Full wwPDB NMR Structure Validation Report (i)

Nov 6, 2023 – 08:01 PM EST

PDB ID	:	2MBZ
BMRB ID	:	19421
Title	:	Structural Basis of a Thiopeptide Antibiotic Multidrug Resistance System from Streptomyces lividans:Promothiocin A in Complex with TipAS
Authors	:	Habazettl, J.; Allan, M.G.; Jensen, P.; Sass, H.; Grzesiek, S.
Deposited on	:	2013-08-12

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 (i) 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 (i)) were used in the production of this report:

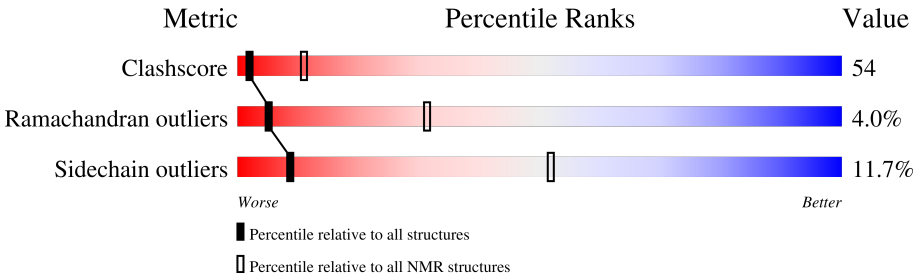
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
SOLUTION NMR

The overall completeness of chemical shifts assignment is 89%.

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	144	28% 53% 6% 12% •
2	B	12	42% 8% 50%

2 Ensemble composition and analysis (i)

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: *lowest energy*.

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:113-A:126, A:142-A:253, B:501-B:501, B:503-B:504, B:506-B:506, B:508-B:508, B:511-B:511 (132)	0.62	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 1 clusters and 1 single-model cluster was found.

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

3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 2302 atoms, of which 1091 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called HTH-type transcriptional activator TipA.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	143	2207	706	1053	204	237	7	0

- Molecule 2 is a protein called Promothiocin A.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
2	B	12	95	36	38	11	8	2	1

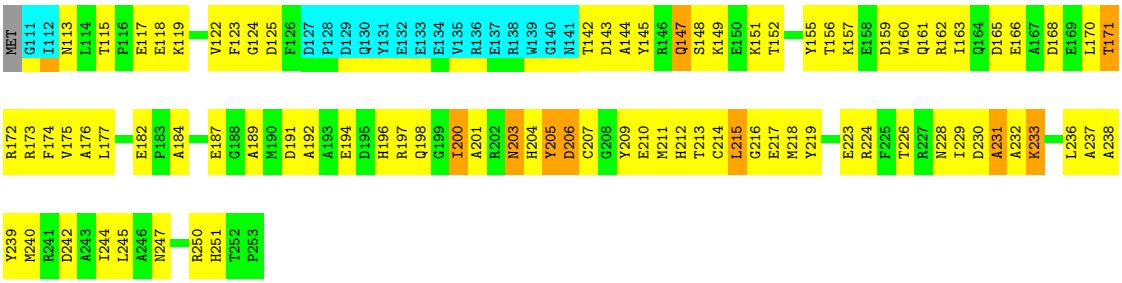
4 Residue-property plots (i)

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.

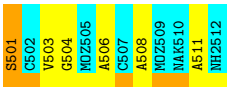
• Molecule 1: HTH-type transcriptional activator TipA

Chain A: 28% 53% 6% 12%



• Molecule 2: Promothiocin A

Chain B: 42% 8% 50%



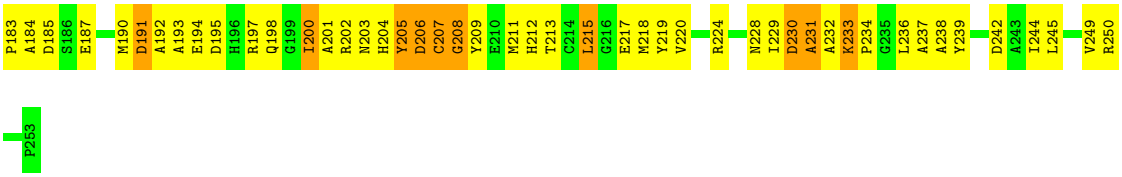
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

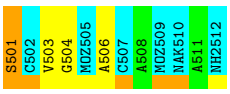
• Molecule 1: HTH-type transcriptional activator TipA

Chain A: 33% 43% 12% 12%



• Molecule 2: Promothiocin A

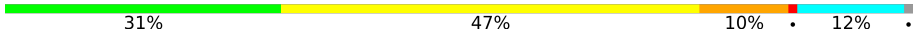
Chain B:

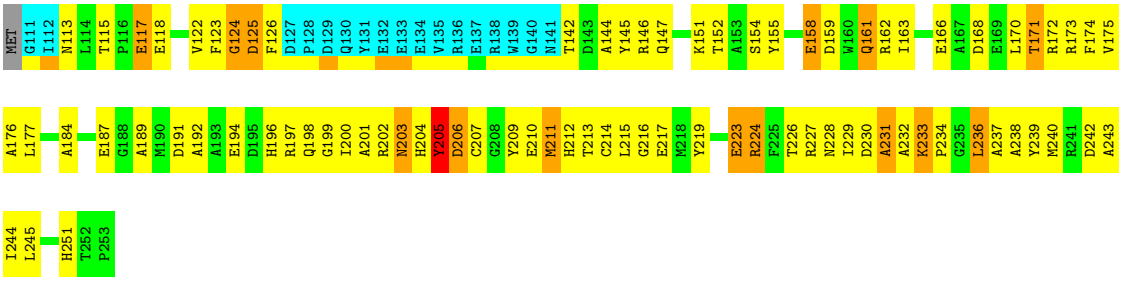


4.2.2 Score per residue for model 2 (medoid)

• Molecule 1: HTH-type transcriptional activator TipA

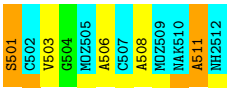
Chain A:





• Molecule 2: Promothiocin A

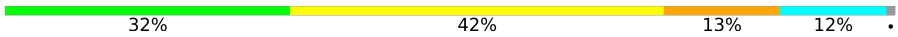
Chain B:

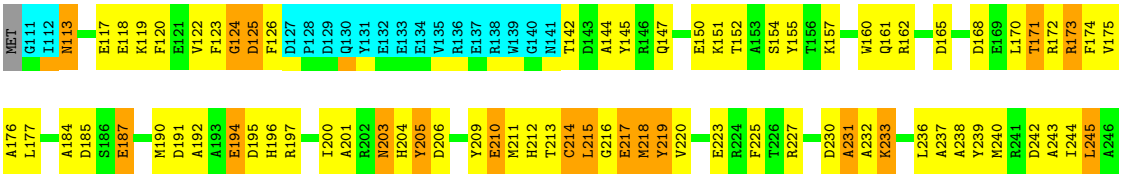


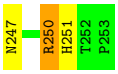
4.2.3 Score per residue for model 3

• Molecule 1: HTH-type transcriptional activator TipA

Chain A:

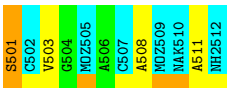






• Molecule 2: Promothiocin A

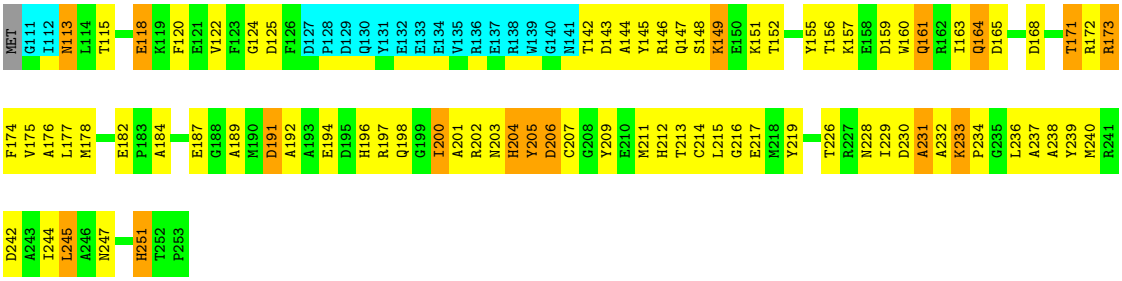
Chain B:



4.2.4 Score per residue for model 4

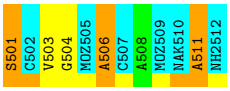
• Molecule 1: HTH-type transcriptional activator TipA

Chain A:



• Molecule 2: Promothiocin A

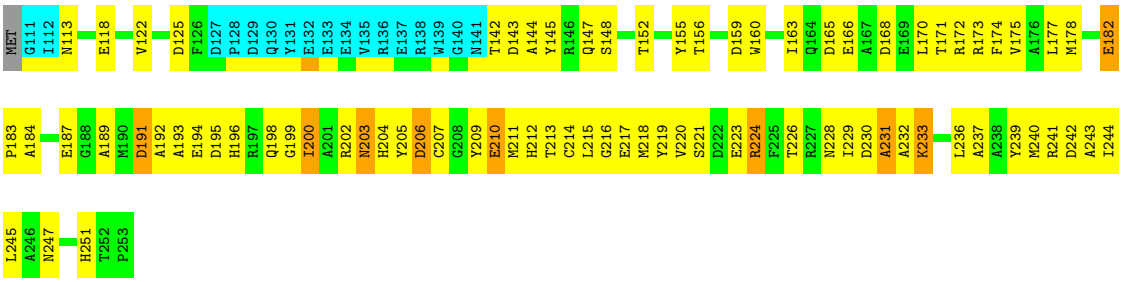
Chain B:



4.2.5 Score per residue for model 5

• Molecule 1: HTH-type transcriptional activator TipA

Chain A:



• Molecule 2: Promothiocin A

Chain B: 8% 25% 17% 50%

S501 C502 V503 G504 MQZ505 A506 C507 A508 MQZ509 NAK510 A511 NH2512

4.2.6 Score per residue for model 6

- Molecule 1: HTH-type transcriptional activator TipA

Chain A: 33% 46% 8% 12%

MET G111 I112 N113 L114 T115 E118 K119 F120 E121 V122 F123 G124 D125 F126 D127 P128 D129 Q130 Y131 E132 E133 E134 V135 R136 E137 R138 W139 G140 N141 T142 D143 A144 Y145 R146 Q147 S148 T152 Y155 T156 K157 E158 D159 W160 Q161 R162 D165 E166 A167 D168 E169 L170 T171 R172 R173 F174

V175 A176 L177 M178 A184 E187 M190 D191 E194 D195 H196 R197 I200 A201 R202 N203 H204 Y205 D206 C207 G208 Y209 E210 M211 H212 T213 C214 L215 G216 E217 M218 Y219 D222 E223 R224 F225 T226 R227 N228 I229 D230 A231 A232 K233 L236 A237 A238 Y239 D242 A243 I244 L245

A246 N247 R250 H251 T252 P253

- Molecule 2: Promothiocin A

Chain B: 8% 33% 8% 50%

S501 C502 V503 G504 MQZ505 A506 C507 A508 MQZ509 NAK510 A511 NH2512

4.2.7 Score per residue for model 7

- Molecule 1: HTH-type transcriptional activator TipA

Chain A: 33% 47% 8% 12%

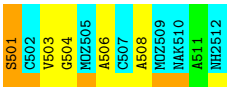
MET G111 I112 N113 L114 E118 K119 F120 E121 V122 F123 G124 D125 F126 D127 P128 D129 Q130 Y131 E132 E133 E134 V135 R136 E137 R138 W139 G140 N141 T142 D143 A144 Y145 R146 Q147 S148 K149 E150 K151 T152 A153 T156 W160 Q161 R162 I163 Q164 D165 E166 A167 D168 T171 R172 R173 F174 V175

A176 L177 M178 D179 A180 G181 E182 P183 A184 D185 S186 E187 G188 A189 M190 D191 A192 A193 E194 D195 H196 R197 Q198 G199 I200 A201 R202 N203 H204 Y205 D206 C207 G208 Y209 E210 M211 H212 T213 C214 L215 M218 Y219 D222 E223 R224 N228 I229 D230 A231 A232 K233 L236 A237 A238 Y239 M240

R241 D242 A243 I244 L245 R250 P253

- Molecule 2: Promothiocin A

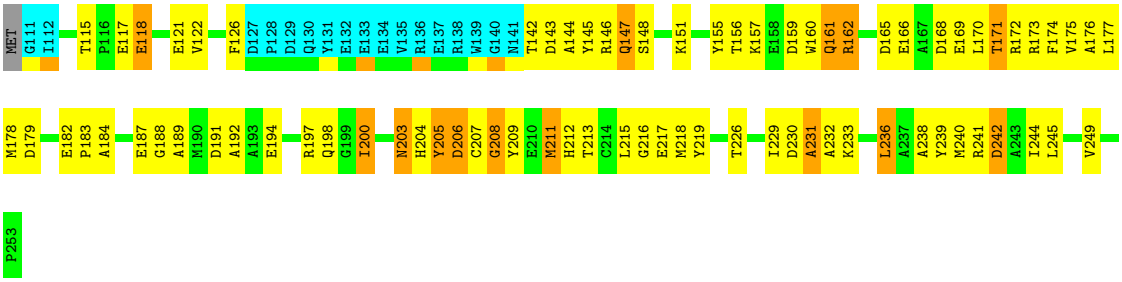
Chain B: 8% 33% 8% 50%



4.2.8 Score per residue for model 8

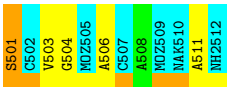
- Molecule 1: HTH-type transcriptional activator TipA

Chain A:



- Molecule 2: Promothiocin A

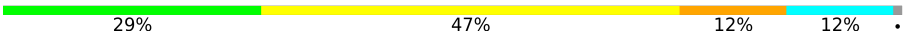
Chain B:

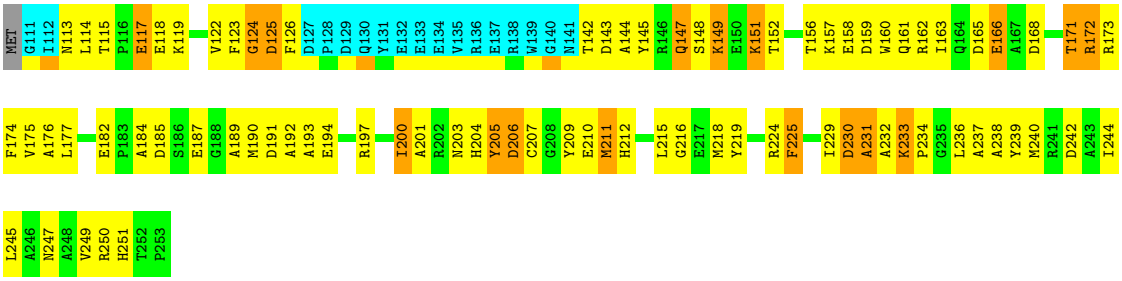


4.2.9 Score per residue for model 9

- Molecule 1: HTH-type transcriptional activator TipA

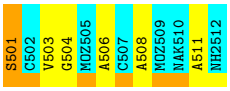
Chain A:





- Molecule 2: Promothiocin A

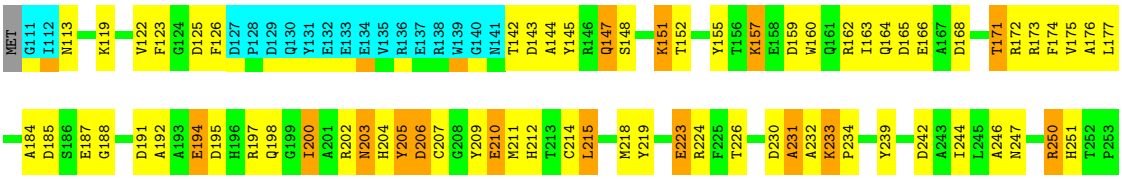
Chain B:



4.2.10 Score per residue for model 10

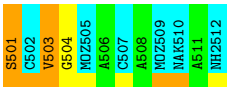
- Molecule 1: HTH-type transcriptional activator TipA

Chain A:



- Molecule 2: Promothiocin A

Chain B:



5 Refinement protocol and experimental data overview (i)

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	2.30
X-PLOR NIH	refinement	2.30

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	1737
Number of shifts mapped to atoms	1733
Number of unparsed shifts	0
Number of shifts with mapping errors	4
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	89%

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: NAK, MOZ, NH2, BB9

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	0.28±0.01	0±0/1027 (0.0± 0.0%)	0.41±0.01	0±0/1384 (0.0± 0.0%)
2	B	2.61±0.06	1±0/21 (4.8± 0.0%)	1.36±0.05	1±0/22 (4.5± 0.0%)
All	All	0.46	10/10480 (0.1%)	0.44	10/14060 (0.1%)

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
2	B	0.4±0.5	0.0±0.0
All	All	4	0

All unique bond outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	B	501	SER	CA-CB	-11.03	1.36	1.52	10	10

All unique angle outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	B	501	SER	CB-CA-C	5.97	121.44	110.10	3	10

All unique chiral outliers are listed below.

Mol	Chain	Res	Type	Atoms	Models (Total)
2	B	501	SER	CA	4

There are no planarity outliers.

6.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	1007	929	928	106±12
2	B	26	27	27	5±2
All	All	10330	9560	9550	1075

