Full wwPDB NMR Structure Validation Report (i)

Mar 5, 2022 – 10:41 AM EST

PDB ID	:	2K2G
Title	:	Solution structure of the wild-type catalytic domain of human matrix metalloproteinase 12 (MMP-12) in complex with a tight-binding inhibitor
Authors	:	Markus, M.A.; Dwyer, B.; Wolfrom, S.; Li, J.; Li, W.; Malakian, K.; Wilhelm, J.; Tsao, D.H.H.
Deposited on	:	2008-04-01

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

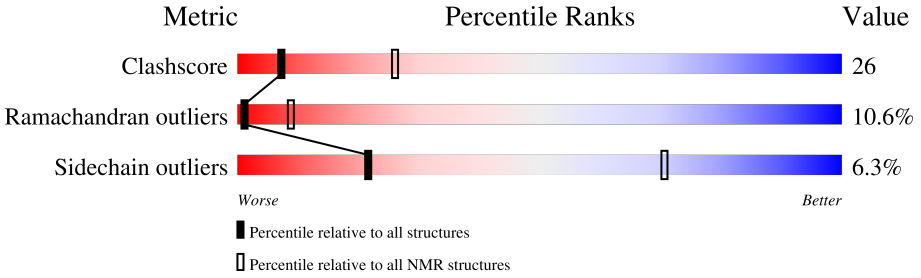
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.27
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.27

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	165	45% 41% • 10%

2 Ensemble composition and analysis (i)

This entry contains 17 models. Model 5 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:111-A:185, A:191-A:263 (148)	0.65	5

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 3 clusters and 3 single-model clusters were found.

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

3 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 2581 atoms, of which 1256 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Macrophage metalloelastase.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	165	2539	831	1240	226	237	5	0

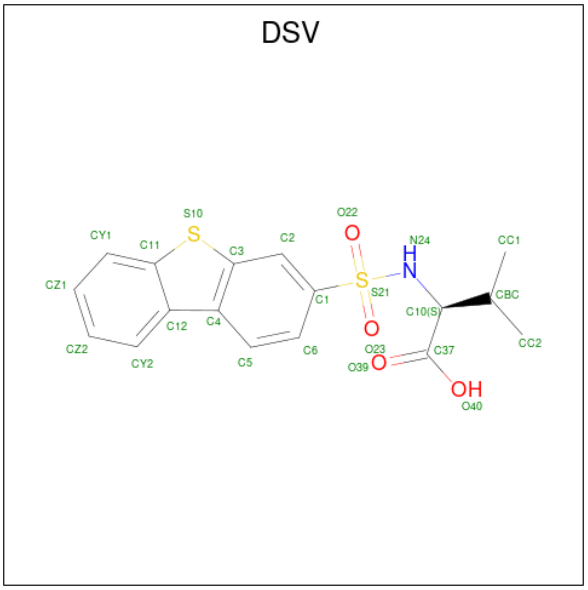
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	99	MET	-	initiating methionine	UNP P39900

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

Mol	Chain	Residues	Atoms	
			Total	Zn
2	A	2	2	2

- Molecule 3 is N-(dibenzo[b,d]thiophen-3-ylsulfonyl)-L-valine (three-letter code: DSV) (formula: $C_{17}H_{17}NO_4S_2$).



Mol	Chain	Residues	Atoms					
			Total	C	H	N	O	S
3	A	1	40	17	16	1	4	2

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: Macrophage metalloelastase

Chain A: 45% 41% • 10%

M99 F100 R101 E102 M103 P104 G105 G106 P107 V108 W109 R110 K111 H112 Y113 I114 T115 Y116 R117 I118 N119 N120 Y121 T122 P123 D124 D131 F138 F149 N153 T154 G155 M156 A157 D158 I159 L160 F163 G166 A167 H168 G169 D170 F171 H172 A173 F174 D175 H183 G186 P187 G188

S189 G190 I191 G192 G193 D194 A195 H196 F197 D198 E199 D200 E201 H206 S207 G208 G209 T210 N211 H218 E219 G225 H228 S229 S230 D231 P232 K233 A234 V235 M236 F237 P238 T239 Y240 K241 Y242 V243 D244 F248 I258 Q259 S260 L261 Y262 G263

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: Macrophage metalloelastase

Chain A: 53% 30% 7% 10%

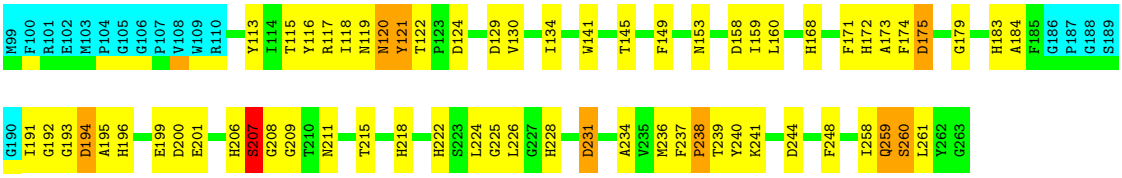
M99 F100 R101 E102 M103 P104 G105 G106 P107 V108 W109 R110 K111 H112 T115 Y116 R117 I118 N119 N120 Y121 T122 P123 D124 R127 D131 R135 K136 A137 F138 D158 I159 L160 F163 A164 R165 H168 G169 D170 F171 H172 A173 F174 H183 A184 F185 G186 P187 G188 S189 G190 I191

G192 G193 D194 A195 H196 F197 D198 E199 D200 E201 F202 W203 H206 S207 G208 G209 T210 N211 L214 H222 G227 H228 S229 S230 A234 V235 M236 F237 Y240 K241 D244 F248 I258 Q259 S260 L261 Y262 G263

4.2.2 Score per residue for model 2

• Molecule 1: Macrophage metalloelastase

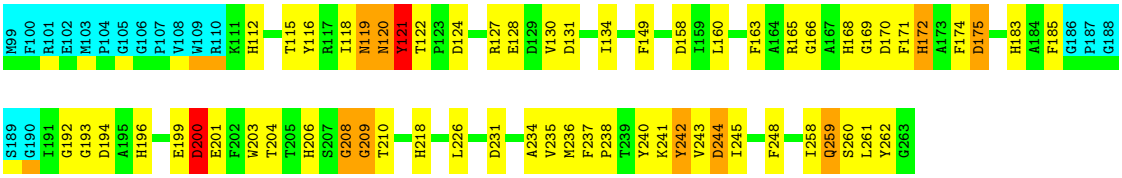
Chain A: 51% 33% 5% • 10%



4.2.3 Score per residue for model 3

- Molecule 1: Macrophage metalloelastase

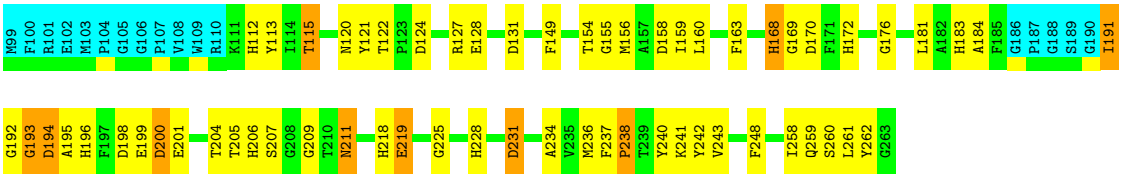
Chain A:



4.2.4 Score per residue for model 4

- Molecule 1: Macrophage metalloelastase

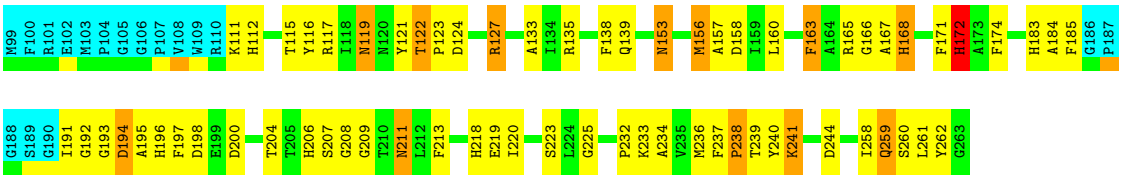
Chain A:



4.2.5 Score per residue for model 5 (medoid)

- Molecule 1: Macrophage metalloelastase

Chain A:



4.2.6 Score per residue for model 6

- Molecule 1: Macrophage metalloelastase

Chain A: 54% 29% 6% • 10%

M99 F100 R101 E102 M103 P104 G105 G106 P107 V108 W109 R110 K111 H112 Y113 I114 T115 I118 N119 N120 Y121 T122 N126 D129 V130 D131 R135 F149 S150 K151 I152 G155 M156 A157 D158 I159 L160 G166 D170 F174 G178 H183 G186 P187 G188 S189 G190

