Full wwPDB NMR Structure Validation Report (i)

Jun 15, 2024 – 08:40 PM EDT

PDB ID	:	2KSQ
Title	:	The myristoylated yeast ARF1 in a GTP and bicelle bound conformation
Authors	:	Liu, Y.; Kahn, R.; Prestegard, J.
Deposited on	:	2010-01-12

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:

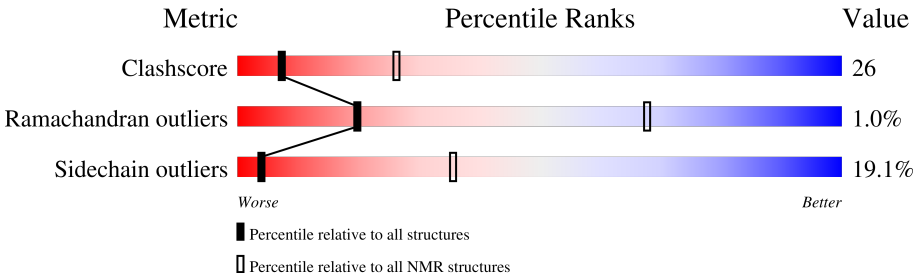
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

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

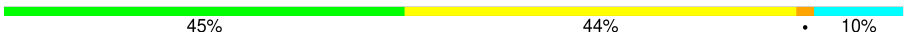
The overall completeness of chemical shifts assignment was not calculated.

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	181	

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 19 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:2-A:10 (9)	0.15	8
2	A:17-A:68, A:72-A:78, A:84-A:178 (154)	0.53	19

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 5 clusters. No single-model clusters were found.

Cluster number	Models
1	5, 10, 11, 13, 16, 19
2	1, 4, 8, 14, 17, 18
3	2, 3, 6, 12
4	7, 20
5	9, 15

3 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 3315 atoms, of which 1665 are hydrogens and 0 are deuteriums.

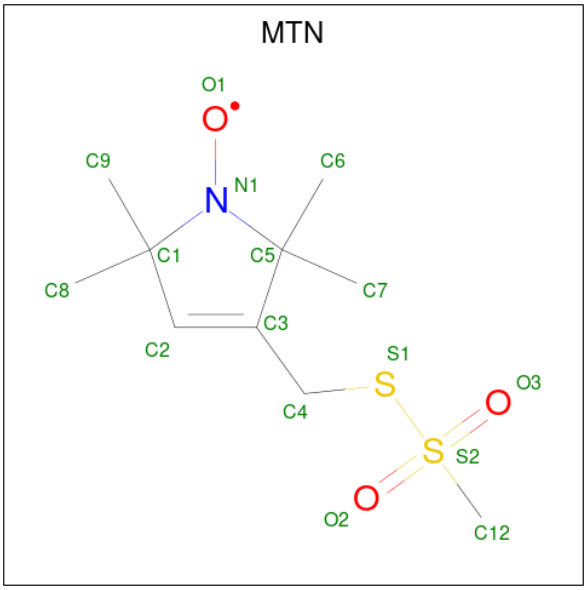
- Molecule 1 is a protein called ADP-ribosylation factor 1.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	181	2867	915	1429	244	268	11	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MYR	-	SEE REMARK 999	UNP P11076
A	55	CYS	THR	SEE REMARK 999	UNP P11076
A	59	CYS	LYS	SEE REMARK 999	UNP P11076
A	83	CYS	ARG	SEE REMARK 999	UNP P11076
A	117	CYS	ARG	SEE REMARK 999	UNP P11076
A	176	CYS	SER	SEE REMARK 999	UNP P11076

- Molecule 2 is S-[(1-oxyl-2,2,5,5-tetramethyl-2,5-dihydro-1H-pyrrol-3-yl)methyl] methanesulf onothioate (three-letter code: MTN) (formula: $C_{10}H_{18}NO_3S_2$).



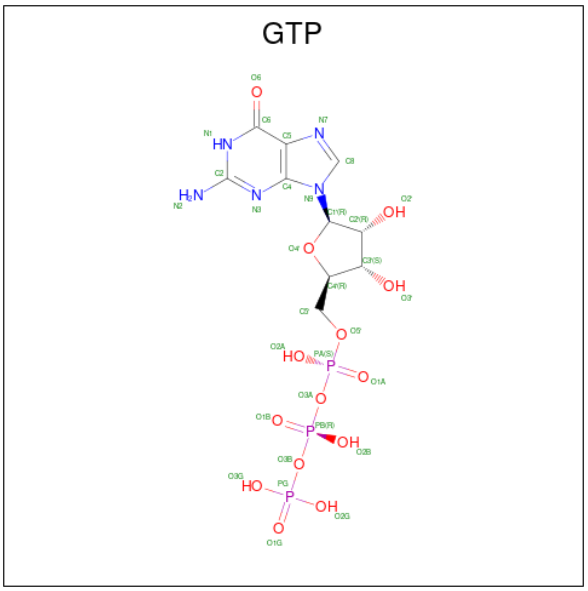
Mol	Chain	Residues	Atoms					
			Total	C	H	N	O	S
2	A	1	81	27	45	3	3	3
2	A	1	81	27	45	3	3	3

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					
			Total	C	H	N	O	S
2	A	1	81	27	45	3	3	3
			Total	C	H	N	O	S
2	A	1	81	27	45	3	3	3
			Total	C	H	N	O	S
2	A	1	81	27	45	3	3	3

- Molecule 3 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



Mol	Chain	Residues	Atoms					
			Total	C	H	N	O	P
3	A	1	43	10	11	5	14	3

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: ADP-ribosylation factor 1

Chain A: 45% 44% • 10%

MYR1 F4 F9 S10 N11 L12 F13 G14 N15 K16 E17 M18 R19 I20 L21 M22 V23 G24 L25 A28 G29 K30 T31 T32 V33 L34 Y35 K36 L37 K38 V42 I43 T44 T45 I49 V53 E54 Y58 C59 N60 I61 S62 F63 T64 V65 W66 D67 V68 G69 G70 Q71 I74

L77 W78 R79 H80 Y81 Y82 C83 N84 T85 E86 G87 V88 I89 F90 V91 V92 D93 S94 R97 I100 G101 E102 A103 R104 E105 V106 M110 L111 D114 E115 L116 C117 A120 W121 L122 V123 F124 A125 N126 K127 Q128 D129 L130 A133 M134 S135 I139 T140 L143 G144 L145

I148 R151 P152 W153 F154 I155 Q156 A157 A160 T161 L166 L170 L173 C176 L177 K178 N179 S180 T181

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: ADP-ribosylation factor 1

Chain A: 45% 38% 7% 10%

MYR1 F4 K7 L8 F9 S10 N11 L12 F13 G14 N15 K16 R19 I20 L21 L25 A28 G29 K30 T31 T32 V33 L34 Y35 K36 L37 K38 L39 V42 I43 T44 T45 V53 E54 Y58 C59 N60 I61 S62 F63 T64 V65 W66 D67 V68 G69 G70 Q71 I74 R79

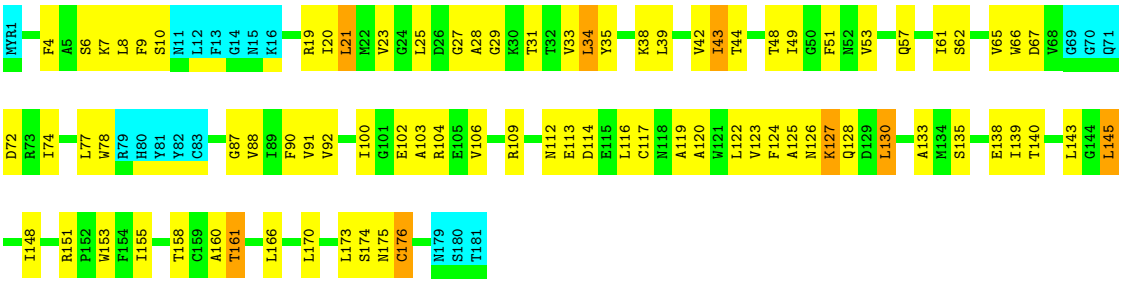
H80 Y81 Y82 C83 N84 T85 E86 G87 V88 I89 F90 V91 V92 D93 R97 I100 G101 E102 A103 R104 E105 V106 L111 D114 E115 L116 C117 N118 A119 A120 W121 F124 A125 N126 K127 Q128 D129 A133 M134 S135 I139 T140 E141 K142 L143 G144 L145 H146 S147 I148 R151 P152

W153 F154 I155 T158 C159 A160 T161 S162 G163 L166 Y167 E168 G169 L170 L173 S174 N175 C176 L177 K178 N179 S180 T181

4.2.2 Score per residue for model 2

- Molecule 1: ADP-ribosylation factor 1

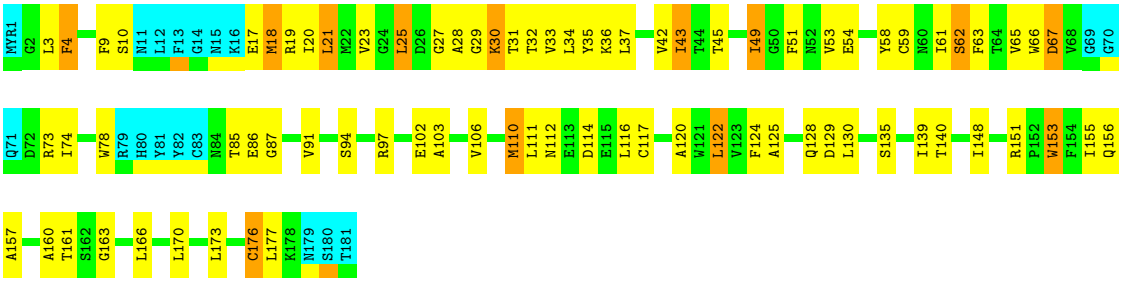
Chain A: 44% 41% • 10%



4.2.3 Score per residue for model 3

- Molecule 1: ADP-ribosylation factor 1

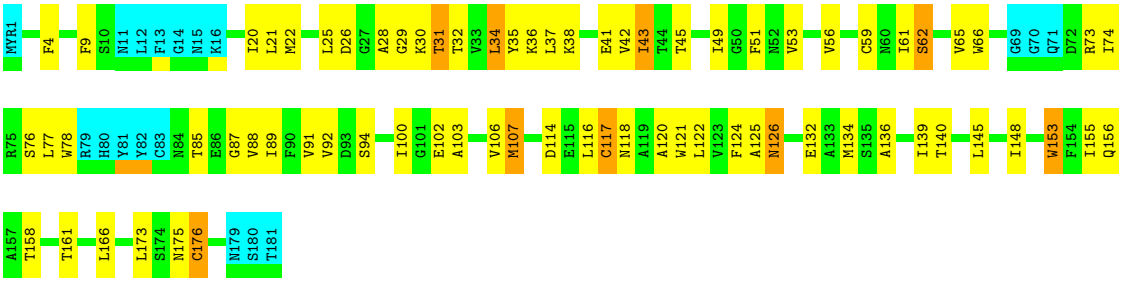
Chain A: 46% 36% 7% 10%



4.2.4 Score per residue for model 4

- Molecule 1: ADP-ribosylation factor 1

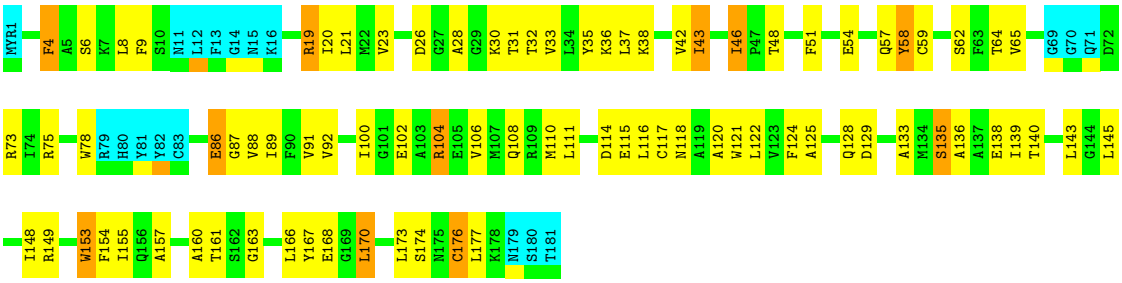
Chain A: 50% 35% 5% 10%



4.2.5 Score per residue for model 5

- Molecule 1: ADP-ribosylation factor 1

Chain A: 44% 40% 6% 10%



4.2.6 Score per residue for model 6

- Molecule 1: ADP-ribosylation factor 1

Chain A: 46% 39% 6% 10%

4.2.7 Score per residue for model 7

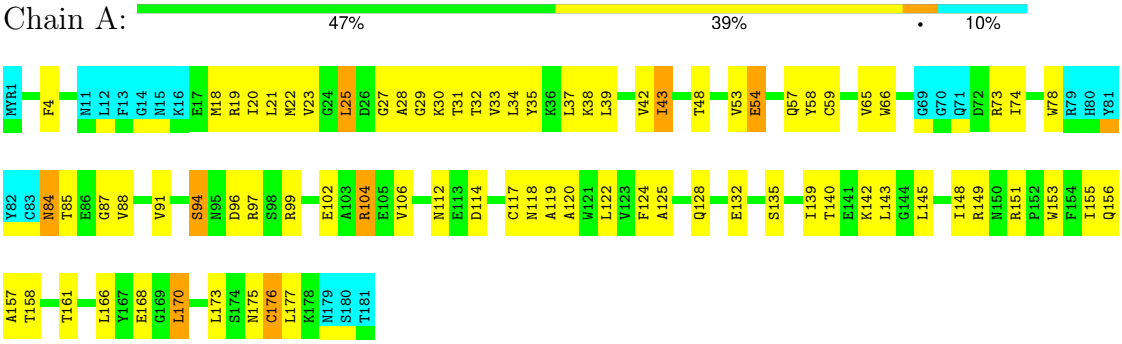
- Molecule 1: ADP-ribosylation factor 1

Chain A: 45% 38% 7% 10%

4.2.8 Score per residue for model 8

- Molecule 1: ADP-ribosylation factor 1

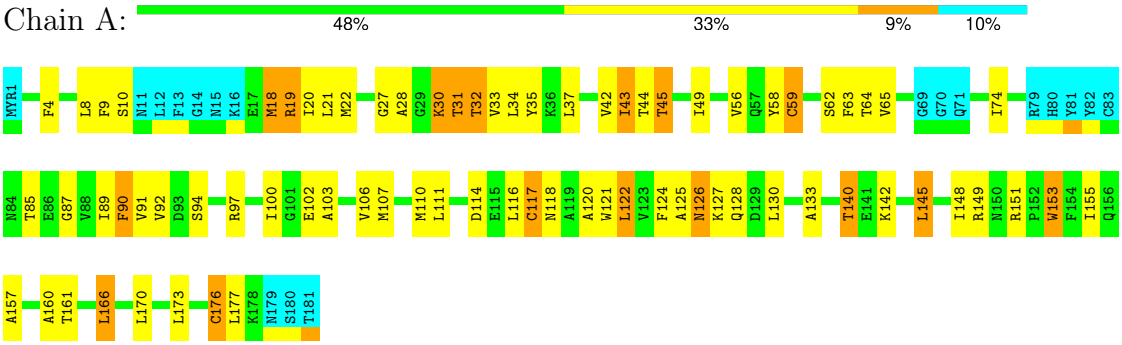
Chain A:



4.2.9 Score per residue for model 9

- Molecule 1: ADP-ribosylation factor 1

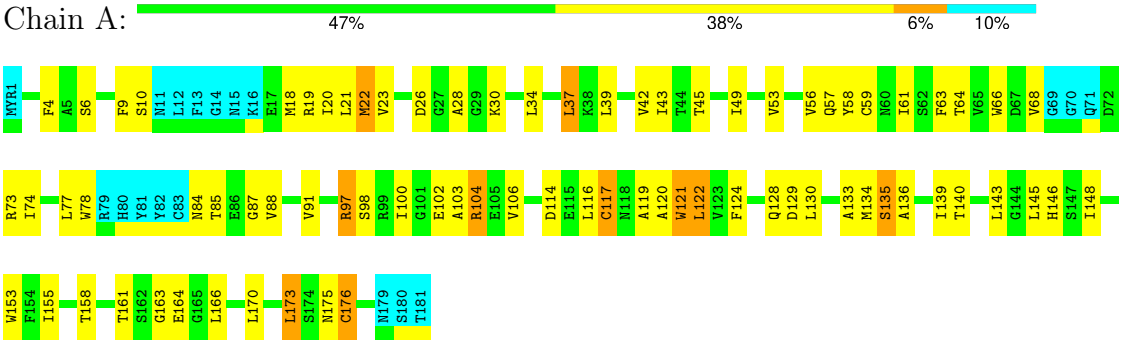
Chain A:



4.2.10 Score per residue for model 10

- Molecule 1: ADP-ribosylation factor 1

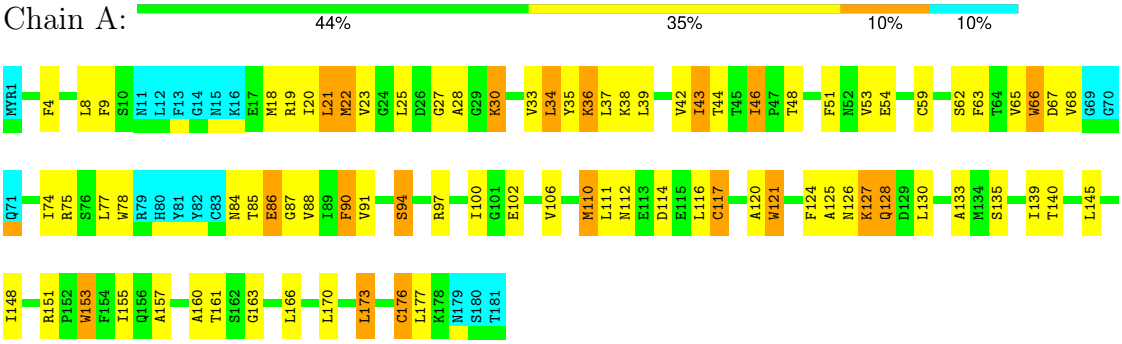
Chain A:



4.2.11 Score per residue for model 11

- Molecule 1: ADP-ribosylation factor 1

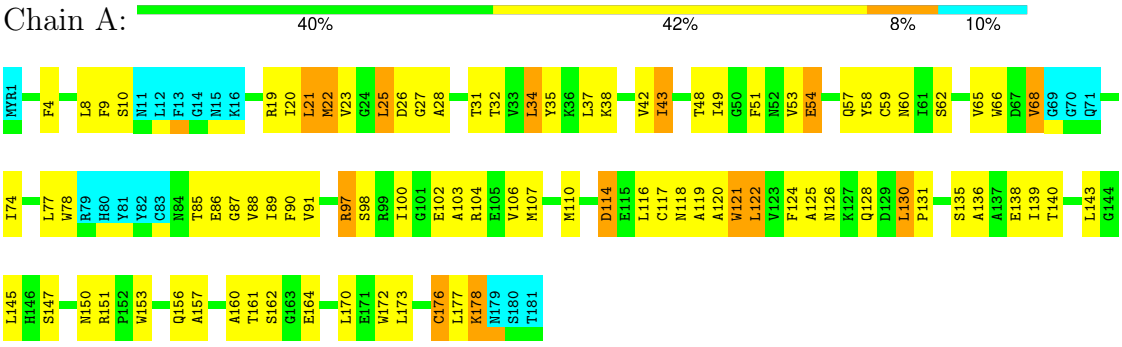
Chain A:



4.2.12 Score per residue for model 12

- Molecule 1: ADP-ribosylation factor 1

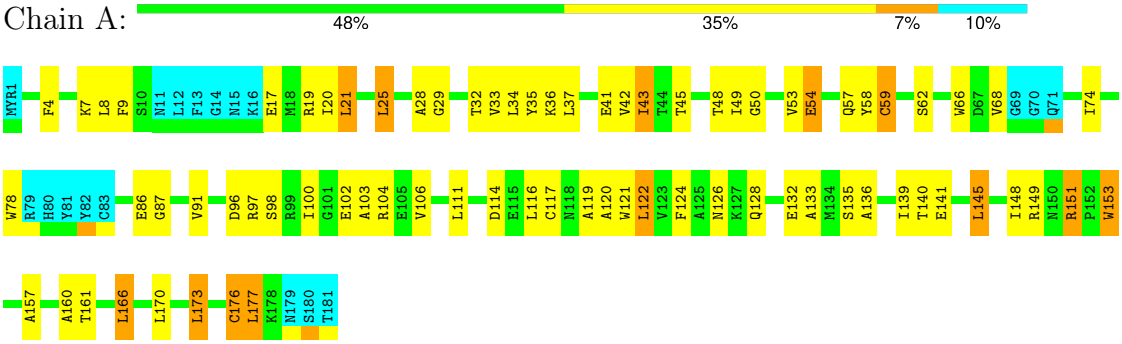
Chain A:



4.2.13 Score per residue for model 13

- Molecule 1: ADP-ribosylation factor 1

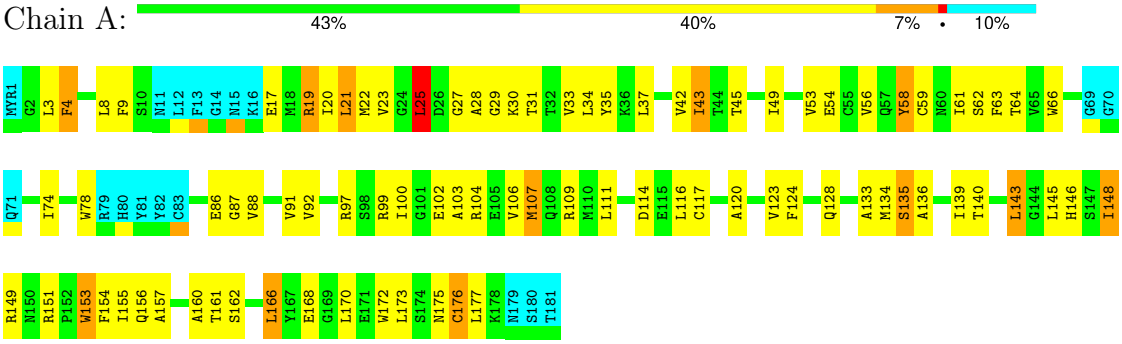
Chain A:



4.2.14 Score per residue for model 14

- Molecule 1: ADP-ribosylation factor 1

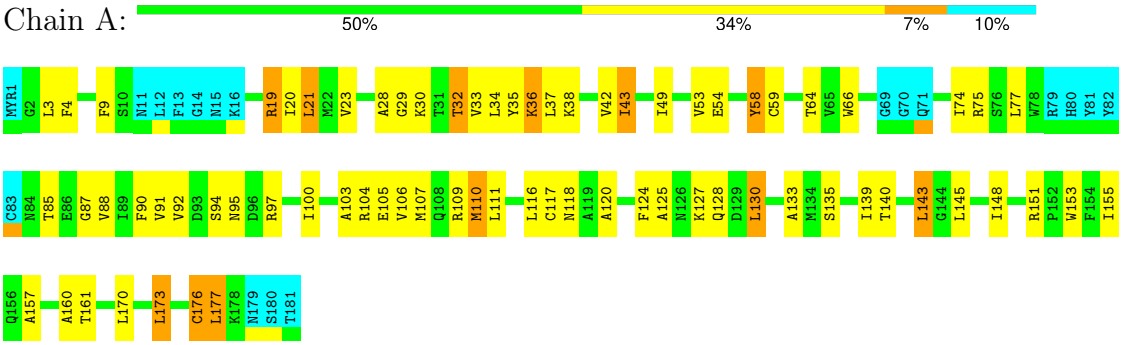
Chain A:



4.2.15 Score per residue for model 15

- Molecule 1: ADP-ribosylation factor 1

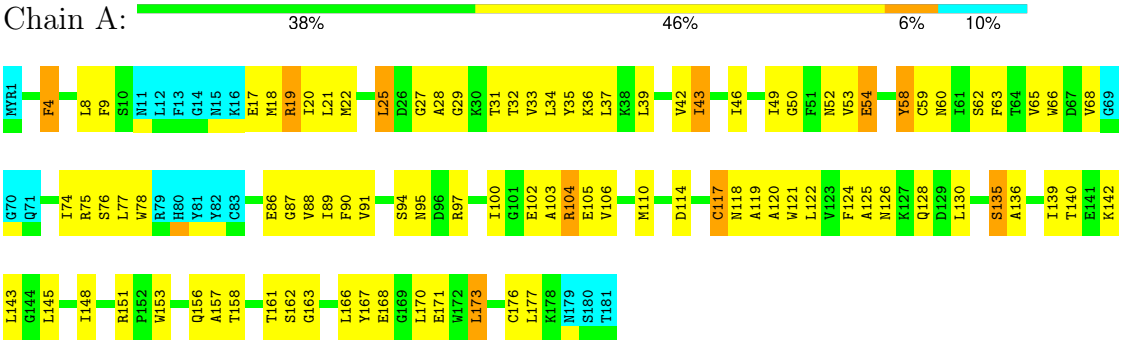
Chain A:



4.2.16 Score per residue for model 16

- Molecule 1: ADP-ribosylation factor 1

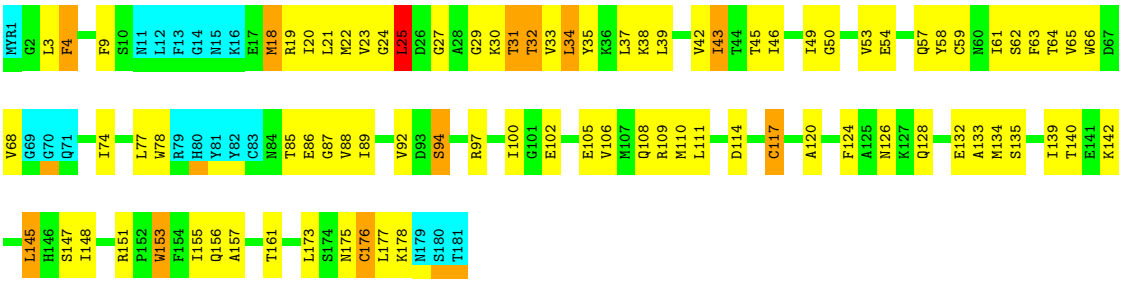
Chain A:



4.2.17 Score per residue for model 17

- Molecule 1: ADP-ribosylation factor 1

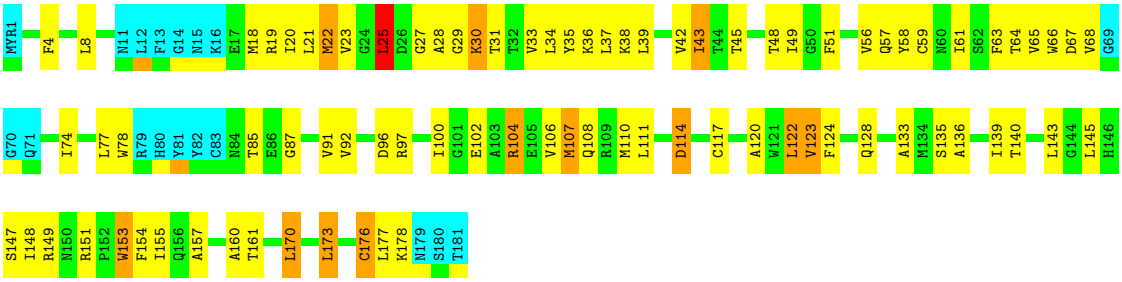
Chain A: 43% 41% 6% • 10%



4.2.18 Score per residue for model 18

- Molecule 1: ADP-ribosylation factor 1

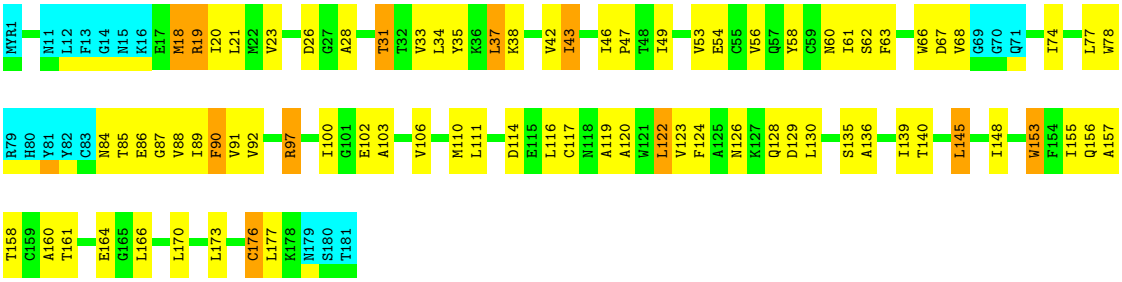
Chain A: 44% 39% 7% • 10%



4.2.19 Score per residue for model 19 (medoid)

- Molecule 1: ADP-ribosylation factor 1

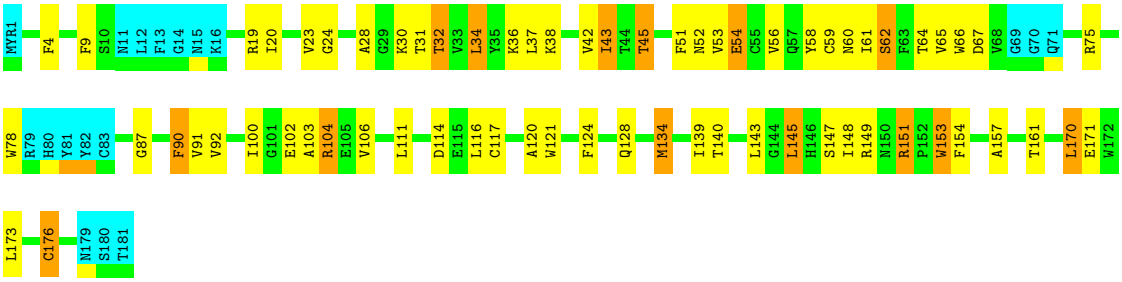
Chain A: 46% 38% 6% 10%



4.2.20 Score per residue for model 20

- Molecule 1: ADP-ribosylation factor 1

Chain A:



5 Refinement protocol and experimental data overview (i)

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

Of the 280 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
X-PLOR NIH	structure solution	
X-PLOR NIH	refinement	

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, MTN, GTP

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	1285	1279	1277	66±6
2	A	180	225	225	19±3
3	A	32	11	12	3±2
All	All	29940	30300	30280	1586

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 26.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:A:185[A]:MTN:H71	2:A:185[A]:MTN:S1	1.39	1.55	3	4
2:A:186[A]:MTN:H71	2:A:186[A]:MTN:S1	1.35	1.61	11	2
2:A:185[A]:MTN:S1	2:A:185[A]:MTN:C7	1.31	2.15	9	7
2:A:186[C]:MTN:S1	2:A:186[C]:MTN:C7	1.17	2.32	9	1
2:A:185[A]:MTN:S1	2:A:185[A]:MTN:H71	1.13	1.82	20	3
2:A:185[C]:MTN:H61	2:A:185[C]:MTN:S1	1.10	1.86	3	2
2:A:186[A]:MTN:S1	2:A:186[A]:MTN:C7	1.10	2.38	11	1
1:A:140:THR:HG22	1:A:155:ILE:HG21	1.07	1.26	4	4
1:A:25:LEU:HD11	1:A:103:ALA:HB2	1.04	1.29	13	5
2:A:185[A]:MTN:S1	2:A:185[A]:MTN:H73	1.04	1.93	16	3

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:A:186[C]:MTN:S1	2:A:186[C]:MTN:H72	1.01	1.92	9	1
2:A:184[C]:MTN:H61	2:A:184[C]:MTN:S1	1.00	1.94	13	2
1:A:21:LEU:HD12	1:A:85:THR:HG21	0.97	1.33	1	3
2:A:184[A]:MTN:S1	2:A:184[A]:MTN:C6	0.95	2.54	7	1
1:A:74:ILE:HG23	1:A:77:LEU:HD12	0.95	1.38	6	5
1:A:28:ALA:HB1	1:A:91:VAL:HG12	0.93	1.41	13	13
2:A:183[C]:MTN:S1	2:A:183[C]:MTN:H71	0.93	2.04	2	2
2:A:185[C]:MTN:H71	2:A:185[C]:MTN:S1	0.92	2.04	8	2
2:A:184[C]:MTN:H71	2:A:184[C]:MTN:S1	0.91	2.06	17	3
2:A:186[C]:MTN:S1	2:A:186[C]:MTN:H71	0.91	2.01	9	1
2:A:185[A]:MTN:H73	2:A:185[A]:MTN:S1	0.90	2.06	18	1
2:A:184[A]:MTN:S1	2:A:184[A]:MTN:H62	0.87	2.09	7	1
1:A:63:PHE:CE1	1:A:170:LEU:HD11	0.87	2.05	18	2
1:A:32:THR:HG23	1:A:45:THR:HG21	0.86	1.48	20	2
1:A:88:VAL:HG23	1:A:119:ALA:HB1	0.85	1.49	16	6
2:A:183[A]:MTN:H71	2:A:183[A]:MTN:S1	0.85	2.12	10	2
2:A:185[C]:MTN:S1	2:A:185[C]:MTN:C6	0.84	2.66	3	2
1:A:20:ILE:HD12	1:A:173:LEU:HD21	0.83	1.48	10	2
1:A:94:SER:HG	1:A:125:ALA:HB1	0.83	1.33	9	1
1:A:31:THR:HG23	3:A:187:GTP:O2B	0.82	1.74	5	4
1:A:102:GLU:O	1:A:106:VAL:HG23	0.81	1.76	3	9
1:A:32:THR:HG21	3:A:187:GTP:C8	0.81	2.09	17	1
3:A:187:GTP:H3'	3:A:187:GTP:O1A	0.80	1.76	6	1
1:A:35:TYR:HB3	1:A:43:ILE:HD11	0.80	1.52	19	14
1:A:35:TYR:CB	1:A:43:ILE:HD11	0.80	2.06	5	13
1:A:49:ILE:HG23	1:A:74:ILE:HD11	0.80	1.52	18	1
1:A:53:VAL:HG22	1:A:66:TRP:CE2	0.79	2.13	11	2
1:A:23:VAL:HG23	1:A:90:PHE:CD2	0.79	2.13	12	2
1:A:88:VAL:HG22	1:A:120:ALA:O	0.78	1.79	11	4
1:A:53:VAL:HG13	1:A:66:TRP:CD1	0.78	2.13	4	5
1:A:21:LEU:CD1	1:A:85:THR:HG21	0.78	2.08	1	3
1:A:28:ALA:HB1	1:A:91:VAL:HG22	0.78	1.55	6	5
1:A:53:VAL:HG22	1:A:66:TRP:CD2	0.78	2.14	3	6
2:A:184[C]:MTN:S1	2:A:184[C]:MTN:C6	0.77	2.73	13	3
1:A:176:CYS:O	2:A:186[C]:MTN:H61	0.77	1.80	1	2
1:A:145:LEU:HD22	1:A:153:TRP:CZ2	0.76	2.14	17	3
2:A:186[B]:MTN:H61	2:A:186[B]:MTN:S1	0.76	2.19	16	2
1:A:29:GLY:O	1:A:33:VAL:HG23	0.76	1.81	6	8
1:A:158:THR:HG23	1:A:166:LEU:CD2	0.76	2.10	8	3
1:A:38:LYS:HD2	1:A:56:VAL:HG12	0.75	1.58	20	1
1:A:94:SER:OG	1:A:125:ALA:HB1	0.75	1.80	9	5

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:114:ASP:HA	2:A:185[C]:MTN:H72	0.75	1.59	14	2
1:A:74:ILE:CG2	1:A:77:LEU:HD12	0.75	2.12	6	2
1:A:122:LEU:HD22	1:A:124:PHE:CE1	0.75	2.17	18	4
1:A:92:VAL:HG12	1:A:103:ALA:HB1	0.75	1.59	19	1
1:A:145:LEU:HD12	1:A:153:TRP:CE3	0.74	2.18	8	2
1:A:34:LEU:HD11	1:A:54:GLU:CB	0.74	2.13	16	2
1:A:28:ALA:HB1	1:A:91:VAL:CG1	0.74	2.12	8	12
1:A:140:THR:OG1	1:A:155:ILE:HG21	0.74	1.82	1	3
1:A:23:VAL:HG11	1:A:110:MET:SD	0.74	2.23	18	2
2:A:184[B]:MTN:S1	2:A:184[B]:MTN:H61	0.74	2.22	14	2
1:A:23:VAL:HG13	1:A:78:TRP:CZ2	0.74	2.17	14	3
1:A:36:LYS:CE	1:A:160:ALA:HB1	0.74	2.13	15	2
1:A:19:ARG:O	1:A:20:ILE:HD13	0.74	1.83	9	10
1:A:175:ASN:O	2:A:186[B]:MTN:H62	0.74	1.82	4	1
1:A:42:VAL:HG21	1:A:161:THR:O	0.73	1.81	13	18
1:A:114:ASP:HB3	2:A:185[A]:MTN:H61	0.73	1.59	5	1
1:A:117:CYS:SG	2:A:185[B]:MTN:H71	0.73	2.22	4	4
1:A:143:LEU:HB2	1:A:145:LEU:HD23	0.73	1.60	8	2
1:A:114:ASP:OD1	2:A:185[C]:MTN:H62	0.73	1.84	2	1
1:A:34:LEU:HD11	1:A:65:VAL:HB	0.73	1.61	18	5
1:A:37:LEU:HD13	1:A:37:LEU:O	0.73	1.83	9	3
1:A:116:LEU:HD23	1:A:121:TRP:CH2	0.73	2.17	20	2
1:A:19:ARG:C	1:A:20:ILE:HD12	0.73	2.04	16	8
2:A:185[B]:MTN:S1	2:A:185[B]:MTN:H71	0.72	2.24	19	2
1:A:23:VAL:HG23	1:A:90:PHE:CE1	0.72	2.19	19	1
1:A:21:LEU:HD13	1:A:85:THR:HG21	0.72	1.61	7	3
1:A:31:THR:HG22	1:A:45:THR:HG22	0.72	1.60	14	1
1:A:34:LEU:HD21	1:A:54:GLU:HB2	0.72	1.60	1	4
2:A:184[C]:MTN:S1	2:A:184[C]:MTN:H71	0.72	2.25	4	2
1:A:111:LEU:HD12	1:A:151:ARG:HG3	0.72	1.61	14	1
1:A:104:ARG:HG3	1:A:143:LEU:HD13	0.71	1.62	2	2
1:A:18:MET:CE	1:A:173:LEU:HD11	0.71	2.15	10	1
1:A:25:LEU:CD1	1:A:103:ALA:HB2	0.71	2.12	13	1
1:A:116:LEU:HD13	1:A:119:ALA:HB3	0.71	1.61	1	1
1:A:176:CYS:O	2:A:186[A]:MTN:H71	0.70	1.86	7	6
1:A:128:GLN:OE1	1:A:157:ALA:HB1	0.70	1.86	20	5
1:A:58:TYR:CD2	1:A:170:LEU:HD12	0.70	2.21	9	1
1:A:68:VAL:HG21	1:A:78:TRP:NE1	0.70	2.02	17	2
1:A:53:VAL:HG22	1:A:66:TRP:CE3	0.70	2.21	17	4
1:A:58:TYR:CG	1:A:170:LEU:HD23	0.69	2.22	20	6
1:A:145:LEU:HD12	1:A:153:TRP:CH2	0.69	2.21	6	4