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 54.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:204:HIS:O	1:A:205:TYR:CD2	1.07	2.06	7	1
1:A:215:LEU:HD12	1:A:216:GLY:N	0.96	1.74	9	5
1:A:236:LEU:HD23	1:A:237:ALA:H	0.95	1.21	6	8
1:A:204:HIS:O	1:A:205:TYR:CG	0.94	2.19	7	1
1:A:229:ILE:HG22	1:A:236:LEU:HD11	0.90	1.44	7	7
1:A:204:HIS:HD1	1:A:205:TYR:N	0.89	1.65	8	1
1:A:171:THR:O	1:A:175:VAL:HG23	0.88	1.67	5	10
1:A:184:ALA:HB2	1:A:239:TYR:CE1	0.87	2.05	9	7
1:A:200:ILE:HD13	1:A:200:ILE:O	0.86	1.68	4	7
1:A:174:PHE:CE1	1:A:192:ALA:HB1	0.84	2.07	4	9
1:A:177:LEU:HD13	1:A:182:GLU:OE2	0.84	1.73	8	1
1:A:236:LEU:HD23	1:A:237:ALA:N	0.82	1.89	2	6
1:A:147:GLN:NE2	1:A:147:GLN:H	0.81	1.74	10	1
1:A:198:GLN:NE2	1:A:199:GLY:N	0.80	2.30	5	1
1:A:184:ALA:HB2	1:A:239:TYR:CD1	0.80	2.12	9	8
1:A:147:GLN:HE21	1:A:147:GLN:H	0.80	1.18	6	2
1:A:230:ASP:O	1:A:230:ASP:OD1	0.79	1.99	8	3
1:A:118:GLU:O	1:A:122:VAL:HG23	0.79	1.77	5	9
1:A:196:HIS:O	1:A:200:ILE:HG22	0.78	1.78	4	4
1:A:173:ARG:O	1:A:177:LEU:HG	0.77	1.78	9	6
1:A:209:TYR:O	1:A:213:THR:HG23	0.77	1.80	7	8
1:A:148:SER:O	1:A:152:THR:HG23	0.76	1.80	10	4
1:A:204:HIS:CE1	1:A:205:TYR:CZ	0.76	2.73	4	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:147:GLN:H	1:A:147:GLN:HE21	0.76	1.24	10	1
1:A:182:GLU:OE1	1:A:183:PRO:O	0.76	2.02	1	3
1:A:205:TYR:CE1	1:A:207:CYS:SG	0.76	2.78	2	2
1:A:205:TYR:O	1:A:207:CYS:N	0.76	2.19	6	4
1:A:162:ARG:O	1:A:165:ASP:OD1	0.75	2.04	7	7
1:A:239:TYR:O	1:A:242:ASP:OD1	0.75	2.04	8	9
1:A:197:ARG:HH21	1:A:247:ASN:ND2	0.75	1.80	3	1
1:A:205:TYR:CD2	1:A:206:ASP:N	0.74	2.55	9	3
1:A:168:ASP:OD1	1:A:169:GLU:N	0.74	2.21	6	3
1:A:204:HIS:ND1	1:A:205:TYR:N	0.74	2.34	8	2
1:A:204:HIS:ND1	1:A:205:TYR:CD1	0.73	2.56	8	1
1:A:166:GLU:O	1:A:170:LEU:HD13	0.73	1.84	6	1
1:A:159:ASP:O	1:A:163:ILE:HD13	0.72	1.84	9	3
1:A:147:GLN:H	1:A:147:GLN:NE2	0.71	1.83	6	2
1:A:204:HIS:CE1	1:A:205:TYR:CE2	0.71	2.79	4	1
1:A:144:ALA:HB1	1:A:205:TYR:CZ	0.70	2.21	1	5
1:A:200:ILE:C	1:A:200:ILE:HD12	0.70	2.07	3	2
1:A:203:ASN:HD22	1:A:204:HIS:N	0.70	1.85	3	5
1:A:217:GLU:O	1:A:220:VAL:HG22	0.69	1.87	1	2
1:A:200:ILE:O	1:A:203:ASN:ND2	0.69	2.26	3	5
1:A:226:THR:O	1:A:230:ASP:N	0.69	2.26	10	3
1:A:203:ASN:ND2	1:A:204:HIS:ND1	0.68	2.42	5	1
1:A:204:HIS:ND1	2:B:508:ALA:CB	0.68	2.57	3	1
1:A:158:GLU:OE1	1:A:159:ASP:N	0.68	2.25	2	2
1:A:165:ASP:O	1:A:168:ASP:OD1	0.67	2.12	7	3
1:A:147:GLN:NE2	1:A:147:GLN:N	0.67	2.43	6	3
1:A:197:ARG:NH1	1:A:209:TYR:CE2	0.67	2.63	9	1
1:A:229:ILE:CG2	1:A:236:LEU:HD11	0.67	2.20	2	6
1:A:204:HIS:ND1	1:A:205:TYR:CD2	0.66	2.63	4	1
1:A:233:LYS:NZ	1:A:236:LEU:N	0.66	2.43	4	1
1:A:215:LEU:O	1:A:219:TYR:CD1	0.66	2.47	10	8
1:A:177:LEU:HD12	1:A:178:MET:N	0.66	2.05	5	4
1:A:164:GLN:NE2	1:A:165:ASP:N	0.66	2.42	4	2
1:A:197:ARG:NH1	1:A:209:TYR:CD2	0.66	2.62	9	1
1:A:200:ILE:O	1:A:204:HIS:CD2	0.66	2.49	8	1
1:A:205:TYR:CD1	1:A:206:ASP:N	0.66	2.64	4	2
1:A:205:TYR:CG	1:A:206:ASP:N	0.65	2.64	3	4
1:A:147:GLN:HE21	1:A:147:GLN:N	0.65	1.90	9	3
1:A:238:ALA:O	1:A:242:ASP:OD1	0.65	2.15	6	5
1:A:201:ALA:HB2	1:A:207:CYS:SG	0.65	2.32	6	1
1:A:200:ILE:HD13	1:A:200:ILE:C	0.65	2.12	7	7

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:174:PHE:O	1:A:178:MET:SD	0.65	2.54	4	1
1:A:197:ARG:NH2	1:A:198:GLN:HE21	0.65	1.90	8	3
1:A:229:ILE:HG22	1:A:236:LEU:HD21	0.65	1.69	1	2
1:A:184:ALA:HB1	1:A:242:ASP:OD1	0.64	1.92	3	3
1:A:184:ALA:HB3	1:A:242:ASP:OD2	0.64	1.91	9	5
1:A:233:LYS:HZ1	1:A:236:LEU:N	0.64	1.90	4	1
1:A:247:ASN:OD1	1:A:251:HIS:NE2	0.64	2.31	10	1
1:A:212:HIS:NE2	1:A:244:ILE:HD13	0.64	2.07	5	10
1:A:142:THR:HG22	2:B:511:ALA:H	0.64	1.53	4	3
1:A:187:GLU:N	1:A:187:GLU:OE1	0.64	2.31	3	1
1:A:114:LEU:O	1:A:119:LYS:NZ	0.63	2.31	1	1
1:A:120:PHE:CD1	1:A:124:GLY:O	0.63	2.51	4	3
1:A:233:LYS:HZ3	1:A:233:LYS:HB3	0.63	1.52	10	1
1:A:164:GLN:HE21	1:A:165:ASP:N	0.63	1.90	1	1
1:A:233:LYS:HB2	1:A:233:LYS:HZ3	0.63	1.52	1	2
1:A:115:THR:OG1	1:A:118:GLU:OE1	0.63	2.16	4	3
1:A:203:ASN:ND2	1:A:204:HIS:CD2	0.63	2.67	9	2
1:A:197:ARG:NH2	1:A:209:TYR:CE1	0.63	2.67	7	2
1:A:204:HIS:NE2	1:A:207:CYS:SG	0.63	2.69	8	1
1:A:197:ARG:NH1	1:A:247:ASN:ND2	0.63	2.47	9	1
1:A:214:CYS:O	1:A:218:MET:SD	0.63	2.56	3	1
1:A:197:ARG:NH2	1:A:198:GLN:NE2	0.63	2.47	2	3
1:A:203:ASN:ND2	1:A:204:HIS:NE2	0.63	2.46	1	1
1:A:148:SER:OG	1:A:205:TYR:CD2	0.63	2.51	5	1
1:A:165:ASP:OD1	1:A:166:GLU:N	0.63	2.32	6	5
1:A:145:TYR:N	2:B:501:SER:CB	0.62	2.62	6	10
1:A:209:TYR:CZ	1:A:251:HIS:CD2	0.62	2.87	2	2
1:A:144:ALA:HB2	1:A:211:MET:SD	0.62	2.35	1	2
1:A:245:LEU:O	1:A:249:VAL:HG23	0.62	1.94	9	3
1:A:210:GLU:OE1	1:A:211:MET:N	0.62	2.32	10	2
1:A:223:GLU:OE1	1:A:224:ARG:N	0.62	2.33	10	2
1:A:144:ALA:HB3	2:B:501:SER:CB	0.62	2.25	5	6
1:A:197:ARG:HH21	1:A:247:ASN:HD22	0.62	1.38	3	1
1:A:230:ASP:O	1:A:233:LYS:N	0.61	2.33	4	10
1:A:197:ARG:NE	1:A:209:TYR:CZ	0.61	2.67	4	2
1:A:236:LEU:CD1	1:A:240:MET:SD	0.61	2.88	8	1
1:A:170:LEU:HD21	1:A:196:HIS:CD2	0.61	2.29	3	1
1:A:185:ASP:OD1	1:A:246:ALA:HB1	0.61	1.94	10	1
1:A:205:TYR:O	1:A:206:ASP:CB	0.61	2.48	4	3
1:A:230:ASP:O	1:A:232:ALA:N	0.61	2.34	3	10
1:A:177:LEU:HD12	1:A:177:LEU:C	0.61	2.16	5	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:190:MET:SD	1:A:250:ARG:NH2	0.61	2.74	7	2
1:A:197:ARG:NH1	1:A:198:GLN:NE2	0.61	2.49	7	3
1:A:151:LYS:HD3	1:A:204:HIS:O	0.61	1.96	4	3
1:A:237:ALA:O	1:A:240:MET:HG2	0.60	1.96	7	4
1:A:161:GLN:NE2	1:A:161:GLN:C	0.60	2.55	8	2
1:A:197:ARG:CZ	1:A:198:GLN:HE21	0.60	2.10	2	3
1:A:204:HIS:CD2	1:A:205:TYR:CE2	0.60	2.89	4	1
1:A:205:TYR:HH	1:A:207:CYS:HG	0.60	1.34	1	1
1:A:197:ARG:NH2	1:A:209:TYR:CD1	0.60	2.70	6	2
1:A:155:TYR:CD2	1:A:159:ASP:OD2	0.60	2.55	4	3
1:A:178:MET:SD	1:A:233:LYS:NZ	0.60	2.74	5	2
1:A:188:GLY:O	1:A:191:ASP:OD1	0.60	2.19	10	2
1:A:220:VAL:HG22	1:A:237:ALA:HB1	0.60	1.73	3	1
1:A:205:TYR:O	1:A:206:ASP:CG	0.60	2.41	8	1
1:A:170:LEU:HD11	1:A:174:PHE:CE1	0.59	2.32	3	1
1:A:203:ASN:ND2	1:A:203:ASN:C	0.59	2.56	10	5
1:A:196:HIS:O	1:A:200:ILE:HG23	0.59	1.98	3	2
1:A:175:VAL:HG13	1:A:233:LYS:HD2	0.59	1.74	8	1
1:A:171:THR:O	1:A:175:VAL:CG2	0.59	2.50	6	10
1:A:197:ARG:NH1	1:A:247:ASN:HD21	0.59	1.94	9	1
1:A:200:ILE:CD1	1:A:207:CYS:SG	0.59	2.91	1	2
1:A:233:LYS:NZ	1:A:236:LEU:H	0.59	1.95	4	1
1:A:204:HIS:CG	1:A:205:TYR:CD2	0.59	2.90	4	1
1:A:200:ILE:HD12	1:A:201:ALA:N	0.59	2.13	2	2
1:A:217:GLU:H	1:A:217:GLU:CD	0.59	2.00	3	1
1:A:210:GLU:N	1:A:210:GLU:OE1	0.59	2.35	3	1
1:A:233:LYS:O	1:A:236:LEU:HD22	0.59	1.98	3	2
1:A:203:ASN:C	1:A:203:ASN:HD22	0.59	1.99	10	2
1:A:214:CYS:SG	1:A:218:MET:SD	0.59	3.01	7	1
1:A:200:ILE:HD13	1:A:204:HIS:NE2	0.59	2.12	8	1
1:A:197:ARG:NE	1:A:209:TYR:CD2	0.59	2.70	10	1
1:A:164:GLN:NE2	1:A:164:GLN:C	0.58	2.56	1	2
1:A:185:ASP:OD1	1:A:185:ASP:O	0.58	2.22	7	4
1:A:174:PHE:O	1:A:177:LEU:HG	0.58	1.98	5	3
1:A:170:LEU:C	1:A:170:LEU:HD23	0.58	2.19	5	1
1:A:190:MET:SD	1:A:250:ARG:NE	0.58	2.75	6	1
1:A:117:GLU:N	1:A:117:GLU:OE1	0.58	2.36	2	3
1:A:250:ARG:HH11	1:A:251:HIS:CE1	0.58	2.15	10	1
1:A:200:ILE:CD1	1:A:204:HIS:CD2	0.58	2.87	4	1
1:A:203:ASN:OD1	1:A:204:HIS:CD2	0.58	2.57	6	1
1:A:151:LYS:NZ	1:A:204:HIS:O	0.58	2.37	3	4