G193 D194 A195 H196 F197 D198 E199 D200 E201 F202 W203 T204 T205 H206 S207 G208 G209 T210 H218 E219 G225 L226 G227 H228 D231 A234 V235 M236 Y240 K241 Y242 V243 D244 F248 I258 Q259 S260 L261 Y262 G263

4.2.7 Score per residue for model 7

- Molecule 1: Macrophage metalloelastase

Chain A: 50% 35% • 10%

M99 F100 R101 E102 M103 P104 G105 G106 P107 V108 W109 R110 Y113 I114 T115 Y116 R117 I118 N119 N120 Y121 T122 P123 D124 V130 I134 W141 T145 F149 N153 D158 I159 L160 F163 G166 A167 H168 G169 D170 F171 H172 A173 F174 D175 G179 I180 H183 A184

F185 G186 P187 G188 S189 G190 G193 D194 A195 H196 E199 D200 E201 T204 T205 H206 S207 G208 H218 H222 S223 L224 G225 L226 G227 H228 S229 S230 D231 A234 V235 M236 Y240 K241 Y242 V243 F248 I258 Q259 Y262 G263

4.2.8 Score per residue for model 8

- Molecule 1: Macrophage metalloelastase

Chain A: 36% 43% 9% • 10%

M99 F100 R101 E102 M103 P104 G105 G106 P107 V108 W109 R110 K111 H112 T115 Y116 R117 I118 N119 N120 Y121 T122 P123 D124 V130 D131 Y132 A133 I134 R135 K136 A137 F138 N143 F149 I152 N153 T154 G155 M156 A157 D158 I159 L160 V161 V162 F163 A167 H168 G169 D170 F171 H172 A173

F174 H183 A184 F185 G186 P187 G188 S189 G190 I191 G192 G193 D194 A195 H196 F197 D198 E199 D200 E201 T204 T205 H206 S207 G208 G209 F213 L214 T215 H218 E219 I220 G221 H222 S223 L224 G225 L226 G227 H228 S229 S230 D231 P232 K233 A234 V235 M236 F237 P238 T239 Y240 K241 Y242 V243 D244

I245 F248 R249 D253 R256 G257 I258 Q259 S260 L261 Y262 G263

4.2.9 Score per residue for model 9

- Molecule 1: Macrophage metalloelastase

Chain A: 48% 32% 9% • 10%

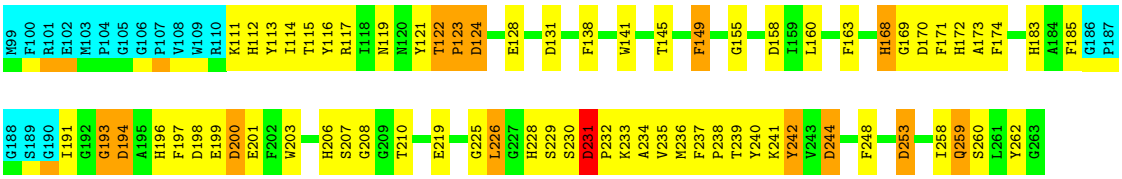
M99 F100 R101 E102 M103 P104 G105 G106 P107 V108 W109 R110 Y113 Y121 T122 P123 D124 Y132 K136 A137 F138 T154 G155 M156 A157 D158 I159 L160 R165 G166 A167 H168 G169 D170 F171 H172 A173 F174 D175 G176 K177 G178 G179 I180 H183 A184 F185 G186 P187 G188 S189 G190

G193 D194 A195 H196 E199 D200 E201 H206 S207 G208 G209 H218 E219 I220 G221 H222 G225 L226 G227 H228 S229 S230 D231 P232 K233 A234 V235 M236 F237 P238 T239 Y240 K241 Y242 V243 D244 T247 F248 R249 I258 Q259 S260 L261 Y262 G263

4.2.10 Score per residue for model 10

- Molecule 1: Macrophage metalloelastase

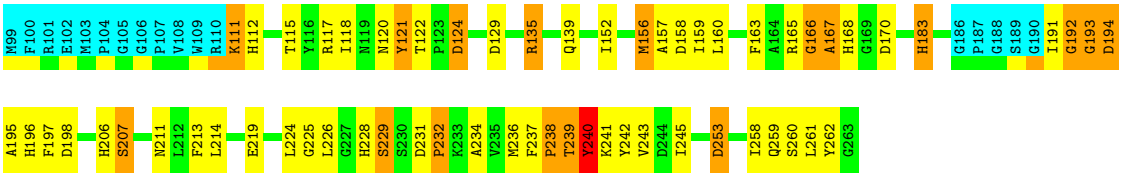
Chain A: 47% 34% 8% • 10%



4.2.11 Score per residue for model 11

- Molecule 1: Macrophage metalloelastase

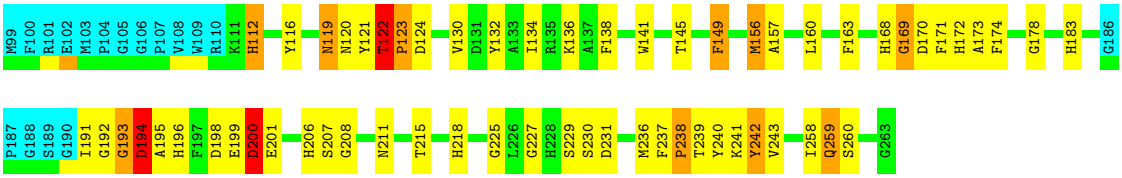
Chain A: 52% 27% 10% • 10%



4.2.12 Score per residue for model 12

- Molecule 1: Macrophage metalloelastase

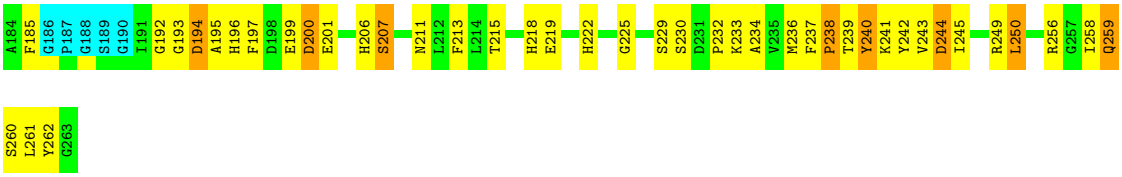
Chain A: 53% 29% 6% • 10%



4.2.13 Score per residue for model 13

- Molecule 1: Macrophage metalloelastase

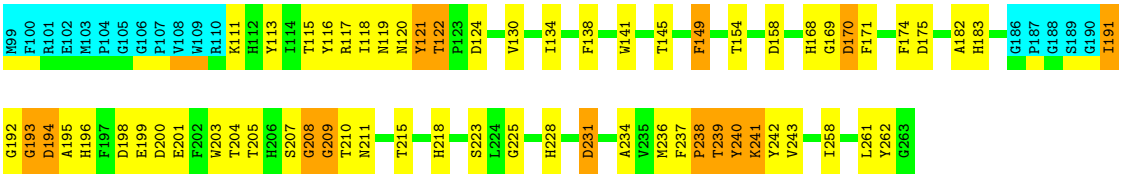
Chain A: 44% 36% 10% 10%



4.2.14 Score per residue for model 14

- Molecule 1: Macrophage metalloelastase

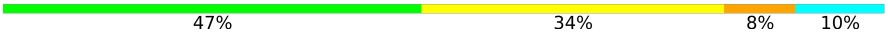
Chain A:

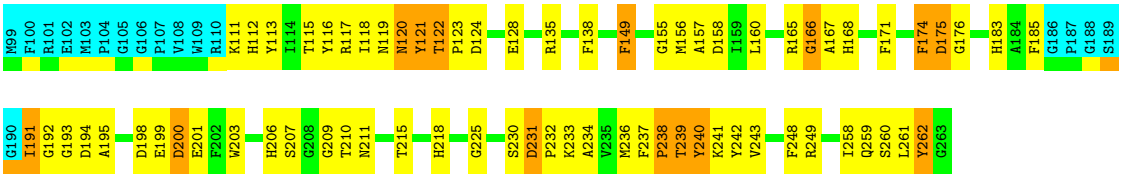


4.2.15 Score per residue for model 15

- Molecule 1: Macrophage metalloelastase

Chain A:

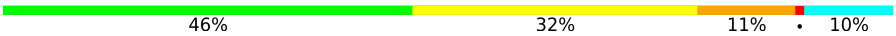


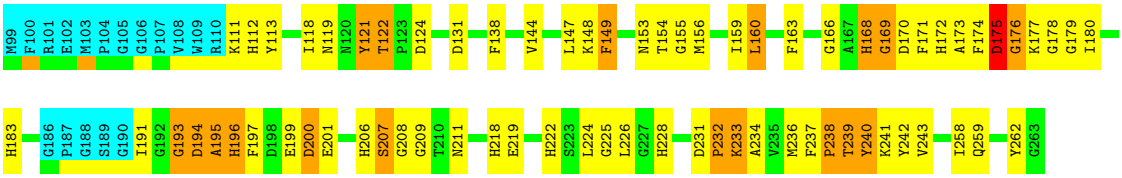


4.2.16 Score per residue for model 16

- Molecule 1: Macrophage metalloelastase

Chain A:

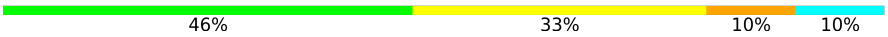


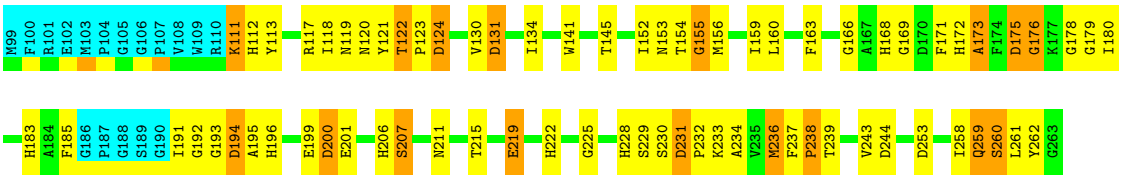


4.2.17 Score per residue for model 17

- Molecule 1: Macrophage metalloelastase

Chain A:


46%
33%
10%
10%


M99
F100
R101
E102
M103
P104
G105
G106
P107
V108
W109
R110
K111
H112
Y113
R117
I118
N119
N120
Y121
T122
P123
D124
V130
D131
I134
W141
T145
I152
N153
T154
G155
M156
I159
L160
F163
G166
A167
H168
G169
D170
F171
H172
A173
F174
D175
G176
K177
G178
G179
I180
H183
A184
F185
G186
P187
G188
S189
G190
I191
G192
G193
D194
A195
H196
E199
D200
E201
H206
S207
N211
T215
E219
H222
G225
H228
S229
S230
D231
P232
K233
A234
V235
M236
F237
P238
T239
V243
D244
D253
I258
Q259
S260
L261
Y262
G263

5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *DGSA-distance geometry simulated annealing, simulated annealing.*

Of the 100 calculated structures, 17 were deposited, based on the following criterion: *structures with the least restraint violations.*

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: ZN, DSV

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	1173	1119	1110	61±8
3	A	24	16	16	3±2
All	All	20383	19295	19141	1047

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
1:A:241:LYS:O	1:A:243:VAL:HG22	0.79	1.77	3	3
1:A:231:ASP:O	1:A:233:LYS:N	0.75	2.19	16	1
1:A:114:ILE:HD12	1:A:114:ILE:N	0.73	1.98	10	1
1:A:193:GLY:O	1:A:195:ALA:N	0.72	2.23	14	15
1:A:240:TYR:CD1	1:A:240:TYR:N	0.66	2.63	13	2
1:A:242:TYR:CG	1:A:243:VAL:N	0.63	2.67	11	2
1:A:183:HIS:ND1	1:A:184:ALA:N	0.63	2.47	4	3
1:A:117:ARG:NE	1:A:119:ASN:ND2	0.62	2.47	7	4
1:A:171:PHE:CE2	1:A:172:HIS:NE2	0.62	2.67	17	1
1:A:183:HIS:CD2	1:A:184:ALA:N	0.62	2.67	7	2
1:A:168:HIS:CD2	1:A:169:GLY:N	0.62	2.67	9	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:132:TYR:CZ	1:A:136:LYS:NZ	0.62	2.68	9	2
1:A:237:PHE:O	1:A:238:PRO:O	0.62	2.16	14	11
1:A:168:HIS:CG	1:A:169:GLY:N	0.62	2.67	4	9
1:A:168:HIS:CE1	1:A:174:PHE:CE1	0.61	2.88	2	1
1:A:168:HIS:CE1	1:A:183:HIS:NE2	0.61	2.67	8	1
1:A:168:HIS:ND1	1:A:174:PHE:CZ	0.61	2.68	15	3
1:A:242:TYR:CD1	1:A:243:VAL:N	0.61	2.68	16	3
1:A:239:THR:O	1:A:241:LYS:N	0.61	2.33	14	4
1:A:168:HIS:CE1	1:A:174:PHE:CZ	0.61	2.88	1	4
1:A:183:HIS:CG	1:A:184:ALA:N	0.61	2.68	2	4
1:A:121:TYR:N	1:A:121:TYR:CD1	0.61	2.68	16	5
1:A:240:TYR:CG	1:A:241:LYS:N	0.61	2.68	6	11
1:A:117:ARG:HE	1:A:119:ASN:ND2	0.61	1.94	7	1
1:A:171:PHE:CZ	1:A:183:HIS:CE1	0.61	2.88	1	1
1:A:118:ILE:HG22	1:A:120:ASN:O	0.60	1.96	6	2
1:A:113:TYR:CE1	1:A:148:LYS:NZ	0.60	2.69	16	1
1:A:228:HIS:CD2	1:A:236:MET:SD	0.60	2.95	14	3
1:A:240:TYR:CD1	1:A:241:LYS:N	0.60	2.70	7	7
1:A:135:ARG:NH2	1:A:136:LYS:NZ	0.60	2.50	1	1
1:A:156:MET:SD	1:A:157:ALA:N	0.60	2.75	5	2
1:A:218:HIS:CE1	1:A:236:MET:SD	0.59	2.95	15	1
1:A:236:MET:SD	1:A:237:PHE:N	0.59	2.76	2	10
1:A:228:HIS:NE2	1:A:236:MET:SD	0.59	2.76	7	1
1:A:117:ARG:NE	1:A:119:ASN:HD21	0.59	1.96	17	4
1:A:180:ILE:HD12	1:A:180:ILE:N	0.58	2.13	7	1
1:A:228:HIS:ND1	1:A:236:MET:SD	0.58	2.76	8	1
1:A:152:ILE:HD11	1:A:156:MET:O	0.58	1.98	6	3
1:A:218:HIS:CE1	1:A:222:HIS:NE2	0.58	2.70	7	1
1:A:231:ASP:N	1:A:232:PRO:CD	0.58	2.66	11	5
1:A:218:HIS:CD2	1:A:236:MET:SD	0.58	2.96	12	1
1:A:117:ARG:NH1	1:A:119:ASN:HD21	0.58	1.96	10	1
1:A:154:THR:O	1:A:156:MET:N	0.58	2.37	17	2
1:A:116:TYR:CD1	1:A:138:PHE:CE2	0.57	2.92	12	2
1:A:218:HIS:NE2	1:A:236:MET:SD	0.57	2.77	15	1
1:A:116:TYR:CE1	1:A:138:PHE:CE2	0.57	2.92	12	1
1:A:119:ASN:ND2	1:A:119:ASN:N	0.57	2.53	12	1
1:A:118:ILE:HG21	1:A:121:TYR:CE1	0.57	2.34	1	1
1:A:117:ARG:HE	1:A:119:ASN:HD21	0.57	1.41	2	4
1:A:222:HIS:HE2	1:A:228:HIS:CD2	0.57	2.16	17	1
1:A:119:ASN:HD22	1:A:119:ASN:N	0.56	1.98	5	1
1:A:168:HIS:CE1	1:A:172:HIS:CD2	0.56	2.93	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:138:PHE:CD1	1:A:149:PHE:CD2	0.56	2.93	8	1
1:A:119:ASN:N	1:A:119:ASN:ND2	0.56	2.53	5	1
1:A:132:TYR:CE1	1:A:136:LYS:NZ	0.56	2.73	9	1
1:A:149:PHE:CD1	1:A:149:PHE:N	0.56	2.73	15	11
1:A:261:LEU:HD12	1:A:261:LEU:N	0.56	2.16	11	2
1:A:163:PHE:CD1	1:A:163:PHE:N	0.56	2.73	5	11
1:A:206:HIS:CG	1:A:207:SER:N	0.56	2.74	8	4
1:A:206:HIS:CG	1:A:207:SER:H	0.56	2.19	10	2
1:A:256:ARG:NH1	1:A:259:GLN:HE22	0.56	1.99	8	1
1:A:119:ASN:N	1:A:119:ASN:HD22	0.56	1.98	12	1
1:A:204:THR:HG22	1:A:205:THR:N	0.56	2.16	14	1
1:A:135:ARG:HH22	1:A:136:LYS:NZ	0.56	1.99	1	1
1:A:183:HIS:CE1	1:A:196:HIS:O	0.56	2.59	3	3
1:A:171:PHE:O	1:A:172:HIS:CG	0.55	2.59	7	1
1:A:229:SER:OG	1:A:230:SER:N	0.55	2.39	7	3
1:A:171:PHE:O	1:A:173:ALA:N	0.55	2.40	10	5
1:A:191:ILE:HG23	1:A:191:ILE:O	0.55	2.01	5	3
1:A:168:HIS:ND1	1:A:172:HIS:O	0.55	2.39	8	2
1:A:191:ILE:O	1:A:193:GLY:N	0.55	2.36	11	5
1:A:178:GLY:O	1:A:180:ILE:N	0.55	2.39	17	3
1:A:228:HIS:CD2	1:A:228:HIS:N	0.55	2.74	14	1
1:A:120:ASN:O	1:A:122:THR:N	0.55	2.40	14	1
1:A:222:HIS:CE1	1:A:228:HIS:NE2	0.55	2.74	17	3
1:A:114:ILE:N	1:A:114:ILE:CD1	0.55	2.69	10	1
1:A:228:HIS:CG	1:A:236:MET:SD	0.55	2.99	14	2
1:A:183:HIS:CD2	1:A:196:HIS:O	0.54	2.61	1	5
1:A:111:LYS:O	1:A:112:HIS:ND1	0.54	2.40	5	2
1:A:258:ILE:O	1:A:260:SER:N	0.54	2.41	15	14
1:A:171:PHE:CE2	1:A:172:HIS:CD2	0.54	2.95	17	1
1:A:204:THR:O	1:A:206:HIS:N	0.54	2.41	8	4
1:A:258:ILE:HG23	1:A:259:GLN:N	0.54	2.17	5	12
1:A:171:PHE:CZ	1:A:172:HIS:NE2	0.54	2.76	17	1
1:A:194:ASP:O	1:A:196:HIS:CE1	0.54	2.61	9	12
1:A:174:PHE:CE1	1:A:183:HIS:CE1	0.54	2.96	6	2
1:A:203:TRP:CZ3	1:A:210:THR:HG22	0.54	2.38	15	3
1:A:194:ASP:O	1:A:196:HIS:CD2	0.54	2.61	4	7
1:A:121:TYR:CE2	1:A:131:ASP:OD1	0.54	2.62	3	2
1:A:208:GLY:N	1:A:242:TYR:OH	0.53	2.41	6	2
1:A:211:ASN:ND2	1:A:239:THR:OG1	0.53	2.41	13	1
1:A:199:GLU:O	1:A:201:GLU:N	0.53	2.41	12	15
1:A:194:ASP:O	1:A:196:HIS:NE2	0.53	2.40	7	7