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:74:ILE:HG23	1:A:77:LEU:HD22	0.69	1.63	16	4
1:A:102:GLU:O	1:A:106:VAL:HG13	0.69	1.88	4	7
1:A:145:LEU:HD12	1:A:153:TRP:CZ2	0.69	2.23	11	5
1:A:114:ASP:CB	2:A:185[C]:MTN:H63	0.69	2.18	1	2
1:A:49:ILE:HD12	1:A:74:ILE:HD11	0.69	1.65	10	5
1:A:104:ARG:CG	1:A:143:LEU:HD13	0.69	2.17	16	1
1:A:114:ASP:OD1	2:A:185[C]:MTN:H72	0.69	1.86	20	1
1:A:127:LYS:HB3	1:A:130:LEU:HD13	0.69	1.65	15	3
1:A:95:ASN:ND2	1:A:130:LEU:HD23	0.69	2.03	16	1
1:A:45:THR:HG21	3:A:187:GTP:O5'	0.68	1.87	18	1
1:A:114:ASP:HB3	2:A:185[C]:MTN:H63	0.68	1.63	1	1
1:A:21:LEU:CB	1:A:88:VAL:HG12	0.68	2.18	2	4
1:A:32:THR:OG1	1:A:45:THR:HG21	0.68	1.86	7	2
1:A:122:LEU:HD22	1:A:124:PHE:CZ	0.68	2.23	7	5
1:A:97:ARG:O	1:A:100:ILE:HG22	0.68	1.87	13	11
1:A:160:ALA:HB3	3:A:187:GTP:O6	0.68	1.89	14	10
1:A:37:LEU:HD23	1:A:37:LEU:O	0.68	1.89	18	13
1:A:18:MET:HG2	1:A:177:LEU:HD12	0.68	1.64	9	2
1:A:122:LEU:HD22	1:A:124:PHE:CE2	0.68	2.24	9	2
1:A:32:THR:HB	1:A:45:THR:HG21	0.68	1.66	17	1
1:A:74:ILE:HG23	1:A:77:LEU:CD1	0.67	2.16	6	1
1:A:25:LEU:HD21	1:A:103:ALA:HA	0.67	1.65	3	2
1:A:88:VAL:CG2	1:A:119:ALA:HB1	0.67	2.18	16	3
1:A:140:THR:HG23	1:A:145:LEU:HD22	0.67	1.65	20	5
1:A:21:LEU:HD13	1:A:85:THR:CG2	0.67	2.19	15	2
1:A:114:ASP:HB2	2:A:185[B]:MTN:H92	0.67	1.64	16	1
1:A:145:LEU:HD22	1:A:153:TRP:CD2	0.67	2.24	16	1
1:A:48:THR:HG22	3:A:187:GTP:O1G	0.67	1.90	2	2
1:A:114:ASP:HB3	2:A:185[B]:MTN:H92	0.67	1.66	9	1
1:A:92:VAL:HG13	1:A:103:ALA:CB	0.67	2.20	6	4
1:A:3:LEU:HD12	1:A:4:PHE:N	0.67	2.05	17	4
1:A:114:ASP:HB3	2:A:185[A]:MTN:H73	0.67	1.66	13	1
1:A:19:ARG:C	1:A:20:ILE:HD13	0.66	2.11	15	7
1:A:140:THR:HG22	1:A:155:ILE:CG2	0.66	2.13	4	4
1:A:34:LEU:HD21	1:A:54:GLU:CB	0.66	2.20	1	2
2:A:184[A]:MTN:S1	2:A:184[A]:MTN:H61	0.66	2.30	7	1
1:A:140:THR:CG2	1:A:145:LEU:HD22	0.66	2.20	20	1
1:A:114:ASP:HB2	2:A:185[A]:MTN:H73	0.66	1.67	11	1
1:A:135:SER:O	1:A:139:ILE:HD12	0.66	1.91	2	16
1:A:148:ILE:HG21	1:A:153:TRP:CZ2	0.65	2.26	5	2
1:A:158:THR:HG23	1:A:166:LEU:CD1	0.65	2.21	4	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:A:185[C]:MTN:S1	2:A:185[C]:MTN:C7	0.65	2.85	2	2
1:A:20:ILE:CD1	1:A:173:LEU:HD21	0.65	2.21	10	1
1:A:88:VAL:HG11	1:A:110:MET:CE	0.65	2.22	7	1
1:A:74:ILE:HG23	1:A:77:LEU:HD21	0.65	1.68	19	1
1:A:143:LEU:CB	1:A:145:LEU:HD23	0.65	2.21	8	2
2:A:184[C]:MTN:S1	2:A:184[C]:MTN:C7	0.65	2.84	17	3
1:A:34:LEU:HD12	1:A:54:GLU:HG3	0.65	1.68	17	1
1:A:148:ILE:HD12	1:A:153:TRP:NE1	0.65	2.07	13	2
1:A:34:LEU:HD11	1:A:54:GLU:HB3	0.65	1.66	16	1
1:A:34:LEU:HD13	1:A:54:GLU:OE1	0.65	1.91	20	1
1:A:128:GLN:HG2	1:A:157:ALA:HB1	0.65	1.69	9	2
1:A:45:THR:HG21	3:A:187:GTP:PA	0.65	2.32	18	1
1:A:53:VAL:HG22	1:A:66:TRP:CD1	0.64	2.28	16	1
1:A:34:LEU:HD21	1:A:65:VAL:O	0.64	1.91	18	2
1:A:116:LEU:CD1	1:A:119:ALA:HB3	0.64	2.21	1	1
1:A:125:ALA:HB3	1:A:128:GLN:OE1	0.64	1.93	6	4
1:A:140:THR:CG2	1:A:155:ILE:HG21	0.64	2.21	8	7
2:A:183[C]:MTN:S1	2:A:183[C]:MTN:C7	0.64	2.83	2	1
1:A:128:GLN:CD	1:A:157:ALA:HB1	0.64	2.13	15	7
1:A:63:PHE:CD2	1:A:170:LEU:HD11	0.64	2.28	10	2
1:A:128:GLN:HG3	1:A:157:ALA:HB1	0.64	1.69	14	4
1:A:140:THR:CG2	1:A:155:ILE:HD13	0.63	2.23	8	2
1:A:38:LYS:CD	1:A:56:VAL:HG12	0.63	2.22	20	1
1:A:50:GLY:O	1:A:68:VAL:HG13	0.63	1.93	16	3
1:A:114:ASP:CG	2:A:185[C]:MTN:H72	0.63	2.14	20	1
1:A:111:LEU:HD12	1:A:151:ARG:CG	0.63	2.23	14	2
1:A:87:GLY:HA2	1:A:120:ALA:HB3	0.63	1.68	11	20
1:A:31:THR:HG22	1:A:35:TYR:CE2	0.63	2.28	9	3
1:A:25:LEU:HD21	1:A:103:ALA:CA	0.62	2.23	12	3
1:A:58:TYR:CG	1:A:170:LEU:HD12	0.62	2.28	13	1
1:A:28:ALA:CB	1:A:91:VAL:HG13	0.62	2.23	2	4
1:A:145:LEU:HA	1:A:148:ILE:HD12	0.62	1.70	16	6
1:A:104:ARG:HB3	1:A:143:LEU:HD23	0.62	1.71	8	1
1:A:140:THR:OG1	1:A:145:LEU:HD22	0.62	1.95	12	1
1:A:104:ARG:CG	1:A:143:LEU:HD22	0.62	2.25	14	1
1:A:148:ILE:HD12	1:A:153:TRP:CZ2	0.62	2.30	4	7
1:A:91:VAL:HG22	1:A:124:PHE:CZ	0.61	2.30	5	1
1:A:114:ASP:CB	2:A:185[C]:MTN:H92	0.61	2.25	1	1
1:A:32:THR:CG2	1:A:45:THR:HG21	0.61	2.24	3	3
1:A:145:LEU:HD23	1:A:153:TRP:CZ3	0.61	2.31	2	2
1:A:134:MET:HB3	1:A:139:ILE:HD11	0.61	1.71	20	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:87:GLY:CA	1:A:120:ALA:HB3	0.61	2.26	11	11
1:A:129:ASP:OD1	1:A:130:LEU:HD22	0.61	1.96	19	2
1:A:139:ILE:CG2	1:A:155:ILE:HD11	0.61	2.26	1	4
1:A:18:MET:CG	1:A:177:LEU:HD12	0.60	2.26	3	1
1:A:140:THR:HG23	1:A:155:ILE:HD13	0.60	1.71	8	3
1:A:107:MET:O	1:A:111:LEU:HD23	0.60	1.96	14	1
1:A:89:ILE:HG23	1:A:122:LEU:O	0.60	1.97	4	4
1:A:117:CYS:SG	2:A:185[C]:MTN:H71	0.60	2.36	9	1
1:A:114:ASP:HB3	2:A:185[B]:MTN:H73	0.60	1.73	17	1
1:A:22:MET:HG3	1:A:34:LEU:HD11	0.60	1.73	7	1
2:A:183[A]:MTN:S1	2:A:183[A]:MTN:C7	0.60	2.89	10	2
1:A:45:THR:HG21	3:A:187:GTP:O2A	0.60	1.96	1	1
1:A:122:LEU:HD21	1:A:124:PHE:CZ	0.60	2.32	4	1
1:A:114:ASP:CG	2:A:185[C]:MTN:H92	0.60	2.17	6	1
2:A:184[B]:MTN:C7	2:A:184[B]:MTN:S1	0.60	2.89	11	1
1:A:148:ILE:HG23	1:A:153:TRP:CD1	0.60	2.31	14	1
1:A:34:LEU:O	1:A:34:LEU:HD23	0.60	1.97	3	2
1:A:111:LEU:HD11	1:A:151:ARG:CB	0.60	2.27	17	3
1:A:18:MET:SD	1:A:177:LEU:HD22	0.60	2.37	8	1
1:A:31:THR:CG2	1:A:45:THR:HG22	0.60	2.25	14	1
1:A:18:MET:HE3	1:A:173:LEU:HD11	0.60	1.73	10	1
1:A:18:MET:SD	1:A:177:LEU:HD12	0.60	2.37	16	1
1:A:33:VAL:HG22	1:A:160:ALA:HB2	0.60	1.74	3	3
1:A:49:ILE:CD1	1:A:74:ILE:HD11	0.60	2.26	3	2
1:A:114:ASP:CA	2:A:185[C]:MTN:H72	0.59	2.26	14	2
1:A:114:ASP:CB	2:A:185[B]:MTN:H92	0.59	2.27	9	2
1:A:111:LEU:HD11	1:A:151:ARG:HG3	0.59	1.73	15	2
1:A:110:MET:HG2	1:A:116:LEU:HD13	0.59	1.75	3	1
1:A:115:GLU:C	1:A:116:LEU:HD22	0.59	2.18	7	2
1:A:170:LEU:O	1:A:170:LEU:HD13	0.59	1.97	13	2
1:A:20:ILE:HG22	1:A:65:VAL:HG13	0.59	1.75	11	2
1:A:104:ARG:HG2	1:A:143:LEU:HD13	0.59	1.74	16	1
1:A:49:ILE:HG23	1:A:74:ILE:CD1	0.59	2.28	18	1
1:A:74:ILE:CG2	1:A:77:LEU:HD21	0.59	2.28	19	1
1:A:39:LEU:O	1:A:39:LEU:HD23	0.58	1.98	2	5
1:A:32:THR:HG23	1:A:45:THR:CG2	0.58	2.26	20	2
1:A:114:ASP:OD1	2:A:185[A]:MTN:H42	0.58	1.97	11	1
1:A:111:LEU:HD12	1:A:121:TRP:CD2	0.58	2.33	1	1
1:A:114:ASP:OD1	2:A:185[C]:MTN:H92	0.58	1.97	6	1
1:A:36:LYS:HE3	1:A:160:ALA:HB1	0.58	1.76	15	1
1:A:145:LEU:HD12	1:A:153:TRP:CZ3	0.58	2.33	8	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:86:GLU:CG	1:A:177:LEU:HD21	0.58	2.29	1	3
1:A:23:VAL:HG12	1:A:78:TRP:CE2	0.58	2.34	2	1
1:A:21:LEU:HB3	1:A:88:VAL:HG13	0.58	1.75	7	2
1:A:22:MET:O	1:A:68:VAL:HG22	0.58	1.99	11	1
1:A:88:VAL:HG11	1:A:110:MET:HE3	0.58	1.76	7	1
1:A:94:SER:HB2	1:A:125:ALA:HB1	0.58	1.76	4	2
1:A:114:ASP:OD2	2:A:185[C]:MTN:H92	0.57	1.98	18	1
1:A:114:ASP:HB2	2:A:185[C]:MTN:H83	0.57	1.75	20	1
1:A:114:ASP:OD1	2:A:185[A]:MTN:H73	0.57	2.00	12	1
1:A:158:THR:HG23	1:A:166:LEU:HD21	0.57	1.76	8	1
1:A:140:THR:OG1	1:A:155:ILE:HD11	0.57	1.99	9	2
1:A:95:ASN:CG	1:A:130:LEU:HD23	0.57	2.20	16	1
1:A:110:MET:HG3	1:A:116:LEU:HD13	0.57	1.76	9	1
1:A:34:LEU:HD11	1:A:54:GLU:CG	0.57	2.30	14	1
1:A:53:VAL:HG23	1:A:66:TRP:CD1	0.57	2.35	20	5
2:A:184[C]:MTN:S1	2:A:184[C]:MTN:H61	0.57	2.40	11	1
1:A:21:LEU:O	1:A:88:VAL:HG23	0.56	1.98	10	1
1:A:21:LEU:HD13	1:A:85:THR:HB	0.56	1.77	19	1
1:A:140:THR:HG23	1:A:145:LEU:CB	0.56	2.30	1	1
1:A:151:ARG:NH2	2:A:185[C]:MTN:S1	0.56	2.79	3	1
1:A:21:LEU:CB	1:A:85:THR:HG21	0.56	2.30	10	1
1:A:34:LEU:HD12	1:A:54:GLU:CB	0.56	2.30	12	1
1:A:143:LEU:HB3	1:A:145:LEU:HD13	0.56	1.76	15	1
1:A:34:LEU:HD21	1:A:65:VAL:HG23	0.56	1.78	3	2
1:A:111:LEU:HD11	1:A:151:ARG:HB2	0.56	1.76	17	2
1:A:151:ARG:NH2	2:A:185[B]:MTN:S1	0.56	2.79	18	3
1:A:136:ALA:O	1:A:140:THR:HG22	0.56	2.01	12	4
1:A:38:LYS:HD2	1:A:56:VAL:HG22	0.56	1.77	19	1
1:A:58:TYR:CD1	1:A:170:LEU:HD12	0.56	2.35	13	1
1:A:175:ASN:OD1	2:A:186[C]:MTN:H91	0.56	2.01	7	1
1:A:34:LEU:HD13	1:A:54:GLU:HG3	0.56	1.77	11	1
1:A:91:VAL:HG23	1:A:126:ASN:ND2	0.55	2.16	6	1
1:A:104:ARG:CB	1:A:143:LEU:HD13	0.55	2.32	12	1
1:A:151:ARG:NH2	2:A:185[B]:MTN:H41	0.55	2.16	20	1
1:A:20:ILE:HG21	1:A:89:ILE:HD11	0.55	1.78	17	2
1:A:175:ASN:O	2:A:186[C]:MTN:H63	0.55	2.00	1	2
1:A:129:ASP:OD2	1:A:161:THR:HG23	0.55	2.01	6	1
1:A:145:LEU:HD22	1:A:148:ILE:HD11	0.55	1.78	13	1
1:A:21:LEU:HD12	1:A:66:TRP:O	0.55	2.02	4	1
1:A:22:MET:O	1:A:23:VAL:HG13	0.55	2.01	8	1
1:A:20:ILE:HB	1:A:65:VAL:HG13	0.55	1.78	9	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:A:184[B]:MTN:S1	2:A:184[B]:MTN:H71	0.55	2.41	11	2
1:A:53:VAL:HG23	1:A:66:TRP:NE1	0.55	2.17	15	4
1:A:103:ALA:O	1:A:106:VAL:HG22	0.55	2.02	19	7
1:A:32:THR:HG22	1:A:36:LYS:HZ3	0.55	1.62	15	1
1:A:91:VAL:HG13	1:A:126:ASN:ND2	0.55	2.16	19	1
1:A:23:VAL:HG13	1:A:78:TRP:CE2	0.55	2.36	3	4
1:A:28:ALA:CB	1:A:91:VAL:HG12	0.55	2.26	13	2
1:A:127:LYS:HB3	1:A:130:LEU:HD12	0.54	1.78	11	1
1:A:63:PHE:CE1	1:A:170:LEU:HD21	0.54	2.37	14	1
1:A:18:MET:HG3	1:A:177:LEU:HD22	0.54	1.77	19	1
1:A:68:VAL:HG11	1:A:78:TRP:CD1	0.54	2.36	11	2
1:A:136:ALA:O	1:A:140:THR:HG23	0.54	2.02	19	5
1:A:30:LYS:HA	1:A:91:VAL:HG21	0.54	1.80	1	1
2:A:186[C]:MTN:H71	2:A:186[C]:MTN:S1	0.54	2.43	5	1
1:A:34:LEU:HD22	1:A:67:ASP:HB3	0.54	1.80	18	1
1:A:21:LEU:HD12	1:A:85:THR:CG2	0.54	2.22	1	2
1:A:46:ILE:HD13	1:A:46:ILE:N	0.54	2.18	11	2
1:A:175:ASN:OD1	2:A:186[B]:MTN:H81	0.54	2.03	10	1
1:A:21:LEU:HB2	1:A:88:VAL:HG12	0.54	1.78	15	2
1:A:21:LEU:HB3	1:A:88:VAL:HG12	0.53	1.79	14	4
1:A:34:LEU:HD21	1:A:65:VAL:HB	0.53	1.79	9	1
1:A:111:LEU:HD23	1:A:121:TRP:CE3	0.53	2.38	11	1
1:A:114:ASP:HB2	2:A:185[A]:MTN:H81	0.53	1.80	1	1
1:A:148:ILE:HD13	1:A:153:TRP:CZ2	0.53	2.37	3	2
1:A:114:ASP:O	2:A:185[B]:MTN:S1	0.53	2.66	4	7
1:A:49:ILE:HG23	1:A:49:ILE:O	0.53	2.04	10	6
1:A:35:TYR:O	1:A:39:LEU:HD12	0.53	2.03	6	1
1:A:116:LEU:HD23	1:A:121:TRP:CZ2	0.53	2.38	4	2
1:A:33:VAL:HG21	1:A:124:PHE:CE2	0.53	2.38	15	2
1:A:53:VAL:CG2	1:A:64:THR:HG22	0.53	2.34	10	1
2:A:186[B]:MTN:S1	2:A:186[B]:MTN:C6	0.53	2.95	16	1
1:A:114:ASP:CA	2:A:185[C]:MTN:H73	0.53	2.33	2	1
1:A:127:LYS:HG3	1:A:130:LEU:HD12	0.53	1.78	2	1
1:A:111:LEU:O	1:A:111:LEU:HD23	0.53	2.03	13	2
1:A:25:LEU:HD11	1:A:102:GLU:HB3	0.53	1.80	14	2
1:A:51:PHE:CZ	1:A:68:VAL:HG22	0.53	2.39	7	1
1:A:163:GLY:HA2	1:A:166:LEU:HD22	0.53	1.80	3	6
1:A:20:ILE:HD12	1:A:20:ILE:N	0.53	2.19	18	8
1:A:114:ASP:CB	2:A:185[A]:MTN:H61	0.53	2.34	5	1
1:A:114:ASP:CG	2:A:185[C]:MTN:H63	0.53	2.24	6	1
1:A:74:ILE:CG2	1:A:77:LEU:HD22	0.53	2.33	12	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:34:LEU:HD11	1:A:54:GLU:HG3	0.53	1.79	14	1
1:A:176:CYS:O	2:A:186[A]:MTN:S1	0.53	2.67	10	20
1:A:32:THR:CA	1:A:45:THR:HG21	0.53	2.34	6	1
2:A:185[B]:MTN:S1	2:A:185[B]:MTN:C7	0.53	2.96	19	2
1:A:36:LYS:HD2	1:A:42:VAL:HG22	0.53	1.80	15	1
1:A:43:ILE:HD12	1:A:43:ILE:H	0.52	1.64	19	13
1:A:36:LYS:HE2	1:A:42:VAL:HG23	0.52	1.81	20	3
1:A:111:LEU:HD21	1:A:151:ARG:HD2	0.52	1.82	1	1
1:A:53:VAL:HG13	1:A:66:TRP:NE1	0.52	2.19	2	1
1:A:20:ILE:CG2	1:A:65:VAL:HG12	0.52	2.34	5	1
1:A:74:ILE:O	1:A:74:ILE:HG22	0.52	2.02	6	3
1:A:88:VAL:HG12	1:A:120:ALA:O	0.52	2.04	10	1
1:A:36:LYS:HG3	1:A:42:VAL:HG12	0.52	1.80	11	1
1:A:95:ASN:CB	1:A:130:LEU:HD22	0.52	2.34	15	1
1:A:20:ILE:CG1	1:A:173:LEU:HD21	0.52	2.35	18	1
1:A:117:CYS:SG	2:A:185[B]:MTN:H62	0.52	2.43	10	1
1:A:176:CYS:HA	2:A:186[C]:MTN:H71	0.52	1.80	5	1
1:A:103:ALA:O	1:A:106:VAL:HG12	0.52	2.04	15	1
1:A:176:CYS:O	2:A:186[C]:MTN:H71	0.52	2.04	6	1
1:A:117:CYS:O	2:A:185[B]:MTN:S1	0.52	2.68	5	9
1:A:114:ASP:O	2:A:185[C]:MTN:S1	0.51	2.68	1	1
1:A:34:LEU:HD11	1:A:65:VAL:O	0.51	2.05	2	4
1:A:34:LEU:HD21	1:A:65:VAL:CG2	0.51	2.35	3	1
1:A:148:ILE:HG21	1:A:153:TRP:HZ2	0.51	1.65	3	2
1:A:111:LEU:HD23	1:A:151:ARG:CB	0.51	2.35	9	1
1:A:49:ILE:HG22	1:A:49:ILE:O	0.51	2.05	15	3
1:A:117:CYS:O	2:A:185[C]:MTN:S1	0.51	2.68	9	4
1:A:158:THR:HG23	1:A:166:LEU:HD12	0.51	1.82	4	2
1:A:173:LEU:O	1:A:173:LEU:HD12	0.51	2.05	18	6
1:A:37:LEU:HD21	1:A:170:LEU:HD22	0.51	1.81	12	1
1:A:22:MET:CG	1:A:34:LEU:HD11	0.51	2.36	7	2
1:A:114:ASP:HA	2:A:185[C]:MTN:H42	0.51	1.83	18	1
1:A:114:ASP:O	2:A:185[A]:MTN:S1	0.51	2.68	1	1
1:A:114:ASP:HA	2:A:185[C]:MTN:H61	0.51	1.80	19	1
1:A:114:ASP:OD1	2:A:185[C]:MTN:H73	0.51	2.05	3	1
1:A:45:THR:HG23	3:A:187:GTP:H3'	0.51	1.82	7	1
1:A:145:LEU:HD12	1:A:153:TRP:CD2	0.51	2.40	10	2
1:A:36:LYS:NZ	1:A:160:ALA:HB1	0.51	2.21	15	1
1:A:34:LEU:HD13	1:A:67:ASP:HB2	0.50	1.83	1	1
1:A:116:LEU:HD22	1:A:116:LEU:N	0.50	2.21	5	2
1:A:34:LEU:HD22	1:A:67:ASP:OD1	0.50	2.06	6	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:86:GLU:HB3	1:A:177:LEU:HD21	0.50	1.82	19	3
1:A:140:THR:HG21	1:A:155:ILE:HG21	0.50	1.81	8	2
1:A:21:LEU:HB2	1:A:85:THR:HG21	0.50	1.83	18	4
1:A:173:LEU:HD13	1:A:173:LEU:O	0.50	2.06	5	3
1:A:114:ASP:CB	2:A:185[C]:MTN:H72	0.50	2.37	14	1
1:A:18:MET:HE1	1:A:173:LEU:HD11	0.50	1.83	10	1
1:A:34:LEU:HD12	1:A:54:GLU:CG	0.50	2.37	17	1
1:A:25:LEU:HD21	1:A:103:ALA:N	0.50	2.21	12	1
1:A:34:LEU:HD13	1:A:34:LEU:C	0.50	2.28	14	1
1:A:117:CYS:HB2	2:A:185[C]:MTN:H61	0.50	1.84	19	1
1:A:68:VAL:HG11	1:A:77:LEU:HD11	0.49	1.85	19	1
3:A:187:GTP:O1G	3:A:187:GTP:O2B	0.49	2.29	1	2
1:A:22:MET:CE	1:A:89:ILE:HD12	0.49	2.38	9	1
1:A:25:LEU:HD21	1:A:103:ALA:HB2	0.49	1.82	12	1
1:A:114:ASP:HA	2:A:185[C]:MTN:H73	0.49	1.83	2	1
1:A:173:LEU:C	1:A:173:LEU:HD13	0.49	2.27	4	2
1:A:114:ASP:CB	2:A:185[A]:MTN:H73	0.49	2.35	11	1
1:A:34:LEU:HD11	1:A:65:VAL:CG1	0.49	2.37	17	1
1:A:38:LYS:CG	1:A:56:VAL:HG22	0.49	2.37	4	1
1:A:33:VAL:CG2	1:A:166:LEU:HD11	0.49	2.37	9	1
1:A:43:ILE:H	1:A:43:ILE:HD13	0.49	1.67	1	4
1:A:173:LEU:HD12	1:A:173:LEU:C	0.49	2.28	16	6
1:A:36:LYS:HE2	1:A:160:ALA:HB1	0.49	1.83	13	1
1:A:114:ASP:HB3	2:A:185[C]:MTN:N1	0.48	2.23	5	2
1:A:117:CYS:SG	2:A:185[B]:MTN:H83	0.48	2.47	10	1
1:A:58:TYR:CB	1:A:170:LEU:HD23	0.48	2.38	12	1
1:A:128:GLN:HA	1:A:133:ALA:HB1	0.48	1.84	18	12
1:A:29:GLY:N	3:A:187:GTP:O1B	0.48	2.46	8	5
1:A:92:VAL:CG1	1:A:103:ALA:HB1	0.48	2.35	19	1
1:A:86:GLU:HG3	1:A:177:LEU:HD21	0.48	1.84	1	3
1:A:89:ILE:HG22	1:A:124:PHE:CE1	0.48	2.43	5	1
1:A:104:ARG:HG2	1:A:143:LEU:HD22	0.48	1.84	14	1
1:A:177:LEU:HD22	1:A:177:LEU:N	0.48	2.24	18	3
1:A:173:LEU:HD23	1:A:173:LEU:O	0.48	2.09	12	9
1:A:148:ILE:HD12	1:A:153:TRP:CE2	0.48	2.43	13	2
1:A:92:VAL:HG13	1:A:125:ALA:HA	0.48	1.84	5	1
1:A:114:ASP:CG	2:A:185[A]:MTN:H73	0.48	2.29	12	1
1:A:33:VAL:HG21	1:A:124:PHE:HE2	0.48	1.67	15	1
1:A:28:ALA:HB3	1:A:91:VAL:HG13	0.48	1.84	6	2
1:A:139:ILE:HG22	1:A:155:ILE:CD1	0.48	2.37	1	2
1:A:114:ASP:OD2	2:A:185[A]:MTN:H82	0.48	2.08	11	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:25:LEU:HD21	1:A:103:ALA:CB	0.48	2.38	12	1
1:A:34:LEU:HD11	1:A:65:VAL:CB	0.48	2.38	17	1
1:A:114:ASP:HA	2:A:185[C]:MTN:S1	0.48	2.49	1	1
1:A:45:THR:HG21	3:A:187:GTP:H2'	0.48	1.86	7	1
1:A:35:TYR:HB2	1:A:43:ILE:HD11	0.48	1.83	9	1
1:A:21:LEU:HD23	1:A:22:MET:N	0.47	2.23	8	2
1:A:130:LEU:HD23	1:A:131:PRO:HD2	0.47	1.84	12	1
1:A:33:VAL:CG1	1:A:166:LEU:HD11	0.47	2.39	13	2
1:A:110:MET:SD	1:A:116:LEU:HD13	0.47	2.49	15	1
1:A:25:LEU:HD13	1:A:103:ALA:HA	0.47	1.85	1	2
1:A:134:MET:HB2	1:A:139:ILE:HD11	0.47	1.86	4	1
1:A:104:ARG:HB2	1:A:143:LEU:HD13	0.47	1.86	12	1
1:A:23:VAL:HG21	1:A:110:MET:CE	0.47	2.39	15	2
1:A:124:PHE:HB3	1:A:158:THR:HG21	0.47	1.85	1	2
1:A:111:LEU:C	1:A:111:LEU:HD23	0.47	2.30	5	1
1:A:160:ALA:HB3	3:A:187:GTP:C6	0.47	2.44	7	5
1:A:34:LEU:HD12	1:A:67:ASP:CG	0.47	2.30	3	2
1:A:45:THR:CG2	3:A:187:GTP:O1A	0.47	2.63	3	1
1:A:30:LYS:CG	1:A:91:VAL:HG11	0.47	2.40	7	1
1:A:56:VAL:CG1	1:A:63:PHE:CZ	0.47	2.98	14	4
1:A:20:ILE:CG2	1:A:65:VAL:HG13	0.47	2.40	16	1
1:A:130:LEU:CD1	3:A:187:GTP:N2	0.47	2.78	3	1
1:A:139:ILE:O	1:A:143:LEU:HD23	0.47	2.09	12	2
1:A:102:GLU:O	1:A:106:VAL:HG12	0.47	2.09	7	3
1:A:36:LYS:CD	1:A:160:ALA:HB1	0.47	2.40	13	1
1:A:31:THR:HG22	1:A:45:THR:CG2	0.47	2.36	14	1
1:A:34:LEU:HD21	1:A:54:GLU:OE1	0.47	2.10	19	1
1:A:20:ILE:CG2	1:A:89:ILE:HD12	0.47	2.38	4	2
1:A:36:LYS:HE3	1:A:42:VAL:HG22	0.47	1.86	13	1
1:A:68:VAL:CG1	1:A:77:LEU:HD11	0.47	2.39	19	1
1:A:8:LEU:C	1:A:8:LEU:HD23	0.47	2.30	2	2
1:A:139:ILE:HD13	1:A:139:ILE:N	0.47	2.25	20	3
1:A:34:LEU:HD11	1:A:54:GLU:HB2	0.47	1.87	6	2
1:A:34:LEU:HD13	1:A:65:VAL:HB	0.47	1.87	6	1
1:A:117:CYS:O	2:A:185[A]:MTN:S1	0.47	2.72	17	1
1:A:37:LEU:HD23	1:A:37:LEU:C	0.47	2.30	1	8
1:A:116:LEU:HD22	1:A:119:ALA:HB3	0.47	1.86	2	1
1:A:20:ILE:HD12	1:A:173:LEU:CD1	0.47	2.40	6	1
1:A:170:LEU:HD13	1:A:170:LEU:C	0.47	2.30	9	1
1:A:35:TYR:HB3	1:A:43:ILE:HD12	0.47	1.87	18	3
1:A:23:VAL:HG21	1:A:110:MET:HE2	0.47	1.86	15	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:148:ILE:HD12	1:A:153:TRP:CD1	0.47	2.45	20	1
1:A:77:LEU:HD12	1:A:77:LEU:N	0.46	2.25	2	2
1:A:30:LYS:NZ	3:A:187:GTP:PB	0.46	2.88	6	1
2:A:183[B]:MTN:H71	2:A:183[B]:MTN:S1	0.46	2.50	6	1
1:A:56:VAL:CG1	1:A:63:PHE:CE2	0.46	2.98	10	1
1:A:30:LYS:NZ	3:A:187:GTP:O3G	0.46	2.48	11	2
1:A:107:MET:CG	1:A:121:TRP:CZ2	0.46	2.98	12	1
1:A:91:VAL:HG13	1:A:126:ASN:OD1	0.46	2.10	13	1
1:A:173:LEU:HD23	1:A:173:LEU:C	0.46	2.29	12	6
1:A:58:TYR:CG	1:A:170:LEU:CD2	0.46	2.99	5	3
1:A:124:PHE:CE1	1:A:156:GLN:CB	0.46	2.98	14	3
1:A:122:LEU:HD22	1:A:124:PHE:CD1	0.46	2.44	19	1
1:A:148:ILE:HD12	1:A:153:TRP:HZ2	0.46	1.69	17	5
1:A:151:ARG:CZ	2:A:185[B]:MTN:S1	0.46	3.03	13	1
3:A:187:GTP:O1A	3:A:187:GTP:O2G	0.46	2.33	16	1
1:A:56:VAL:CG1	1:A:63:PHE:CE1	0.46	2.98	18	1
1:A:140:THR:HB	1:A:155:ILE:HG21	0.46	1.86	5	1
1:A:175:ASN:O	2:A:186[A]:MTN:H62	0.46	2.10	17	1
1:A:18:MET:HG3	1:A:177:LEU:HD12	0.46	1.87	3	1
1:A:129:ASP:OD1	1:A:130:LEU:HD12	0.46	2.11	3	1
1:A:176:CYS:O	2:A:186[A]:MTN:H2	0.46	2.11	14	1
1:A:118:ASN:N	2:A:185[A]:MTN:S1	0.46	2.89	1	1
1:A:175:ASN:O	2:A:186[C]:MTN:H92	0.46	2.11	7	2
1:A:23:VAL:CG1	1:A:78:TRP:CE2	0.46	2.99	20	3
1:A:45:THR:CB	3:A:187:GTP:O1A	0.46	2.64	4	1
1:A:30:LYS:CG	1:A:91:VAL:HG21	0.46	2.41	5	1
1:A:25:LEU:HD21	1:A:102:GLU:HB3	0.46	1.86	18	2
1:A:145:LEU:HD22	1:A:153:TRP:CE2	0.46	2.46	17	1
1:A:38:LYS:CD	1:A:56:VAL:HG22	0.46	2.41	19	1
1:A:126:ASN:ND2	3:A:187:GTP:N7	0.46	2.64	1	4
1:A:127:LYS:CB	1:A:130:LEU:HD13	0.46	2.39	15	3
1:A:111:LEU:HD11	1:A:151:ARG:CG	0.46	2.40	15	2
1:A:20:ILE:O	1:A:21:LEU:HD12	0.46	2.11	19	1
1:A:111:LEU:CD1	1:A:153:TRP:CH2	0.46	2.99	5	1
1:A:34:LEU:HD21	1:A:54:GLU:CG	0.46	2.40	15	1
1:A:110:MET:SD	1:A:116:LEU:HD22	0.46	2.51	19	1
1:A:21:LEU:CG	1:A:85:THR:HG21	0.46	2.41	1	2
1:A:148:ILE:HD13	1:A:153:TRP:HZ2	0.46	1.70	5	2
1:A:46:ILE:HD13	1:A:46:ILE:H	0.46	1.70	11	2
1:A:88:VAL:CG2	1:A:121:TRP:CE3	0.46	2.99	5	1
1:A:140:THR:HG22	1:A:145:LEU:CB	0.46	2.41	20	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:122:LEU:HD23	1:A:123:VAL:N	0.45	2.26	2	1
1:A:122:LEU:CD2	1:A:124:PHE:CZ	0.45	2.99	12	6
1:A:111:LEU:HD22	1:A:151:ARG:CB	0.45	2.41	11	1
1:A:30:LYS:NZ	3:A:187:GTP:O1B	0.45	2.50	18	1
1:A:92:VAL:HG13	1:A:92:VAL:O	0.45	2.10	5	1
1:A:110:MET:CE	1:A:116:LEU:HD13	0.45	2.42	12	1
2:A:184[B]:MTN:S1	2:A:184[B]:MTN:C6	0.45	2.98	14	2
1:A:145:LEU:CD2	1:A:153:TRP:CZ3	0.45	3.00	15	1
1:A:18:MET:HG2	1:A:177:LEU:HD22	0.45	1.87	17	1
1:A:20:ILE:HB	1:A:65:VAL:HG12	0.45	1.88	3	1
1:A:92:VAL:O	1:A:92:VAL:HG13	0.45	2.11	17	5
1:A:49:ILE:HD12	1:A:74:ILE:CD1	0.45	2.39	10	1
1:A:145:LEU:CD1	1:A:153:TRP:CD2	0.45	2.99	8	2
1:A:94:SER:HB3	1:A:125:ALA:HB1	0.45	1.88	15	1
1:A:173:LEU:C	1:A:173:LEU:HD23	0.45	2.32	2	3
1:A:173:LEU:HD13	1:A:173:LEU:C	0.45	2.32	5	1
1:A:122:LEU:CD2	1:A:124:PHE:CE1	0.45	3.00	10	2
1:A:117:CYS:CB	2:A:185[C]:MTN:H61	0.45	2.41	19	1
1:A:124:PHE:CE2	1:A:156:GLN:CB	0.45	2.99	19	1
1:A:111:LEU:HD21	1:A:151:ARG:CD	0.45	2.40	1	1
1:A:63:PHE:CE2	1:A:173:LEU:HD12	0.45	2.47	19	2
1:A:114:ASP:CB	2:A:185[C]:MTN:H62	0.45	2.42	3	1
1:A:134:MET:CB	1:A:139:ILE:HD11	0.45	2.42	4	1
1:A:51:PHE:CZ	1:A:68:VAL:CG2	0.45	2.99	7	1
1:A:56:VAL:HG11	1:A:63:PHE:CZ	0.45	2.47	10	2
1:A:90:PHE:CD1	1:A:107:MET:CG	0.45	3.00	15	1
1:A:75:ARG:CG	1:A:78:TRP:CZ3	0.45	3.00	20	1
1:A:104:ARG:HG3	1:A:143:LEU:HD23	0.45	1.87	5	2
1:A:23:VAL:CG1	1:A:78:TRP:CZ2	0.45	2.99	10	3
1:A:175:ASN:O	2:A:186[B]:MTN:H91	0.45	2.11	10	1
1:A:68:VAL:CG2	1:A:78:TRP:CD1	0.45	2.99	12	1
1:A:31:THR:OG1	1:A:45:THR:HG22	0.45	2.11	20	1
1:A:63:PHE:CD2	1:A:170:LEU:HD21	0.45	2.46	7	3
1:A:25:LEU:HD21	1:A:102:GLU:CB	0.45	2.41	7	1
1:A:92:VAL:O	1:A:92:VAL:HG23	0.45	2.12	15	1
1:A:167:TYR:CD1	1:A:168:GLU:N	0.45	2.85	7	3
1:A:23:VAL:CG2	1:A:90:PHE:CZ	0.45	3.00	2	1
1:A:58:TYR:CD2	1:A:170:LEU:CD2	0.45	3.00	3	1
1:A:122:LEU:HD21	1:A:124:PHE:HZ	0.45	1.71	4	1
1:A:176:CYS:O	2:A:186[A]:MTN:H41	0.45	2.11	5	1
1:A:148:ILE:CD1	1:A:153:TRP:CZ2	0.45	3.00	4	3

