ASP:O	1:A:63:LYS:N	0.48	2.47	5	8
1:A:93:THR:O	1:A:93:THR:CG2	0.48	2.60	12	3
1:A:70:PHE:CE1	1:A:81:LEU:HD21	0.48	2.43	10	2
1:A:179:ASN:HB3	1:A:182:ILE:HD12	0.48	1.84	20	1
1:A:32:TYR:O	1:A:36:LEU:HD12	0.48	2.07	22	2
1:A:177:LEU:CD2	1:A:177:LEU:N	0.48	2.77	20	3
1:A:158:PHE:HB3	1:A:182:ILE:HD11	0.48	1.86	1	1
1:A:39:CYS:SG	1:A:41:SER:N	0.48	2.85	4	3
1:A:72:SER:CB	1:A:132:MET:O	0.48	2.62	8	1
1:A:19:LEU:O	1:A:20:ASN:CB	0.47	2.62	22	2
1:A:138:THR:C	1:A:140:HIS:H	0.47	2.12	20	1
1:A:102:LEU:O	1:A:104:TRP:N	0.47	2.47	10	2
1:A:102:LEU:HD13	1:A:176:THR:OG1	0.47	2.09	6	2
1:A:156:TRP:CD1	1:A:162:LYS:O	0.47	2.67	9	1
1:A:188:PHE:O	1:A:189:GLU:CB	0.47	2.61	10	1
1:A:99:ASN:HD22	1:A:99:ASN:H	0.47	1.50	1	1
1:A:88:ILE:CG2	1:A:125:ILE:HG23	0.47	2.39	8	3
1:A:168:THR:OG1	1:A:171:GLU:CG	0.47	2.63	10	1
1:A:25:GLU:OE2	1:A:26:GLU:OE1	0.47	2.32	17	1
1:A:183:LEU:CD1	1:A:187:GLN:HE21	0.47	2.21	18	1
1:A:91:HIS:C	1:A:93:THR:H	0.47	2.13	12	1
1:A:92:MET:O	1:A:93:THR:CG2	0.47	2.62	1	1
1:A:119:LYS:O	1:A:122:VAL:N	0.47	2.48	17	7
1:A:46:ARG:C	1:A:48:GLU:N	0.47	2.68	3	5
1:A:186:ILE:C	1:A:188:PHE:H	0.47	2.13	8	2
1:A:88:ILE:HG22	1:A:89:ALA:N	0.47	2.25	19	3
1:A:3:ASN:OD1	1:A:4:SER:N	0.47	2.48	19	1
1:A:114:ASN:C	1:A:116:THR:N	0.47	2.68	3	1
1:A:23:PHE:CD1	1:A:23:PHE:N	0.47	2.82	3	4
1:A:186:ILE:C	1:A:186:ILE:CD1	0.47	2.83	20	1
1:A:114:ASN:OD1	1:A:115:GLY:N	0.47	2.48	18	1
1:A:162:LYS:O	1:A:164:ASP:N	0.46	2.48	13	1
1:A:159:PHE:CD2	1:A:182:ILE:HD13	0.46	2.46	6	2
1:A:98:THR:C	1:A:100:GLN:H	0.46	2.14	10	7

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:162:LYS:C	1:A:164:ASP:N	0.46	2.68	13	1
1:A:82:ASP:CG	1:A:85:GLU:OE1	0.46	2.54	14	2
1:A:161:LYS:O	1:A:161:LYS:CG	0.46	2.63	14	1
1:A:146:ASN:N	1:A:146:ASN:HD22	0.46	2.08	17	1
1:A:46:ARG:HG3	1:A:47:GLN:N	0.46	2.26	18	6
1:A:137:ASP:OD1	1:A:137:ASP:N	0.46	2.47	2	2
1:A:140:HIS:CD2	1:A:140:HIS:N	0.46	2.83	22	2
1:A:146:ASN:O	1:A:146:ASN:ND2	0.46	2.49	4	1
1:A:32:TYR:CE2	1:A:36:LEU:HD11	0.46	2.46	7	5
1:A:24:THR:OG1	1:A:25:GLU:OE2	0.46	2.34	13	3
1:A:170:LYS:O	1:A:174:GLU:N	0.46	2.48	15	3
1:A:168:THR:H	1:A:171:GLU:HB2	0.46	1.71	21	2
1:A:25:GLU:OE2	1:A:26:GLU:OE2	0.46	2.33	15	1
1:A:188:PHE:CE2	1:A:189:GLU:OE1	0.46	2.68	9	1
1:A:102:LEU:C	1:A:104:TRP:N	0.46	2.67	10	2