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:204:HIS:CG	1:A:205:TYR:CE2	0.58	2.91	4	1
2:B:503:VAL:HG12	2:B:504:GLY:N	0.58	2.13	9	6
1:A:223:GLU:OE1	1:A:223:GLU:C	0.58	2.42	2	3
1:A:184:ALA:HB2	1:A:239:TYR:CE2	0.58	2.33	7	1
1:A:236:LEU:HD12	1:A:236:LEU:C	0.58	2.20	8	1
1:A:115:THR:HG23	1:A:118:GLU:OE1	0.57	1.99	6	1
1:A:207:CYS:SG	1:A:211:MET:SD	0.57	3.02	8	3
1:A:245:LEU:C	1:A:245:LEU:HD23	0.57	2.19	6	3
1:A:191:ASP:O	1:A:194:GLU:HG3	0.57	1.99	3	2
1:A:182:GLU:O	1:A:182:GLU:OE1	0.57	2.21	5	1
1:A:205:TYR:O	1:A:205:TYR:CD1	0.57	2.57	6	3
1:A:155:TYR:CE2	1:A:159:ASP:OD2	0.57	2.57	8	3
1:A:151:LYS:CE	1:A:204:HIS:O	0.57	2.52	10	1
1:A:205:TYR:O	1:A:206:ASP:C	0.57	2.43	10	2
1:A:122:VAL:CG2	1:A:157:LYS:NZ	0.57	2.68	3	1
1:A:118:GLU:OE1	1:A:118:GLU:N	0.57	2.37	4	2
1:A:177:LEU:HD11	1:A:239:TYR:CE2	0.57	2.34	6	2
1:A:197:ARG:CZ	1:A:209:TYR:CE1	0.57	2.87	7	1
1:A:236:LEU:CD2	1:A:237:ALA:N	0.57	2.67	6	3
1:A:194:GLU:O	1:A:194:GLU:OE1	0.57	2.23	6	2
1:A:168:ASP:CG	1:A:172:ARG:HH21	0.56	2.04	2	1
1:A:143:ASP:OD1	1:A:144:ALA:N	0.56	2.39	6	3
1:A:197:ARG:CZ	1:A:209:TYR:CZ	0.56	2.88	4	3
1:A:205:TYR:OH	1:A:211:MET:SD	0.56	2.63	1	2
1:A:250:ARG:HD3	1:A:251:HIS:ND1	0.56	2.15	10	1
1:A:201:ALA:HB1	1:A:206:ASP:HA	0.56	1.77	1	2
1:A:190:MET:SD	1:A:250:ARG:CZ	0.56	2.94	9	2
1:A:200:ILE:O	1:A:204:HIS:NE2	0.56	2.38	8	1
1:A:114:LEU:HB2	1:A:119:LYS:HZ2	0.56	1.61	1	1
1:A:174:PHE:O	1:A:178:MET:HG3	0.56	2.00	8	2
1:A:162:ARG:NH2	1:A:165:ASP:OD1	0.56	2.38	7	1
1:A:168:ASP:OD1	1:A:172:ARG:CZ	0.56	2.54	5	1
1:A:178:MET:SD	1:A:239:TYR:CG	0.56	2.99	6	1
1:A:198:GLN:O	1:A:202:ARG:NH1	0.56	2.39	10	1
1:A:170:LEU:HD23	1:A:170:LEU:O	0.56	2.00	5	1
1:A:178:MET:SD	1:A:239:TYR:CD2	0.56	2.98	6	1
1:A:162:ARG:NH1	1:A:166:GLU:CG	0.56	2.69	2	1
1:A:205:TYR:CE2	1:A:206:ASP:O	0.56	2.59	8	1
1:A:224:ARG:O	1:A:228:ASN:ND2	0.55	2.39	1	1
1:A:216:GLY:O	1:A:220:VAL:HG23	0.55	2.00	3	1
1:A:184:ALA:CB	1:A:242:ASP:OD1	0.55	2.54	8	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:211:MET:C	1:A:211:MET:SD	0.55	2.85	9	1
1:A:242:ASP:OD1	1:A:242:ASP:N	0.55	2.39	1	1
1:A:158:GLU:CD	1:A:159:ASP:N	0.55	2.59	9	1
1:A:245:LEU:C	1:A:245:LEU:HD13	0.55	2.22	1	4
1:A:122:VAL:HG23	1:A:157:LYS:NZ	0.55	2.17	3	1
1:A:197:ARG:NH2	1:A:247:ASN:HD22	0.55	1.98	3	1
1:A:120:PHE:CE1	1:A:124:GLY:O	0.55	2.60	7	3
1:A:210:GLU:CD	1:A:211:MET:N	0.55	2.60	5	2
1:A:217:GLU:OE1	1:A:241:ARG:NH1	0.55	2.40	8	1
1:A:233:LYS:NZ	1:A:234:PRO:O	0.55	2.40	4	5
1:A:144:ALA:O	1:A:147:GLN:N	0.55	2.39	4	3
1:A:168:ASP:O	1:A:171:THR:OG1	0.55	2.23	9	9
1:A:203:ASN:HD22	1:A:203:ASN:C	0.55	2.04	3	4
1:A:211:MET:SD	1:A:211:MET:C	0.55	2.85	8	2
1:A:205:TYR:CD1	1:A:207:CYS:SG	0.55	2.99	10	1
1:A:189:ALA:O	1:A:192:ALA:HB3	0.54	2.02	5	6
1:A:168:ASP:OD1	1:A:172:ARG:NH1	0.54	2.41	9	1
1:A:164:GLN:NE2	1:A:168:ASP:OD2	0.54	2.41	4	1
1:A:226:THR:O	1:A:230:ASP:OD1	0.54	2.25	6	3
1:A:144:ALA:HB1	1:A:205:TYR:CD2	0.54	2.37	2	1
1:A:214:CYS:SG	2:B:511:ALA:O	0.54	2.65	5	3
1:A:233:LYS:HB3	1:A:233:LYS:NZ	0.54	2.16	10	1
1:A:147:GLN:N	1:A:147:GLN:OE1	0.54	2.40	1	2
1:A:230:ASP:C	1:A:232:ALA:N	0.54	2.61	3	10
1:A:142:THR:HG22	2:B:511:ALA:N	0.54	2.17	4	5
1:A:151:LYS:NZ	1:A:151:LYS:CB	0.54	2.71	3	2
1:A:247:ASN:O	1:A:251:HIS:CE1	0.54	2.60	4	2
1:A:223:GLU:H	1:A:223:GLU:CD	0.54	2.07	6	1
1:A:187:GLU:H	1:A:187:GLU:CD	0.54	2.07	6	3
1:A:214:CYS:SG	1:A:218:MET:CE	0.53	2.96	7	1
1:A:187:GLU:O	1:A:191:ASP:OD1	0.53	2.26	4	4
1:A:187:GLU:O	1:A:191:ASP:OD2	0.53	2.27	9	3
1:A:197:ARG:NE	1:A:209:TYR:CE2	0.53	2.77	1	2
1:A:230:ASP:OD1	1:A:236:LEU:CD2	0.53	2.57	1	1
1:A:247:ASN:O	1:A:251:HIS:ND1	0.53	2.41	4	5
1:A:204:HIS:CE1	1:A:205:TYR:CE1	0.53	2.97	4	2
1:A:125:ASP:O	1:A:125:ASP:OD1	0.53	2.27	6	3
1:A:178:MET:CG	1:A:239:TYR:CD2	0.53	2.90	6	1
1:A:172:ARG:O	1:A:176:ALA:CB	0.53	2.57	10	9
1:A:144:ALA:HB1	1:A:205:TYR:CE2	0.53	2.38	4	2
1:A:218:MET:SD	1:A:218:MET:C	0.53	2.87	8	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:194:GLU:O	1:A:198:GLN:OE1	0.53	2.26	10	1
1:A:161:GLN:NE2	1:A:161:GLN:O	0.53	2.42	1	1
1:A:168:ASP:O	1:A:172:ARG:NE	0.53	2.41	2	1
1:A:201:ALA:O	1:A:205:TYR:C	0.53	2.47	2	3
1:A:184:ALA:HB2	1:A:239:TYR:CD2	0.53	2.39	7	1
1:A:122:VAL:O	1:A:164:GLN:OE1	0.53	2.27	10	1
1:A:179:ASP:OD1	1:A:180:ALA:N	0.53	2.42	7	1
1:A:197:ARG:NH2	1:A:209:TYR:OH	0.53	2.42	8	3
1:A:124:GLY:O	1:A:125:ASP:C	0.53	2.47	2	3
1:A:215:LEU:O	1:A:219:TYR:CE2	0.52	2.62	3	1
1:A:144:ALA:CB	1:A:205:TYR:CZ	0.52	2.93	4	2
1:A:156:THR:O	1:A:160:TRP:CD1	0.52	2.61	4	6
1:A:201:ALA:CB	1:A:207:CYS:H	0.52	2.17	4	1
1:A:197:ARG:NE	1:A:209:TYR:CD1	0.52	2.77	7	1
1:A:211:MET:SD	1:A:211:MET:O	0.52	2.67	9	2
1:A:143:ASP:O	1:A:147:GLN:NE2	0.52	2.42	9	3
1:A:173:ARG:HH12	1:A:195:ASP:CB	0.52	2.17	10	1
1:A:242:ASP:OD1	1:A:243:ALA:N	0.52	2.42	3	3
1:A:203:ASN:O	1:A:204:HIS:ND1	0.52	2.42	5	1
1:A:142:THR:HG21	2:B:511:ALA:N	0.52	2.19	9	1
1:A:158:GLU:OE1	1:A:159:ASP:OD1	0.52	2.27	9	1
1:A:166:GLU:OE1	1:A:166:GLU:O	0.52	2.28	9	1
1:A:205:TYR:O	1:A:206:ASP:HB2	0.52	2.05	9	2
1:A:217:GLU:N	1:A:217:GLU:OE1	0.52	2.42	6	1
1:A:142:THR:CG2	2:B:511:ALA:N	0.52	2.72	8	2
1:A:197:ARG:CZ	1:A:209:TYR:CE2	0.52	2.92	9	2
1:A:191:ASP:OD1	1:A:192:ALA:N	0.52	2.43	8	1
1:A:163:ILE:CG1	1:A:203:ASN:OD1	0.52	2.58	4	1
1:A:168:ASP:OD2	1:A:172:ARG:NH2	0.52	2.42	2	1
1:A:212:HIS:O	1:A:215:LEU:HG	0.51	2.05	10	4
1:A:144:ALA:O	1:A:148:SER:OG	0.51	2.27	5	1
1:A:200:ILE:C	1:A:200:ILE:CD1	0.51	2.79	3	4
1:A:164:GLN:CD	1:A:165:ASP:N	0.51	2.64	4	1
1:A:175:VAL:HG13	1:A:233:LYS:HG3	0.51	1.83	3	1
1:A:149:LYS:CB	1:A:149:LYS:NZ	0.51	2.74	9	2
1:A:161:GLN:OE1	1:A:161:GLN:O	0.51	2.28	4	2
1:A:203:ASN:OD1	1:A:203:ASN:O	0.51	2.29	6	1
1:A:239:TYR:C	1:A:242:ASP:OD1	0.51	2.49	7	5
1:A:203:ASN:CG	1:A:204:HIS:ND1	0.51	2.64	5	1
1:A:172:ARG:O	1:A:176:ALA:HB2	0.51	2.06	10	7
1:A:151:LYS:C	1:A:153:ALA:H	0.51	2.08	7	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:205:TYR:CZ	1:A:207:CYS:SG	0.51	2.94	1	2