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:185:PHE:CG	1:A:185:PHE:O	0.53	2.61	17	2
1:A:207:SER:OG	1:A:208:GLY:N	0.53	2.39	10	2
1:A:183:HIS:O	1:A:183:HIS:CG	0.53	2.60	11	4
1:A:261:LEU:N	1:A:261:LEU:CD1	0.53	2.71	11	1
1:A:153:ASN:HD22	1:A:153:ASN:N	0.53	2.02	13	1
1:A:240:TYR:OH	1:A:248:PHE:CE2	0.53	2.62	10	4
1:A:219:GLU:N	1:A:219:GLU:OE1	0.53	2.42	4	1
1:A:197:PHE:CE2	1:A:219:GLU:OE2	0.53	2.62	8	5
1:A:185:PHE:CD2	1:A:192:GLY:O	0.53	2.62	17	2
1:A:117:ARG:NH2	1:A:155:GLY:O	0.53	2.42	10	1
1:A:222:HIS:NE2	1:A:228:HIS:CD2	0.53	2.76	17	1
1:A:116:TYR:CG	1:A:138:PHE:CE2	0.53	2.97	1	2
1:A:185:PHE:CD1	1:A:192:GLY:O	0.53	2.61	3	2
1:A:168:HIS:CG	1:A:169:GLY:H	0.53	2.22	12	4
1:A:135:ARG:NH1	1:A:139:GLN:OE1	0.53	2.42	5	1
1:A:138:PHE:CD1	1:A:149:PHE:CG	0.53	2.97	8	5
1:A:167:ALA:O	1:A:174:PHE:CD2	0.53	2.62	8	1
1:A:177:LYS:N	1:A:200:ASP:OD2	0.53	2.42	16	2
1:A:159:ILE:HG23	1:A:159:ILE:O	0.53	2.03	7	5
1:A:111:LYS:N	1:A:111:LYS:CD	0.53	2.72	6	1
1:A:253:ASP:N	1:A:253:ASP:OD1	0.53	2.42	10	1
1:A:172:HIS:O	1:A:172:HIS:ND1	0.53	2.42	5	1
1:A:117:ARG:NE	1:A:119:ASN:OD1	0.53	2.42	15	3
1:A:218:HIS:CE1	3:A:1:DSV:HN24	0.53	2.21	8	1
1:A:118:ILE:O	1:A:121:TYR:CZ	0.52	2.63	8	6
1:A:120:ASN:ND2	1:A:163:PHE:O	0.52	2.42	12	1
1:A:175:ASP:N	1:A:175:ASP:OD1	0.52	2.42	3	1
1:A:167:ALA:O	1:A:174:PHE:CE2	0.52	2.63	8	2
1:A:166:GLY:O	1:A:174:PHE:CD2	0.52	2.63	6	1
1:A:170:ASP:O	1:A:172:HIS:N	0.52	2.42	13	4
1:A:232:PRO:O	1:A:234:ALA:N	0.52	2.42	16	1
1:A:117:ARG:NH1	1:A:119:ASN:OD1	0.52	2.42	10	2
1:A:222:HIS:O	1:A:225:GLY:N	0.52	2.42	8	3
1:A:112:HIS:N	1:A:112:HIS:ND1	0.52	2.57	12	1
1:A:171:PHE:CE1	1:A:183:HIS:CE1	0.52	2.97	1	1
1:A:197:PHE:CZ	1:A:219:GLU:OE1	0.52	2.62	6	5
1:A:152:ILE:HD12	1:A:152:ILE:O	0.52	2.04	8	1
1:A:168:HIS:O	1:A:170:ASP:N	0.52	2.42	1	1
1:A:197:PHE:CE2	1:A:219:GLU:OE1	0.52	2.63	5	1
1:A:172:HIS:O	1:A:174:PHE:CD2	0.52	2.62	16	1
1:A:211:ASN:N	1:A:211:ASN:OD1	0.52	2.42	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:130:VAL:CG1	1:A:163:PHE:CZ	0.52	2.92	13	2
1:A:197:PHE:CE1	1:A:219:GLU:OE1	0.52	2.62	8	2
1:A:228:HIS:O	1:A:229:SER:CB	0.52	2.57	11	1
1:A:174:PHE:CG	1:A:198:ASP:OD1	0.52	2.63	12	1
1:A:218:HIS:CE1	3:A:1:DSV:C5	0.52	2.92	6	5
1:A:218:HIS:ND1	3:A:1:DSV:C5	0.52	2.73	4	3
1:A:119:ASN:HD22	1:A:119:ASN:H	0.52	1.46	5	2
1:A:122:THR:O	1:A:124:ASP:N	0.52	2.42	10	4
1:A:199:GLU:OE2	1:A:203:TRP:CD1	0.51	2.63	14	1
1:A:117:ARG:NH1	1:A:155:GLY:O	0.51	2.43	15	1
1:A:117:ARG:NH1	1:A:119:ASN:ND2	0.51	2.59	1	2
1:A:244:ASP:OD1	1:A:245:ILE:N	0.51	2.43	3	1
3:A:1:DSV:O40	3:A:1:DSV:HC2B	0.51	2.05	17	1
1:A:124:ASP:OD2	1:A:165:ARG:NH2	0.51	2.43	3	2
1:A:259:GLN:O	1:A:262:TYR:N	0.51	2.40	17	5
1:A:218:HIS:CE1	3:A:1:DSV:C6	0.51	2.93	2	3
1:A:178:GLY:N	1:A:201:GLU:OE2	0.51	2.43	6	2
1:A:117:ARG:NH1	1:A:153:ASN:O	0.51	2.43	7	2
1:A:224:LEU:O	1:A:226:LEU:N	0.51	2.44	16	3
1:A:174:PHE:CE1	1:A:198:ASP:OD1	0.51	2.63	10	1
1:A:183:HIS:HD1	1:A:184:ALA:N	0.51	2.03	5	2
1:A:197:PHE:CZ	1:A:219:GLU:OE2	0.51	2.63	13	1
1:A:183:HIS:NE2	1:A:196:HIS:O	0.51	2.43	16	3
1:A:171:PHE:O	1:A:171:PHE:CD2	0.51	2.64	2	3
1:A:228:HIS:N	1:A:228:HIS:CD2	0.51	2.78	10	2
1:A:258:ILE:O	1:A:261:LEU:N	0.51	2.44	14	4
1:A:170:ASP:N	1:A:170:ASP:OD1	0.51	2.42	14	1
1:A:111:LYS:O	1:A:112:HIS:CG	0.51	2.64	17	1
1:A:131:ASP:OD1	1:A:131:ASP:N	0.51	2.42	4	4
1:A:218:HIS:HE2	3:A:1:DSV:C37	0.51	2.19	12	1
1:A:218:HIS:CD2	3:A:1:DSV:C5	0.51	2.94	3	3
1:A:230:SER:OG	1:A:231:ASP:N	0.50	2.44	10	2
1:A:201:GLU:N	1:A:201:GLU:OE1	0.50	2.43	2	1
1:A:220:ILE:N	1:A:220:ILE:CD1	0.50	2.74	8	1
1:A:193:GLY:O	1:A:194:ASP:C	0.50	2.50	2	6
1:A:172:HIS:O	1:A:174:PHE:CE2	0.50	2.64	16	1
1:A:154:THR:HG22	1:A:155:GLY:N	0.50	2.21	17	1
1:A:234:ALA:O	1:A:236:MET:N	0.50	2.45	10	15
1:A:118:ILE:O	1:A:121:TYR:CE2	0.50	2.64	2	3
1:A:183:HIS:O	1:A:183:HIS:CD2	0.50	2.64	6	2
1:A:156:MET:SD	1:A:157:ALA:O	0.50	2.70	11	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:206:HIS:CD2	1:A:207:SER:H	0.50	2.24	6	2
1:A:183:HIS:CD2	1:A:183:HIS:O	0.50	2.65	15	2
1:A:211:ASN:O	1:A:215:THR:HG23	0.50	2.06	17	3
1:A:121:TYR:CD2	1:A:131:ASP:OD1	0.50	2.64	3	1
1:A:206:HIS:O	1:A:207:SER:CB	0.50	2.58	11	6
1:A:118:ILE:O	1:A:121:TYR:CE1	0.50	2.65	14	2
1:A:203:TRP:CZ3	1:A:210:THR:O	0.50	2.65	1	2
1:A:234:ALA:C	1:A:236:MET:N	0.50	2.65	14	16
1:A:218:HIS:CD2	3:A:1:DSV:C6	0.50	2.94	16	1
1:A:218:HIS:HD1	3:A:1:DSV:C5	0.50	2.19	14	2
1:A:132:TYR:OH	1:A:136:LYS:NZ	0.50	2.44	8	2
1:A:170:ASP:O	1:A:172:HIS:CD2	0.50	2.65	9	1
1:A:166:GLY:O	1:A:174:PHE:CE2	0.49	2.65	3	2
1:A:222:HIS:CE1	1:A:228:HIS:HE2	0.49	2.17	16	1
1:A:230:SER:O	1:A:231:ASP:CB	0.49	2.61	8	4
1:A:168:HIS:CD2	1:A:169:GLY:H	0.49	2.25	14	2
1:A:196:HIS:N	1:A:196:HIS:ND1	0.49	2.60	1	1
1:A:120:ASN:OD1	1:A:121:TYR:N	0.49	2.45	4	1
1:A:195:ALA:O	1:A:196:HIS:CD2	0.49	2.65	7	1
1:A:135:ARG:O	1:A:135:ARG:NE	0.49	2.44	11	1
1:A:222:HIS:CE1	1:A:228:HIS:CE1	0.49	3.00	2	1
1:A:121:TYR:CD1	1:A:121:TYR:N	0.49	2.80	10	3
1:A:168:HIS:CE1	1:A:170:ASP:OD2	0.49	2.65	3	1
1:A:183:HIS:ND1	1:A:183:HIS:C	0.49	2.66	4	2
1:A:170:ASP:OD1	1:A:171:PHE:N	0.49	2.45	10	1
1:A:198:ASP:OD1	1:A:198:ASP:N	0.49	2.42	10	1
1:A:171:PHE:CZ	1:A:172:HIS:CD2	0.49	3.01	17	1
1:A:258:ILE:CG2	1:A:259:GLN:N	0.49	2.76	6	10
1:A:126:ASN:ND2	1:A:126:ASN:N	0.49	2.58	6	1
1:A:120:ASN:C	1:A:121:TYR:CG	0.49	2.86	11	1
1:A:248:PHE:O	1:A:249:ARG:NE	0.49	2.46	8	2
1:A:240:TYR:O	1:A:242:TYR:N	0.49	2.44	14	1
1:A:258:ILE:C	1:A:260:SER:N	0.49	2.66	10	12
1:A:244:ASP:N	1:A:244:ASP:OD1	0.49	2.45	17	2
1:A:229:SER:O	1:A:236:MET:SD	0.49	2.71	17	1
1:A:171:PHE:O	1:A:172:HIS:CB	0.48	2.61	3	1
1:A:151:LYS:NZ	1:A:151:LYS:CB	0.48	2.76	13	2
1:A:228:HIS:CE1	1:A:236:MET:SD	0.48	3.05	7	2
1:A:132:TYR:O	1:A:135:ARG:N	0.48	2.44	8	1
1:A:248:PHE:O	1:A:249:ARG:CZ	0.48	2.61	8	1
1:A:116:TYR:CD1	1:A:116:TYR:N	0.48	2.82	1	8