1:A:133:ILE:CG2	1:A:134:SER:N	0.46	2.79	22	1
1:A:92:MET:O	1:A:93:THR:C	0.46	2.54	8	6
1:A:19:LEU:N	1:A:19:LEU:HD23	0.46	2.26	15	7
1:A:21:THR:CG2	1:A:21:THR:O	0.46	2.64	12	1
1:A:69:VAL:HG22	1:A:132:MET:HE2	0.46	1.86	1	2
1:A:137:ASP:C	1:A:139:LYS:N	0.46	2.69	22	2
1:A:31:TRP:CH2	1:A:35:PHE:CD2	0.46	3.04	10	1
1:A:91:HIS:O	1:A:93:THR:N	0.46	2.48	12	1
1:A:139:LYS:HZ1	1:A:140:HIS:CE1	0.46	2.28	4	1
1:A:87:VAL:HG13	1:A:91:HIS:CE1	0.46	2.45	10	4
1:A:130:PHE:CZ	1:A:138:THR:CG2	0.46	2.99	17	1
1:A:32:TYR:CE1	1:A:36:LEU:HD12	0.46	2.45	20	1
1:A:65:TYR:CG	1:A:66:ALA:N	0.45	2.82	20	2
1:A:17:LEU:HD23	1:A:18:GLN:CB	0.45	2.41	11	1
1:A:154:LYS:O	1:A:158:PHE:CD1	0.45	2.70	6	1
1:A:168:THR:C	1:A:170:LYS:N	0.45	2.69	20	2
1:A:22:LYS:C	1:A:23:PHE:CG	0.45	2.90	20	1
1:A:144:ASP:OD2	1:A:145:GLU:OE2	0.45	2.34	1	1
1:A:156:TRP:NE1	1:A:162:LYS:O	0.45	2.49	9	2
1:A:10:SER:OG	1:A:104:TRP:NE1	0.45	2.49	8	1
1:A:169:GLU:O	1:A:173:ILE:CG1	0.45	2.65	8	1
1:A:67:GLN:HG3	1:A:68:HIS:N	0.45	2.25	9	2
1:A:88:ILE:HD11	1:A:108:LEU:HD23	0.45	1.88	15	1
1:A:97:LYS:N	1:A:97:LYS:HD3	0.45	2.26	19	1
1:A:98:THR:O	1:A:101:LYS:N	0.45	2.49	7	3
1:A:154:LYS:O	1:A:158:PHE:CD2	0.45	2.69	16	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:21:THR:OG1	1:A:23:PHE:CD2	0.45	2.69	3	1
1:A:94:SER:O	1:A:101:LYS:NZ	0.45	2.50	9	1
1:A:60:ALA:O	1:A:61:ASP:CB	0.45	2.64	11	3
1:A:11:LYS:CE	1:A:25:GLU:OE1	0.45	2.64	16	1
1:A:31:TRP:O	1:A:33:GLN:N	0.45	2.50	22	1
1:A:17:LEU:C	1:A:19:LEU:N	0.45	2.70	14	2
1:A:146:ASN:OD1	1:A:146:ASN:N	0.45	2.48	12	1
1:A:63:LYS:O	1:A:63:LYS:CD	0.45	2.63	21	1
1:A:125:ILE:HG22	1:A:129:ILE:HD11	0.45	1.86	1	1
1:A:119:LYS:HG2	1:A:156:TRP:CD2	0.45	2.47	2	1
1:A:179:ASN:HD22	1:A:182:ILE:HD12	0.45	1.72	14	1
1:A:138:THR:C	1:A:140:HIS:N	0.45	2.70	20	2
1:A:46:ARG:HH21	1:A:47:GLN:NE2	0.45	2.10	9	1
1:A:17:LEU:CD1	1:A:90:LEU:HD11	0.45	2.42	10	1
1:A:109:TYR:OH	1:A:125:ILE:CG1	0.45	2.65	21	2
1:A:87:VAL:HG12	1:A:88:ILE:N	0.45	2.26	19	2
1:A:102:LEU:N	1:A:102:LEU:HD23	0.44	2.27	2	6
1:A:24:THR:OG1	1:A:25:GLU:CD	0.44	2.56	1	1
1:A:155:ILE:HG22	1:A:159:PHE:CZ	0.44	2.47	1	2
1:A:22:LYS:C	1:A:23:PHE:CD2	0.44	2.91	20	1
1:A:69:VAL:CG1	1:A:86:TYR:CE2	0.44	3.00	1	2
1:A:98:THR:O	1:A:99:ASN:C	0.44	2.56	7	4