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:18:MET:CB	1:A:63:PHE:CE1	0.45	3.00	6	1
1:A:30:LYS:CE	3:A:187:GTP:O3G	0.45	2.64	9	1
1:A:23:VAL:CG1	1:A:78:TRP:CH2	0.45	3.00	14	3
1:A:173:LEU:HD11	1:A:177:LEU:HD11	0.45	1.87	15	1
1:A:117:CYS:SG	2:A:185[C]:MTN:H63	0.45	2.51	19	1
1:A:145:LEU:HD22	1:A:153:TRP:CH2	0.44	2.47	17	1
1:A:175:ASN:O	2:A:186[C]:MTN:H91	0.44	2.13	17	1
1:A:92:VAL:HG23	1:A:103:ALA:CB	0.44	2.43	4	1
1:A:121:TRP:CZ3	1:A:151:ARG:CG	0.44	3.00	6	1
1:A:104:ARG:CG	1:A:143:LEU:HD23	0.44	2.42	7	4
1:A:4:PHE:O	1:A:8:LEU:HD13	0.44	2.13	14	1
1:A:94:SER:OG	1:A:139:ILE:HD11	0.44	2.12	17	1
1:A:107:MET:CE	1:A:121:TRP:CE3	0.44	3.00	4	1
1:A:45:THR:CG2	3:A:187:GTP:PA	0.44	3.05	18	1
1:A:90:PHE:CE2	1:A:92:VAL:HG22	0.44	2.47	1	1
1:A:129:ASP:OD2	1:A:161:THR:HG21	0.44	2.12	5	2
1:A:58:TYR:CG	1:A:170:LEU:CD1	0.44	2.99	13	1
1:A:123:VAL:HG12	1:A:154:PHE:O	0.44	2.12	14	1
1:A:158:THR:OG1	1:A:166:LEU:HD23	0.44	2.12	19	1
1:A:36:LYS:CE	1:A:42:VAL:HG23	0.44	2.42	20	1
1:A:23:VAL:HG21	1:A:90:PHE:CZ	0.44	2.48	2	1
1:A:90:PHE:CG	1:A:107:MET:CE	0.44	3.00	9	1
1:A:58:TYR:O	1:A:61:ILE:CG1	0.44	2.66	17	4
1:A:23:VAL:CG2	1:A:90:PHE:CD2	0.44	3.00	11	1
1:A:85:THR:HG22	1:A:87:GLY:O	0.44	2.11	18	1
1:A:53:VAL:CG2	1:A:66:TRP:CD2	0.44	3.00	8	1
1:A:86:GLU:HG2	1:A:177:LEU:HD22	0.44	1.88	13	1
1:A:32:THR:HG22	1:A:36:LYS:NZ	0.44	2.26	15	1
1:A:86:GLU:CG	1:A:177:LEU:HD13	0.44	2.42	3	1
1:A:51:PHE:CE2	1:A:68:VAL:HG22	0.44	2.47	7	1
1:A:139:ILE:O	1:A:143:LEU:HD12	0.44	2.13	8	1
1:A:158:THR:HG23	1:A:166:LEU:HD11	0.44	1.88	10	1
1:A:35:TYR:CD2	1:A:43:ILE:HD11	0.43	2.48	1	1
1:A:21:LEU:HD22	1:A:66:TRP:HB2	0.43	1.90	14	1
1:A:114:ASP:HB2	2:A:185[C]:MTN:H92	0.43	1.89	1	1
1:A:117:CYS:N	2:A:185[A]:MTN:S1	0.43	2.91	1	1
3:A:187:GTP:O1B	3:A:187:GTP:H5'	0.43	2.13	8	1
1:A:167:TYR:CE2	1:A:168:GLU:CG	0.43	3.00	16	1
1:A:20:ILE:HG12	1:A:173:LEU:HD21	0.43	1.90	18	1
2:A:184[C]:MTN:H92	2:A:184[C]:MTN:H63	0.43	1.91	20	20
2:A:185[A]:MTN:H93	2:A:185[A]:MTN:H62	0.43	1.91	1	20

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:49:ILE:HD12	1:A:74:ILE:HD13	0.43	1.89	9	1
1:A:21:LEU:C	1:A:88:VAL:HG23	0.43	2.34	10	1
2:A:182[C]:MTN:H63	2:A:182[C]:MTN:H92	0.43	1.90	14	20
2:A:183[C]:MTN:H92	2:A:183[C]:MTN:H63	0.43	1.91	3	20
2:A:186[C]:MTN:H63	2:A:186[C]:MTN:H92	0.43	1.91	2	18
1:A:26:ASP:O	3:A:187:GTP:PG	0.43	2.76	7	1
1:A:34:LEU:HD21	1:A:65:VAL:HG12	0.43	1.91	17	2
1:A:37:LEU:HD13	1:A:37:LEU:C	0.43	2.34	9	1
2:A:186[A]:MTN:H93	2:A:186[A]:MTN:H62	0.43	1.91	9	19
2:A:182[A]:MTN:H93	2:A:182[A]:MTN:H62	0.43	1.91	13	20
2:A:183[A]:MTN:H62	2:A:183[A]:MTN:H93	0.43	1.91	9	20
1:A:153:TRP:CE3	1:A:153:TRP:O	0.43	2.71	2	5
1:A:4:PHE:O	1:A:8:LEU:HD23	0.43	2.13	16	2
1:A:111:LEU:HD23	1:A:111:LEU:O	0.43	2.13	5	1
1:A:86:GLU:OE2	1:A:177:LEU:HD23	0.43	2.14	14	1
1:A:124:PHE:CD2	1:A:158:THR:HG21	0.43	2.49	1	1
1:A:66:TRP:CD1	1:A:66:TRP:N	0.43	2.86	2	3
1:A:21:LEU:HD23	1:A:88:VAL:HG21	0.43	1.91	10	1
2:A:186[A]:MTN:H62	2:A:186[A]:MTN:H93	0.43	1.91	17	1
1:A:161:THR:HG23	3:A:187:GTP:C2	0.43	2.49	20	1
2:A:185[C]:MTN:H63	2:A:185[C]:MTN:H92	0.43	1.91	12	18
1:A:145:LEU:O	1:A:153:TRP:CZ2	0.43	2.72	10	6
1:A:53:VAL:HG22	1:A:66:TRP:CG	0.43	2.49	12	1
1:A:74:ILE:HG23	1:A:77:LEU:CD2	0.43	2.40	19	1
1:A:114:ASP:CB	2:A:185[C]:MTN:C6	0.43	2.97	6	1
1:A:33:VAL:HG13	1:A:34:LEU:N	0.43	2.29	8	4
1:A:58:TYR:CD2	1:A:170:LEU:CD1	0.43	3.00	9	1
1:A:36:LYS:HE3	1:A:42:VAL:HG13	0.43	1.89	13	1
1:A:58:TYR:CD2	1:A:170:LEU:HD23	0.43	2.49	1	2
2:A:186[C]:MTN:H92	2:A:186[C]:MTN:H63	0.43	1.91	13	2
1:A:107:MET:CE	1:A:153:TRP:CE3	0.43	3.02	18	1
1:A:34:LEU:HD13	1:A:67:ASP:OD1	0.43	2.14	19	1
1:A:61:ILE:HG22	1:A:62:SER:N	0.42	2.29	2	7
1:A:20:ILE:HG23	1:A:87:GLY:O	0.42	2.13	3	2
1:A:88:VAL:HG13	1:A:121:TRP:CE3	0.42	2.49	4	1
1:A:36:LYS:CE	1:A:42:VAL:HG13	0.42	2.44	13	1
1:A:126:ASN:OD1	3:A:187:GTP:C5	0.42	2.72	16	1
1:A:23:VAL:HG12	1:A:24:GLY:N	0.42	2.29	17	2
1:A:49:ILE:HG22	1:A:50:GLY:N	0.42	2.29	17	1
1:A:114:ASP:HB3	2:A:185[C]:MTN:H92	0.42	1.91	1	1
1:A:126:ASN:OD1	3:A:187:GTP:N7	0.42	2.53	9	3