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:203:TRP:CE3	1:A:210:THR:O	0.48	2.66	1	2
1:A:211:ASN:CG	1:A:242:TYR:CD1	0.48	2.87	11	1
1:A:115:THR:N	1:A:158:ASP:OD2	0.48	2.43	3	5
1:A:129:ASP:N	1:A:129:ASP:OD1	0.48	2.46	2	1
1:A:174:PHE:CD1	1:A:198:ASP:OD2	0.48	2.66	10	1
1:A:218:HIS:NE2	3:A:1:DSV:C37	0.48	2.77	12	1
1:A:197:PHE:CE2	1:A:219:GLU:CD	0.48	2.87	6	4
1:A:153:ASN:N	1:A:153:ASN:ND2	0.48	2.62	13	1
1:A:238:PRO:O	3:A:1:DSV:CZ2	0.48	2.62	12	11
1:A:168:HIS:NE2	1:A:170:ASP:OD2	0.48	2.47	3	1
1:A:197:PHE:CZ	1:A:219:GLU:CD	0.48	2.87	13	2
1:A:258:ILE:HG23	1:A:259:GLN:H	0.48	1.69	16	1
1:A:191:ILE:HG23	1:A:192:GLY:N	0.48	2.23	17	1
1:A:233:LYS:NZ	1:A:253:ASP:OD1	0.48	2.46	17	1
1:A:224:LEU:C	1:A:226:LEU:N	0.48	2.67	11	3
1:A:201:GLU:N	1:A:201:GLU:CD	0.47	2.67	15	3
1:A:113:TYR:O	1:A:113:TYR:CD2	0.47	2.67	17	4
1:A:211:ASN:ND2	1:A:211:ASN:N	0.47	2.62	5	1
1:A:199:GLU:CD	1:A:203:TRP:CD1	0.47	2.88	14	1
1:A:259:GLN:O	1:A:261:LEU:N	0.47	2.47	17	5
1:A:196:HIS:ND1	1:A:196:HIS:N	0.47	2.63	6	2
1:A:247:THR:O	1:A:249:ARG:NH1	0.47	2.47	9	1
1:A:156:MET:CE	1:A:157:ALA:O	0.47	2.63	15	2
3:A:1:DSV:HC2B	3:A:1:DSV:O39	0.47	2.08	13	1
1:A:259:GLN:C	1:A:261:LEU:N	0.47	2.67	17	6
1:A:128:GLU:N	1:A:128:GLU:CD	0.47	2.68	3	4
1:A:174:PHE:CD1	1:A:198:ASP:CG	0.47	2.88	5	2
1:A:133:ALA:CB	1:A:213:PHE:CE2	0.47	2.97	8	2
1:A:220:ILE:N	1:A:220:ILE:HD12	0.47	2.23	8	1
1:A:182:ALA:N	3:A:1:DSV:O22	0.47	2.48	14	1
1:A:185:PHE:CD1	1:A:185:PHE:C	0.47	2.88	1	1
1:A:185:PHE:CB	1:A:192:GLY:O	0.47	2.63	5	1
1:A:117:ARG:CZ	1:A:155:GLY:O	0.47	2.62	15	1
1:A:117:ARG:NH1	1:A:119:ASN:CG	0.47	2.68	5	2
1:A:119:ASN:N	1:A:119:ASN:OD1	0.47	2.48	1	1
1:A:180:ILE:N	1:A:180:ILE:CD1	0.47	2.78	7	1
1:A:121:TYR:O	1:A:122:THR:C	0.47	2.53	14	3
1:A:131:ASP:N	1:A:131:ASP:OD1	0.47	2.46	1	4
1:A:261:LEU:O	1:A:262:TYR:CB	0.47	2.62	3	3
1:A:204:THR:O	1:A:206:HIS:O	0.47	2.33	8	1
1:A:120:ASN:C	1:A:121:TYR:CD1	0.47	2.89	11	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:239:THR:C	1:A:241:LYS:N	0.47	2.68	11	3
1:A:195:ALA:C	1:A:196:HIS:CG	0.47	2.89	16	1
1:A:211:ASN:HD21	3:A:1:DSV:CY1	0.46	2.23	4	1
1:A:199:GLU:O	1:A:199:GLU:CG	0.46	2.63	7	2
1:A:166:GLY:N	1:A:200:ASP:OD1	0.46	2.41	17	1
1:A:120:ASN:ND2	1:A:121:TYR:N	0.46	2.64	1	1
1:A:198:ASP:N	1:A:198:ASP:OD1	0.46	2.48	1	2
1:A:199:GLU:C	1:A:201:GLU:N	0.46	2.67	2	14
1:A:261:LEU:C	1:A:262:TYR:CG	0.46	2.87	5	1
1:A:207:SER:OG	1:A:207:SER:O	0.46	2.32	9	2
1:A:175:ASP:CG	1:A:176:GLY:N	0.46	2.68	17	1
1:A:130:VAL:O	1:A:134:ILE:HD12	0.46	2.11	14	3
1:A:204:THR:C	1:A:206:HIS:N	0.46	2.67	8	3
1:A:117:ARG:CZ	1:A:119:ASN:OD1	0.46	2.63	15	2
1:A:229:SER:OG	1:A:234:ALA:CB	0.46	2.63	9	1
1:A:113:TYR:O	1:A:113:TYR:CG	0.46	2.68	15	2
1:A:113:TYR:CD1	1:A:113:TYR:O	0.46	2.69	9	3
1:A:159:ILE:CG1	1:A:193:GLY:O	0.46	2.64	17	4
1:A:135:ARG:NE	1:A:135:ARG:C	0.46	2.68	11	1
1:A:153:ASN:OD1	1:A:153:ASN:N	0.46	2.45	5	2
1:A:239:THR:O	1:A:239:THR:OG1	0.46	2.34	17	2
1:A:120:ASN:O	1:A:120:ASN:ND2	0.46	2.48	15	1
1:A:242:TYR:O	1:A:243:VAL:HG13	0.46	2.11	6	5
1:A:168:HIS:HD1	1:A:172:HIS:CB	0.46	2.23	7	1
1:A:120:ASN:CG	1:A:121:TYR:N	0.45	2.70	4	1
1:A:122:THR:C	1:A:124:ASP:H	0.45	2.14	5	3
1:A:226:LEU:O	1:A:227:GLY:O	0.45	2.34	9	2
1:A:236:MET:SD	1:A:236:MET:C	0.45	2.95	4	8
1:A:214:LEU:HD12	1:A:214:LEU:N	0.45	2.27	11	2
1:A:120:ASN:O	1:A:121:TYR:C	0.45	2.55	14	4
1:A:156:MET:C	1:A:156:MET:SD	0.45	2.95	12	2
1:A:120:ASN:OD1	1:A:163:PHE:O	0.45	2.33	17	1
1:A:218:HIS:CE1	3:A:1:DSV:H6	0.45	2.47	2	1
1:A:172:HIS:C	1:A:172:HIS:ND1	0.45	2.68	8	1
1:A:243:VAL:HG22	1:A:244:ASP:H	0.45	1.71	9	1
1:A:159:ILE:O	1:A:159:ILE:CG2	0.45	2.64	9	2
1:A:115:THR:OG1	1:A:158:ASP:N	0.45	2.42	6	1
1:A:133:ALA:HB2	1:A:213:PHE:CE2	0.45	2.47	8	1
1:A:206:HIS:CG	1:A:206:HIS:O	0.45	2.69	13	1
1:A:199:GLU:O	1:A:201:GLU:O	0.45	2.34	4	11
1:A:174:PHE:CD1	1:A:174:PHE:N	0.45	2.84	8	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:226:LEU:N	1:A:226:LEU:CD2	0.45	2.80	10	1
1:A:168:HIS:HE2	1:A:170:ASP:CG	0.45	2.15	12	1
1:A:203:TRP:CH2	1:A:210:THR:CG2	0.45	3.00	14	1
1:A:236:MET:C	1:A:236:MET:SD	0.45	2.95	13	3
1:A:172:HIS:O	1:A:172:HIS:CG	0.45	2.68	5	1
1:A:181:LEU:CD2	1:A:201:GLU:OE2	0.45	2.64	13	1
1:A:156:MET:CG	1:A:157:ALA:N	0.45	2.80	9	1
1:A:168:HIS:CD2	1:A:196:HIS:CB	0.45	3.00	9	1
1:A:120:ASN:CG	1:A:163:PHE:H	0.45	2.15	17	1
1:A:174:PHE:CD2	1:A:198:ASP:OD1	0.45	2.70	6	2
1:A:199:GLU:O	1:A:200:ASP:C	0.45	2.54	9	1
1:A:258:ILE:O	1:A:258:ILE:HD13	0.45	2.12	9	1
1:A:168:HIS:CE1	1:A:170:ASP:O	0.45	2.69	4	1
1:A:127:ARG:H	1:A:127:ARG:CD	0.45	2.24	5	1
1:A:174:PHE:CZ	1:A:183:HIS:CE1	0.45	3.04	6	1
1:A:118:ILE:HG21	1:A:121:TYR:CE2	0.45	2.47	13	2
1:A:198:ASP:OD1	1:A:200:ASP:N	0.44	2.45	5	1
1:A:232:PRO:O	1:A:233:LYS:C	0.44	2.55	16	6
1:A:117:ARG:NH1	1:A:152:ILE:O	0.44	2.50	11	1
1:A:168:HIS:CD2	1:A:196:HIS:CG	0.44	3.06	2	1
1:A:154:THR:OG1	1:A:155:GLY:N	0.44	2.50	9	1
1:A:206:HIS:ND1	1:A:206:HIS:O	0.44	2.50	9	1
1:A:154:THR:CG2	1:A:155:GLY:N	0.44	2.80	17	1
1:A:141:TRP:O	1:A:145:THR:OG1	0.44	2.33	17	6
1:A:175:ASP:OD1	1:A:175:ASP:N	0.44	2.51	2	1
1:A:119:ASN:ND2	1:A:160:LEU:HD21	0.44	2.26	6	2
1:A:262:TYR:CD1	1:A:262:TYR:O	0.44	2.71	15	1
1:A:206:HIS:O	1:A:206:HIS:CG	0.44	2.70	1	1
1:A:112:HIS:ND1	1:A:112:HIS:N	0.44	2.66	4	1
1:A:211:ASN:O	1:A:215:THR:OG1	0.44	2.33	14	2
1:A:121:TYR:CE2	1:A:131:ASP:CG	0.44	2.91	3	1
1:A:166:GLY:H	1:A:200:ASP:CG	0.44	2.16	15	1
1:A:130:VAL:O	1:A:134:ILE:CG1	0.44	2.66	17	4
1:A:198:ASP:O	1:A:198:ASP:OD1	0.44	2.36	11	3
1:A:124:ASP:N	1:A:124:ASP:OD1	0.44	2.51	11	2
1:A:121:TYR:O	1:A:123:PRO:N	0.44	2.51	12	1
1:A:127:ARG:O	1:A:131:ASP:OD1	0.44	2.35	1	3
1:A:200:ASP:N	1:A:200:ASP:OD1	0.44	2.50	8	2
1:A:206:HIS:O	1:A:207:SER:O	0.44	2.36	8	1
1:A:242:TYR:CD1	1:A:242:TYR:C	0.44	2.90	10	1
1:A:183:HIS:NE2	1:A:196:HIS:ND1	0.44	2.66	14	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:153:ASN:O	1:A:154:THR:HG23	0.44	2.11	16	1
1:A:154:THR:C	1:A:156:MET:N	0.44	2.70	17	2
1:A:120:ASN:ND2	1:A:121:TYR:O	0.44	2.51	1	1
1:A:118:ILE:HG22	1:A:121:TYR:H	0.44	1.72	3	1
1:A:122:THR:C	1:A:124:ASP:N	0.44	2.71	13	2
1:A:185:PHE:O	1:A:185:PHE:CD1	0.44	2.71	5	1
1:A:120:ASN:HB3	1:A:162:VAL:HG13	0.44	1.90	8	1
1:A:194:ASP:O	1:A:194:ASP:OD1	0.44	2.35	8	2
1:A:218:HIS:NE2	3:A:1:DSV:O40	0.44	2.51	12	1
1:A:248:PHE:C	1:A:248:PHE:CD1	0.43	2.91	7	3
1:A:117:ARG:HH11	1:A:119:ASN:CG	0.43	2.15	5	1
1:A:240:TYR:C	1:A:242:TYR:H	0.43	2.15	14	1
1:A:115:THR:OG1	1:A:158:ASP:OD2	0.43	2.36	4	1
1:A:238:PRO:O	1:A:240:TYR:N	0.43	2.49	8	1
1:A:206:HIS:O	1:A:207:SER:OG	0.43	2.36	17	2
1:A:118:ILE:CG2	1:A:121:TYR:CE2	0.43	3.01	16	1
1:A:168:HIS:CD2	1:A:168:HIS:C	0.43	2.91	17	1
1:A:191:ILE:CG2	1:A:192:GLY:N	0.43	2.80	17	1
1:A:218:HIS:NE2	3:A:1:DSV:O39	0.43	2.51	6	1
1:A:231:ASP:N	1:A:232:PRO:HD2	0.43	2.29	11	2
1:A:234:ALA:C	1:A:236:MET:H	0.43	2.17	10	9
1:A:172:HIS:O	1:A:173:ALA:O	0.43	2.36	17	1
1:A:183:HIS:CG	1:A:184:ALA:H	0.43	2.31	2	1
1:A:181:LEU:O	1:A:198:ASP:OD1	0.43	2.36	4	1
1:A:200:ASP:O	1:A:200:ASP:OD1	0.43	2.36	5	1
1:A:194:ASP:O	1:A:195:ALA:C	0.43	2.56	7	1
1:A:211:ASN:ND2	1:A:242:TYR:CE1	0.43	2.87	15	1
1:A:115:THR:OG1	1:A:158:ASP:OD1	0.43	2.37	15	8
1:A:200:ASP:O	1:A:201:GLU:CG	0.43	2.66	9	1
1:A:224:LEU:C	1:A:226:LEU:H	0.43	2.17	11	1
1:A:174:PHE:CG	1:A:198:ASP:CG	0.43	2.92	12	1
1:A:168:HIS:O	1:A:168:HIS:CG	0.43	2.72	15	1
1:A:207:SER:OG	1:A:242:TYR:OH	0.43	2.36	8	1
1:A:213:PHE:CG	1:A:245:ILE:CG2	0.43	3.02	8	1
1:A:243:VAL:O	1:A:244:ASP:C	0.43	2.57	13	1
1:A:128:GLU:CD	1:A:128:GLU:H	0.43	2.17	3	1
1:A:215:THR:OG1	3:A:1:DSV:CY1	0.43	2.67	13	3
1:A:228:HIS:O	1:A:229:SER:OG	0.43	2.35	11	1
1:A:175:ASP:O	1:A:176:GLY:O	0.43	2.36	16	1
1:A:248:PHE:CD1	1:A:248:PHE:C	0.43	2.92	10	3
1:A:222:HIS:CE1	1:A:228:HIS:CD2	0.43	3.07	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:156:MET:SD	1:A:160:LEU:HD11	0.43	2.54	6	1
1:A:256:ARG:HH11	1:A:259:GLN:HE22	0.43	1.57	8	1
1:A:165:ARG:O	1:A:166:GLY:O	0.43	2.37	11	3
1:A:174:PHE:CD2	1:A:198:ASP:CG	0.43	2.92	14	1
1:A:204:THR:CG2	1:A:205:THR:N	0.43	2.81	14	1
1:A:208:GLY:O	1:A:209:GLY:O	0.42	2.37	14	2
1:A:135:ARG:C	1:A:135:ARG:HE	0.42	2.16	11	1
1:A:168:HIS:ND1	1:A:168:HIS:N	0.42	2.66	11	1
1:A:239:THR:OG1	1:A:240:TYR:N	0.42	2.49	14	1
1:A:218:HIS:ND1	3:A:1:DSV:H5	0.42	2.28	15	1
1:A:166:GLY:O	1:A:175:ASP:OD1	0.42	2.36	16	1
1:A:122:THR:OG1	1:A:199:GLU:OE2	0.42	2.37	16	2
1:A:170:ASP:O	1:A:171:PHE:O	0.42	2.37	1	1
1:A:166:GLY:O	1:A:167:ALA:O	0.42	2.36	11	3
1:A:160:LEU:O	1:A:195:ALA:O	0.42	2.37	9	1
1:A:117:ARG:NH2	1:A:119:ASN:OD1	0.42	2.52	8	1
1:A:203:TRP:CH2	1:A:210:THR:HG21	0.42	2.49	14	1
1:A:113:TYR:C	1:A:114:ILE:HD12	0.42	2.35	10	1
1:A:120:ASN:O	1:A:121:TYR:O	0.42	2.38	15	1
1:A:153:ASN:O	1:A:154:THR:OG1	0.42	2.36	17	1
1:A:215:THR:O	1:A:219:GLU:OE2	0.42	2.37	17	1
1:A:129:ASP:O	1:A:129:ASP:OD1	0.42	2.38	6	1
1:A:218:HIS:CE1	1:A:222:HIS:CD2	0.42	3.07	7	1
1:A:171:PHE:C	1:A:173:ALA:H	0.42	2.18	13	2
1:A:206:HIS:O	1:A:208:GLY:N	0.42	2.53	6	1
1:A:198:ASP:OD1	1:A:200:ASP:OD1	0.42	2.38	12	1
1:A:213:PHE:CE2	1:A:245:ILE:CD1	0.42	3.03	13	1
1:A:175:ASP:OD1	1:A:175:ASP:C	0.42	2.58	17	1
1:A:176:GLY:O	1:A:200:ASP:OD2	0.42	2.37	4	1
1:A:123:PRO:O	1:A:124:ASP:OD2	0.42	2.38	10	1
1:A:222:HIS:CD2	1:A:222:HIS:N	0.42	2.85	1	1
1:A:172:HIS:ND1	1:A:173:ALA:N	0.42	2.67	2	1
1:A:218:HIS:CE1	3:A:1:DSV:O40	0.42	2.73	5	1
1:A:259:GLN:C	1:A:261:LEU:H	0.42	2.19	17	3
1:A:176:GLY:O	1:A:201:GLU:OE2	0.42	2.38	15	1
1:A:211:ASN:HD21	3:A:1:DSV:HY1	0.41	1.75	4	1
1:A:211:ASN:O	1:A:211:ASN:ND2	0.41	2.42	4	1
1:A:183:HIS:NE2	1:A:196:HIS:N	0.41	2.65	14	1
1:A:118:ILE:CG2	1:A:121:TYR:CE1	0.41	3.02	1	1
1:A:166:GLY:O	1:A:174:PHE:O	0.41	2.38	7	1
1:A:111:LYS:NZ	1:A:111:LYS:CB	0.41	2.84	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:170:ASP:OD1	1:A:170:ASP:O	0.41	2.37	6	2
1:A:138:PHE:CD1	1:A:220:ILE:HD13	0.41	2.50	9	1
1:A:237:PHE:CD1	1:A:237:PHE:C	0.41	2.93	3	2
1:A:242:TYR:O	1:A:243:VAL:CG1	0.41	2.68	7	4
1:A:197:PHE:CD2	1:A:219:GLU:OE2	0.41	2.73	8	1
1:A:220:ILE:O	1:A:223:SER:CB	0.41	2.68	5	1
1:A:224:LEU:O	1:A:225:GLY:C	0.41	2.59	7	2
1:A:231:ASP:OD1	1:A:231:ASP:O	0.41	2.37	11	1
1:A:253:ASP:OD1	1:A:253:ASP:N	0.41	2.53	11	1
1:A:207:SER:OG	1:A:242:TYR:CE1	0.41	2.73	13	1
1:A:258:ILE:C	1:A:260:SER:H	0.41	2.19	2	1
1:A:118:ILE:O	1:A:120:ASN:N	0.41	2.54	3	1
1:A:135:ARG:NH2	1:A:139:GLN:NE2	0.41	2.69	11	1
1:A:183:HIS:O	1:A:183:HIS:ND1	0.41	2.54	11	1
1:A:118:ILE:O	1:A:119:ASN:C	0.41	2.59	3	1
1:A:238:PRO:O	1:A:239:THR:OG1	0.41	2.36	10	1
1:A:213:PHE:CG	1:A:245:ILE:HG22	0.41	2.51	11	1
1:A:194:ASP:OD1	1:A:194:ASP:N	0.41	2.54	12	1
1:A:215:THR:OG1	3:A:1:DSV:C11	0.41	2.68	14	1
1:A:155:GLY:O	1:A:156:MET:C	0.41	2.59	4	2
1:A:183:HIS:CE1	1:A:196:HIS:ND1	0.41	2.88	13	1
1:A:185:PHE:CD2	1:A:192:GLY:C	0.41	2.94	17	1
1:A:123:PRO:O	1:A:124:ASP:CG	0.41	2.59	7	3
1:A:198:ASP:O	1:A:201:GLU:OE1	0.41	2.38	1	1
1:A:129:ASP:OD1	1:A:129:ASP:O	0.41	2.39	11	1
1:A:169:GLY:O	1:A:170:ASP:O	0.41	2.39	14	1
1:A:191:ILE:C	1:A:193:GLY:H	0.41	2.19	14	1
1:A:168:HIS:N	1:A:168:HIS:ND1	0.40	2.68	1	1
1:A:176:GLY:O	1:A:177:LYS:C	0.40	2.60	9	1
1:A:243:VAL:HG22	1:A:244:ASP:N	0.40	2.30	9	1
1:A:239:THR:C	1:A:241:LYS:H	0.40	2.19	13	1
1:A:230:SER:O	1:A:231:ASP:CG	0.40	2.59	15	2
1:A:119:ASN:O	1:A:120:ASN:CB	0.40	2.69	3	1
1:A:113:TYR:CD1	1:A:113:TYR:N	0.40	2.89	6	1
1:A:249:ARG:O	1:A:250:LEU:O	0.40	2.39	13	1
1:A:147:LEU:O	1:A:148:LYS:CG	0.40	2.69	16	1
1:A:165:ARG:CG	1:A:166:GLY:N	0.40	2.84	5	1
1:A:239:THR:O	1:A:240:TYR:C	0.40	2.60	15	1
1:A:211:ASN:ND2	1:A:242:TYR:CD1	0.40	2.89	16	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	147/165 (89%)	108±3 (73±2%)	24±3 (16±2%)	16±3 (11±2%)	1 9
All	All	2499/2805 (89%)	1832 (73%)	401 (16%)	266 (11%)	1 9

All 50 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	194	ASP	15
1	A	200	ASP	15
1	A	259	GLN	14
1	A	238	PRO	13
1	A	207	SER	11
1	A	225	GLY	11
1	A	231	ASP	11
1	A	124	ASP	10
1	A	209	GLY	10
1	A	262	TYR	10
1	A	244	ASP	8
1	A	208	GLY	8
1	A	168	HIS	8
1	A	169	GLY	7
1	A	191	ILE	7
1	A	172	HIS	7
1	A	171	PHE	6
1	A	227	GLY	6
1	A	179	GLY	6
1	A	193	GLY	6
1	A	175	ASP	6
1	A	121	TYR	5
1	A	123	PRO	5
1	A	111	LYS	5
1	A	155	GLY	5
1	A	167	ALA	5
1	A	235	VAL	4

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Mol	Chain	Res	Type	Models (Total)
1	A	205	THR	4
1	A	166	GLY	4
1	A	173	ALA	3
1	A	260	SER	3
1	A	242	TYR	3
1	A	195	ALA	2
1	A	229	SER	2
1	A	170	ASP	2
1	A	232	PRO	2
1	A	240	TYR	2
1	A	174	PHE	2
1	A	176	GLY	2
1	A	119	ASN	1
1	A	120	ASN	1
1	A	156	MET	1
1	A	226	LEU	1
1	A	192	GLY	1
1	A	122	THR	1
1	A	250	LEU	1
1	A	241	LYS	1
1	A	206	HIS	1
1	A	233	LYS	1
1	A	243	VAL	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	121/133 (91%)	113±2 (94±2%)	8±2 (6±2%)	21 70
All	All	2057/2261 (91%)	1927 (94%)	130 (6%)	21 70

All 44 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	122	THR	16
1	A	160	LEU	16

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Mol	Chain	Res	Type	Models (Total)
1	A	149	PHE	7
1	A	239	THR	7
1	A	231	ASP	6
1	A	175	ASP	5
1	A	156	MET	5
1	A	196	HIS	4
1	A	121	TYR	4
1	A	240	TYR	4
1	A	211	ASN	3
1	A	120	ASN	3
1	A	200	ASP	3
1	A	172	HIS	3
1	A	135	ARG	3
1	A	253	ASP	3
1	A	131	ASP	2
1	A	124	ASP	2
1	A	207	SER	2
1	A	154	THR	2
1	A	219	GLU	2
1	A	119	ASN	2
1	A	153	ASN	2
1	A	174	PHE	2
1	A	183	HIS	2
1	A	194	ASP	2
1	A	198	ASP	1
1	A	226	LEU	1
1	A	115	THR	1
1	A	127	ARG	1
1	A	163	PHE	1
1	A	241	LYS	1
1	A	111	LYS	1
1	A	126	ASN	1
1	A	143	ASN	1
1	A	152	ILE	1
1	A	258	ILE	1
1	A	242	TYR	1
1	A	112	HIS	1
1	A	229	SER	1
1	A	244	ASP	1
1	A	256	ARG	1
1	A	144	VAL	1
1	A	236	MET	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)

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 for Mogul analysis.

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
3	DSV	A	1	2	22,26,26	2.63±0.02	8±0 (36±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
3	DSV	A	1	2	27,39,39	1.09±0.01	2±0 (7±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
3	DSV	A	1	2	-	0±0,15,19,19	0±0,3,3,3

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	1	DSV	S21-N24	7.79	1.74	1.61	13	17
3	A	1	DSV	C11-S10	5.31	1.78	1.74	4	17
3	A	1	DSV	C3-S10	5.01	1.78	1.74	6	17
3	A	1	DSV	C2-C1	3.02	1.42	1.36	13	17
3	A	1	DSV	C5-C6	2.82	1.42	1.36	9	17
3	A	1	DSV	CZ2-CY2	2.59	1.42	1.36	9	17
3	A	1	DSV	CZ1-CY1	2.46	1.42	1.36	14	17
3	A	1	DSV	C6-C1	2.27	1.42	1.38	9	17

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
3	A	1	DSV	CY2-C12-C4	2.40	127.88	133.15	12	17
3	A	1	DSV	C5-C4-C12	2.39	127.89	133.15	13	17

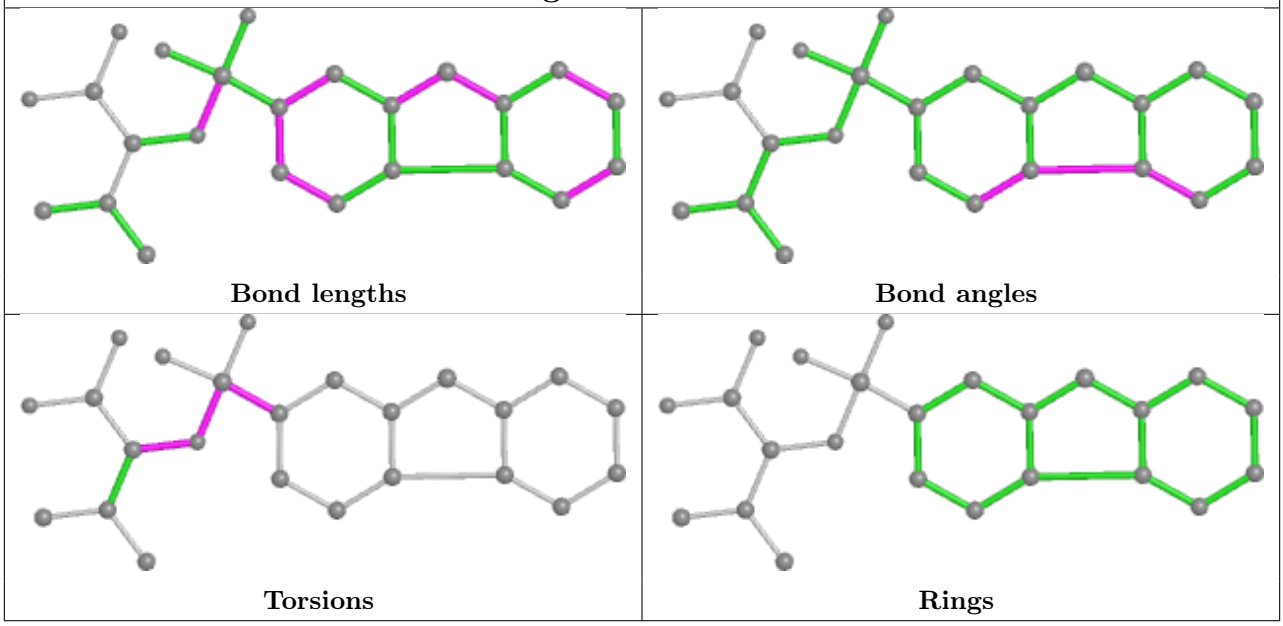
There are no chirality outliers.

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 DSV A 1



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