1:A:170:LYS:H	1:A:170:LYS:HD2	0.44	1.71	4	1
1:A:46:ARG:H	1:A:46:ARG:CD	0.44	2.25	9	1
1:A:145:GLU:O	1:A:147:THR:N	0.44	2.50	10	1
1:A:168:THR:OG1	1:A:171:GLU:OE2	0.44	2.35	14	1
1:A:119:LYS:HE3	1:A:156:TRP:CD1	0.44	2.47	15	1
1:A:121:GLU:N	1:A:121:GLU:CD	0.44	2.71	16	1
1:A:86:TYR:CD1	1:A:86:TYR:C	0.44	2.91	4	3
1:A:188:PHE:CE1	1:A:189:GLU:O	0.44	2.70	5	1
1:A:188:PHE:CD1	1:A:188:PHE:C	0.44	2.90	6	1
1:A:172:PHE:C	1:A:172:PHE:CD1	0.44	2.90	21	1
1:A:106:PHE:CD1	1:A:106:PHE:C	0.44	2.91	16	3
1:A:114:ASN:N	1:A:114:ASN:ND2	0.44	2.65	7	1
1:A:106:PHE:CZ	1:A:169:GLU:CA	0.44	3.01	10	2
1:A:82:ASP:OD1	1:A:85:GLU:OE1	0.44	2.34	14	1
1:A:55:LYS:NZ	1:A:56:PHE:CZ	0.44	2.79	6	1
1:A:106:PHE:CZ	1:A:115:GLY:O	0.44	2.71	8	1
1:A:109:TYR:HE2	1:A:125:ILE:HD11	0.44	1.73	10	1
1:A:13:ILE:O	1:A:16:GLU:N	0.44	2.51	17	1
1:A:32:TYR:CD1	2:A:1:MYR:H72	0.44	2.47	19	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:182:ILE:O	1:A:185:LEU:N	0.44	2.51	21	1
1:A:119:LYS:O	1:A:120:ASN:C	0.44	2.56	17	8
1:A:39:CYS:SG	1:A:43:ARG:O	0.44	2.75	6	1
1:A:179:ASN:CG	1:A:181:GLU:OE1	0.44	2.56	8	1
1:A:19:LEU:HD22	1:A:60:ALA:HB1	0.44	1.90	14	1
1:A:45:THR:HG1	1:A:48:GLU:CD	0.44	2.15	20	1
1:A:59:GLU:OE1	1:A:59:GLU:C	0.44	2.56	2	1
1:A:155:ILE:HD11	1:A:185:LEU:CB	0.44	2.43	7	1
1:A:65:TYR:C	1:A:65:TYR:CD1	0.44	2.89	15	2
1:A:56:PHE:CD1	1:A:56:PHE:N	0.44	2.83	22	1
1:A:159:PHE:CD1	1:A:159:PHE:N	0.44	2.86	1	1
1:A:119:LYS:HG3	1:A:156:TRP:CE2	0.44	2.48	2	1
1:A:93:THR:OG1	1:A:94:SER:N	0.44	2.51	8	1
1:A:109:TYR:C	1:A:111:VAL:N	0.44	2.70	8	1
1:A:82:ASP:OD2	1:A:85:GLU:OE1	0.43	2.36	4	1
1:A:13:ILE:HG22	1:A:14:LEU:N	0.43	2.27	20	1
1:A:42:GLY:O	1:A:83:PHE:N	0.43	2.50	10	2
1:A:3:ASN:ND2	1:A:6:SER:CB	0.43	2.82	13	1
1:A:32:TYR:CD1	2:A:1:MYR:C7	0.43	3.01	19	1
1:A:92:MET:O	1:A:93:THR:HB	0.43	2.14	1	1
1:A:94:SER:O	1:A:95:ALA:CB	0.43	2.66	6	4
1:A:188:PHE:CZ	1:A:189:GLU:O	0.43	2.72	5	1
1:A:62:PRO:C	1:A:63:LYS:CG	0.43	2.85	15	1
1:A:98:THR:HG22	1:A:99:ASN:N	0.43	2.29	13	1
1:A:126:VAL:HG13	1:A:151:ARG:NE	0.43	2.28	21	1
1:A:92:MET:SD	1:A:101:LYS:CG	0.43	3.07	4	2
1:A:163:ASP:C	1:A:165:ASP:N	0.43	2.71	7	3
1:A:19:LEU:HD13	1:A:57:PHE:CE2	0.43	2.48	12	1
1:A:110:ASP:OD1	1:A:110:ASP:C	0.43	2.56	14	1
1:A:48:GLU:HG3	1:A:49:PHE:N	0.43	2.29	3	1