1:A:197:ARG:HH11	1:A:198:GLN:NE2	0.51	2.04	7	1
1:A:168:ASP:C	1:A:172:ARG:NH1	0.50	2.65	9	1
1:A:161:GLN:OE1	1:A:161:GLN:C	0.50	2.50	2	2
1:A:184:ALA:CB	1:A:242:ASP:OD2	0.50	2.60	6	3
1:A:166:GLU:OE1	1:A:166:GLU:C	0.50	2.50	9	1
1:A:161:GLN:O	1:A:165:ASP:OD1	0.50	2.29	9	3
1:A:204:HIS:NE2	1:A:205:TYR:CZ	0.50	2.80	4	1
1:A:204:HIS:CE1	1:A:207:CYS:HG	0.50	2.20	8	1
1:A:215:LEU:HD12	1:A:216:GLY:CA	0.50	2.37	9	5
1:A:213:THR:O	1:A:217:GLU:OE2	0.50	2.29	3	1
1:A:214:CYS:O	1:A:217:GLU:OE2	0.50	2.30	3	1
1:A:168:ASP:CG	1:A:172:ARG:NH1	0.50	2.65	9	1
1:A:114:LEU:HD22	1:A:157:LYS:HD3	0.49	1.84	9	1
1:A:215:LEU:CD1	1:A:216:GLY:N	0.49	2.66	5	5
1:A:162:ARG:HH21	1:A:165:ASP:CG	0.49	2.11	7	1
1:A:168:ASP:O	1:A:172:ARG:NH1	0.49	2.44	9	1
1:A:124:GLY:O	1:A:126:PHE:N	0.49	2.46	2	3
1:A:168:ASP:CG	1:A:172:ARG:NH2	0.49	2.65	2	1
1:A:170:LEU:HD23	1:A:174:PHE:CD1	0.49	2.43	2	2
1:A:204:HIS:CE1	1:A:205:TYR:CD1	0.49	3.01	8	1
1:A:212:HIS:NE2	1:A:244:ILE:CD1	0.49	2.75	10	9
1:A:174:PHE:CZ	1:A:192:ALA:HB1	0.49	2.42	1	3
1:A:230:ASP:OD1	1:A:233:LYS:C	0.49	2.50	8	2
1:A:245:LEU:O	1:A:245:LEU:HD13	0.49	2.07	9	1
1:A:210:GLU:OE1	1:A:210:GLU:C	0.49	2.51	9	3
1:A:203:ASN:C	1:A:203:ASN:ND2	0.49	2.64	7	1
1:A:245:LEU:HD13	1:A:245:LEU:O	0.49	2.07	8	5
1:A:117:GLU:O	1:A:121:GLU:HG3	0.49	2.08	8	1
1:A:230:ASP:O	1:A:231:ALA:C	0.49	2.51	3	10
1:A:207:CYS:SG	1:A:211:MET:CE	0.49	3.01	8	1
1:A:162:ARG:HH12	1:A:166:GLU:CD	0.48	2.11	2	1
1:A:184:ALA:CB	1:A:239:TYR:CE1	0.48	2.90	9	3
1:A:217:GLU:OE1	1:A:217:GLU:C	0.48	2.52	2	1
1:A:178:MET:CB	1:A:233:LYS:HZ3	0.48	2.20	8	1
1:A:197:ARG:CD	1:A:209:TYR:CD2	0.48	2.96	10	1
1:A:173:ARG:NH1	1:A:195:ASP:OD2	0.48	2.46	1	1
1:A:197:ARG:HH22	1:A:198:GLN:NE2	0.48	2.05	8	2
1:A:224:ARG:O	1:A:228:ASN:OD1	0.48	2.31	2	2
1:A:151:LYS:NZ	1:A:151:LYS:HB3	0.48	2.23	3	1
1:A:163:ILE:HD13	1:A:203:ASN:CG	0.48	2.29	7	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:204:HIS:CD2	2:B:508:ALA:CB	0.48	2.97	5	2
1:A:204:HIS:NE2	1:A:205:TYR:CE2	0.48	2.82	4	1
1:A:162:ARG:NH2	1:A:165:ASP:CG	0.48	2.67	7	1
1:A:205:TYR:O	1:A:206:ASP:HB3	0.48	2.08	1	1
1:A:151:LYS:NZ	1:A:204:HIS:C	0.48	2.66	9	3
1:A:115:THR:O	1:A:118:GLU:N	0.48	2.47	6	2
1:A:182:GLU:O	1:A:239:TYR:OH	0.48	2.30	4	4
1:A:218:MET:SD	1:A:218:MET:O	0.48	2.71	8	1
1:A:154:SER:O	1:A:155:TYR:C	0.48	2.51	2	3
1:A:206:ASP:O	1:A:206:ASP:OD1	0.48	2.32	3	4
1:A:230:ASP:HA	1:A:236:LEU:HD22	0.48	1.85	1	1
1:A:151:LYS:HB3	1:A:151:LYS:HZ3	0.48	1.67	3	1
1:A:113:ASN:O	1:A:113:ASN:OD1	0.48	2.31	10	2
1:A:211:MET:SD	1:A:215:LEU:HD23	0.48	2.48	9	2
1:A:162:ARG:NH1	1:A:166:GLU:CD	0.48	2.66	2	1
1:A:230:ASP:CG	1:A:236:LEU:CD2	0.48	2.82	5	1
1:A:212:HIS:CD2	1:A:244:ILE:HD13	0.48	2.44	5	10
1:A:178:MET:CG	1:A:239:TYR:CE2	0.48	2.97	6	1
1:A:152:THR:HA	1:A:155:TYR:CD1	0.48	2.44	10	6
1:A:241:ARG:O	1:A:245:LEU:N	0.48	2.32	5	1
1:A:205:TYR:O	1:A:206:ASP:OD1	0.48	2.31	8	1
1:A:233:LYS:NZ	1:A:234:PRO:C	0.47	2.67	4	1
1:A:250:ARG:NH1	1:A:251:HIS:ND1	0.47	2.61	10	1
1:A:223:GLU:OE1	1:A:223:GLU:O	0.47	2.32	2	1
1:A:204:HIS:CE1	1:A:207:CYS:SG	0.47	3.08	8	1
1:A:233:LYS:HZ3	1:A:234:PRO:C	0.47	2.13	4	1
1:A:197:ARG:NH1	1:A:198:GLN:HE22	0.47	2.07	7	1
1:A:118:GLU:O	1:A:122:VAL:N	0.47	2.45	2	1
1:A:173:ARG:CB	1:A:173:ARG:NH1	0.47	2.78	8	6
1:A:251:HIS:ND1	1:A:251:HIS:N	0.47	2.61	4	3
1:A:205:TYR:OH	1:A:207:CYS:SG	0.47	2.60	1	1
1:A:233:LYS:HB2	1:A:233:LYS:NZ	0.47	2.25	1	2
1:A:197:ARG:CZ	1:A:198:GLN:NE2	0.47	2.76	2	2
1:A:201:ALA:O	1:A:205:TYR:N	0.47	2.41	2	1
1:A:203:ASN:C	1:A:204:HIS:ND1	0.47	2.68	5	1
1:A:230:ASP:OD1	1:A:233:LYS:O	0.47	2.33	8	1
1:A:209:TYR:CE2	1:A:251:HIS:NE2	0.47	2.83	2	2
1:A:198:GLN:O	1:A:202:ARG:HG2	0.47	2.09	4	1
1:A:198:GLN:NE2	1:A:199:GLY:CA	0.47	2.78	5	1
1:A:204:HIS:CD2	2:B:508:ALA:HB2	0.47	2.45	2	2
1:A:228:ASN:ND2	2:B:506:ALA:HB2	0.47	2.24	4	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:151:LYS:C	1:A:153:ALA:N	0.47	2.67	7	1
1:A:200:ILE:HD11	1:A:204:HIS:CD2	0.47	2.45	4	1
1:A:175:VAL:O	1:A:179:ASP:OD1	0.47	2.33	8	1
1:A:115:THR:OG1	1:A:118:GLU:HG2	0.46	2.10	1	2
1:A:209:TYR:CE2	1:A:251:HIS:CD2	0.46	3.04	2	1
1:A:222:ASP:OD1	1:A:223:GLU:N	0.46	2.48	7	1
2:B:503:VAL:CG1	2:B:504:GLY:N	0.46	2.79	9	5
1:A:118:GLU:O	1:A:122:VAL:CG2	0.46	2.63	6	2
1:A:200:ILE:CD1	1:A:204:HIS:NE2	0.46	2.78	8	1
1:A:188:GLY:C	1:A:191:ASP:OD1	0.46	2.54	10	1
1:A:247:ASN:O	1:A:251:HIS:NE2	0.46	2.49	10	1
1:A:165:ASP:O	1:A:168:ASP:OD2	0.46	2.33	1	1
1:A:203:ASN:HD21	1:A:204:HIS:CD2	0.46	2.29	8	1
1:A:227:ARG:HA	1:A:230:ASP:OD1	0.46	2.10	6	2
1:A:157:LYS:O	1:A:161:GLN:N	0.46	2.46	4	2
1:A:159:ASP:O	1:A:163:ILE:CD1	0.46	2.63	4	2
1:A:190:MET:O	1:A:193:ALA:HB3	0.46	2.11	1	1
1:A:191:ASP:O	1:A:194:GLU:HG2	0.46	2.10	1	1
1:A:200:ILE:O	1:A:200:ILE:CD1	0.46	2.62	5	1
1:A:123:PHE:O	1:A:124:GLY:O	0.46	2.34	2	3
1:A:206:ASP:O	1:A:208:GLY:N	0.46	2.48	1	1
1:A:182:GLU:OE1	1:A:239:TYR:OH	0.46	2.33	5	1
1:A:144:ALA:HB1	1:A:205:TYR:CE1	0.46	2.46	8	1
1:A:203:ASN:HD22	1:A:204:HIS:CD2	0.46	2.28	1	1
1:A:220:VAL:HG12	1:A:220:VAL:O	0.46	2.11	3	1
1:A:191:ASP:O	1:A:195:ASP:OD1	0.46	2.33	5	1
1:A:114:LEU:O	1:A:119:LYS:HE3	0.46	2.11	9	1
1:A:217:GLU:C	1:A:219:TYR:N	0.45	2.70	1	1
1:A:203:ASN:O	1:A:204:HIS:CD2	0.45	2.69	3	1
1:A:157:LYS:HB2	1:A:157:LYS:NZ	0.45	2.25	10	1
1:A:207:CYS:O	1:A:208:GLY:O	0.45	2.33	1	2
1:A:193:ALA:HB1	1:A:244:ILE:HG12	0.45	1.89	9	2
1:A:230:ASP:OD1	1:A:230:ASP:C	0.45	2.54	8	1
1:A:203:ASN:ND2	1:A:204:HIS:N	0.45	2.62	3	2
1:A:201:ALA:HA	1:A:207:CYS:H	0.45	1.72	7	1
1:A:197:ARG:HB3	1:A:197:ARG:NH1	0.45	2.27	1	1
1:A:115:THR:OG1	1:A:118:GLU:OE2	0.45	2.35	9	1
1:A:202:ARG:CB	1:A:202:ARG:NH1	0.45	2.80	5	2
1:A:200:ILE:C	1:A:203:ASN:ND2	0.45	2.70	2	1
1:A:197:ARG:NH2	1:A:209:TYR:CZ	0.45	2.85	8	1
1:A:250:ARG:CB	1:A:250:ARG:NH1	0.45	2.80	6	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:151:LYS:C	1:A:151:LYS:HD3	0.45	2.32	9	1