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:88:VAL:HG23	1:A:120:ALA:O	0.42	2.14	17	1
1:A:151:ARG:O	1:A:153:TRP:CD1	0.42	2.73	14	2
1:A:49:ILE:HG23	1:A:74:ILE:HG21	0.42	1.90	13	1
1:A:35:TYR:CB	1:A:43:ILE:HD12	0.42	2.44	18	1
1:A:34:LEU:HD12	1:A:67:ASP:HB2	0.42	1.89	20	1
1:A:151:ARG:HH22	2:A:185[B]:MTN:H2	0.42	1.75	13	1
1:A:46:ILE:C	1:A:46:ILE:HD12	0.42	2.34	16	1
1:A:117:CYS:N	2:A:185[B]:MTN:S1	0.42	2.92	12	2
1:A:116:LEU:HG	1:A:119:ALA:HB3	0.42	1.91	10	1
1:A:34:LEU:HD12	1:A:67:ASP:OD1	0.42	2.14	2	1
1:A:25:LEU:HD11	1:A:103:ALA:CB	0.42	2.21	13	1
1:A:111:LEU:HD23	1:A:151:ARG:HB2	0.42	1.92	9	1
1:A:31:THR:OG1	3:A:187:GTP:O2B	0.42	2.38	19	1
1:A:53:VAL:HG22	1:A:54:GLU:N	0.42	2.29	6	1
1:A:86:GLU:HG2	1:A:177:LEU:HD13	0.42	1.90	16	1
1:A:23:VAL:CG2	1:A:90:PHE:CE1	0.41	3.03	2	2
1:A:49:ILE:HG23	1:A:74:ILE:HD13	0.41	1.92	13	1
1:A:63:PHE:CZ	1:A:170:LEU:HD11	0.41	2.50	14	1
1:A:61:ILE:CD1	1:A:63:PHE:CZ	0.41	3.03	17	1
1:A:116:LEU:HD23	1:A:121:TRP:HH2	0.41	1.69	20	1
1:A:176:CYS:C	2:A:186[C]:MTN:H61	0.41	2.35	1	1
1:A:26:ASP:CA	3:A:187:GTP:O2G	0.41	2.68	5	1
2:A:185[C]:MTN:H92	2:A:185[C]:MTN:H63	0.41	1.91	18	2
1:A:111:LEU:HD12	1:A:121:TRP:CD1	0.41	2.51	7	1
1:A:68:VAL:CG2	1:A:78:TRP:NE1	0.41	2.80	11	1
1:A:23:VAL:HG21	1:A:110:MET:SD	0.41	2.55	12	1
1:A:46:ILE:HD12	1:A:46:ILE:O	0.41	2.15	16	1
1:A:46:ILE:N	1:A:46:ILE:CD1	0.41	2.84	5	2
1:A:32:THR:OG1	3:A:187:GTP:H2'	0.41	2.14	7	1
1:A:36:LYS:CG	1:A:42:VAL:HG12	0.41	2.45	11	1
1:A:175:ASN:O	2:A:186[A]:MTN:H91	0.41	2.15	14	1
1:A:21:LEU:HD23	1:A:22:MET:H	0.41	1.75	12	1
1:A:89:ILE:CG2	1:A:124:PHE:CD2	0.41	3.04	12	2
1:A:42:VAL:HG21	1:A:161:THR:C	0.41	2.35	19	4
1:A:22:MET:SD	1:A:34:LEU:HD13	0.41	2.55	18	1
1:A:111:LEU:C	1:A:111:LEU:HD12	0.41	2.36	20	1
2:A:185[C]:MTN:S1	2:A:185[C]:MTN:H71	0.41	2.56	3	1
1:A:116:LEU:O	1:A:121:TRP:CH2	0.41	2.74	11	1
1:A:30:LYS:HG2	3:A:187:GTP:O2B	0.41	2.16	14	1
1:A:153:TRP:CD1	1:A:153:TRP:N	0.41	2.87	14	1
1:A:43:ILE:HD12	1:A:43:ILE:N	0.41	2.30	19	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:187:GTP:O2B	3:A:187:GTP:O1G	0.41	2.38	20	1
1:A:51:PHE:HB3	1:A:68:VAL:HG12	0.41	1.93	18	1
1:A:51:PHE:CE2	1:A:66:TRP:CZ3	0.41	3.08	20	1
1:A:42:VAL:HG11	1:A:161:THR:HA	0.41	1.90	11	1
1:A:107:MET:HG2	1:A:121:TRP:CZ2	0.41	2.51	12	1
1:A:20:ILE:CG2	1:A:89:ILE:CD1	0.41	2.99	5	1
1:A:23:VAL:CG1	1:A:78:TRP:CZ3	0.41	3.04	5	1
1:A:119:ALA:O	1:A:121:TRP:CZ3	0.41	2.74	13	2
1:A:75:ARG:HG3	1:A:78:TRP:CZ3	0.41	2.51	20	1
1:A:118:ASN:N	2:A:185[B]:MTN:S1	0.41	2.94	12	2
1:A:34:LEU:HD12	1:A:54:GLU:HB2	0.41	1.91	12	1
1:A:148:ILE:HG23	1:A:153:TRP:NE1	0.41	2.31	14	1
1:A:168:GLU:O	1:A:172:TRP:CD1	0.41	2.74	14	1
1:A:115:GLU:O	1:A:116:LEU:HD13	0.40	2.17	7	1
1:A:110:MET:O	1:A:121:TRP:CZ2	0.40	2.74	11	1
1:A:111:LEU:CD2	1:A:151:ARG:CD	0.40	3.00	1	1
1:A:140:THR:OG1	1:A:155:ILE:HD13	0.40	2.16	2	1
1:A:26:ASP:OD2	3:A:187:GTP:O2G	0.40	2.39	6	1
1:A:120:ALA:O	1:A:121:TRP:CE3	0.40	2.74	7	1
1:A:53:VAL:CG2	1:A:66:TRP:CE3	0.40	3.02	8	1
1:A:45:THR:HG23	3:A:187:GTP:H5"	0.40	1.93	9	1
1:A:151:ARG:HB2	1:A:153:TRP:CH2	0.40	2.52	13	1
1:A:43:ILE:HD13	1:A:43:ILE:H	0.40	1.75	16	1
1:A:46:ILE:CG1	1:A:47:PRO:HD2	0.40	2.46	19	1
1:A:104:ARG:CG	1:A:143:LEU:CD2	0.40	3.00	7	1
1:A:153:TRP:O	1:A:153:TRP:CE3	0.40	2.74	7	2
1:A:30:LYS:HE2	3:A:187:GTP:O3G	0.40	2.16	9	1
1:A:123:VAL:HG23	1:A:154:PHE:O	0.40	2.17	18	1
1:A:30:LYS:HB3	1:A:91:VAL:HG21	0.40	1.93	3	1
1:A:166:LEU:N	1:A:166:LEU:CD1	0.40	2.85	5	1
1:A:21:LEU:O	1:A:89:ILE:N	0.40	2.53	9	1
1:A:111:LEU:HD11	1:A:121:TRP:CG	0.40	2.51	9	1
1:A:63:PHE:CE2	1:A:170:LEU:CD2	0.40	3.04	10	1
1:A:36:LYS:CD	1:A:42:VAL:HG22	0.40	2.46	15	1
1:A:87:GLY:HA2	1:A:120:ALA:CB	0.40	2.46	16	1
1:A:117:CYS:CB	2:A:185[C]:MTN:C6	0.40	3.00	19	1
1:A:26:ASP:O	3:A:187:GTP:O2G	0.40	2.39	4	1
1:A:29:GLY:CA	3:A:187:GTP:O1B	0.40	2.70	4	1
1:A:177:LEU:N	1:A:177:LEU:CD2	0.40	2.85	6	2
1:A:53:VAL:CG2	1:A:66:TRP:NE1	0.40	2.85	15	1
1:A:37:LEU:C	1:A:37:LEU:HD23	0.40	2.37	16	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:23:VAL:O	1:A:90:PHE:CD1	0.40	2.74	20	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	162/181 (90%)	151±2 (93±1%)	10±2 (6±1%)	2±1 (1±1%)	20	68
All	All	3240/3620 (90%)	3015 (93%)	194 (6%)	31 (1%)	20	68

All 6 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	27	GLY	10
1	A	25	LEU	9
1	A	84	ASN	6
1	A	59	CYS	4
1	A	149	ARG	1
1	A	133	ALA	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	140/154 (91%)	113±4 (81±3%)	27±4 (19±3%)	4	36
All	All	2800/3080 (91%)	2264 (81%)	536 (19%)	4	36

All 110 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	43	ILE	20
1	A	4	PHE	19
1	A	176	CYS	19
1	A	9	PHE	17
1	A	59	CYS	16
1	A	153	TRP	13
1	A	62	SER	12
1	A	30	LYS	11
1	A	32	THR	10
1	A	145	LEU	10
1	A	22	MET	10
1	A	64	THR	9
1	A	31	THR	9
1	A	57	GLN	9
1	A	21	LEU	8
1	A	54	GLU	8
1	A	97	ARG	8
1	A	151	ARG	8
1	A	38	LYS	8
1	A	122	LEU	8
1	A	117	CYS	8
1	A	104	ARG	8
1	A	100	ILE	7
1	A	118	ASN	7
1	A	34	LEU	7
1	A	18	MET	7
1	A	58	TYR	6
1	A	36	LYS	6
1	A	73	ARG	6
1	A	110	MET	6
1	A	156	GLN	6
1	A	19	ARG	6
1	A	149	ARG	6
1	A	90	PHE	6
1	A	173	LEU	6
1	A	44	THR	5
1	A	124	PHE	5
1	A	109	ARG	5
1	A	170	LEU	5
1	A	96	ASP	5
1	A	142	LYS	5
1	A	121	TRP	5
1	A	146	HIS	4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	112	ASN	4
1	A	17	GLU	4
1	A	132	GLU	4
1	A	75	ARG	4
1	A	108	GLN	4
1	A	135	SER	4
1	A	26	ASP	4
1	A	94	SER	4
1	A	25	LEU	4
1	A	48	THR	4
1	A	8	LEU	4
1	A	134	MET	4
1	A	60	ASN	4
1	A	147	SER	4
1	A	7	LYS	3
1	A	111	LEU	3
1	A	141	GLU	3
1	A	6	SER	3
1	A	127	LYS	3
1	A	130	LEU	3
1	A	138	GLU	3
1	A	76	SER	3
1	A	107	MET	3
1	A	126	ASN	3
1	A	46	ILE	3
1	A	86	GLU	3
1	A	154	PHE	3
1	A	66	TRP	3
1	A	39	LEU	3
1	A	45	THR	3
1	A	166	LEU	3
1	A	98	SER	3
1	A	164	GLU	3
1	A	162	SER	3
1	A	178	LYS	3
1	A	105	GLU	3
1	A	116	LEU	2
1	A	174	SER	2
1	A	67	ASP	2
1	A	41	GLU	2
1	A	150	ASN	2
1	A	128	GLN	2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	99	ARG	2
1	A	37	LEU	2
1	A	114	ASP	2
1	A	177	LEU	2
1	A	143	LEU	2
1	A	52	ASN	2
1	A	171	GLU	2
1	A	123	VAL	2
1	A	93	ASP	1
1	A	72	ASP	1
1	A	113	GLU	1
1	A	161	THR	1
1	A	49	ILE	1
1	A	55	CYS	1
1	A	35	TYR	1
1	A	84	ASN	1
1	A	168	GLU	1
1	A	175	ASN	1
1	A	140	THR	1
1	A	10	SER	1
1	A	85	THR	1
1	A	68	VAL	1
1	A	172	TRP	1
1	A	148	ILE	1
1	A	3	LEU	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 (i)

16 ligands 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	MTN	A	182[A]	1	9,12,16	1.23±0.02	2±0 (22±0%)
2	MTN	A	184[A]	1	9,12,16	1.25±0.02	2±0 (22±0%)
2	MTN	A	183[C]	1	9,12,16	1.21±0.02	2±0 (22±0%)
2	MTN	A	185[A]	1	9,12,16	1.21±0.02	2±0 (22±0%)
2	MTN	A	185[B]	1	9,12,16	1.23±0.01	2±0 (22±0%)
2	MTN	A	185[C]	1	9,12,16	1.25±0.02	2±0 (22±0%)
2	MTN	A	186[C]	1	9,12,16	1.20±0.02	2±0 (22±0%)
2	MTN	A	183[B]	1	9,12,16	1.23±0.02	2±0 (22±0%)
2	MTN	A	182[B]	1	9,12,16	1.21±0.01	2±0 (22±0%)
2	MTN	A	184[C]	1	9,12,16	1.21±0.01	2±0 (22±0%)
2	MTN	A	184[B]	1	9,12,16	1.23±0.01	2±0 (22±0%)
2	MTN	A	186[A]	1	9,12,16	1.21±0.02	2±0 (22±0%)
2	MTN	A	186[B]	1	9,12,16	1.20±0.02	2±0 (22±0%)
2	MTN	A	182[C]	1	9,12,16	1.27±0.02	2±0 (22±0%)
2	MTN	A	183[A]	1	9,12,16	1.23±0.01	2±0 (22±0%)
3	GTP	A	187	-	29,34,34	1.42±0.01	5±0 (17±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	MTN	A	182[A]	1	11,20,27	3.47±0.02	5±0 (45±0%)

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
2	MTN	A	184[A]	1	11,20,27	3.46±0.02	5±0 (45±0%)
2	MTN	A	183[C]	1	11,20,27	3.44±0.02	5±0 (45±0%)
2	MTN	A	185[A]	1	11,20,27	3.47±0.02	5±0 (45±0%)
2	MTN	A	185[B]	1	11,20,27	3.47±0.02	5±0 (45±0%)
2	MTN	A	185[C]	1	11,20,27	3.47±0.02	5±0 (45±0%)
2	MTN	A	186[C]	1	11,20,27	3.46±0.02	5±0 (45±0%)
2	MTN	A	183[B]	1	11,20,27	3.47±0.01	5±0 (45±0%)
2	MTN	A	182[B]	1	11,20,27	3.45±0.02	5±0 (45±0%)
2	MTN	A	184[C]	1	11,20,27	3.45±0.02	5±0 (45±0%)
2	MTN	A	184[B]	1	11,20,27	3.45±0.02	5±0 (45±0%)
2	MTN	A	186[A]	1	11,20,27	3.46±0.02	5±0 (45±0%)
2	MTN	A	186[B]	1	11,20,27	3.45±0.02	5±0 (45±0%)
2	MTN	A	182[C]	1	11,20,27	3.46±0.02	5±0 (45±0%)
2	MTN	A	183[A]	1	11,20,27	3.45±0.02	5±0 (45±0%)
3	GTP	A	187	-	35,54,54	0.66±0.01	1±0 (2±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	MTN	A	185[C]	1	-	0±0,0,25,29	0±0,1,1,1
2	MTN	A	183[C]	1	-	0±0,0,25,29	0±0,1,1,1
2	MTN	A	182[C]	1	-	0±0,0,25,29	0±0,1,1,1
2	MTN	A	184[B]	1	-	0±0,0,25,29	0±0,1,1,1
2	MTN	A	185[B]	1	-	0±0,0,25,29	0±0,1,1,1
2	MTN	A	184[A]	1	-	0±0,0,25,29	0±0,1,1,1
2	MTN	A	182[B]	1	-	0±0,0,25,29	0±0,1,1,1
2	MTN	A	183[A]	1	-	0±0,0,25,29	0±0,1,1,1
2	MTN	A	186[B]	1	-	0±0,0,25,29	0±0,1,1,1
2	MTN	A	185[A]	1	-	0±0,0,25,29	0±0,1,1,1
2	MTN	A	182[A]	1	-	0±0,0,25,29	0±0,1,1,1
2	MTN	A	186[C]	1	-	0±0,0,25,29	0±0,1,1,1
3	GTP	A	187	-	-	0±0,18,38,38	0±0,3,3,3
2	MTN	A	183[B]	1	-	0±0,0,25,29	0±0,1,1,1
2	MTN	A	184[C]	1	-	0±0,0,25,29	0±0,1,1,1
2	MTN	A	186[A]	1	-	0±0,0,25,29	0±0,1,1,1

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
3	A	187	GTP	PG-O1G	3.05	1.60	1.50	17	20
3	A	187	GTP	C8-N7	2.76	1.30	1.34	8	20
3	A	187	GTP	C5-C6	2.75	1.42	1.47	1	20
2	A	185[B]	MTN	C5-N1	2.74	1.47	1.50	19	20
2	A	182[C]	MTN	C5-N1	2.73	1.47	1.50	15	20
2	A	184[A]	MTN	C5-N1	2.73	1.47	1.50	10	20
2	A	185[C]	MTN	C5-N1	2.69	1.47	1.50	17	20
2	A	184[B]	MTN	C5-N1	2.68	1.47	1.50	1	20
2	A	182[A]	MTN	C5-N1	2.68	1.47	1.50	6	20
2	A	183[A]	MTN	C5-N1	2.67	1.47	1.50	14	20
2	A	183[B]	MTN	C5-N1	2.62	1.47	1.50	8	20
3	A	187	GTP	PA-O1A	2.61	1.59	1.50	11	20
2	A	186[A]	MTN	C5-N1	2.61	1.47	1.50	18	20
2	A	186[B]	MTN	C5-N1	2.61	1.47	1.50	5	20
3	A	187	GTP	PB-O1B	2.60	1.59	1.50	9	20
2	A	185[A]	MTN	C5-N1	2.59	1.47	1.50	11	20
2	A	183[C]	MTN	C5-N1	2.57	1.47	1.50	17	20
2	A	182[B]	MTN	C5-N1	2.55	1.47	1.50	9	20
2	A	184[C]	MTN	C5-N1	2.54	1.47	1.50	3	20
2	A	186[C]	MTN	C5-N1	2.53	1.47	1.50	20	20
2	A	183[B]	MTN	O1-N1	2.08	1.32	1.43	10	20
2	A	186[B]	MTN	O1-N1	2.08	1.32	1.43	10	20
2	A	186[C]	MTN	O1-N1	2.07	1.32	1.43	3	20
2	A	183[A]	MTN	O1-N1	2.07	1.32	1.43	19	20
2	A	183[C]	MTN	O1-N1	2.07	1.32	1.43	19	20
2	A	185[C]	MTN	O1-N1	2.07	1.32	1.43	19	20
2	A	185[A]	MTN	O1-N1	2.07	1.32	1.43	19	20
2	A	185[B]	MTN	O1-N1	2.07	1.32	1.43	6	20
2	A	184[B]	MTN	O1-N1	2.07	1.32	1.43	11	20
2	A	182[C]	MTN	O1-N1	2.06	1.32	1.43	20	20
2	A	184[C]	MTN	O1-N1	2.06	1.32	1.43	9	20
2	A	182[A]	MTN	O1-N1	2.06	1.32	1.43	3	20
2	A	184[A]	MTN	O1-N1	2.06	1.32	1.43	7	20
2	A	186[A]	MTN	O1-N1	2.06	1.32	1.43	17	20
2	A	182[B]	MTN	O1-N1	2.05	1.32	1.43	5	20

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	A	185[A]	MTN	C2-C1-N1	8.65	105.38	99.43	16	20
2	A	186[A]	MTN	C2-C1-N1	8.64	105.38	99.43	13	20
2	A	182[C]	MTN	C2-C1-N1	8.64	105.38	99.43	6	20
2	A	185[C]	MTN	C2-C1-N1	8.63	105.37	99.43	10	20
2	A	185[B]	MTN	C2-C1-N1	8.62	105.36	99.43	9	20
2	A	184[C]	MTN	C2-C1-N1	8.62	105.36	99.43	12	20
2	A	183[B]	MTN	C2-C1-N1	8.61	105.36	99.43	15	20
2	A	182[A]	MTN	C2-C1-N1	8.61	105.36	99.43	13	20
2	A	184[A]	MTN	C2-C1-N1	8.58	105.34	99.43	7	20
2	A	182[B]	MTN	C2-C1-N1	8.58	105.34	99.43	14	20
2	A	186[B]	MTN	C2-C1-N1	8.57	105.33	99.43	1	20
2	A	186[C]	MTN	C2-C1-N1	8.57	105.33	99.43	13	20
2	A	183[A]	MTN	C2-C1-N1	8.57	105.33	99.43	1	20
2	A	184[B]	MTN	C2-C1-N1	8.56	105.32	99.43	11	20
2	A	183[C]	MTN	C2-C1-N1	8.54	105.31	99.43	9	20
2	A	185[C]	MTN	C8-C1-C2	4.80	108.21	112.77	12	20
2	A	186[B]	MTN	C8-C1-C2	4.79	108.22	112.77	3	20
2	A	184[B]	MTN	C8-C1-C2	4.76	108.25	112.77	12	20
2	A	182[A]	MTN	C8-C1-C2	4.74	108.27	112.77	9	20
2	A	183[A]	MTN	C8-C1-C2	4.73	108.27	112.77	16	20
2	A	185[A]	MTN	C8-C1-C2	4.73	108.28	112.77	15	20
2	A	185[B]	MTN	C8-C1-C2	4.73	108.28	112.77	15	20
2	A	183[B]	MTN	C8-C1-C2	4.73	108.28	112.77	7	20
2	A	186[C]	MTN	C8-C1-C2	4.73	108.28	112.77	3	20
2	A	184[C]	MTN	C8-C1-C2	4.73	108.28	112.77	18	20
2	A	186[A]	MTN	C8-C1-C2	4.73	108.28	112.77	16	20
2	A	183[C]	MTN	C8-C1-C2	4.72	108.29	112.77	9	20
2	A	182[B]	MTN	C8-C1-C2	4.71	108.30	112.77	1	20
2	A	184[A]	MTN	C8-C1-C2	4.71	108.30	112.77	7	20
2	A	182[C]	MTN	C8-C1-C2	4.71	108.30	112.77	10	20
2	A	183[B]	MTN	C1-C2-C3	3.88	109.97	113.48	12	20
2	A	185[C]	MTN	C1-C2-C3	3.88	109.97	113.48	15	20
2	A	182[A]	MTN	C1-C2-C3	3.87	109.99	113.48	5	20
2	A	184[A]	MTN	C1-C2-C3	3.87	109.99	113.48	1	20
2	A	185[A]	MTN	C1-C2-C3	3.82	110.03	113.48	5	20
2	A	186[C]	MTN	C1-C2-C3	3.82	110.03	113.48	1	20
2	A	182[C]	MTN	C1-C2-C3	3.80	110.05	113.48	14	20
2	A	182[B]	MTN	C1-C2-C3	3.79	110.06	113.48	12	20
2	A	184[B]	MTN	C1-C2-C3	3.78	110.06	113.48	8	20
2	A	183[C]	MTN	C1-C2-C3	3.75	110.09	113.48	20	20
2	A	185[B]	MTN	C1-C2-C3	3.75	110.09	113.48	15	20
2	A	183[A]	MTN	C1-C2-C3	3.74	110.10	113.48	16	20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	A	186[A]	MTN	C1-C2-C3	3.74	110.10	113.48	4	20
2	A	186[B]	MTN	C1-C2-C3	3.74	110.10	113.48	1	20
2	A	184[C]	MTN	C1-C2-C3	3.73	110.11	113.48	19	20
2	A	183[B]	MTN	C8-C1-N1	3.39	113.94	110.05	11	20
2	A	185[A]	MTN	C8-C1-N1	3.39	113.94	110.05	11	20
2	A	184[A]	MTN	C8-C1-N1	3.39	113.94	110.05	16	20
2	A	184[B]	MTN	C8-C1-N1	3.38	113.93	110.05	20	20
2	A	182[A]	MTN	C8-C1-N1	3.38	113.92	110.05	6	20
2	A	182[C]	MTN	C8-C1-N1	3.38	113.92	110.05	15	20
2	A	183[A]	MTN	C8-C1-N1	3.37	113.92	110.05	10	20
2	A	186[B]	MTN	C8-C1-N1	3.38	113.92	110.05	7	20
2	A	186[C]	MTN	C8-C1-N1	3.38	113.92	110.05	15	20
2	A	185[C]	MTN	C8-C1-N1	3.37	113.92	110.05	10	20
2	A	182[B]	MTN	C8-C1-N1	3.36	113.90	110.05	18	20
2	A	184[C]	MTN	C8-C1-N1	3.35	113.89	110.05	2	20
2	A	185[B]	MTN	C8-C1-N1	3.35	113.88	110.05	2	20
2	A	183[C]	MTN	C8-C1-N1	3.34	113.88	110.05	14	20
2	A	186[A]	MTN	C8-C1-N1	3.34	113.88	110.05	6	20
2	A	184[C]	MTN	C9-C1-C2	2.76	110.15	112.77	14	20
2	A	182[A]	MTN	C9-C1-C2	2.75	110.16	112.77	6	20
2	A	182[C]	MTN	C9-C1-C2	2.75	110.16	112.77	15	20
2	A	182[B]	MTN	C9-C1-C2	2.74	110.17	112.77	18	20
2	A	184[A]	MTN	C9-C1-C2	2.74	110.17	112.77	3	20
2	A	185[B]	MTN	C9-C1-C2	2.74	110.17	112.77	1	20
2	A	185[A]	MTN	C9-C1-C2	2.73	110.17	112.77	12	20
2	A	184[B]	MTN	C9-C1-C2	2.73	110.18	112.77	1	20
2	A	186[C]	MTN	C9-C1-C2	2.73	110.18	112.77	12	20
2	A	183[B]	MTN	C9-C1-C2	2.72	110.18	112.77	10	20
2	A	185[C]	MTN	C9-C1-C2	2.72	110.18	112.77	10	20
2	A	186[B]	MTN	C9-C1-C2	2.72	110.19	112.77	17	20
2	A	186[A]	MTN	C9-C1-C2	2.70	110.20	112.77	12	20
2	A	183[C]	MTN	C9-C1-C2	2.70	110.20	112.77	14	20
2	A	183[A]	MTN	C9-C1-C2	2.70	110.20	112.77	14	20
3	A	187	GTP	O6-C6-C5	2.21	128.71	124.32	6	20

There are no chirality outliers.

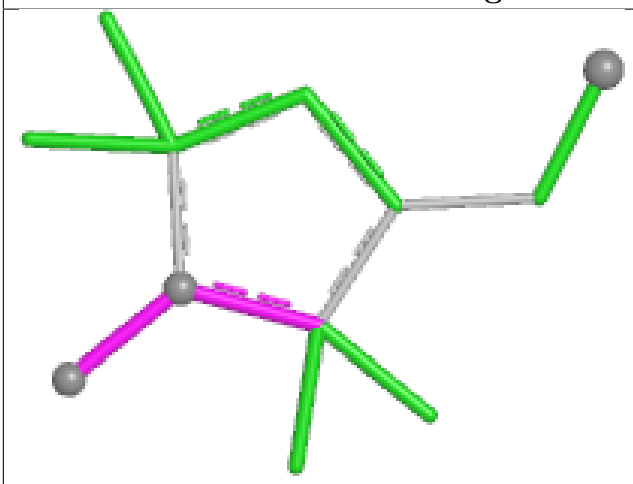
There are no torsion outliers.

There are no ring outliers.

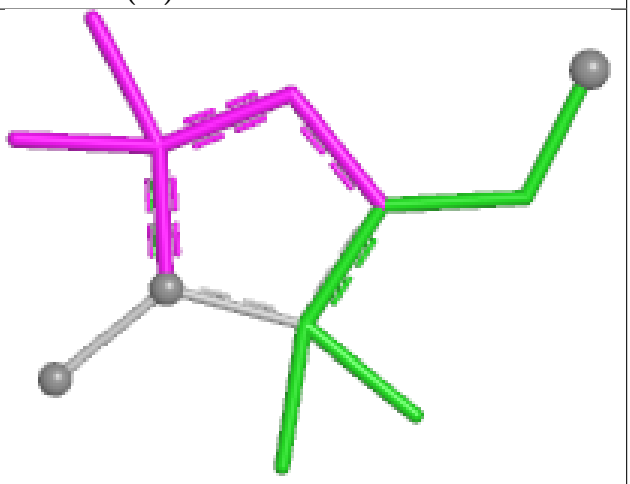
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

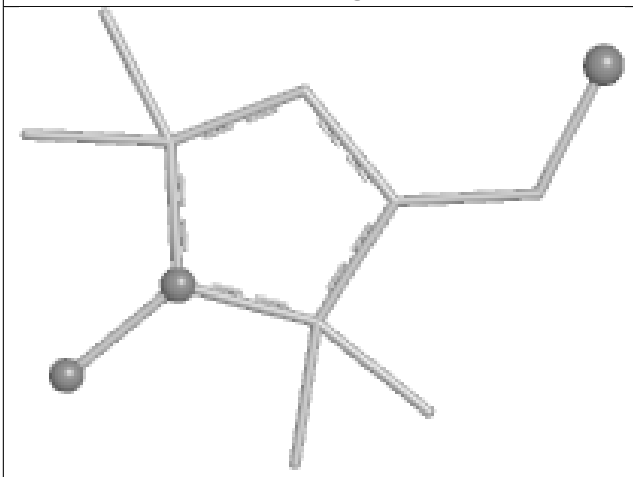
Ligand MTN A 185 (C)



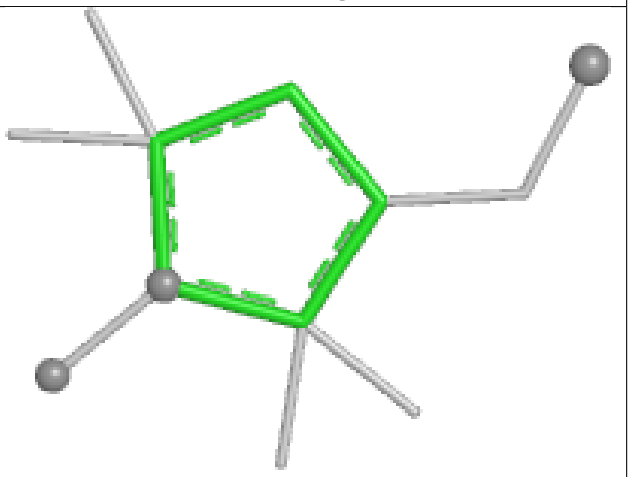
Bond lengths



Bond angles

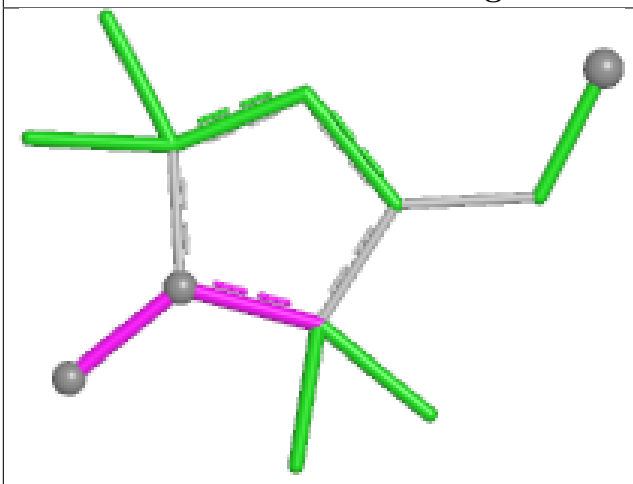


Torsions

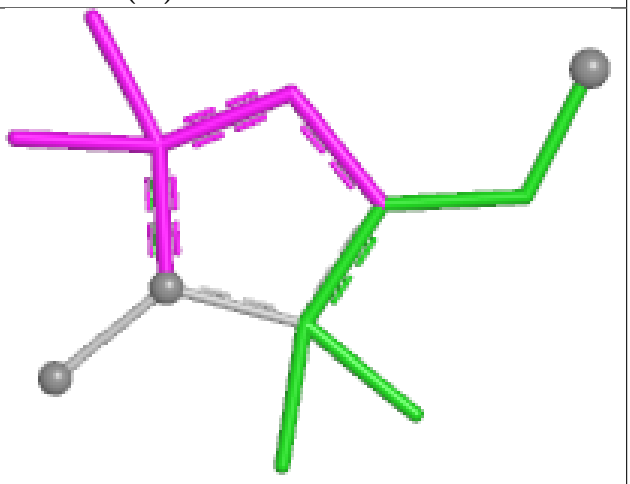


Rings

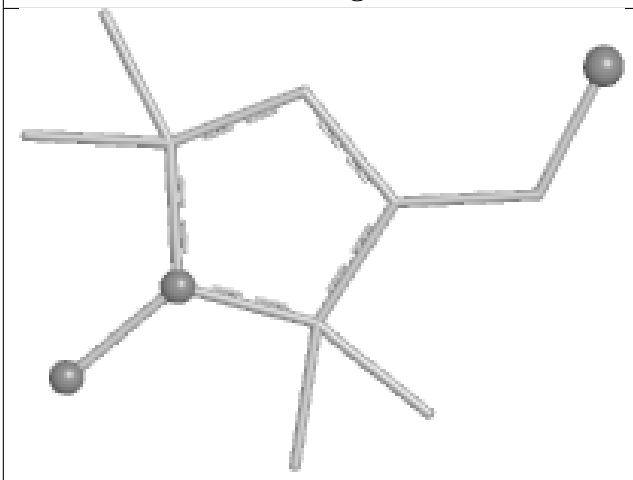
Ligand MTN A 183 (C)



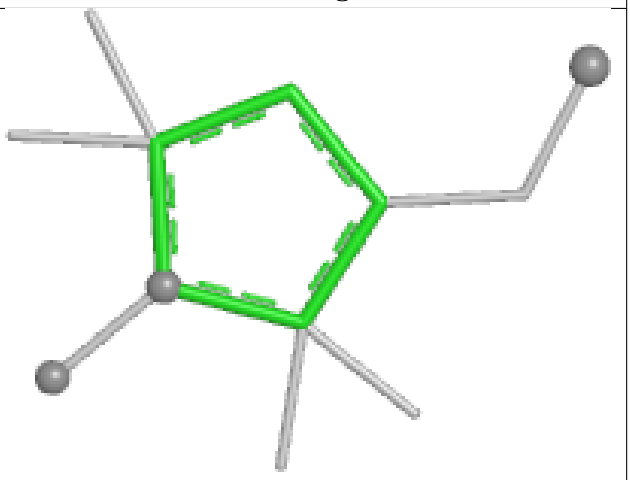
Bond lengths



Bond angles

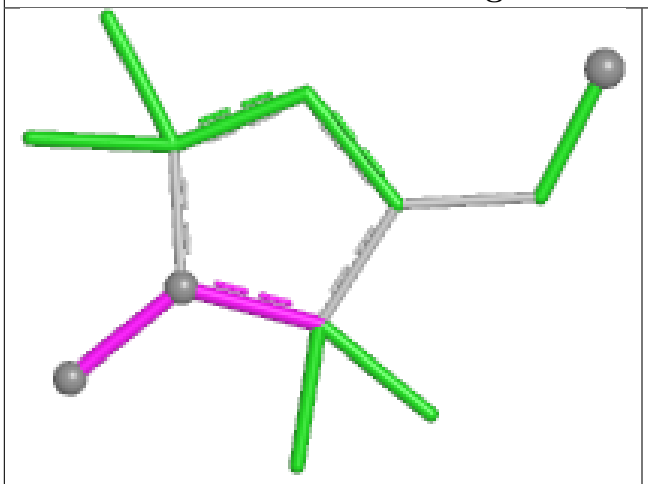


Torsions

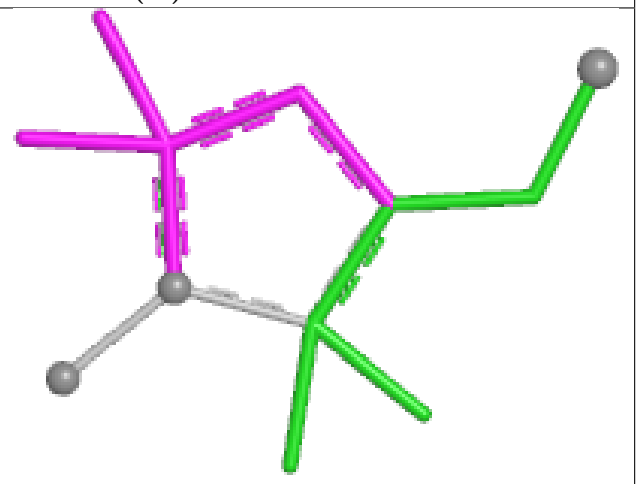


Rings

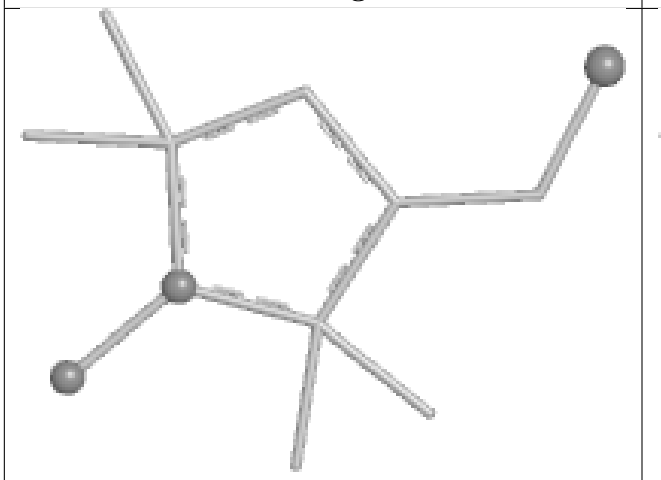
Ligand MTN A 182 (C)



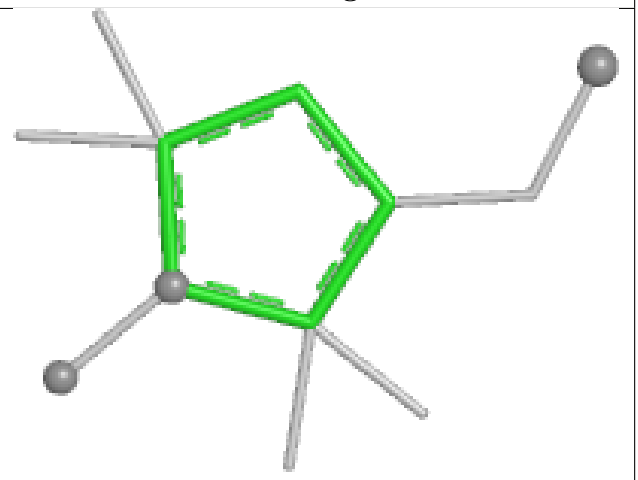
Bond lengths



Bond angles

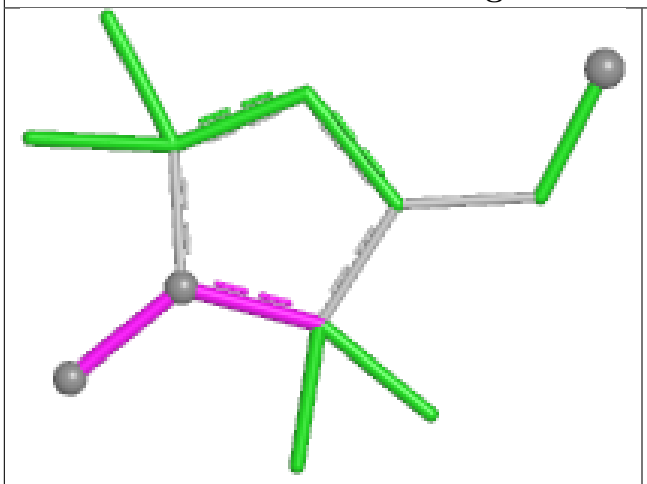


Torsions

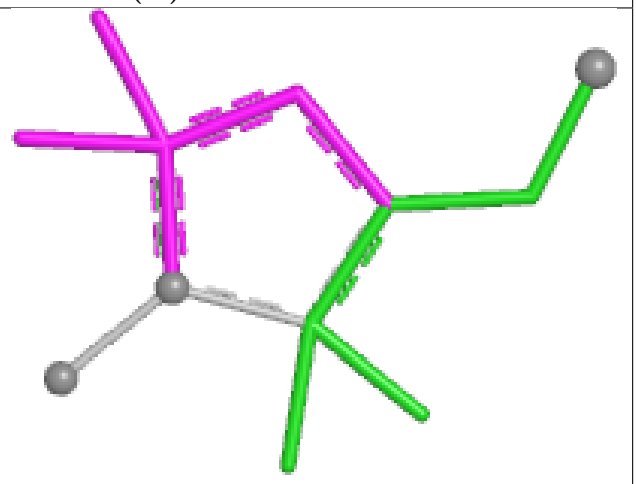


Rings

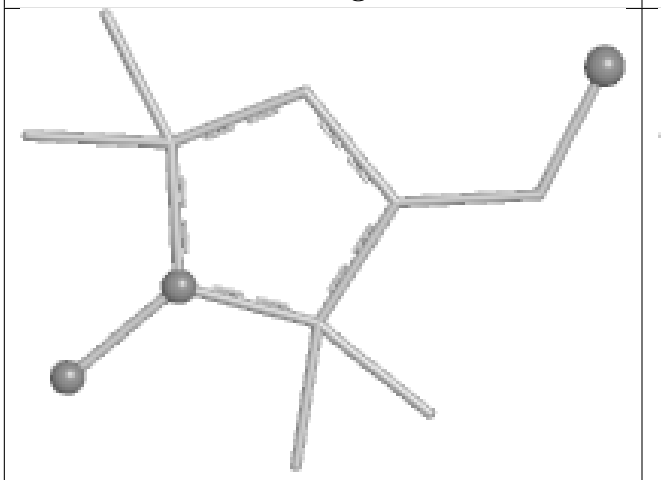
Ligand MTN A 184 (B)



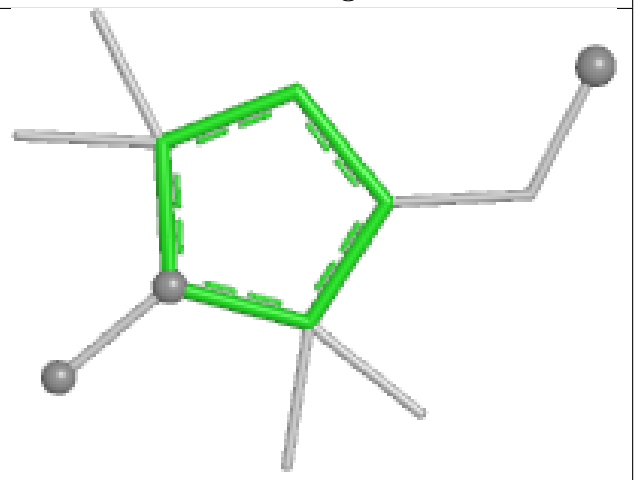
Bond lengths



Bond angles

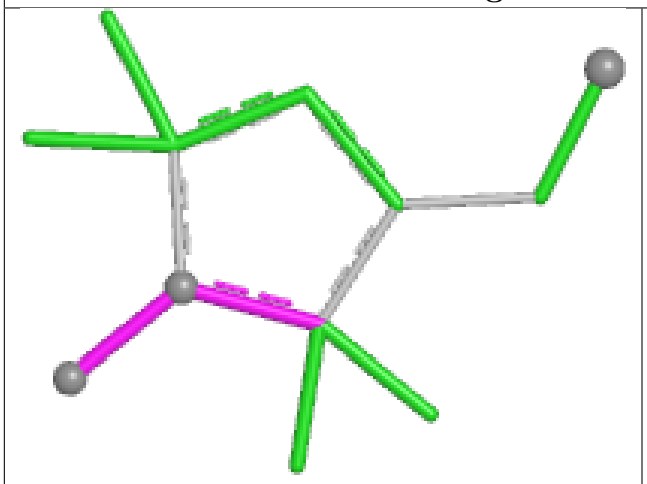


Torsions

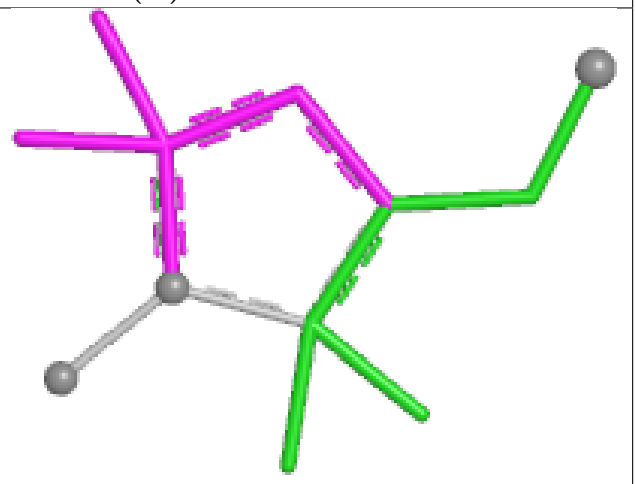


Rings

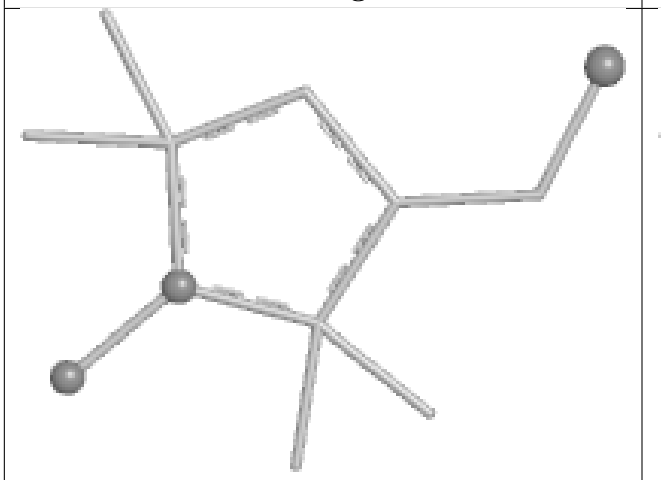
Ligand MTN A 185 (B)



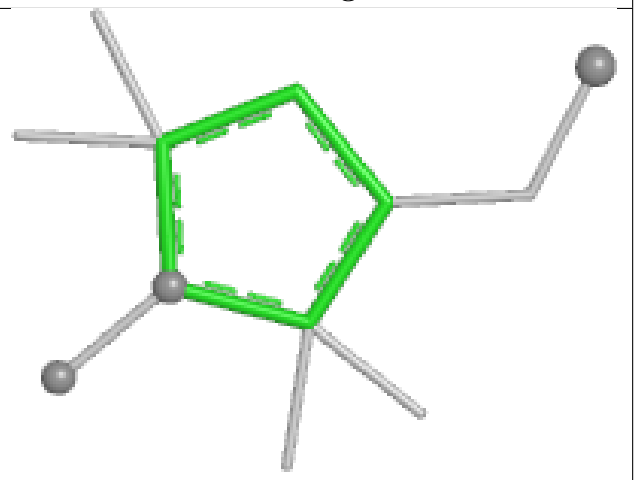
Bond lengths



Bond angles

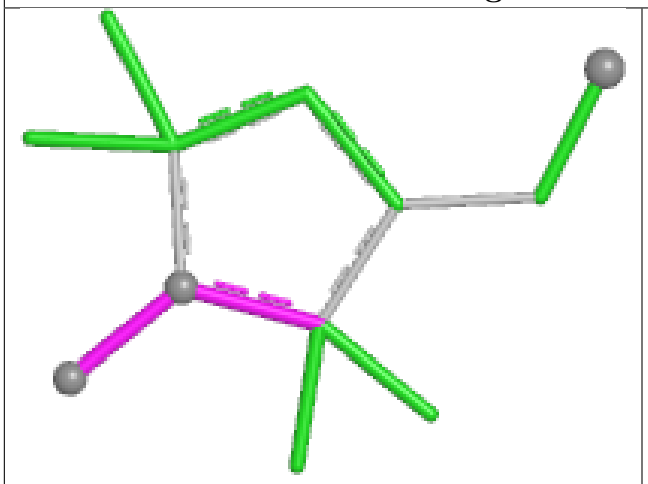


Torsions

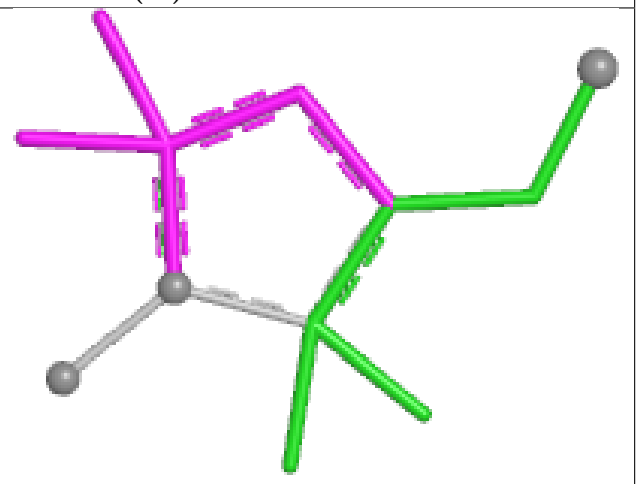


Rings

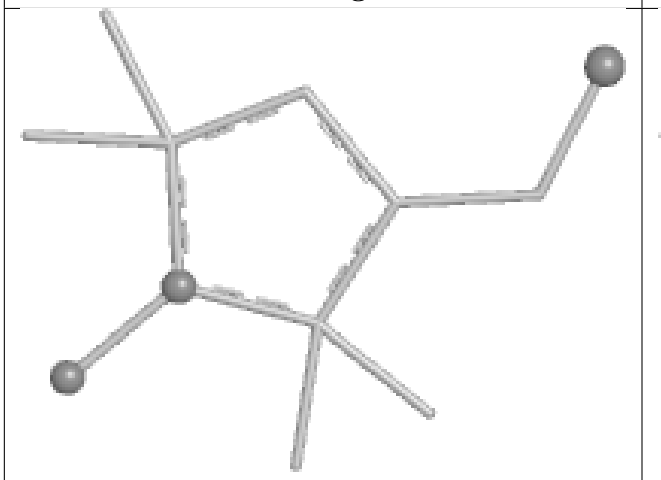
Ligand MTN A 184 (A)



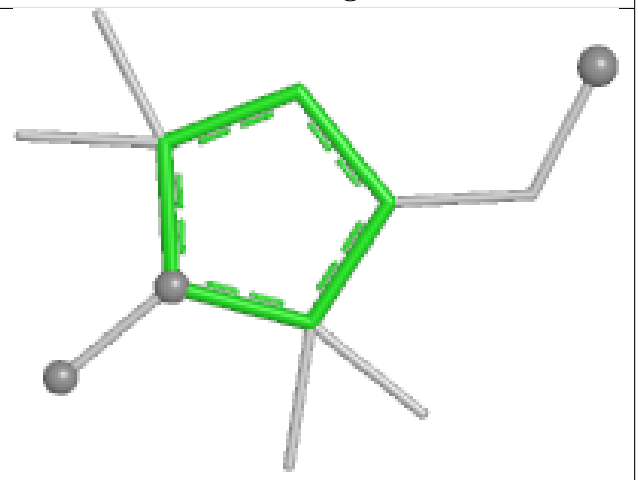
Bond lengths



Bond angles

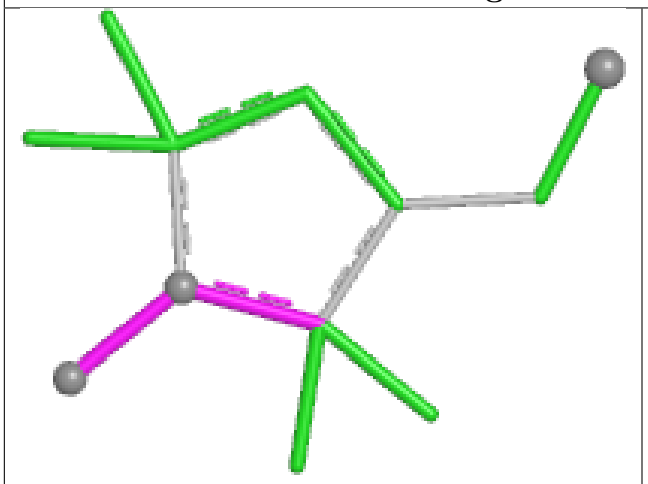


Torsions

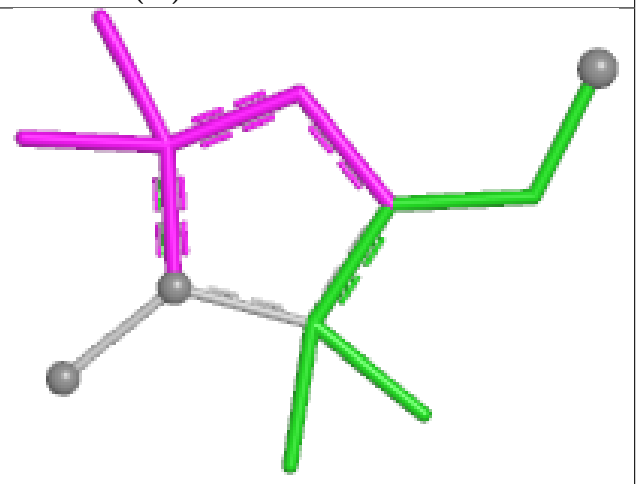


Rings

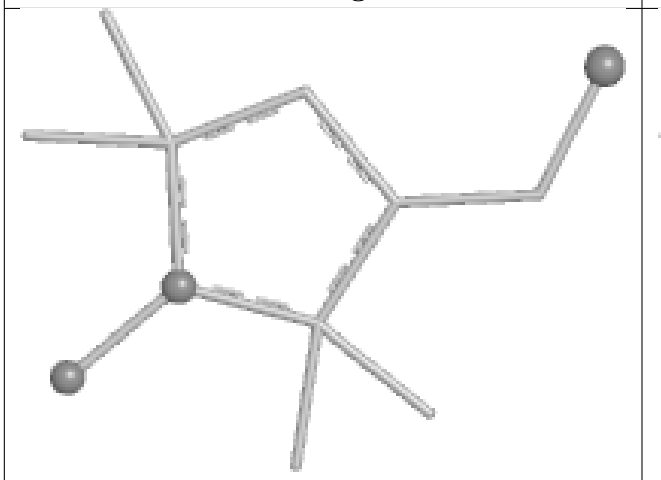
Ligand MTN A 182 (B)



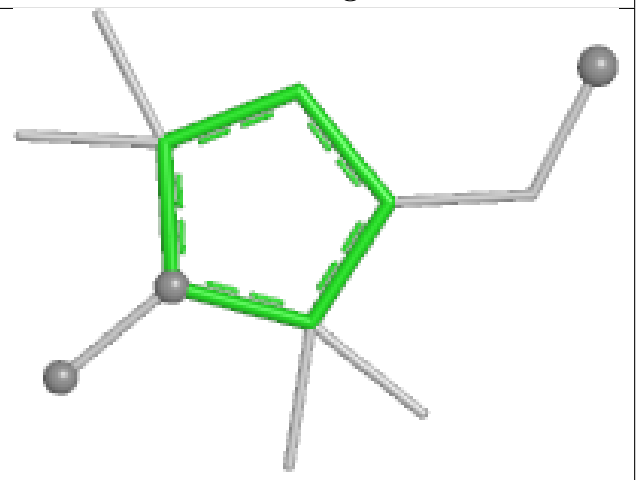
Bond lengths



Bond angles

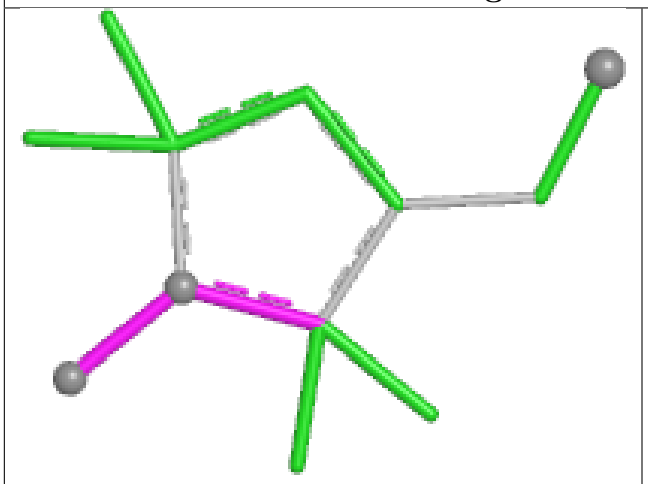


Torsions

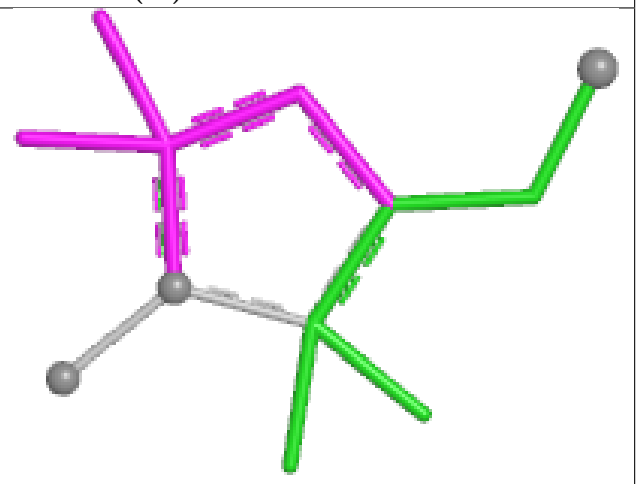


Rings

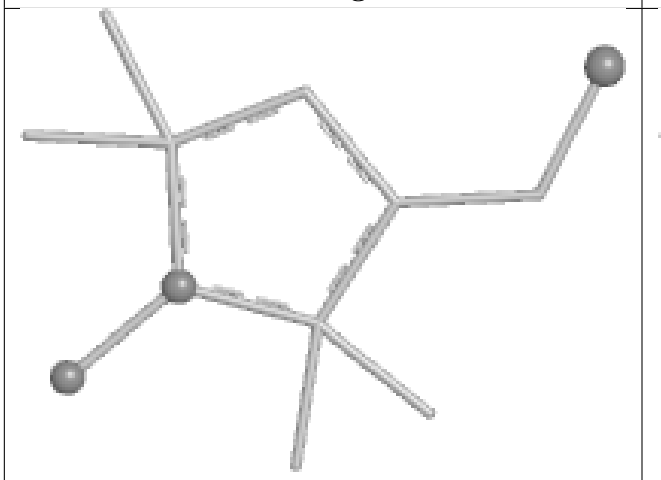
Ligand MTN A 183 (A)



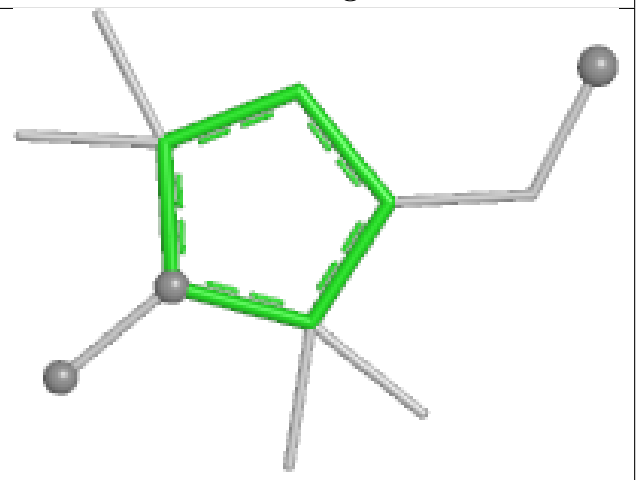
Bond lengths



Bond angles

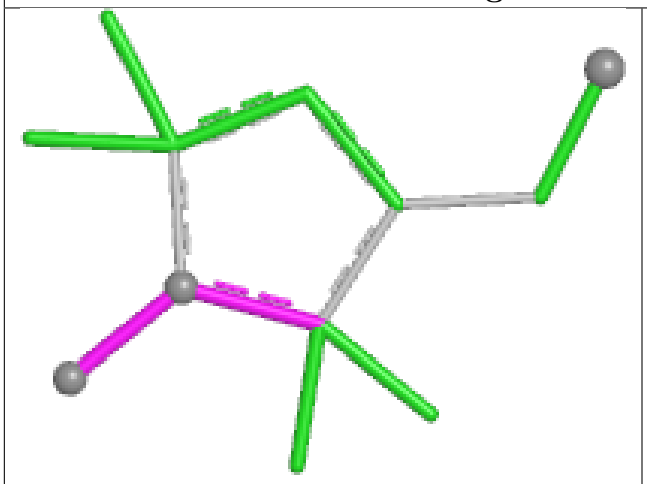


Torsions

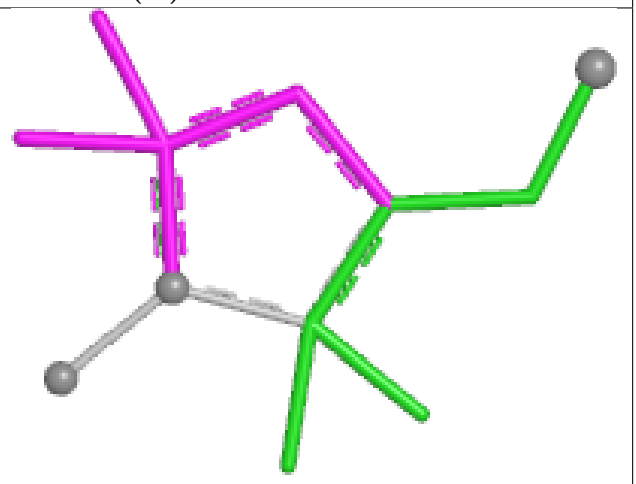


Rings

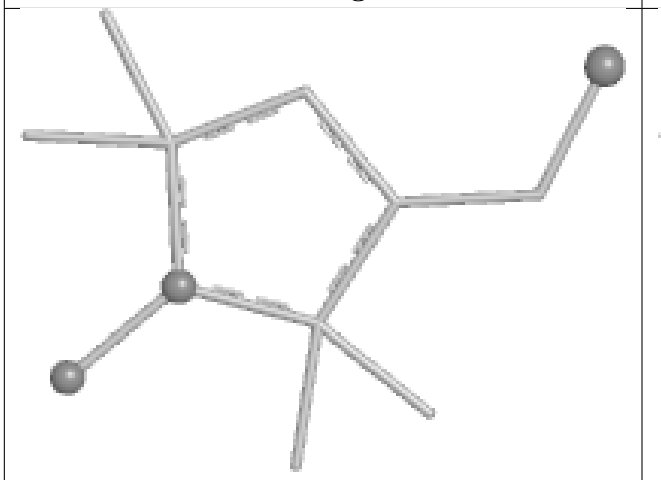
Ligand MTN A 186 (B)



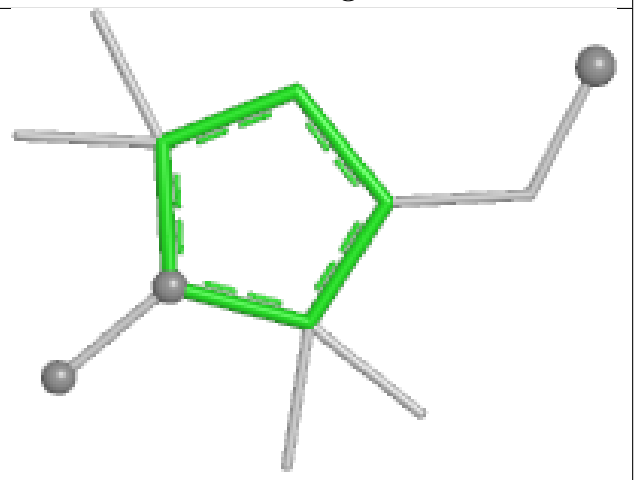
Bond lengths



Bond angles

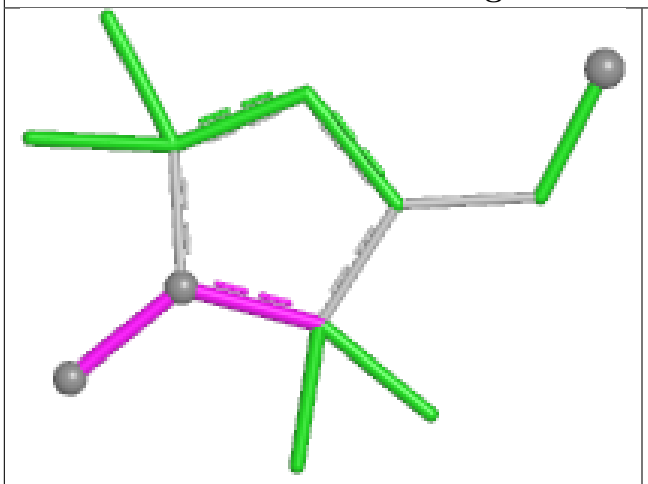


Torsions

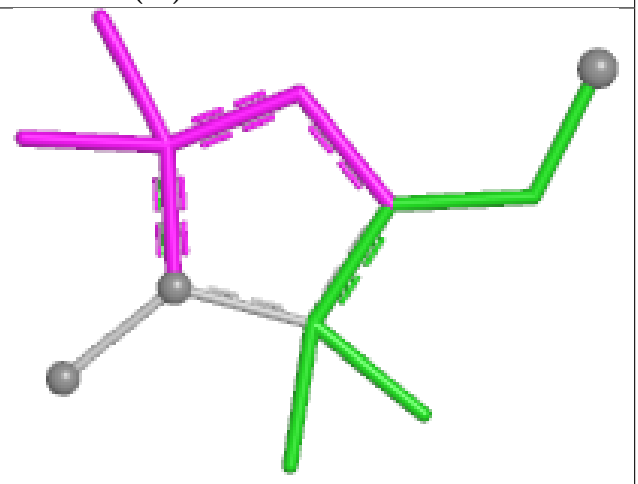


Rings

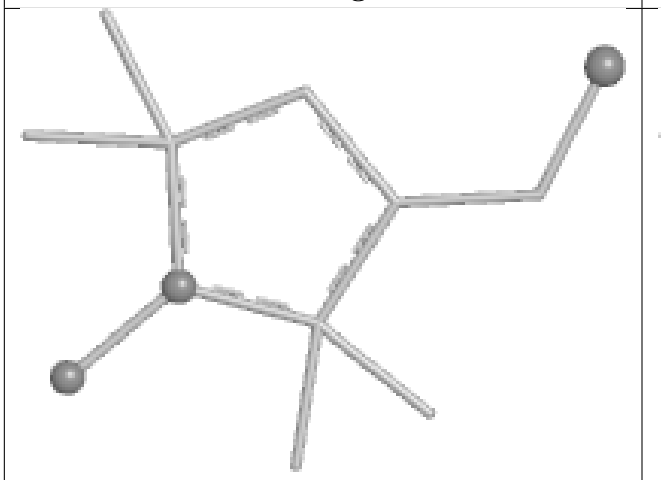
Ligand MTN A 185 (A)



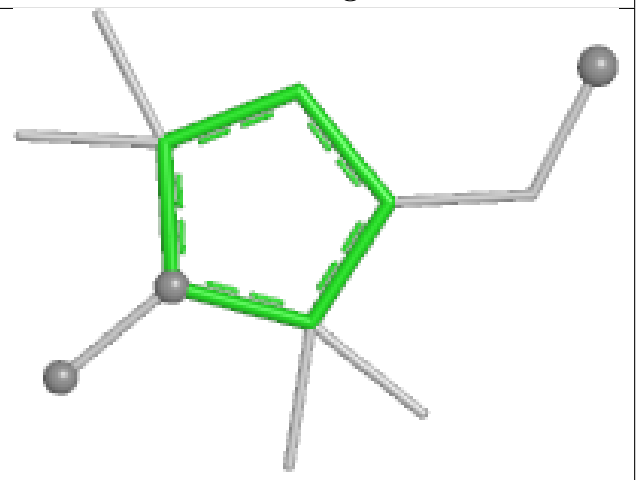
Bond lengths



Bond angles

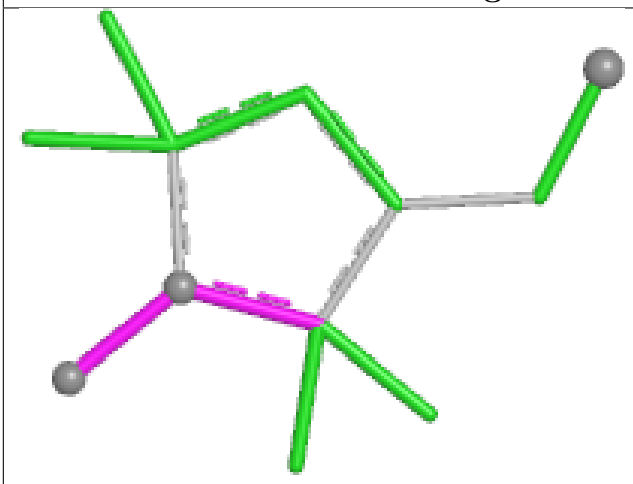


Torsions

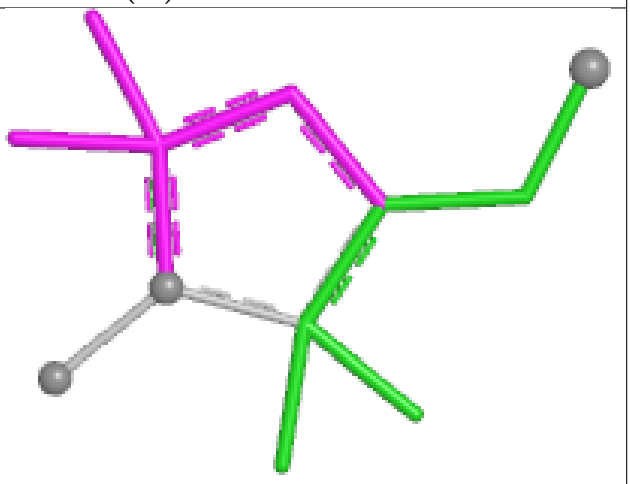


Rings

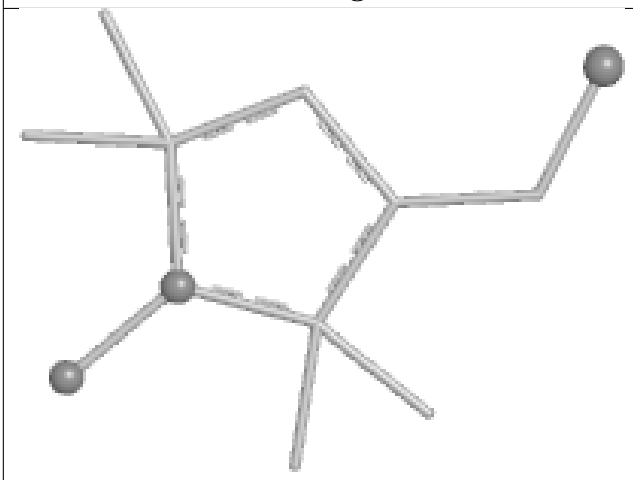
Ligand MTN A 182 (A)



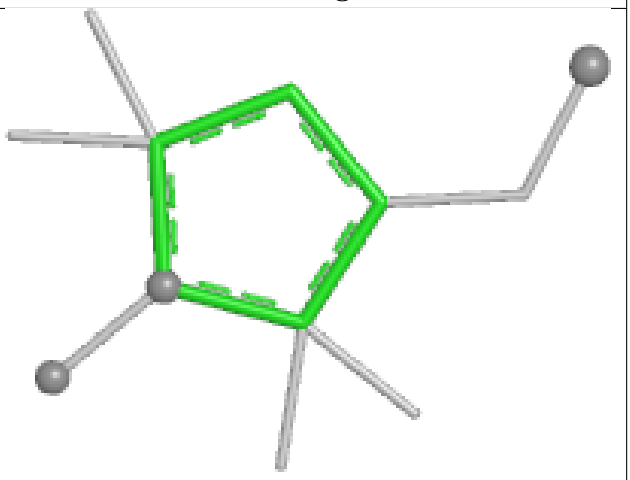
Bond lengths



Bond angles

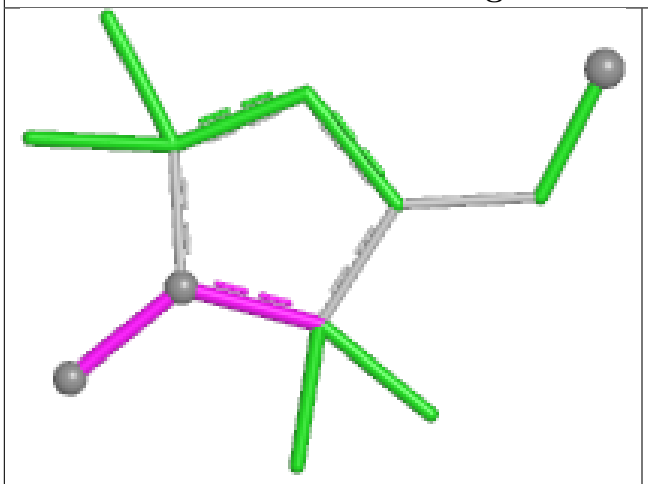


Torsions

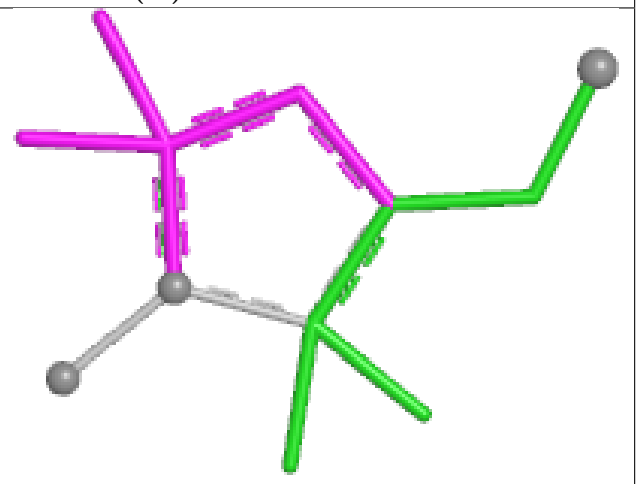


Rings

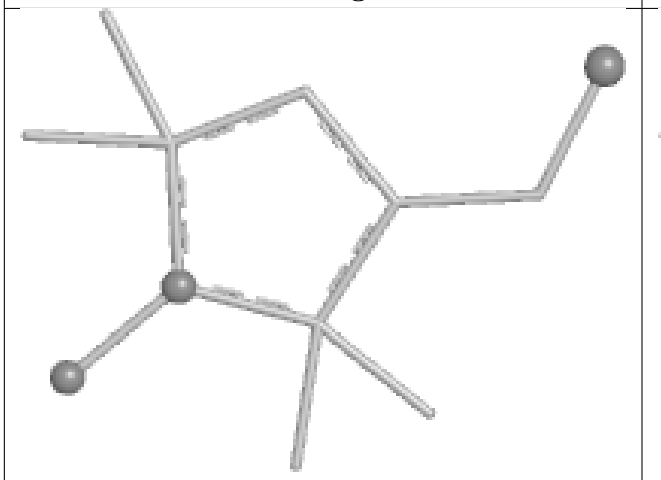
Ligand MTN A 186 (C)



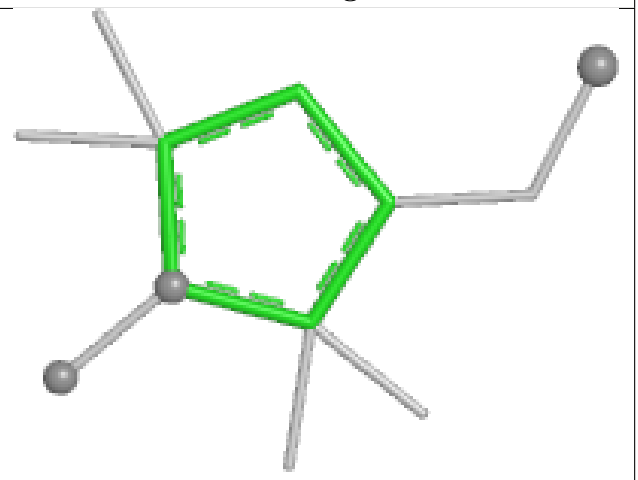
Bond lengths



Bond angles

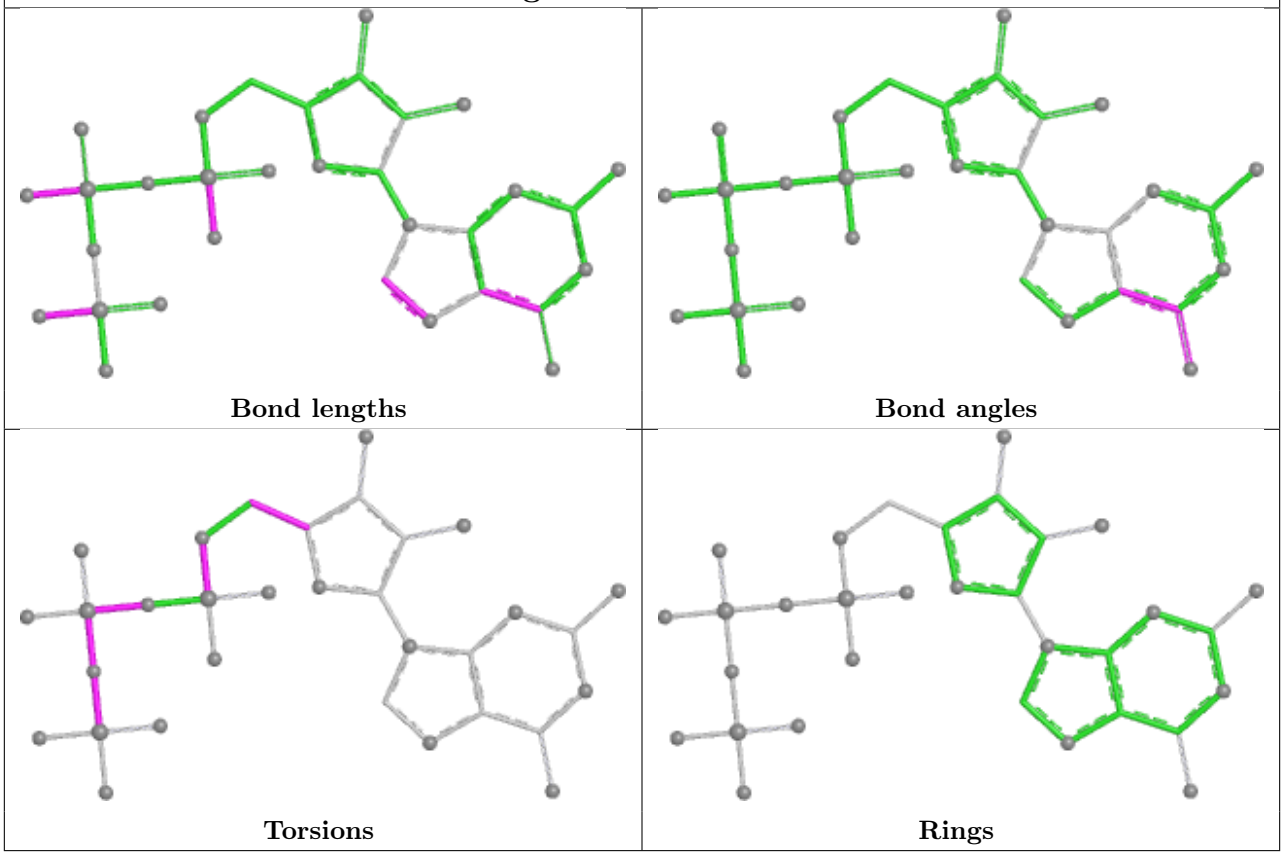


Torsions

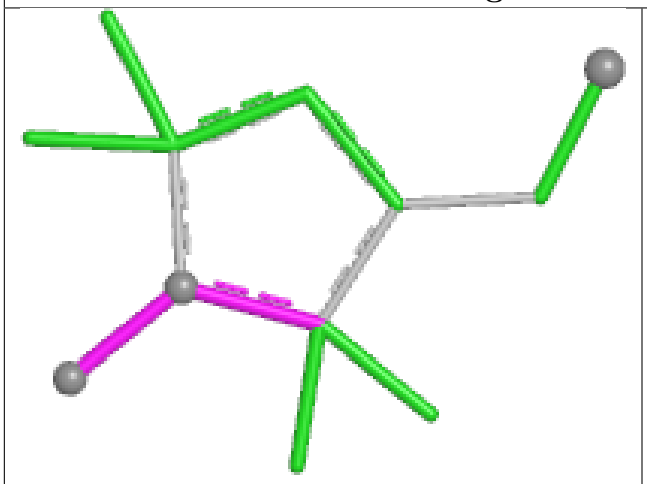


Rings

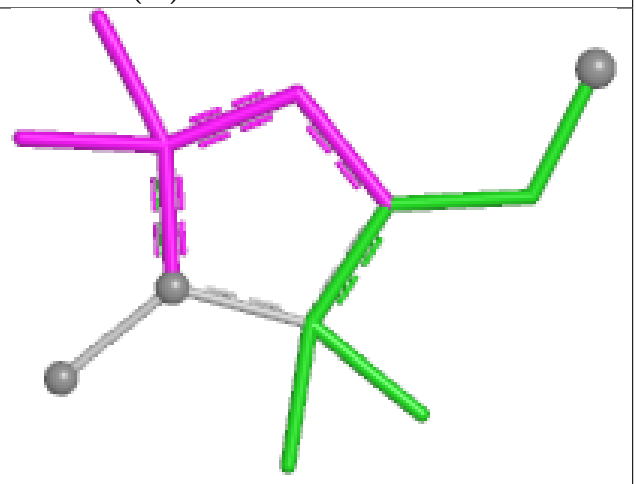
Ligand GTP A 187



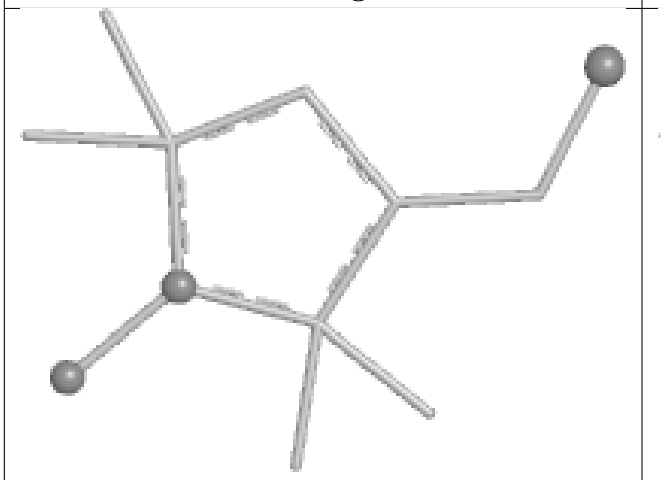
Ligand MTN A 183 (B)



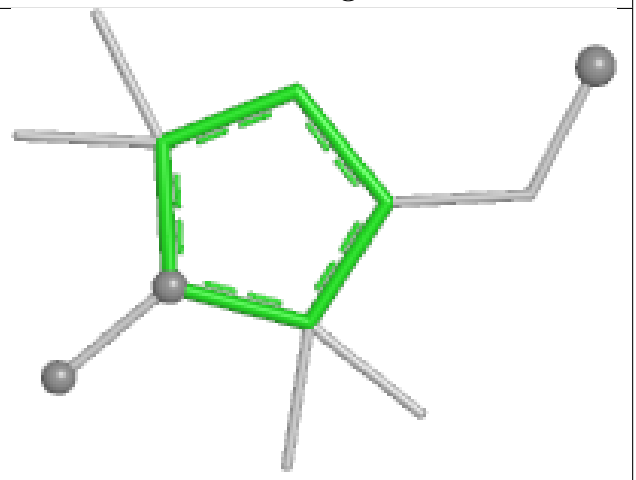
Bond lengths



Bond angles

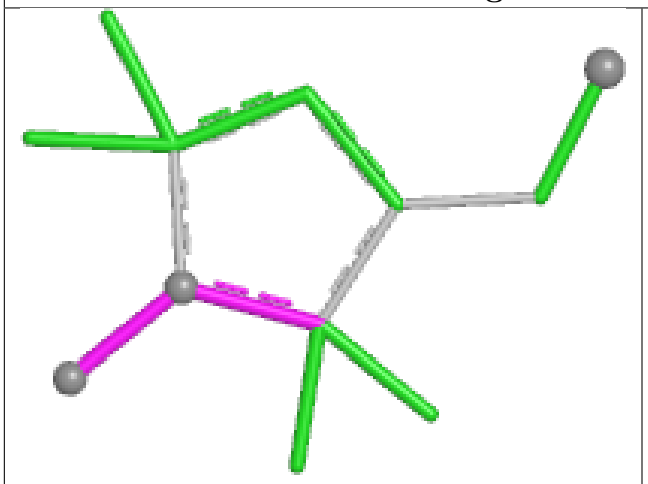


Torsions

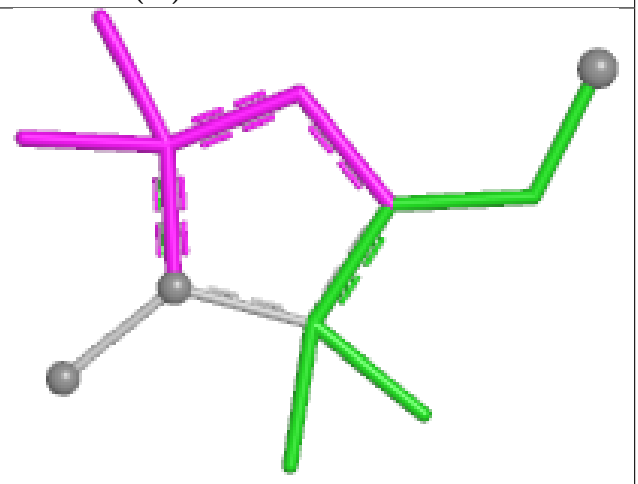


Rings

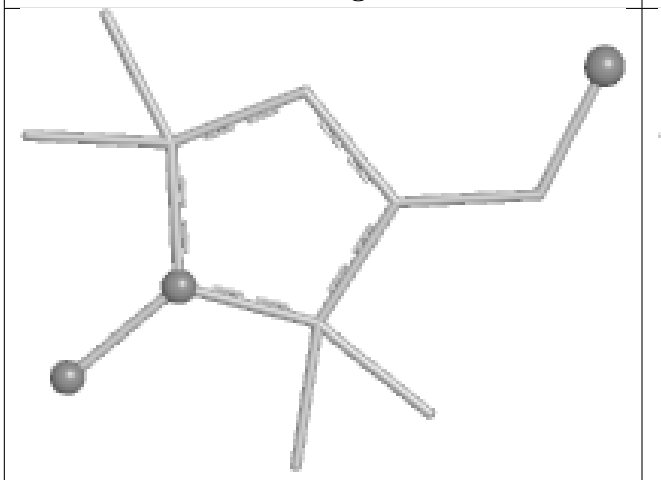
Ligand MTN A 184 (C)



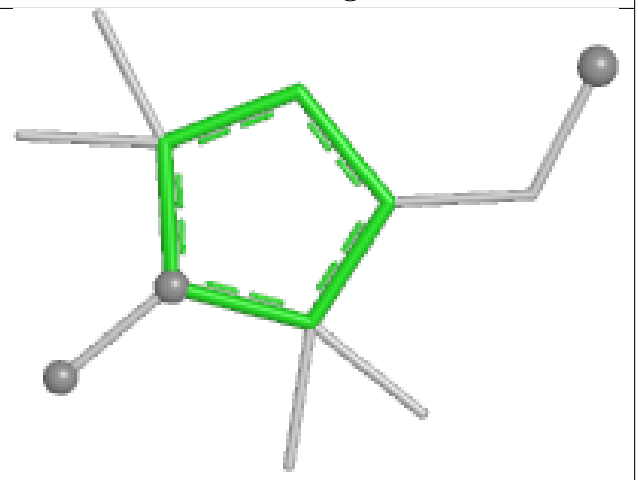
Bond lengths



Bond angles

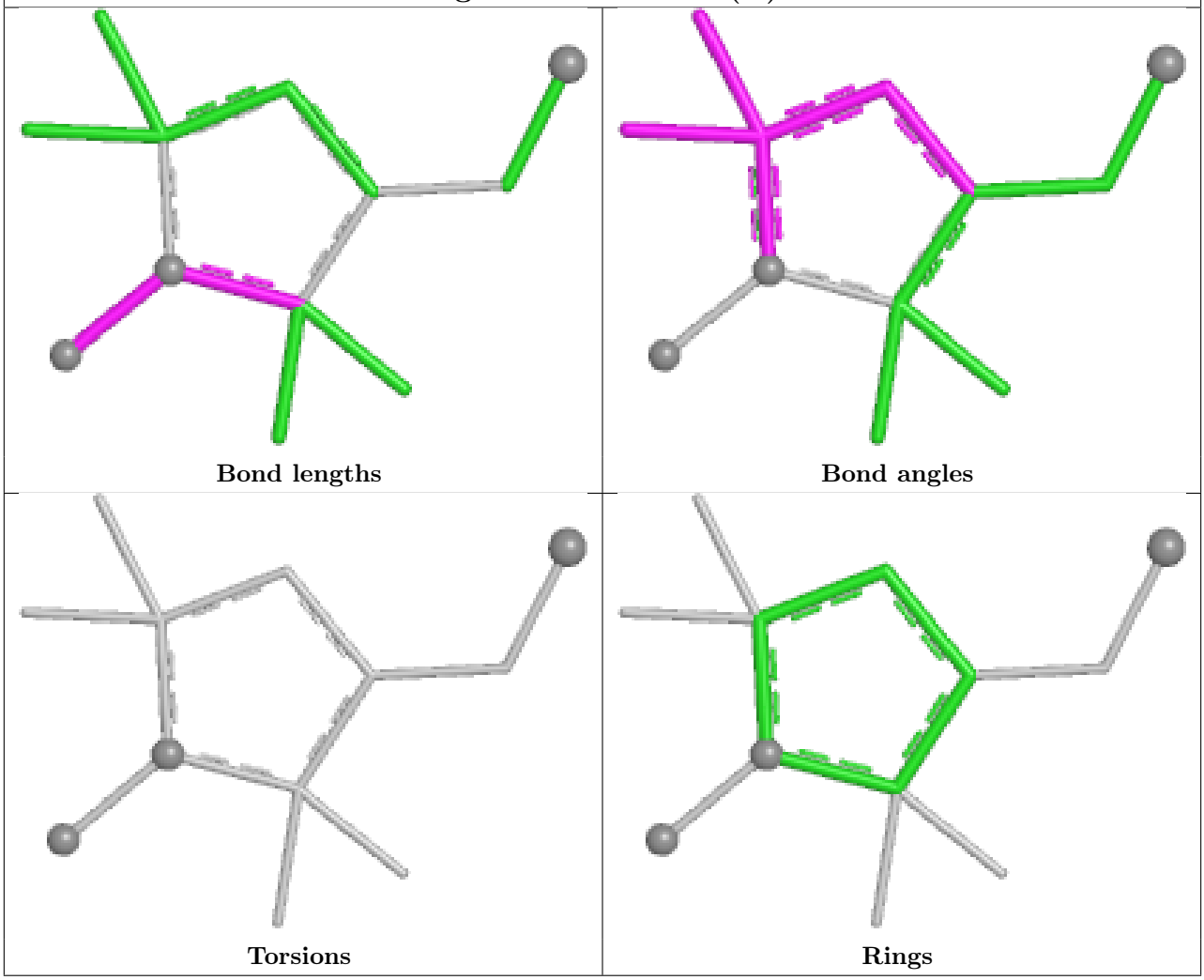


Torsions



Rings

Ligand MTN A 186 (A)



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)

No chemical shift data were provided