1:A:181:GLU:O	1:A:184:ARG:N	0.43	2.51	6	4
1:A:24:THR:HG23	1:A:27:GLU:H	0.43	1.73	13	1
1:A:179:ASN:N	1:A:179:ASN:HD22	0.43	2.10	15	1
1:A:145:GLU:O	1:A:146:ASN:C	0.43	2.57	1	1
1:A:169:GLU:CD	1:A:169:GLU:C	0.43	2.76	2	1
1:A:85:GLU:CD	1:A:85:GLU:N	0.43	2.72	7	1
1:A:19:LEU:HD11	1:A:53:TYR:CZ	0.43	2.48	9	2
1:A:57:PHE:CD1	1:A:57:PHE:N	0.43	2.83	9	1
1:A:31:TRP:O	1:A:32:TYR:C	0.43	2.57	22	2
1:A:186:ILE:HD12	1:A:187:GLN:N	0.43	2.29	13	1
1:A:111:VAL:CG1	1:A:112:ASP:N	0.43	2.82	20	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:92:MET:CE	1:A:105:ALA:HB2	0.43	2.44	21	1
1:A:20:ASN:OD1	1:A:20:ASN:N	0.43	2.51	6	1
1:A:59:GLU:C	1:A:61:ASP:N	0.43	2.72	10	1
1:A:5:LYS:HG2	1:A:6:SER:N	0.43	2.29	13	1
1:A:28:LEU:CD2	1:A:56:PHE:CZ	0.43	3.02	15	1
1:A:170:LYS:O	1:A:171:GLU:C	0.43	2.58	19	5
1:A:187:GLN:O	1:A:188:PHE:C	0.43	2.58	17	5
1:A:123:LEU:HD11	1:A:148:PRO:HB2	0.43	1.90	7	2
1:A:70:PHE:CZ	1:A:81:LEU:HD21	0.43	2.49	15	1
1:A:117:ILE:HG13	1:A:118:SER:N	0.43	2.29	14	1
1:A:70:PHE:CD1	1:A:70:PHE:O	0.42	2.72	8	1
1:A:53:TYR:O	1:A:57:PHE:CD2	0.42	2.72	9	1
1:A:176:THR:OG1	1:A:177:LEU:N	0.42	2.50	10	1
1:A:49:PHE:O	1:A:52:ILE:N	0.42	2.52	14	3
1:A:144:ASP:OD1	1:A:144:ASP:C	0.42	2.57	13	1
1:A:5:LYS:C	1:A:7:GLY:N	0.42	2.72	18	1
1:A:91:HIS:O	1:A:92:MET:C	0.42	2.58	20	2
1:A:145:GLU:OE1	1:A:185:LEU:HD22	0.42	2.13	22	1
1:A:16:GLU:C	1:A:18:GLN:N	0.42	2.72	2	2
1:A:49:PHE:HZ	1:A:86:TYR:HH	0.42	1.55	15	1
1:A:136:GLU:N	1:A:136:GLU:OE1	0.42	2.52	18	1
1:A:187:GLN:CG	1:A:187:GLN:O	0.42	2.66	4	1
1:A:85:GLU:N	1:A:85:GLU:OE1	0.42	2.51	7	1
1:A:176:THR:C	1:A:178:ALA:H	0.42	2.16	13	1
1:A:10:SER:OG	1:A:14:LEU:CD1	0.42	2.68	18	1
1:A:53:TYR:CE1	1:A:57:PHE:CE2	0.42	3.08	2	1
1:A:113:GLY:O	1:A:114:ASN:ND2	0.42	2.53	2	1
1:A:56:PHE:C	1:A:57:PHE:CD1	0.42	2.93	3	1
1:A:163:ASP:OD1	1:A:164:ASP:N	0.42	2.51	6	1
1:A:182:ILE:O	1:A:186:ILE:HG23	0.42	2.15	13	1
1:A:163:ASP:O	1:A:164:ASP:CG	0.42	2.58	20	1
1:A:46:ARG:O	1:A:47:GLN:C	0.42	2.58	22	6
1:A:119:LYS:HG2	1:A:120:ASN:N	0.42	2.30	4	1
1:A:45:THR:CG2	1:A:80:THR:HG22	0.42	2.43	10	1
1:A:35:PHE:CD1	1:A:39:CYS:SG	0.42	3.12	9	1
1:A:8:ALA:O	1:A:11:LYS:N	0.42	2.53	13	1
1:A:13:ILE:HD13	1:A:101:LYS:NZ	0.42	2.30	17	1
1:A:156:TRP:CZ3	1:A:167:LEU:CD1	0.42	3.02	5	1