1:A:191:ASP:O	1:A:194:GLU:OE2	0.45	2.35	3	1
1:A:227:ARG:CB	1:A:227:ARG:NH1	0.45	2.80	3	1
1:A:217:GLU:O	1:A:217:GLU:CD	0.45	2.55	4	1
1:A:144:ALA:HB1	1:A:205:TYR:CD1	0.45	2.47	6	1
1:A:146:ARG:CG	1:A:147:GLN:N	0.44	2.80	2	2
1:A:245:LEU:HD23	1:A:245:LEU:O	0.44	2.12	6	3
1:A:237:ALA:O	1:A:240:MET:CG	0.44	2.65	2	2
1:A:151:LYS:CD	1:A:204:HIS:O	0.44	2.65	10	3
1:A:143:ASP:O	1:A:147:GLN:OE1	0.44	2.35	5	1
1:A:155:TYR:CE2	1:A:159:ASP:OD1	0.44	2.71	6	2
1:A:113:ASN:C	1:A:113:ASN:HD22	0.44	2.15	4	2
1:A:194:GLU:OE2	1:A:195:ASP:N	0.44	2.50	3	1
1:A:157:LYS:NZ	1:A:157:LYS:CB	0.44	2.80	10	1
1:A:238:ALA:O	1:A:242:ASP:OD2	0.44	2.34	8	3
1:A:149:LYS:NZ	1:A:149:LYS:HB3	0.44	2.28	4	1
1:A:173:ARG:O	1:A:177:LEU:CG	0.44	2.63	4	2
1:A:142:THR:HG21	2:B:511:ALA:H	0.44	1.71	9	1
1:A:158:GLU:OE1	1:A:159:ASP:CA	0.44	2.66	2	1
1:A:157:LYS:HG3	1:A:161:GLN:HE21	0.44	1.72	3	1
1:A:165:ASP:OD1	1:A:165:ASP:C	0.44	2.56	8	2
1:A:230:ASP:OD1	1:A:234:PRO:N	0.44	2.50	9	1
1:A:190:MET:SD	1:A:250:ARG:NH1	0.44	2.91	1	1
1:A:204:HIS:NE2	2:B:508:ALA:HB2	0.44	2.28	6	1
1:A:119:LYS:O	1:A:123:PHE:N	0.44	2.49	1	4
1:A:182:GLU:OE2	1:A:239:TYR:OH	0.44	2.36	1	1
1:A:224:ARG:N	1:A:224:ARG:HD3	0.44	2.28	2	1
1:A:203:ASN:OD1	1:A:204:HIS:NE2	0.44	2.50	6	1
1:A:188:GLY:HA2	1:A:191:ASP:OD2	0.44	2.12	8	1
1:A:222:ASP:OD1	1:A:223:GLU:OE2	0.43	2.36	6	1
1:A:195:ASP:O	1:A:198:GLN:NE2	0.43	2.37	5	1
1:A:201:ALA:CB	1:A:207:CYS:SG	0.43	3.06	6	1
1:A:144:ALA:HB1	1:A:205:TYR:CG	0.43	2.49	6	1
1:A:233:LYS:HZ3	1:A:234:PRO:HD2	0.43	1.74	1	2
1:A:145:TYR:H	2:B:501:SER:CB	0.43	2.25	5	1
1:A:144:ALA:O	1:A:145:TYR:C	0.43	2.56	8	1
1:A:242:ASP:OD1	1:A:242:ASP:C	0.43	2.57	10	1
1:A:226:THR:O	1:A:230:ASP:OD2	0.43	2.37	2	1
1:A:163:ILE:HD13	1:A:203:ASN:OD1	0.43	2.14	7	1
1:A:158:GLU:OE2	1:A:159:ASP:OD1	0.43	2.37	9	1
1:A:223:GLU:O	1:A:227:ARG:NH1	0.43	2.51	3	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:218:MET:O	1:A:221:SER:OG	0.43	2.37	5	1
1:A:182:GLU:OE1	1:A:182:GLU:O	0.43	2.36	8	1
1:A:162:ARG:C	1:A:165:ASP:OD1	0.43	2.57	1	3
1:A:113:ASN:C	1:A:113:ASN:ND2	0.43	2.71	4	2
1:A:187:GLU:O	1:A:191:ASP:CG	0.43	2.57	7	3
1:A:215:LEU:O	1:A:219:TYR:CD2	0.43	2.72	3	1
1:A:144:ALA:O	1:A:147:GLN:CG	0.43	2.67	7	1
1:A:230:ASP:CG	1:A:233:LYS:O	0.43	2.56	10	1
1:A:182:GLU:OE1	1:A:182:GLU:C	0.43	2.58	1	3
1:A:194:GLU:OE1	1:A:198:GLN:OE1	0.43	2.36	10	1
1:A:170:LEU:O	1:A:174:PHE:CD1	0.43	2.72	1	1
1:A:194:GLU:CD	1:A:194:GLU:C	0.43	2.78	3	1
1:A:217:GLU:O	1:A:217:GLU:OE2	0.43	2.37	4	1
1:A:185:ASP:O	1:A:185:ASP:CG	0.43	2.57	10	1
1:A:215:LEU:O	1:A:219:TYR:CG	0.43	2.72	10	1
1:A:226:THR:HG22	1:A:230:ASP:OD2	0.42	2.14	2	1
1:A:200:ILE:CD1	1:A:200:ILE:C	0.42	2.88	4	1
1:A:245:LEU:C	1:A:245:LEU:CD2	0.42	2.87	6	1
1:A:215:LEU:HD23	1:A:215:LEU:N	0.42	2.29	1	1
1:A:204:HIS:CE1	1:A:205:TYR:CD2	0.42	3.08	4	1
1:A:149:LYS:NZ	1:A:149:LYS:HB2	0.42	2.29	7	1
1:A:149:LYS:HB2	1:A:149:LYS:NZ	0.42	2.30	1	1
1:A:230:ASP:OD1	1:A:230:ASP:N	0.42	2.53	1	1
1:A:230:ASP:OD1	1:A:236:LEU:HD21	0.42	2.15	1	1
1:A:215:LEU:HD12	1:A:215:LEU:C	0.42	2.32	5	1
1:A:199:GLY:O	1:A:203:ASN:CG	0.42	2.57	5	2
1:A:147:GLN:O	1:A:150:GLU:CG	0.42	2.68	3	1
1:A:245:LEU:C	1:A:245:LEU:CD1	0.42	2.88	1	3
1:A:215:LEU:O	1:A:218:MET:N	0.42	2.53	8	1
1:A:204:HIS:ND1	1:A:205:TYR:CE2	0.42	2.87	4	1
1:A:168:ASP:OD1	1:A:172:ARG:NE	0.42	2.53	2	1
1:A:210:GLU:O	1:A:213:THR:OG1	0.42	2.36	2	2
1:A:247:ASN:O	1:A:250:ARG:CG	0.42	2.68	3	1
1:A:203:ASN:CG	1:A:203:ASN:O	0.42	2.58	4	1
1:A:179:ASP:OD1	1:A:179:ASP:C	0.42	2.58	7	1
1:A:229:ILE:HG22	1:A:236:LEU:CD1	0.42	2.32	7	1
1:A:233:LYS:C	1:A:233:LYS:HD3	0.41	2.36	1	2
1:A:197:ARG:NH1	1:A:212:HIS:HB3	0.41	2.30	3	1
1:A:206:ASP:OD1	1:A:206:ASP:C	0.41	2.58	9	1
1:A:219:TYR:CD2	1:A:229:ILE:CD1	0.41	3.03	8	1
1:A:151:LYS:NZ	1:A:151:LYS:HB2	0.41	2.29	10	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:168:ASP:OD1	1:A:168:ASP:C	0.41	2.58	1	1
1:A:173:ARG:CG	1:A:174:PHE:N	0.41	2.83	5	1
1:A:177:LEU:C	1:A:177:LEU:CD1	0.41	2.88	5	1
1:A:200:ILE:HA	1:A:203:ASN:ND2	0.41	2.31	5	1
1:A:148:SER:O	1:A:152:THR:CG2	0.41	2.61	10	1
1:A:143:ASP:O	1:A:146:ARG:HB3	0.41	2.15	4	1
1:A:149:LYS:NZ	1:A:149:LYS:CB	0.41	2.84	4	1
1:A:122:VAL:HG13	1:A:161:GLN:HA	0.41	1.91	6	1
1:A:151:LYS:HG3	1:A:204:HIS:O	0.41	2.15	1	1
1:A:159:ASP:O	1:A:163:ILE:HG12	0.41	2.15	2	1
1:A:214:CYS:C	1:A:217:GLU:OE2	0.41	2.59	3	1
1:A:184:ALA:HA	1:A:239:TYR:CZ	0.41	2.51	6	1
1:A:197:ARG:NE	1:A:209:TYR:CE1	0.41	2.88	7	1
1:A:222:ASP:OD1	1:A:224:ARG:N	0.41	2.54	7	1
1:A:187:GLU:CD	1:A:187:GLU:N	0.41	2.74	2	2
1:A:170:LEU:CD1	1:A:174:PHE:CE1	0.41	3.03	3	1
1:A:198:GLN:NE2	1:A:199:GLY:H	0.41	2.09	5	1
1:A:233:LYS:CE	1:A:234:PRO:O	0.41	2.68	2	1
1:A:200:ILE:HD12	1:A:207:CYS:SG	0.41	2.55	1	1
1:A:198:GLN:CD	1:A:199:GLY:N	0.41	2.74	5	1
1:A:204:HIS:CE1	2:B:508:ALA:CB	0.41	3.03	9	1
2:B:503:VAL:HG12	2:B:504:GLY:H	0.41	1.76	9	1
1:A:162:ARG:HH12	1:A:166:GLU:CG	0.41	2.29	2	1
1:A:163:ILE:HD12	1:A:203:ASN:CB	0.41	2.46	5	1
1:A:115:THR:CG2	1:A:118:GLU:OE1	0.41	2.68	6	1
1:A:158:GLU:HG3	1:A:159:ASP:N	0.41	2.31	6	1
1:A:178:MET:CB	1:A:233:LYS:NZ	0.41	2.84	8	1
1:A:214:CYS:O	1:A:218:MET:CB	0.41	2.69	10	1
1:A:151:LYS:O	1:A:155:TYR:CE1	0.41	2.74	1	1
1:A:205:TYR:CE2	1:A:207:CYS:SG	0.41	3.07	1	1
1:A:236:LEU:HD23	1:A:236:LEU:N	0.41	2.31	3	1
1:A:120:PHE:HD1	1:A:125:ASP:H	0.40	1.59	3	1
1:A:194:GLU:OE1	1:A:194:GLU:C	0.40	2.60	6	1
1:A:143:ASP:CG	1:A:144:ALA:N	0.40	2.75	8	1
1:A:142:THR:OG1	1:A:145:TYR:HB2	0.40	2.16	8	1
1:A:177:LEU:CD1	1:A:178:MET:N	0.40	2.83	6	1
1:A:177:LEU:CD1	1:A:239:TYR:OH	0.40	2.70	6	1
1:A:173:ARG:NH1	1:A:195:ASP:CB	0.40	2.84	10	1
1:A:185:ASP:O	1:A:190:MET:CE	0.40	2.70	3	1
1:A:158:GLU:CD	1:A:159:ASP:OD1	0.40	2.59	9	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	125/144 (87%)	114±2 (92±2%)	7±2 (5±1%)	4±1 (3±1%)	7 39
2	B	5/12 (42%)	1±1 (14±20%)	3±1 (60±18%)	1±0 (26±9%)	0 1
All	All	1300/1560 (83%)	1151 (89%)	97 (7%)	52 (4%)	5 31