1:A:11:LYS:O	1:A:15:GLU:CG	0.42	2.68	7	1
1:A:68:HIS:O	1:A:68:HIS:CG	0.42	2.71	7	1
1:A:25:GLU:CD	1:A:25:GLU:H	0.42	2.18	11	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:177:LEU:N	1:A:177:LEU:HD22	0.42	2.29	12	2
1:A:186:ILE:HD12	1:A:186:ILE:C	0.42	2.35	13	1
1:A:166:LYS:HD2	1:A:166:LYS:H	0.42	1.75	21	1
1:A:155:ILE:CG2	1:A:159:PHE:CE2	0.42	3.03	15	3
1:A:58:PRO:O	1:A:59:GLU:C	0.42	2.58	17	2
1:A:151:ARG:HH12	1:A:185:LEU:CB	0.42	2.27	14	1
1:A:162:LYS:CG	1:A:163:ASP:N	0.42	2.82	4	1
1:A:32:TYR:CG	2:A:1:MYR:H51	0.42	2.50	10	2
1:A:22:LYS:O	1:A:23:PHE:C	0.42	2.57	13	1
1:A:46:ARG:N	1:A:46:ARG:HD3	0.42	2.29	9	1
1:A:168:THR:O	1:A:169:GLU:C	0.42	2.58	14	6
1:A:183:LEU:C	1:A:185:LEU:N	0.42	2.73	15	1
1:A:173:ILE:N	1:A:173:ILE:CD1	0.42	2.83	18	1
1:A:119:LYS:HE2	1:A:156:TRP:CD1	0.41	2.49	1	1
1:A:73:PHE:O	1:A:74:ASP:CB	0.41	2.68	2	1
1:A:130:PHE:O	1:A:130:PHE:CD1	0.41	2.73	8	1
1:A:59:GLU:O	1:A:61:ASP:N	0.41	2.53	10	1
1:A:16:GLU:O	1:A:17:LEU:C	0.41	2.58	1	2
1:A:18:GLN:O	1:A:18:GLN:CG	0.41	2.66	21	2
1:A:184:ARG:NH2	1:A:187:GLN:OE1	0.41	2.53	5	1
1:A:180:LYS:HG3	1:A:181:GLU:N	0.41	2.30	16	1
1:A:70:PHE:CE1	1:A:81:LEU:CD2	0.41	3.04	17	1
1:A:46:ARG:O	1:A:49:PHE:N	0.41	2.53	22	1
1:A:57:PHE:N	1:A:58:PRO:HD3	0.41	2.30	5	2
1:A:66:ALA:O	1:A:67:GLN:C	0.41	2.58	10	1
1:A:31:TRP:O	1:A:35:PHE:CB	0.41	2.68	16	1
1:A:10:SER:O	1:A:11:LYS:C	0.41	2.59	17	1
1:A:102:LEU:O	1:A:103:GLU:C	0.41	2.57	19	5
1:A:135:PRO:C	1:A:138:THR:OG1	0.41	2.58	4	1
1:A:129:ILE:O	1:A:132:MET:N	0.41	2.54	7	2
1:A:73:PHE:CZ	1:A:86:TYR:HA	0.41	2.50	8	1
1:A:46:ARG:H	1:A:46:ARG:HD3	0.41	1.76	9	1
1:A:166:LYS:N	1:A:166:LYS:CD	0.41	2.83	20	2
1:A:119:LYS:N	1:A:156:TRP:CH2	0.41	2.89	6	1
1:A:98:THR:HG23	1:A:99:ASN:N	0.41	2.23	7	1
1:A:118:SER:OG	1:A:166:LYS:CE	0.41	2.69	7	1
1:A:174:GLU:O	1:A:178:ALA:HB3	0.41	2.16	8	1
1:A:81:LEU:HD12	1:A:81:LEU:C	0.41	2.36	9	1
1:A:109:TYR:CD2	1:A:117:ILE:CD1	0.41	3.03	12	1
1:A:154:LYS:HG3	1:A:158:PHE:CZ	0.41	2.51	19	1
1:A:125:ILE:O	1:A:128:ALA:N	0.41	2.54	1	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:106:PHE:CD2	1:A:110:ASP:OD2	0.41	2.73	6	1
1:A:21:THR:HG23	1:A:23:PHE:N	0.41	2.31	7	1
1:A:97:LYS:HG3	1:A:98:THR:N	0.41	2.31	12	1
1:A:151:ARG:HH12	1:A:185:LEU:CA	0.41	2.29	14	1
1:A:142:PRO:C	1:A:144:ASP:H	0.41	2.18	17	1
1:A:96:GLY:O	1:A:97:LYS:C	0.41	2.58	22	1
1:A:163:ASP:CG	1:A:164:ASP:H	0.41	2.19	22	1
1:A:168:THR:H	1:A:171:GLU:HB3	0.41	1.75	22	1
1:A:98:THR:CG2	1:A:102:LEU:HD11	0.41	2.46	2	1
1:A:134:SER:O	1:A:138:THR:OG1	0.41	2.39	5	1
1:A:110:ASP:O	1:A:110:ASP:CG	0.41	2.59	8	1
1:A:117:ILE:O	1:A:117:ILE:HG23	0.41	2.15	8	1
1:A:68:HIS:O	1:A:69:VAL:C	0.41	2.59	9	1
1:A:90:LEU:O	1:A:91:HIS:C	0.41	2.59	10	1
1:A:147:THR:C	1:A:149:GLU:N	0.41	2.73	13	1
1:A:13:ILE:O	1:A:14:LEU:C	0.41	2.58	17	1
1:A:174:GLU:HG3	1:A:175:GLY:N	0.41	2.31	18	1
1:A:74:ASP:OD1	1:A:74:ASP:N	0.41	2.54	22	1
1:A:21:THR:O	1:A:22:LYS:C	0.41	2.59	6	1
1:A:69:VAL:HG13	1:A:132:MET:SD	0.41	2.56	11	1
1:A:56:PHE:N	1:A:56:PHE:CD1	0.41	2.89	15	1
1:A:170:LYS:O	1:A:174:GLU:CG	0.41	2.69	18	1
1:A:88:ILE:HD11	1:A:108:LEU:CD2	0.41	2.46	19	1
1:A:92:MET:SD	1:A:101:LYS:HB3	0.41	2.56	1	1
1:A:17:LEU:O	1:A:17:LEU:HD23	0.41	2.16	2	1
1:A:112:ASP:OD1	1:A:112:ASP:C	0.41	2.58	2	1
1:A:142:PRO:O	1:A:146:ASN:ND2	0.41	2.53	2	1
1:A:169:GLU:HG3	1:A:170:LYS:N	0.41	2.31	2	1
1:A:170:LYS:HG2	1:A:171:GLU:N	0.41	2.31	4	1
1:A:120:ASN:CG	1:A:121:GLU:N	0.41	2.73	5	1
1:A:47:GLN:CG	1:A:48:GLU:N	0.41	2.84	6	1
1:A:119:LYS:HB2	1:A:156:TRP:CE2	0.41	2.51	6	2
1:A:136:GLU:O	1:A:139:LYS:N	0.41	2.54	6	1
1:A:21:THR:HG23	1:A:23:PHE:H	0.41	1.75	7	1
1:A:72:SER:C	1:A:74:ASP:H	0.41	2.19	8	1
1:A:113:GLY:O	1:A:114:ASN:CB	0.41	2.66	11	1
1:A:82:ASP:N	1:A:82:ASP:OD1	0.41	2.54	12	1
1:A:106:PHE:CE1	1:A:169:GLU:HB2	0.41	2.51	12	1
1:A:141:LEU:HD23	1:A:141:LEU:N	0.41	2.31	12	1
1:A:68:HIS:O	1:A:72:SER:CB	0.41	2.69	14	1
1:A:65:TYR:CD1	1:A:66:ALA:N	0.41	2.89	15	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:11:LYS:HZ2	1:A:11:LYS:HB2	0.41	1.75	19	1
1:A:97:LYS:H	1:A:97:LYS:HD2	0.41	1.76	5	1
1:A:114:ASN:OD1	1:A:114:ASN:N	0.41	2.54	6	1
1:A:133:ILE:O	1:A:134:SER:C	0.41	2.59	9	1
1:A:109:TYR:CD1	1:A:121:GLU:HG3	0.41	2.51	15	1
1:A:155:ILE:HG23	1:A:159:PHE:CE2	0.41	2.51	15	1
1:A:181:GLU:O	1:A:182:ILE:C	0.40	2.60	7	3
1:A:26:GLU:HG2	1:A:27:GLU:N	0.40	2.30	3	1
1:A:3:ASN:HD22	1:A:4:SER:N	0.40	2.15	4	1
1:A:139:LYS:HZ3	1:A:140:HIS:CD2	0.40	2.34	4	1
1:A:101:LYS:HZ1	1:A:187:GLN:HA	0.40	1.75	15	1
1:A:166:LYS:N	1:A:166:LYS:HE3	0.40	2.31	21	1
1:A:188:PHE:O	1:A:189:GLU:C	0.40	2.60	11	2
1:A:176:THR:HG22	1:A:182:ILE:CG2	0.40	2.46	8	1
1:A:156:TRP:CH2	1:A:167:LEU:HD11	0.40	2.51	9	1
1:A:183:LEU:O	1:A:185:LEU:N	0.40	2.54	15	1
1:A:49:PHE:CD2	1:A:70:PHE:CE2	0.40	3.09	7	1
1:A:141:LEU:N	1:A:141:LEU:HD23	0.40	2.31	10	1
1:A:32:TYR:CD1	2:A:1:MYR:H82	0.40	2.52	16	1
1:A:59:GLU:O	1:A:59:GLU:CG	0.40	2.68	18	1
1:A:130:PHE:O	1:A:133:ILE:N	0.40	2.54	21	1
1:A:177:LEU:O	1:A:178:ALA:C	0.40	2.60	2	1
1:A:56:PHE:HB3	1:A:57:PHE:CE1	0.40	2.51	3	1
1:A:17:LEU:HD23	1:A:17:LEU:C	0.40	2.36	4	1
1:A:182:ILE:O	1:A:186:ILE:N	0.40	2.55	5	1
1:A:46:ARG:HG2	1:A:47:GLN:N	0.40	2.30	9	1
1:A:106:PHE:CZ	1:A:169:GLU:HA	0.40	2.51	14	1
1:A:144:ASP:OD1	1:A:144:ASP:N	0.40	2.53	18	1
1:A:155:ILE:O	1:A:159:PHE:CE1	0.40	2.75	1	1
1:A:13:ILE:C	1:A:15:GLU:H	0.40	2.20	2	1
1:A:179:ASN:ND2	1:A:180:LYS:N	0.40	2.66	4	1
1:A:91:HIS:C	1:A:93:THR:N	0.40	2.74	12	1
1:A:67:GLN:CA	1:A:67:GLN:OE1	0.40	2.68	19	1
1:A:87:VAL:O	1:A:88:ILE:C	0.40	2.60	19	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	181/201 (90%)	134±5 (74±3%)	33±4 (18±2%)	14±3 (8±2%)	2	14
All	All	3982/4422 (90%)	2951 (74%)	721 (18%)	310 (8%)	2	14

All 54 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	18	GLN	20
1	A	66	ALA	20
1	A	92	MET	18
1	A	99	ASN	17
1	A	74	ASP	14
1	A	93	THR	11
1	A	17	LEU	11
1	A	58	PRO	10
1	A	142	PRO	10
1	A	114	ASN	10
1	A	113	GLY	9
1	A	161	LYS	9
1	A	41	SER	9
1	A	61	ASP	8
1	A	112	ASP	8
1	A	62	PRO	7
1	A	97	LYS	7
1	A	110	ASP	7
1	A	164	ASP	7
1	A	111	VAL	6
1	A	20	ASN	6
1	A	162	LYS	6
1	A	169	GLU	6
1	A	188	PHE	6
1	A	115	GLY	5
1	A	47	GLN	5
1	A	94	SER	5
1	A	24	THR	4
1	A	95	ALA	4
1	A	145	GLU	4
1	A	42	GLY	4
1	A	59	GLU	3
1	A	159	PHE	3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	22	LYS	3
1	A	19	LEU	3
1	A	60	ALA	2
1	A	144	ASP	2
1	A	96	GLY	2
1	A	63	LYS	2
1	A	73	PHE	2
1	A	98	THR	2
1	A	40	PRO	1
1	A	173	ILE	1
1	A	137	ASP	1
1	A	187	GLN	1
1	A	103	GLU	1
1	A	146	ASN	1
1	A	4	SER	1
1	A	69	VAL	1
1	A	135	PRO	1
1	A	163	ASP	1
1	A	177	LEU	1
1	A	178	ALA	1
1	A	32	TYR	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	164/180 (91%)	137±3 (83±2%)	27±3 (17±2%)	5 41
All	All	3608/3960 (91%)	3004 (83%)	604 (17%)	5 41

All 113 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	186	ILE	22
1	A	81	LEU	19
1	A	168	THR	19
1	A	138	THR	19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	51	THR	18
1	A	61	ASP	18
1	A	176	THR	17
1	A	147	THR	16
1	A	159	PHE	16
1	A	116	THR	14
1	A	134	SER	14
1	A	25	GLU	13
1	A	90	LEU	12
1	A	18	GLN	9
1	A	73	PHE	9
1	A	177	LEU	9
1	A	37	LYS	9
1	A	174	GLU	9
1	A	22	LYS	8
1	A	139	LYS	8
1	A	179	ASN	8
1	A	24	THR	7
1	A	39	CYS	7
1	A	99	ASN	7
1	A	184	ARG	7
1	A	21	THR	6
1	A	44	ILE	6
1	A	97	LYS	6
1	A	170	LYS	6
1	A	71	ARG	6
1	A	82	ASP	6
1	A	93	THR	6
1	A	166	LYS	6
1	A	54	SER	6
1	A	101	LYS	6
1	A	132	MET	6
1	A	169	GLU	6
1	A	180	LYS	6
1	A	38	GLU	6
1	A	144	ASP	5
1	A	187	GLN	5
1	A	17	LEU	5
1	A	27	GLU	5
1	A	145	GLU	5
1	A	74	ASP	5
1	A	3	ASN	5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	47	GLN	5
1	A	161	LYS	5
1	A	50	GLN	5
1	A	158	PHE	4
1	A	171	GLU	4
1	A	150	LYS	4
1	A	15	GLU	4
1	A	63	LYS	4
1	A	114	ASN	4
1	A	121	GLU	4
1	A	6	SER	4
1	A	11	LYS	4
1	A	146	ASN	4
1	A	20	ASN	4
1	A	29	SER	4
1	A	43	ARG	4
1	A	46	ARG	4
1	A	141	LEU	4
1	A	30	SER	4
1	A	59	GLU	3
1	A	129	ILE	3
1	A	143	GLU	3
1	A	164	ASP	3
1	A	120	ASN	3
1	A	26	GLU	3
1	A	98	THR	3
1	A	112	ASP	3
1	A	111	VAL	3
1	A	162	LYS	3
1	A	137	ASP	3
1	A	92	MET	3
1	A	140	HIS	2
1	A	103	GLU	2
1	A	41	SER	2
1	A	142	PRO	2
1	A	163	ASP	2
1	A	188	PHE	2
1	A	131	LYS	2
1	A	124	GLU	2
1	A	94	SER	2
1	A	189	GLU	2
1	A	151	ARG	2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	67	GLN	2
1	A	10	SER	2
1	A	118	SER	2
1	A	5	LYS	2
1	A	33	GLN	2
1	A	12	GLU	2
1	A	153	GLU	2
1	A	154	LYS	2
1	A	130	PHE	2
1	A	48	GLU	1
1	A	9	LEU	1
1	A	185	LEU	1
1	A	85	GLU	1
1	A	110	ASP	1
1	A	16	GLU	1
1	A	165	ASP	1
1	A	181	GLU	1
1	A	57	PHE	1
1	A	84	LYS	1
1	A	117	ILE	1
1	A	68	HIS	1
1	A	136	GLU	1
1	A	100	GLN	1
1	A	55	LYS	1
1	A	4	SER	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 monosaccharides in this entry.

6.6 Ligand geometry

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	MYR	A	1	1	14,14,15	0.40±0.02	0±0 (0±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	MYR	A	1	1	13,13,15	0.97±0.01	0±0 (0±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	MYR	A	1	1	-	0±0,11,12,13	-

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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

No chemical shift data were provided