All 11 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	231	ALA	10
1	A	206	ASP	9
2	B	506	ALA	8
1	A	205	TYR	7
1	A	125	ASP	6
1	A	124	GLY	3
2	B	511	ALA	3
1	A	208	GLY	2
2	B	503	VAL	2
1	A	207	CYS	1
1	A	113	ASN	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	102/118 (86%)	90±3 (88±2%)	12±3 (12±2%)	8 51
2	B	1/2 (50%)	1±0 (100±0%)	0±0 (0±0%)	100 100
All	All	1030/1200 (86%)	910 (88%)	120 (12%)	9 52

All 45 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	233	LYS	9
1	A	194	GLU	9
1	A	200	ILE	8
1	A	171	THR	8
1	A	203	ASN	7
1	A	147	GLN	5
1	A	215	LEU	5
1	A	149	LYS	4
1	A	161	GLN	4
1	A	210	GLU	4
1	A	191	ASP	3
1	A	151	LYS	3
1	A	211	MET	3
1	A	223	GLU	3
1	A	250	ARG	3
1	A	164	GLN	2
1	A	172	ARG	2
1	A	230	ASP	2
1	A	117	GLU	2
1	A	205	TYR	2
1	A	224	ARG	2
1	A	236	LEU	2
1	A	113	ASN	2
1	A	173	ARG	2
1	A	214	CYS	2
1	A	245	LEU	2
1	A	118	GLU	2
1	A	142	THR	1
1	A	168	ASP	1
1	A	158	GLU	1
1	A	202	ARG	1
1	A	227	ARG	1
1	A	187	GLU	1
1	A	217	GLU	1
1	A	218	MET	1
1	A	219	TYR	1
1	A	204	HIS	1
1	A	251	HIS	1
1	A	182	GLU	1
1	A	162	ARG	1
1	A	242	ASP	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	166	GLU	1
1	A	225	PHE	1
1	A	126	PHE	1
1	A	157	LYS	1

6.3.3 RNA (i)

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues are 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	BB9	B	507	2	3,5,6	1.78±0.06	1±0 (33±0%)
2	MOZ	B	509	2	4,5,7	2.35±0.03	2±0 (50±0%)
2	BB9	B	502	2	3,5,6	1.49±0.07	1±0 (33±0%)
2	MOZ	B	505	2	6,6,7	2.66±0.10	3±0 (46±6%)

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	BB9	B	507	2	1,5,7	3.69±0.27	1±0 (100±0%)
2	MOZ	B	509	2	3,6,9	3.76±0.13	2±0 (66±0%)
2	BB9	B	502	2	1,5,7	3.07±0.14	1±0 (100±0%)

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
2	MOZ	B	505	2	4,7,9	8.84±0.04	4±0 (100±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	BB9	B	507	2	-	0±0,0,4,6	-
2	BB9	B	502	2	-	0±0,0,4,6	-
2	MOZ	B	505	2	-	0±0,0,6,8	-
2	MOZ	B	509	2	-	0±0,0,4,8	-

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	B	505	MOZ	C-CA	4.89	1.53	1.45	1	10
2	B	509	MOZ	OG-CB	4.05	1.42	1.31	10	10
2	B	505	MOZ	OG-CB	3.69	1.41	1.31	2	10
2	B	507	BB9	CA-N	3.11	1.43	1.35	1	10
2	B	509	MOZ	CA-N	2.79	1.40	1.33	8	10
2	B	502	BB9	CA-N	2.48	1.41	1.35	2	10
2	B	505	MOZ	CA-N	2.20	1.41	1.36	5	8

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(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	B	505	MOZ	OG-CB-CA	16.29	106.29	121.10	3	10
2	B	505	MOZ	C6-CB-CA	5.77	132.65	124.02	1	10
2	B	509	MOZ	OG-CB-C6	4.74	124.21	114.59	1	10
2	B	509	MOZ	C-CA-N	4.71	120.43	115.40	4	10
2	B	507	BB9	O-C-CA	4.02	120.28	125.39	9	10
2	B	505	MOZ	O-C-CA	3.51	118.99	125.54	10	10
2	B	502	BB9	O-C-CA	3.30	121.19	125.39	9	10
2	B	505	MOZ	OG-CB-C6	3.22	121.14	114.59	8	10

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6.5 Carbohydrates (i)

There are no monosaccharides in this entry.

6.6 Ligand geometry (i)

There are no ligands in this entry.

6.7 Other polymers (i)

There are no such molecules in this entry.

6.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

7 Chemical shift validation (i)

The completeness of assignment taking into account all chemical shift lists is 89% for the well-defined parts and 88% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping (i)

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

Total number of shifts	1737
Number of shifts mapped to atoms	1733
Number of unparsed shifts	0
Number of shifts with mapping errors	4
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	8

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

- No matching atom found in the structure. All 4 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	B	501	SER	HB2	7.77	0.006	1
1	B	511	DHA	H	5.943	0.008	1
1	B	511	DHA	HB1	2.837	0.001	1
1	B	511	DHA	HB2	2.553	0.004	1

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	143	-0.64 ± 0.18	Should be checked
$^{13}C_{\beta}$	134	0.21 ± 0.05	None needed (< 0.5 ppm)
$^{13}C'$	133	-0.55 ± 0.12	Should be applied
^{15}N	137	0.28 ± 0.33	None needed (< 0.5 ppm)

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 89%, i.e. 1537 atoms were assigned a chemical shift out of a possible 1724. 0 out of 11 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	632/660 (96%)	264/268 (99%)	246/264 (93%)	122/128 (95%)
Sidechain	778/919 (85%)	532/590 (90%)	230/286 (80%)	16/43 (37%)
Aromatic	127/145 (88%)	65/71 (92%)	60/68 (88%)	2/6 (33%)
Overall	1537/1724 (89%)	861/929 (93%)	536/618 (87%)	140/177 (79%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 88%, i.e. 1724 atoms were assigned a chemical shift out of a possible 1957. 0 out of 12 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	711/745 (95%)	298/303 (98%)	276/298 (93%)	137/144 (95%)
Sidechain	866/1046 (83%)	594/668 (89%)	255/327 (78%)	17/51 (33%)
Aromatic	147/166 (89%)	75/81 (93%)	69/78 (88%)	3/7 (43%)
Overall	1724/1957 (88%)	967/1052 (92%)	600/703 (85%)	157/202 (78%)

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.

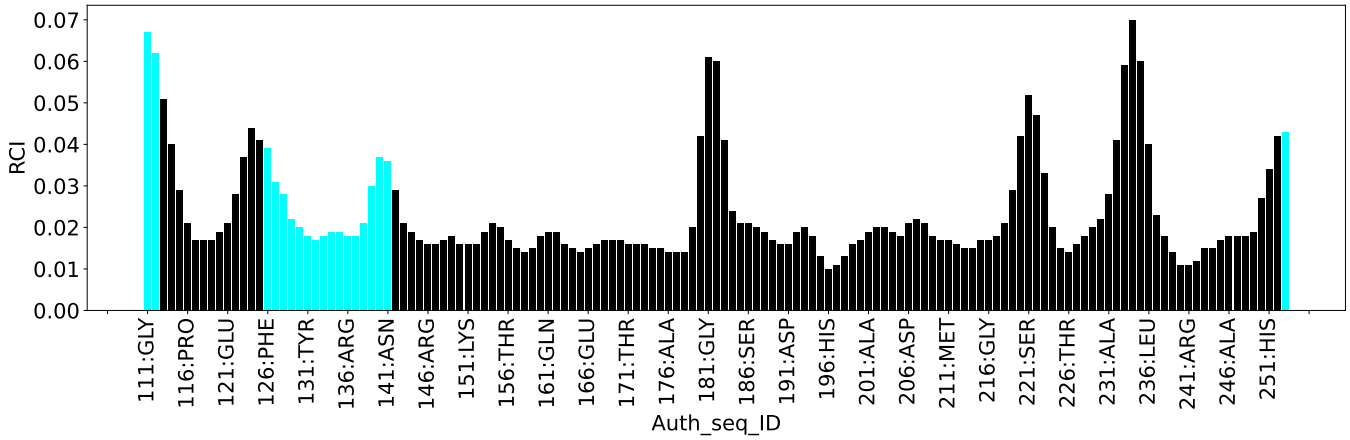
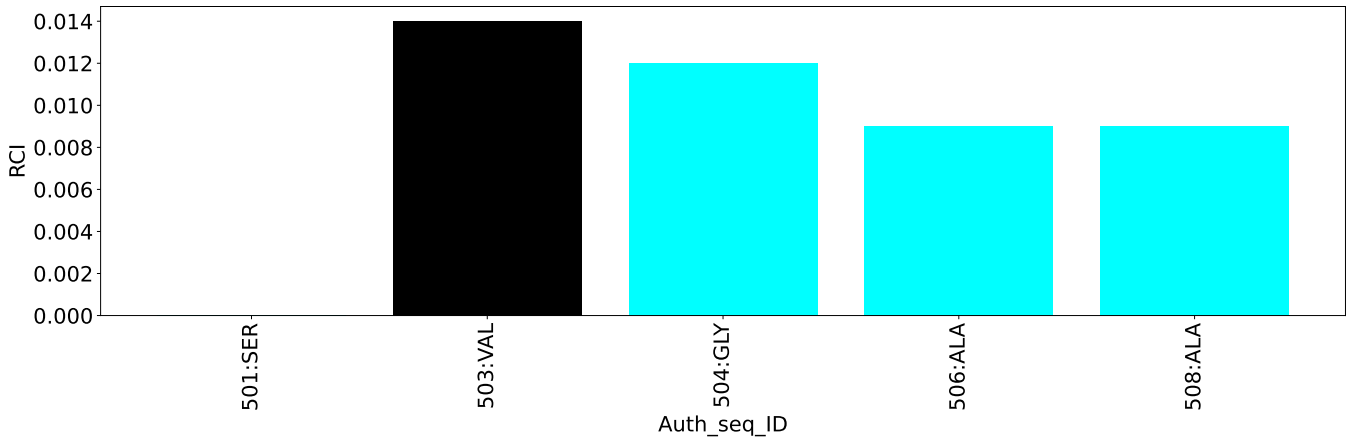
List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	B	501	SER	HB2	7.77	2.61 – 5.13	15.5
1	B	501	SER	HB3	7.77	2.49 – 5.20	14.5
1	A	138	ARG	HB2	-0.06	0.52 – 3.08	-7.2
1	A	138	ARG	HB3	0.02	0.43 – 3.11	-6.5
1	B	503	VAL	HG11	2.42	-0.48 – 2.12	6.1
1	B	503	VAL	HG12	2.42	-0.48 – 2.12	6.1
1	B	503	VAL	HG13	2.42	-0.48 – 2.12	6.1
1	B	504	GLY	HA2	1.79	2.15 – 5.77	-6.0

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:



Random coil index (RCI) for chain B: