Full wwPDB NMR Structure Validation Report (i)

Jun 11, 2024 – 11:32 PM EDT

PDB ID	:	1PUQ
Title	:	Solution Structure of the MutT Pyrophosphohydrolase Complexed with Mg(2+) and 8-oxo-dGMP, a Tightly-bound Product
Authors	:	Massiah, M.A.; Saraswat, V.; Azurmendi, H.F.; Mildvan, A.S.
Deposited on	:	2003-06-25

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:

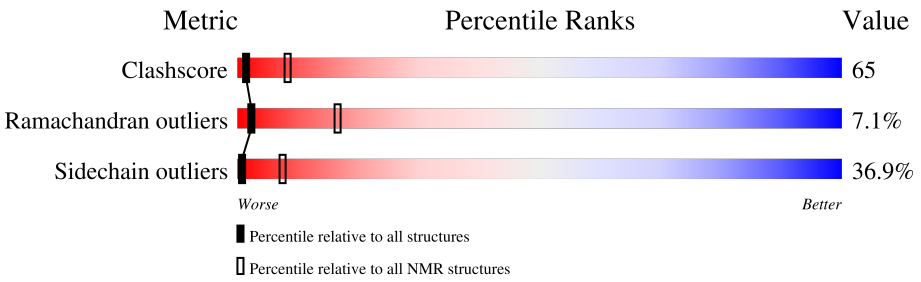
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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	129	22% 47% 23% 7%

2 Ensemble composition and analysis (i)

This entry contains 20 models. The atoms present in the NMR models are not consistent. Some calculations may have failed as a result. All residues are included in the validation scores. Model 2 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	**Residue range (total)**	**Backbone RMSD (Å)**	**Medoid model**
1	A:2-A:22, A:31-A:129 (120)	0.56	2

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

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

The models can be grouped into 2 clusters. No single-model clusters were found.

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

3 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 2135 atoms, of which 1054 are hydrogens and 0 are deuteriums.

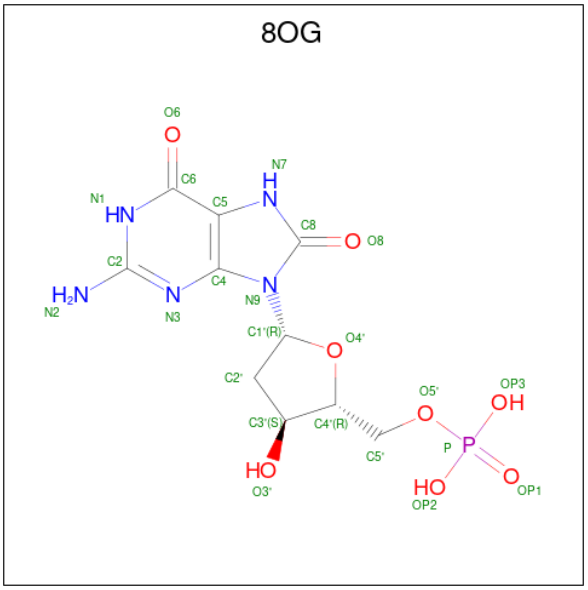
- Molecule 1 is a protein called Mutator mutT protein.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	129	2092	679	1038	180	191	4	0

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	
			Total	Mg
2	A	1	1	1

- Molecule 3 is 8-OXO-2'-DEOXY-GUANOSINE-5'-MONOPHOSPHATE (three-letter code: 8OG) (formula: $C_{10}H_{14}N_5O_8P$).



Mol	Chain	Residues	Atoms					
			Total	C	H	N	O	P
3	A	1	36	10	12	5	8	1

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		
			Total	H	O
4	A	4	6	4	2

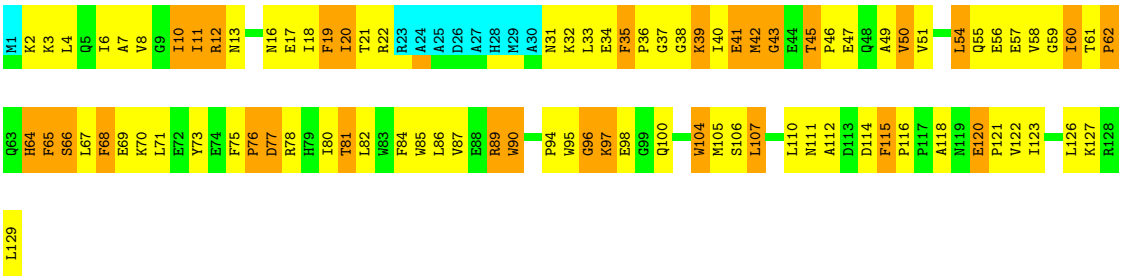
4 Residue-property plots (i)

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: Mutator mutT protein

Chain A: 22% 47% 23% 7%



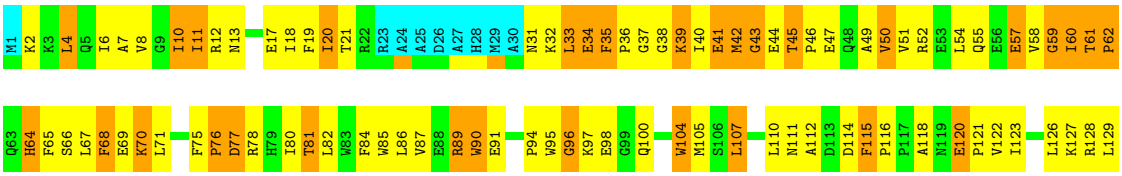
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: Mutator mutT protein

Chain A: 24% 45% 24% 7%



4.2.2 Score per residue for model 2 (medoid)

• Molecule 1: Mutator mutT protein

Chain A: 26% 44% 22% • 7%

M1 K2 K3 I6 A7 V8 G9 I10 I11 R12 N13 E14 I18 F19 I20 T21 R22 R23 A24 A25 D26 A27 H28 M29 A30 N31 K32 L33 E34 F35 P36 G37 G38 K39 I40 E41 M42 G43 E44 T45 P46 E47 Q48 A49 V50 V51 R52 E53 L54 Q55 V58 G59 I60 T61 P62 Q63 H64

F65 S66 L67 F68 E69 K70 L71 E72 Y73 E74 F75 P76 D77 R78 H79 I80 T81 L82 W83 F84 W85 L86 V87 E88 R89 W90 P94 W95 G96 K97 E98 G99 Q100 E103 W104 M105 S106 L107 L110 N111 A112 D113 D114 F115 P116 P117 A118 N119 E120 P121 V122 I123 A124 K125 L126 K127 R128

L129

4.2.3 Score per residue for model 3

- Molecule 1: Mutator mutT protein

Chain A: 26% 45% 21% • 7%

M1 K2 K3 L4 Q5 I6 A7 V8 G9 I10 I11 R12 N13 N16 E17 I18 F19 I20 T21 R22 R23 A24 A25 D26 A27 H28 M29 A30 N31 E34 F35 P36 G37 G38 K39 I40 E41 M42 G43 E44 T45 P46 E47 Q48 A49 V50 V51 L54 E57 V58 G59 I60 T61 P62 Q63 H64

F65 S66 L67 F68 E69 K70 L71 F75 P76 D77 R78 H79 I80 T81 L82 W83 F84 W85 L86 V87 E88 R89 W90 E91 P94 W95 G96 K97 E98 G99 Q100 W104 L107 L110 N111 A112 D113 D114 F115 P116 P117 A118 N119 E120 P121 V122 I123 A124 K125 L126 K127 R128 L129

4.2.4 Score per residue for model 4

- Molecule 1: Mutator mutT protein

Chain A: 27% 40% 23% • 7%

M1 K2 K3 L4 Q5 I6 A7 V8 G9 I10 I11 R12 N13 E14 I18 F19 I20 T21 R22 R23 A24 A25 D26 A27 H28 M29 A30 N31 K32 L33 E34 F35 P36 G37 G38 K39 I40 E41 M42 G43 E44 T45 P46 E47 Q48 A49 V50 V51 R52 E53 L54 Q55 E56 E57 V58 G59 I60 T61 P62

Q63 H64 F65 S66 L67 F68 E69 K70 L71 E72 Y73 E74 F75 P76 D77 R78 H79 I80 T81 L82 W83 F84 W85 L86 V87 E88 R89 W90 P94 W95 G96 K97 E98 W104 M105 S106 L107 L110 N111 A112 D113 D114 F115 P116 P117 A118 N119 E120 P121 V122 I123 L126 K127 R128 L129

4.2.5 Score per residue for model 5

- Molecule 1: Mutator mutT protein

Chain A: 26% 41% 24% • 7%

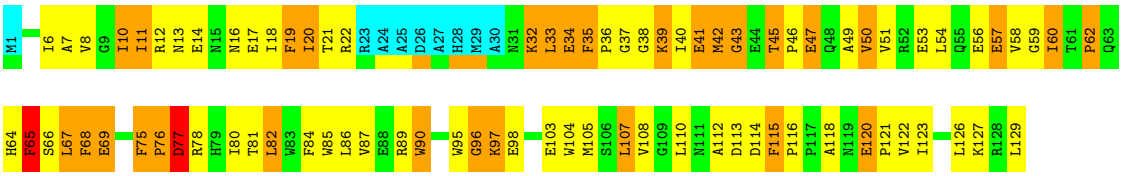
M1 K2 K3 L4 Q5 I6 A7 I10 I11 R12 N13 N16 E17 I18 F19 I20 T21 R22 R23 A24 A25 D26 A27 H28 M29 A30 N31 K32 L33 E34 F35 P36 G37 G38 K39 I40 E41 M42 G43 E44 T45 P46 E47 Q48 A49 V50 V51 R52 E53 L54 Q55 E56 E57 V58 G59 I60 T61 P62

Q63 H64 F65 S66 L67 F68 E69 K70 L71 F75 P76 D77 R78 H79 I80 T81 L82 W83 F84 W85 L86 V87 E88 R89 W90 P94 W95 G96 K97 Q100 W104 M105 S106 L107 L110 N111 A112 D113 D114 F115 P116 P117 A118 N119 E120 P121 V122 I123 L126 L129

4.2.6 Score per residue for model 6

- Molecule 1: Mutator mutT protein

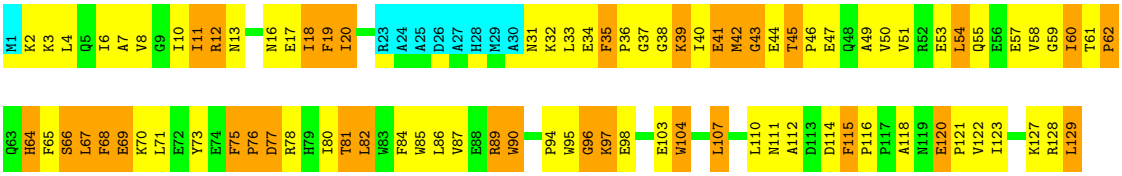
Chain A: 29% 40% 23% • 7%



4.2.7 Score per residue for model 7

- Molecule 1: Mutator mutT protein

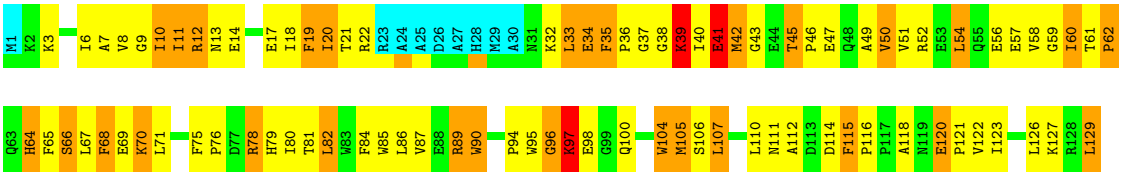
Chain A: 25% 43% 26% 7%



4.2.8 Score per residue for model 8

- Molecule 1: Mutator mutT protein

Chain A: 25% 43% 22% • 7%



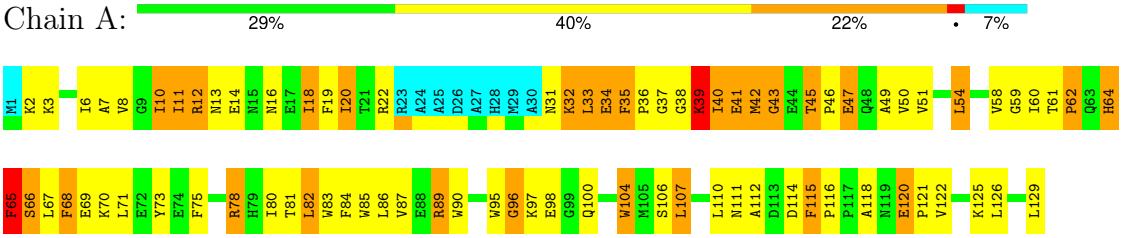
4.2.9 Score per residue for model 9

- Molecule 1: Mutator mutT protein

Chain A: 22% 47% 22% • 7%

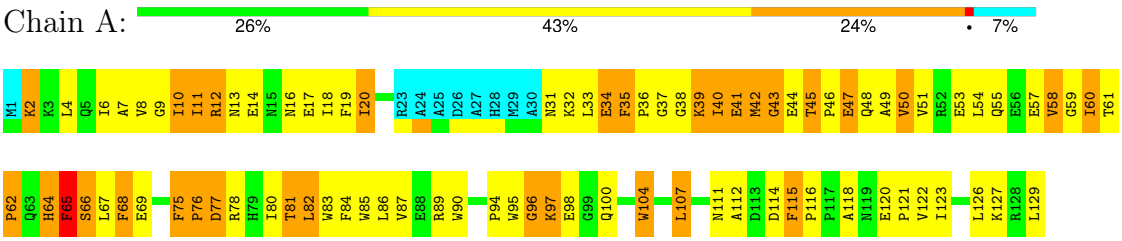
4.2.10 Score per residue for model 10

- Molecule 1: Mutator mutT protein



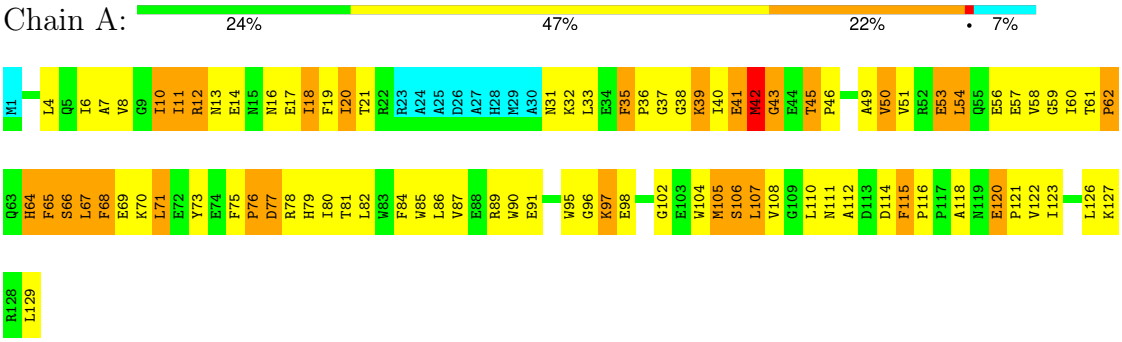
4.2.11 Score per residue for model 11

- Molecule 1: Mutator mutT protein



4.2.12 Score per residue for model 12

- Molecule 1: Mutator mutT protein



4.2.13 Score per residue for model 13

- Molecule 1: Mutator mutT protein

Chain A: 28% 40% 24% • 7%

M1 L4 Q5 I6 A7 V8 G9 I10 I11 R12 N13 E17 I18 F19 I20 T21 R22 R23 A24 A25 D26 A27 H28 M29 A30 N31 K32 L33 E34 F35 P36 G37 G38 K39 I40 E41 M42 G43 E44 T45 P46 E47 Q48 A49 V50 V51 R52 E53 L54 Q55 E56 E57 V58 G59 I60 T61 P62 Q63

H64 F65 S66 L67 F68 E69 K70 L71 F75 P76 D77 R78 H79 I80 T81 F84 W85 L86 V87 E88 R89 W90 P94 W95 G96 K97 W104 M105 S106 L107 V108 G109 L110 N111 A112 D113 D114 F115 P116 N119 E120 P121 V122 I123 L126 K127 R128 L129

4.2.14 Score per residue for model 14

- Molecule 1: Mutator mutT protein

Chain A: 26% 50% 16% • 7%

M1 K2 K3 L4 Q5 I6 A7 V8 G9 I10 I11 R12 N13 E17 I18 F19 I20 T21 R22 R23 A24 A25 D26 A27 H28 M29 A30 N31 K32 L33 E34 F35 P36 G37 G38 K39 I40 E41 M42 G43 E44 T45 P46 A49 V50 V51 L54 Q55 E56 E57 V58 G59 I60 T61 P62 Q63 H64

F65 S66 L67 F68 E69 K70 L71 E72 Y73 E74 F75 R78 H79 I80 T81 L82 W83 F84 W85 L86 V87 E88 R89 W90 E91 G92 E93 P94 W95 G96 K97 E98 W104 M105 S106 L107 V108 G109 L110 N111 D114 F115 P116 P117 A118 N119 E120 P121 V122 I123 L126 K127 R128 L129

4.2.15 Score per residue for model 15

- Molecule 1: Mutator mutT protein

Chain A: 25% 42% 24% • 7%

M1 K2 K3 L4 Q5 I6 A7 V8 G9 I10 I11 R12 N13 E17 I18 F19 I20 T21 R22 R23 A24 A25 D26 A27 H28 M29 A30 N31 K32 L33 E34 F35 P36 G37 G38 K39 I40 E41 M42 G43 E44 T45 P46 E47 Q48 A49 V50 V51 R52 E53 L54 Q55 E56 E57 V58 G59 I60 T61 P62

Q63 H64 F65 S66 L67 F68 E69 K70 L71 E72 Y73 E74 F75 P76 D77 R78 H79 I80 T81 L82 W83 F84 W85 L86 V87 E88 R89 W90 E93 P94 W95 G96 K97 W104 L107 L110 N111 A112 D113 D114 F115 A118 N119 E120 P121 V122 I123 L126 K127 R128 L129

4.2.16 Score per residue for model 16

- Molecule 1: Mutator mutT protein

Chain A: 22% 47% 22% • 7%

M1 K2 K3 L4 Q5 I6 A7 V8 G9 I10 I11 R12 N13 E14 N15 N16 E17 I18 F19 I20 T21 R22 R23 A24 A25 D26 A27 H28 M29 A30 N31 K32 L33 E34 F35 P36 G37 G38 K39 I40 E41 M42 G43 E44 T45 P46 E47 Q48 A49 V50 V51 R52 E53 L54 Q55 E56 E57 V58 G59 I60

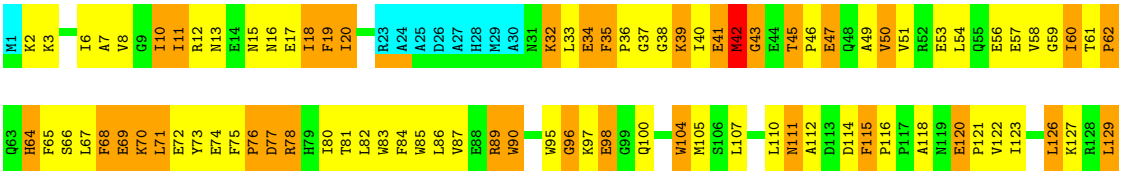
T61 P62 Q63 H64 F65 S66 L67 F68 E69 K70 L71 E72 Y73 R78 H79 I80 T81 L82 W83 F84 W85 L86 V87 E88 R89 W90 E93 P94 W95 G96 K97 E98 G99 Q100 W104 M105 S106 L107 N111 A112 D113 D114 F115 P116 P117 A118 N119 E120 P121 V122 I123 A124 K125 L126 K127 R128

L129

4.2.17 Score per residue for model 17

- Molecule 1: Mutator mutT protein

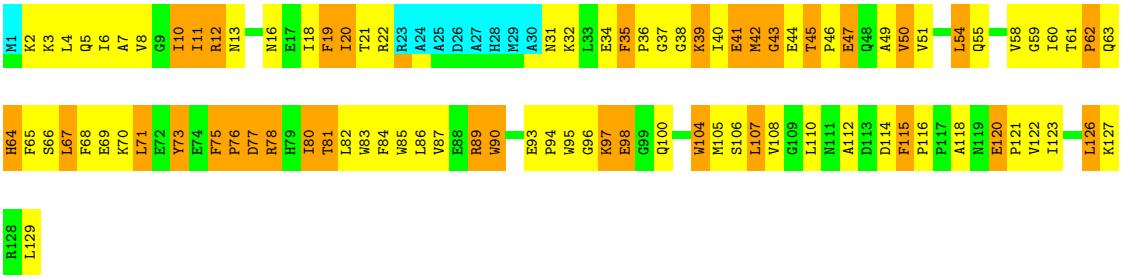
Chain A: 24% 42% 26% • 7%



4.2.18 Score per residue for model 18

- Molecule 1: Mutator mutT protein

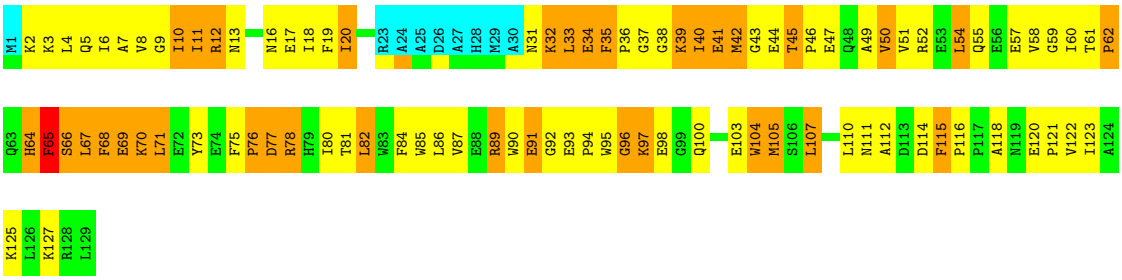
Chain A: 22% 45% 26% 7%



4.2.19 Score per residue for model 19

- Molecule 1: Mutator mutT protein

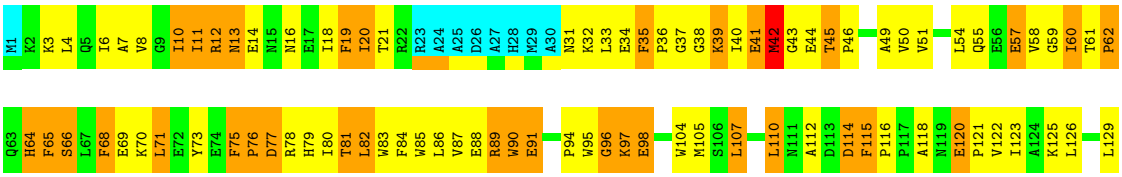
Chain A: 20% 45% 27% • 7%



4.2.20 Score per residue for model 20

- Molecule 1: Mutator mutT protein

Chain A: 25% 41% 26% • 7%


M1
K2
K3
L4
Q5
I6
A7
V8
G9
I10
I11
R12
N13
E14
N15
N16
E17
I18
F19
I20
T21
R22
R23
A24
A25
D26
A27
H28
M29
A30
N31
K32
L33
E34
F35
P36
G37
G38
K39
I40
E41
M42
G43
E44
T45
P46
A49
V50
V51
L54
Q55
E56
E57
V58
G59
I60
T61
P62
Q63
H64
F65
S66
L67
F68
E69
K70
L71
E72
Y73
E74
F75
P76
D77
R78
H79
I80
T81
L82
W83
F84
W85
L86
V87
E88
R89
W90
E91
P94
W95
G96
K97
E98
W104
M105
S106
L107
L110
N111
A112
D113
D114
F115
P116
P117
A118
N119
E120
P121
V122
I123
A124
K125
L126
L129

5 Refinement protocol and experimental data overview (i)

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

Of the 50 calculated structures, 20 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
CNS	structure solution	1.1
CNS	refinement	1.1

No chemical shift data was provided.

6 Model quality (i)

6.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 8OG, MG

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	989	973	971	125±8
3	A	24	12	12	15±3
All	All	20320	19780	19660	2580

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 65.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:7:ALA:HB3	1:A:40:ILE:HG21	1.06	1.16	10	20
1:A:10:ILE:HG22	1:A:18:ILE:HG21	1.06	1.12	9	17
1:A:71:LEU:HD11	1:A:122:VAL:HG22	1.01	1.25	9	5
1:A:40:ILE:HD12	1:A:49:ALA:HB1	0.98	1.30	15	17
1:A:58:VAL:HG12	1:A:60:ILE:HG22	0.97	1.35	19	4
1:A:64:HIS:CD2	1:A:87:VAL:HG22	0.95	1.97	5	6
1:A:4:LEU:HD12	1:A:6:ILE:HD11	0.90	1.39	12	6
1:A:58:VAL:HG12	1:A:60:ILE:HD11	0.89	1.43	16	2
1:A:80:ILE:HD12	3:A:131:8OG:C4	0.88	1.98	14	16
1:A:64:HIS:ND1	1:A:87:VAL:HG22	0.88	1.84	8	8
1:A:54:LEU:O	1:A:58:VAL:HG23	0.88	1.68	9	9

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:107:LEU:HD21	1:A:110:LEU:HD12	0.86	1.46	10	1
1:A:54:LEU:HD11	1:A:64:HIS:CE1	0.85	2.07	3	9
1:A:40:ILE:HD12	1:A:49:ALA:CB	0.84	2.02	15	16
1:A:7:ALA:HB2	1:A:40:ILE:HD13	0.84	1.47	4	17
1:A:54:LEU:HD21	1:A:64:HIS:CD2	0.84	2.08	20	15
1:A:84:PHE:CD1	1:A:122:VAL:HG11	0.84	2.07	12	6
1:A:84:PHE:CE2	1:A:122:VAL:HG11	0.82	2.09	18	14
1:A:64:HIS:CE1	1:A:87:VAL:HG22	0.82	2.09	19	16
1:A:10:ILE:CG2	1:A:18:ILE:HG21	0.82	2.02	9	18
1:A:54:LEU:HD11	1:A:64:HIS:NE2	0.82	1.90	10	9
1:A:58:VAL:HG12	1:A:60:ILE:CD1	0.82	2.05	9	2
1:A:7:ALA:HB1	1:A:50:VAL:HG12	0.81	1.52	3	10
1:A:82:LEU:HD23	1:A:122:VAL:CG2	0.80	2.06	5	2
1:A:58:VAL:HG12	1:A:60:ILE:HG13	0.80	1.53	3	9
1:A:10:ILE:HG22	1:A:18:ILE:CG2	0.80	2.05	2	15
1:A:84:PHE:CZ	1:A:122:VAL:HG11	0.79	2.12	7	11
1:A:110:LEU:HD11	1:A:123:ILE:CG2	0.78	2.08	20	1
1:A:68:PHE:CD1	1:A:126:LEU:HD23	0.78	2.12	18	2
1:A:84:PHE:CE1	1:A:122:VAL:HG11	0.77	2.13	12	11
1:A:82:LEU:HD12	1:A:84:PHE:CE1	0.77	2.13	10	5
1:A:10:ILE:HD11	1:A:68:PHE:CE2	0.77	2.13	18	2
1:A:7:ALA:HB3	1:A:40:ILE:CG2	0.77	2.06	11	18
1:A:68:PHE:CE2	1:A:126:LEU:HD22	0.77	2.13	5	1
1:A:6:ILE:HD13	3:A:131:8OG:H4'	0.77	1.56	4	3
1:A:4:LEU:CD1	1:A:6:ILE:HD11	0.77	2.10	9	6
1:A:118:ALA:HB1	3:A:131:8OG:O6	0.76	1.78	4	18
1:A:10:ILE:HD12	1:A:18:ILE:HD13	0.76	1.56	7	1
1:A:126:LEU:O	1:A:126:LEU:HD13	0.76	1.80	2	12
1:A:107:LEU:O	1:A:107:LEU:HD13	0.75	1.81	17	12
1:A:84:PHE:CE1	1:A:122:VAL:HG21	0.75	2.15	10	4
1:A:20:ILE:HG22	1:A:34:GLU:O	0.75	1.81	15	8
1:A:54:LEU:HD21	1:A:64:HIS:NE2	0.75	1.97	15	7
1:A:84:PHE:CD2	1:A:122:VAL:HG11	0.75	2.16	9	12
1:A:4:LEU:HD13	3:A:131:8OG:O4'	0.75	1.82	5	3
1:A:58:VAL:HG13	1:A:60:ILE:HD12	0.75	1.59	11	1
1:A:45:THR:HG22	1:A:46:PRO:HD2	0.75	1.57	18	20
1:A:64:HIS:CB	1:A:87:VAL:HG13	0.74	2.12	19	20
1:A:71:LEU:HD11	1:A:122:VAL:CG2	0.74	2.11	9	4
1:A:10:ILE:HD12	1:A:85:TRP:O	0.74	1.82	17	2
3:A:131:8OG:OP1	3:A:131:8OG:O3'	0.74	2.05	19	16
1:A:60:ILE:HD11	1:A:91:GLU:O	0.74	1.83	19	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:86:LEU:HD23	1:A:87:VAL:N	0.73	1.98	4	1
1:A:50:VAL:HG11	1:A:85:TRP:NE1	0.73	1.98	14	11
1:A:37:GLY:O	1:A:40:ILE:HG23	0.73	1.83	10	18
1:A:11:ILE:O	1:A:18:ILE:HG23	0.73	1.82	9	16
1:A:54:LEU:HD21	1:A:64:HIS:CG	0.73	2.18	3	5
1:A:64:HIS:HB2	1:A:87:VAL:HG13	0.72	1.61	20	20
1:A:71:LEU:HD21	1:A:73:TYR:CD1	0.72	2.18	20	3
1:A:10:ILE:HD12	1:A:35:PHE:CD2	0.72	2.19	9	1
1:A:11:ILE:HG23	1:A:87:VAL:HG11	0.72	1.60	19	8
1:A:33:LEU:HD13	1:A:111:ASN:HB3	0.72	1.60	2	4
1:A:50:VAL:HG11	1:A:85:TRP:CZ2	0.72	2.20	9	9
1:A:128:ARG:O	1:A:129:LEU:HD12	0.72	1.85	7	3
1:A:40:ILE:HB	1:A:49:ALA:HB1	0.71	1.61	13	14
1:A:73:TYR:OH	1:A:80:ILE:HD13	0.71	1.85	12	7
1:A:6:ILE:HD11	3:A:131:8OG:O4'	0.70	1.86	20	5
1:A:110:LEU:HD23	1:A:123:ILE:HG23	0.70	1.63	9	1
3:A:131:8OG:P	3:A:131:8OG:H3'	0.70	2.26	5	19
1:A:123:ILE:HG22	1:A:127:LYS:HB2	0.69	1.64	9	12
1:A:7:ALA:CB	1:A:50:VAL:HG12	0.69	2.18	1	13
1:A:18:ILE:CG2	1:A:107:LEU:HD23	0.69	2.18	7	3
1:A:21:THR:O	1:A:33:LEU:HD12	0.69	1.88	12	3
1:A:20:ILE:HD12	1:A:33:LEU:HD21	0.68	1.63	9	3
1:A:10:ILE:HG23	1:A:35:PHE:CD2	0.68	2.23	11	13
1:A:71:LEU:CD1	1:A:122:VAL:HG22	0.68	2.12	9	2
1:A:126:LEU:O	1:A:129:LEU:HD22	0.68	1.88	17	4
1:A:107:LEU:CD2	1:A:110:LEU:HD12	0.68	2.17	10	1
1:A:71:LEU:HD22	1:A:72:GLU:N	0.68	2.04	17	1
1:A:22:ARG:HB3	1:A:33:LEU:HD12	0.68	1.62	5	1
1:A:47:GLU:O	1:A:51:VAL:HG23	0.67	1.90	10	15
1:A:82:LEU:HD23	1:A:122:VAL:HG23	0.67	1.64	5	2
1:A:60:ILE:O	1:A:62:PRO:HD3	0.67	1.90	10	5
1:A:67:LEU:HA	1:A:85:TRP:HA	0.67	1.65	18	11
1:A:58:VAL:O	1:A:60:ILE:HG23	0.67	1.90	1	1
1:A:126:LEU:O	1:A:129:LEU:HD12	0.67	1.90	6	4
1:A:54:LEU:HD11	1:A:64:HIS:HE2	0.67	1.47	8	3
1:A:78:ARG:NH2	3:A:131:8OG:N1	0.67	2.43	5	20
1:A:110:LEU:HD23	1:A:123:ILE:HD12	0.67	1.67	18	4
1:A:60:ILE:HD11	1:A:94:PRO:HA	0.67	1.65	9	7
1:A:67:LEU:HD11	1:A:70:LYS:HG2	0.67	1.64	5	2
1:A:10:ILE:HG22	1:A:18:ILE:HG12	0.66	1.66	17	3
1:A:60:ILE:HD11	1:A:91:GLU:C	0.66	2.10	12	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:54:LEU:HD11	1:A:64:HIS:CD2	0.66	2.26	13	2
1:A:82:LEU:HG	1:A:122:VAL:HG21	0.65	1.67	15	1
1:A:60:ILE:HG23	1:A:95:TRP:CD1	0.65	2.26	15	2
1:A:5:GLN:C	1:A:6:ILE:HD12	0.65	2.11	3	3
1:A:54:LEU:HD21	1:A:64:HIS:CE1	0.65	2.27	5	1
1:A:71:LEU:HD22	1:A:73:TYR:CE2	0.65	2.25	18	1
1:A:21:THR:HG22	1:A:98:GLU:OE2	0.64	1.92	20	5
1:A:71:LEU:HD21	1:A:122:VAL:HG22	0.64	1.66	1	2
1:A:71:LEU:HB2	1:A:122:VAL:HG22	0.64	1.69	2	2
1:A:80:ILE:HD13	3:A:131:8OG:C4	0.64	2.22	18	1
1:A:7:ALA:CB	1:A:40:ILE:HD13	0.64	2.21	15	15
1:A:22:ARG:CG	1:A:33:LEU:HD13	0.64	2.22	4	2
1:A:2:LYS:CE	1:A:4:LEU:HD23	0.64	2.22	11	1
1:A:107:LEU:HD11	1:A:110:LEU:HD22	0.64	1.70	18	4
1:A:60:ILE:HG21	1:A:93:GLU:O	0.63	1.93	15	3
1:A:64:HIS:CG	1:A:87:VAL:HG22	0.63	2.28	4	9
1:A:22:ARG:CB	1:A:33:LEU:HD13	0.63	2.23	4	2
1:A:50:VAL:HG11	1:A:85:TRP:CE2	0.63	2.28	9	19
1:A:13:ASN:HB3	1:A:90:TRP:CH2	0.63	2.29	7	6
1:A:12:ARG:O	1:A:89:ARG:HA	0.63	1.94	19	4
1:A:11:ILE:HD11	1:A:36:PRO:HG3	0.62	1.72	13	4
1:A:11:ILE:HG22	1:A:90:TRP:CE3	0.62	2.29	15	16
1:A:38:GLY:O	1:A:39:LYS:CB	0.62	2.48	15	18
1:A:62:PRO:CB	1:A:90:TRP:HA	0.62	2.25	2	18
1:A:10:ILE:HG21	1:A:107:LEU:CD2	0.62	2.24	2	2
1:A:7:ALA:CB	1:A:40:ILE:HG21	0.62	2.10	5	3
1:A:68:PHE:CE2	1:A:126:LEU:HD12	0.62	2.30	17	1
1:A:110:LEU:HD11	1:A:123:ILE:HG21	0.62	1.70	20	1
1:A:54:LEU:HD21	1:A:64:HIS:ND1	0.62	2.10	5	1
1:A:22:ARG:HA	1:A:33:LEU:HD12	0.61	1.72	13	1
1:A:33:LEU:HD13	1:A:111:ASN:CB	0.61	2.26	9	4
1:A:71:LEU:HD13	1:A:71:LEU:N	0.61	2.10	9	1
1:A:58:VAL:HG11	1:A:62:PRO:HG3	0.61	1.71	4	8
1:A:22:ARG:HD2	1:A:33:LEU:HD22	0.61	1.73	4	1
1:A:60:ILE:HD11	1:A:94:PRO:CA	0.61	2.25	20	3
1:A:60:ILE:HD13	1:A:90:TRP:HB2	0.61	1.72	12	1
1:A:72:GLU:HG3	1:A:81:THR:HG22	0.60	1.72	15	1
1:A:58:VAL:N	1:A:96:GLY:HA3	0.60	2.11	19	17
1:A:22:ARG:CB	1:A:33:LEU:HD12	0.60	2.26	5	1
1:A:71:LEU:HD23	1:A:73:TYR:CD1	0.60	2.31	19	2
1:A:58:VAL:CG1	1:A:60:ILE:HG22	0.60	2.25	12	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:82:LEU:HD23	1:A:122:VAL:HG21	0.60	1.72	3	3
1:A:72:GLU:CG	1:A:81:THR:HG22	0.60	2.27	15	1
1:A:67:LEU:HD13	1:A:70:LYS:HD3	0.60	1.74	1	1
1:A:80:ILE:CG2	3:A:131:8OG:N2	0.60	2.65	11	18
1:A:58:VAL:HG13	1:A:94:PRO:HB3	0.60	1.74	13	1
3:A:131:8OG:OP2	3:A:131:8OG:O8	0.59	2.20	15	3
1:A:68:PHE:CE2	1:A:84:PHE:HB3	0.59	2.32	18	3
1:A:10:ILE:O	1:A:87:VAL:HB	0.59	1.97	15	18
1:A:71:LEU:HD21	1:A:122:VAL:HA	0.59	1.73	4	3
1:A:8:VAL:HB	1:A:36:PRO:O	0.59	1.97	15	17
1:A:120:GLU:N	1:A:121:PRO:CD	0.59	2.66	18	20
1:A:67:LEU:HD23	1:A:67:LEU:O	0.59	1.97	2	4
1:A:110:LEU:HD22	1:A:123:ILE:CD1	0.59	2.28	15	1
1:A:71:LEU:HD21	1:A:122:VAL:CG2	0.59	2.28	1	1
1:A:69:GLU:O	1:A:84:PHE:HB2	0.59	1.96	19	10
1:A:10:ILE:HD11	1:A:68:PHE:CD2	0.59	2.32	18	2
1:A:18:ILE:HG21	1:A:107:LEU:HD23	0.59	1.75	12	3
1:A:65:PHE:O	1:A:86:LEU:O	0.59	2.21	14	16
1:A:80:ILE:HD12	3:A:131:8OG:N3	0.59	2.12	7	10
1:A:80:ILE:HD11	1:A:82:LEU:HD13	0.59	1.74	14	4
1:A:7:ALA:HB2	1:A:40:ILE:CD1	0.58	2.28	9	11
1:A:126:LEU:CD2	1:A:129:LEU:HD13	0.58	2.28	2	3
1:A:20:ILE:HG22	1:A:35:PHE:HA	0.58	1.74	20	2
1:A:64:HIS:NE2	1:A:87:VAL:HG22	0.58	2.13	6	2
1:A:18:ILE:HD12	1:A:107:LEU:HB2	0.58	1.76	19	3
1:A:110:LEU:CD2	1:A:126:LEU:HD12	0.58	2.28	20	2
1:A:10:ILE:HG23	1:A:35:PHE:CD1	0.58	2.33	15	2
1:A:66:SER:HB3	1:A:86:LEU:HD21	0.58	1.75	17	1
1:A:107:LEU:HD11	1:A:126:LEU:HD11	0.58	1.73	17	1
1:A:33:LEU:O	1:A:33:LEU:HD23	0.58	1.96	6	2
1:A:80:ILE:HD12	3:A:131:8OG:C5	0.58	2.29	20	3
1:A:17:GLU:C	1:A:18:ILE:HD12	0.58	2.19	15	1
1:A:71:LEU:CB	1:A:122:VAL:HG22	0.58	2.28	16	4
1:A:86:LEU:HD13	1:A:87:VAL:N	0.57	2.13	1	1
1:A:6:ILE:HD13	1:A:80:ILE:HG13	0.57	1.74	3	1
1:A:50:VAL:O	1:A:54:LEU:HB2	0.57	1.99	14	5
1:A:10:ILE:HB	1:A:18:ILE:HD13	0.57	1.73	19	3
1:A:37:GLY:O	1:A:40:ILE:CG2	0.57	2.52	19	18
1:A:18:ILE:HB	1:A:107:LEU:HD23	0.57	1.75	3	6
1:A:82:LEU:CD2	1:A:122:VAL:HG21	0.57	2.29	8	2
1:A:35:PHE:CD1	1:A:35:PHE:N	0.57	2.68	13	17

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:131:8OG:H3'	3:A:131:8OG:OP2	0.57	2.00	20	12
1:A:110:LEU:HD11	1:A:123:ILE:HG23	0.57	1.77	20	1
1:A:40:ILE:CD1	1:A:49:ALA:HB1	0.57	2.30	6	11
1:A:64:HIS:CG	1:A:87:VAL:HG13	0.57	2.35	6	10
1:A:35:PHE:CZ	1:A:110:LEU:HD13	0.57	2.34	15	1
1:A:60:ILE:HG22	1:A:95:TRP:CD1	0.57	2.35	1	1
1:A:18:ILE:HG22	1:A:107:LEU:HD23	0.56	1.76	7	1
1:A:19:PHE:CD1	1:A:19:PHE:C	0.56	2.78	20	2
1:A:6:ILE:HB	1:A:82:LEU:HD23	0.56	1.76	1	3
1:A:13:ASN:CB	1:A:90:TRP:CH2	0.56	2.88	20	8
1:A:71:LEU:HB3	1:A:122:VAL:HG22	0.56	1.76	20	4
1:A:6:ILE:HB	1:A:82:LEU:HD22	0.56	1.76	19	1
1:A:106:SER:HB2	1:A:108:VAL:HG12	0.56	1.78	13	3
1:A:4:LEU:HD12	1:A:4:LEU:O	0.56	2.00	13	5
1:A:54:LEU:O	1:A:58:VAL:CG2	0.56	2.53	16	1
1:A:68:PHE:CD1	1:A:69:GLU:N	0.55	2.74	14	20
1:A:110:LEU:HD22	1:A:123:ILE:HD12	0.55	1.77	8	5
1:A:10:ILE:HD12	1:A:18:ILE:CD1	0.55	2.29	7	1
1:A:41:GLU:O	1:A:43:GLY:N	0.55	2.39	15	18
1:A:76:PRO:O	1:A:77:ASP:CB	0.55	2.54	7	16
1:A:90:TRP:CD1	1:A:90:TRP:O	0.55	2.59	20	16
1:A:10:ILE:HG23	1:A:35:PHE:CE1	0.55	2.36	15	1
1:A:6:ILE:HB	1:A:82:LEU:HD12	0.55	1.77	5	4
1:A:84:PHE:CG	1:A:122:VAL:HG11	0.55	2.36	9	7
1:A:11:ILE:HG22	1:A:90:TRP:HE3	0.55	1.60	5	15
1:A:60:ILE:HG21	1:A:91:GLU:O	0.55	2.01	3	2
1:A:10:ILE:HD12	1:A:35:PHE:CE2	0.55	2.37	9	2
1:A:61:THR:HG23	1:A:91:GLU:CB	0.55	2.32	3	1
1:A:66:SER:O	1:A:86:LEU:N	0.55	2.41	20	5
1:A:71:LEU:HD22	1:A:122:VAL:HG23	0.55	1.78	7	2
1:A:62:PRO:HB3	1:A:90:TRP:CB	0.55	2.32	12	4
1:A:8:VAL:HG11	1:A:84:PHE:CE1	0.54	2.37	9	1
1:A:110:LEU:HD23	1:A:126:LEU:HD12	0.54	1.79	20	2
1:A:112:ALA:HA	1:A:115:PHE:CD1	0.54	2.38	13	15
1:A:40:ILE:HG13	1:A:41:GLU:N	0.54	2.18	10	20
1:A:71:LEU:HD22	1:A:71:LEU:O	0.54	2.03	9	1
1:A:13:ASN:ND2	1:A:90:TRP:CZ2	0.54	2.76	19	5
1:A:41:GLU:O	1:A:42:MET:C	0.54	2.46	10	18
1:A:6:ILE:HD12	1:A:80:ILE:HD11	0.54	1.79	20	3
1:A:107:LEU:HD21	1:A:110:LEU:CD1	0.54	2.28	10	1
1:A:59:GLY:HA3	1:A:95:TRP:CZ2	0.54	2.38	20	20

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:62:PRO:CB	1:A:89:ARG:O	0.54	2.56	3	2
1:A:21:THR:HG23	1:A:36:PRO:HD3	0.54	1.78	9	1
1:A:71:LEU:HD22	1:A:71:LEU:C	0.54	2.22	17	1
1:A:6:ILE:HD12	1:A:82:LEU:HD13	0.54	1.79	5	1
1:A:7:ALA:O	1:A:37:GLY:C	0.53	2.46	20	17
1:A:64:HIS:CE1	1:A:87:VAL:CG2	0.53	2.91	2	14
1:A:6:ILE:HD12	1:A:80:ILE:CD1	0.53	2.34	20	2
1:A:20:ILE:CG2	1:A:35:PHE:CD2	0.53	2.91	9	15
3:A:131:8OG:C3'	3:A:131:8OG:P	0.53	2.97	8	16
1:A:20:ILE:HD11	1:A:105:MET:SD	0.53	2.43	19	1
1:A:59:GLY:HA3	1:A:95:TRP:CE2	0.53	2.39	15	18
1:A:6:ILE:CG2	1:A:82:LEU:HD13	0.53	2.34	10	1
1:A:8:VAL:HG21	1:A:35:PHE:HB2	0.53	1.81	15	1
1:A:50:VAL:CG2	1:A:51:VAL:N	0.53	2.72	3	16
1:A:78:ARG:NH2	3:A:131:8OG:C6	0.53	2.72	18	19
1:A:7:ALA:O	1:A:37:GLY:HA3	0.53	2.04	9	2
1:A:73:TYR:CZ	1:A:80:ILE:HD13	0.53	2.39	12	1
1:A:108:VAL:HG23	1:A:129:LEU:HD21	0.53	1.81	14	1
1:A:107:LEU:CD1	1:A:126:LEU:HD11	0.53	2.34	13	1
1:A:62:PRO:HB2	1:A:89:ARG:O	0.52	2.05	20	6
1:A:67:LEU:HD13	1:A:70:LYS:CD	0.52	2.34	19	2
1:A:54:LEU:O	1:A:58:VAL:HB	0.52	2.04	11	3
1:A:8:VAL:HG21	1:A:35:PHE:CB	0.52	2.35	15	1
1:A:118:ALA:CB	3:A:131:8OG:O6	0.52	2.57	15	12
1:A:12:ARG:HG2	1:A:18:ILE:HD11	0.52	1.82	15	1
1:A:10:ILE:HG23	1:A:35:PHE:HD2	0.52	1.63	19	5
1:A:4:LEU:HD12	1:A:6:ILE:CD1	0.52	2.25	12	5
1:A:127:LYS:O	1:A:129:LEU:HD13	0.52	2.05	12	1
1:A:98:GLU:H	1:A:98:GLU:CD	0.52	2.08	17	1
1:A:86:LEU:O	1:A:86:LEU:HD13	0.52	2.05	12	1
1:A:64:HIS:CD2	1:A:64:HIS:C	0.51	2.83	10	13
1:A:115:PHE:CE2	1:A:123:ILE:HG13	0.51	2.40	13	8
1:A:126:LEU:HD13	1:A:126:LEU:C	0.51	2.26	1	8
1:A:10:ILE:HD13	1:A:10:ILE:N	0.51	2.21	9	4
1:A:80:ILE:CG2	3:A:131:8OG:C2	0.51	2.88	20	20
1:A:50:VAL:O	1:A:54:LEU:N	0.51	2.44	16	11
1:A:13:ASN:CG	1:A:14:GLU:N	0.51	2.64	6	2
1:A:11:ILE:HA	1:A:87:VAL:HB	0.51	1.82	11	4
1:A:68:PHE:CD1	1:A:126:LEU:HD13	0.51	2.41	14	1
1:A:10:ILE:HG22	1:A:18:ILE:CG1	0.51	2.35	17	2
1:A:64:HIS:HB2	1:A:87:VAL:CG1	0.51	2.35	19	15

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:19:PHE:CD1	1:A:19:PHE:O	0.51	2.63	19	9
1:A:59:GLY:CA	1:A:95:TRP:CZ2	0.51	2.94	18	18
1:A:110:LEU:HD21	1:A:123:ILE:HD12	0.51	1.83	9	1
1:A:35:PHE:CZ	1:A:110:LEU:HD11	0.51	2.41	6	2
1:A:123:ILE:O	1:A:127:LYS:CB	0.51	2.59	7	9
1:A:21:THR:HG22	1:A:98:GLU:OE1	0.51	2.05	3	1
1:A:71:LEU:HD12	1:A:71:LEU:O	0.51	2.06	8	3
1:A:71:LEU:CD2	1:A:122:VAL:HG22	0.51	2.35	1	1
1:A:95:TRP:CE3	1:A:96:GLY:N	0.51	2.79	1	15
1:A:58:VAL:HG12	1:A:60:ILE:CG1	0.51	2.34	3	1
1:A:75:PHE:O	1:A:77:ASP:N	0.50	2.44	15	16
1:A:56:GLU:O	1:A:97:LYS:N	0.50	2.44	9	6
1:A:7:ALA:O	1:A:37:GLY:O	0.50	2.29	14	18
1:A:20:ILE:HG21	1:A:35:PHE:CD2	0.50	2.41	18	3
1:A:22:ARG:HB2	1:A:33:LEU:HD13	0.50	1.82	4	2
1:A:71:LEU:HD21	1:A:122:VAL:CA	0.50	2.37	15	1
1:A:45:THR:CG2	1:A:46:PRO:HD2	0.50	2.33	18	3
1:A:80:ILE:HG21	3:A:131:8OG:C2	0.50	2.37	20	12
1:A:35:PHE:CZ	1:A:110:LEU:CD1	0.50	2.94	15	2
1:A:57:GLU:C	1:A:96:GLY:HA3	0.50	2.26	12	5
1:A:5:GLN:O	1:A:6:ILE:HD13	0.50	2.07	14	1
1:A:110:LEU:HD23	1:A:111:ASN:N	0.50	2.22	17	1
1:A:60:ILE:HD11	1:A:90:TRP:HB2	0.50	1.83	1	1
1:A:86:LEU:HD13	1:A:86:LEU:C	0.50	2.26	12	2
1:A:80:ILE:HG22	3:A:131:8OG:N2	0.50	2.21	3	14
1:A:60:ILE:HG12	1:A:93:GLU:O	0.50	2.07	9	2
1:A:104:TRP:CD1	1:A:104:TRP:N	0.50	2.80	11	15
1:A:6:ILE:HD11	3:A:131:8OG:H4'	0.50	1.83	6	4
1:A:80:ILE:CD1	3:A:131:8OG:C4	0.50	2.90	18	2
1:A:19:PHE:CD2	1:A:19:PHE:O	0.50	2.65	13	3
1:A:63:GLN:CG	1:A:63:GLN:O	0.50	2.59	16	1
1:A:67:LEU:HD22	1:A:70:LYS:HE2	0.50	1.84	17	1
1:A:10:ILE:HG21	1:A:107:LEU:HD21	0.49	1.84	19	1
1:A:86:LEU:C	1:A:86:LEU:HD13	0.49	2.27	16	2
1:A:80:ILE:HB	3:A:131:8OG:N3	0.49	2.22	13	17
1:A:110:LEU:CD2	1:A:123:ILE:HD12	0.49	2.37	1	4
1:A:67:LEU:HD12	1:A:67:LEU:O	0.49	2.07	3	1
1:A:110:LEU:HD22	1:A:123:ILE:HG23	0.49	1.84	4	2
1:A:6:ILE:HG22	1:A:82:LEU:HA	0.49	1.83	8	1
1:A:19:PHE:CB	1:A:90:TRP:CH2	0.49	2.96	7	5
1:A:40:ILE:HA	1:A:53:GLU:HG3	0.49	1.84	11	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:10:ILE:CB	1:A:18:ILE:HG21	0.49	2.38	5	6
1:A:82:LEU:HD23	1:A:84:PHE:CE1	0.49	2.42	11	1
1:A:68:PHE:O	1:A:69:GLU:CG	0.49	2.60	14	2
1:A:12:ARG:HB2	1:A:87:VAL:O	0.48	2.07	4	5
1:A:2:LYS:HE3	1:A:4:LEU:HD23	0.48	1.85	11	1
1:A:67:LEU:C	1:A:86:LEU:HD23	0.48	2.28	17	1
1:A:13:ASN:ND2	1:A:90:TRP:CH2	0.48	2.81	16	4
1:A:115:PHE:C	1:A:115:PHE:CD1	0.48	2.87	20	4
1:A:13:ASN:HA	1:A:90:TRP:CZ3	0.48	2.43	6	1
1:A:71:LEU:CD2	1:A:73:TYR:CE2	0.48	2.95	18	1
1:A:110:LEU:HD12	1:A:110:LEU:C	0.48	2.29	20	1
1:A:64:HIS:CA	1:A:87:VAL:HG13	0.48	2.39	3	7
1:A:80:ILE:HD13	3:A:131:8OG:C5	0.48	2.38	18	1
1:A:54:LEU:CD2	1:A:64:HIS:CD2	0.48	2.97	4	5
1:A:71:LEU:HD12	1:A:71:LEU:C	0.48	2.29	3	4
1:A:61:THR:HG23	1:A:91:GLU:HB3	0.48	1.86	3	1
1:A:68:PHE:CD1	1:A:69:GLU:HB2	0.48	2.44	9	3
1:A:10:ILE:HG23	1:A:35:PHE:CG	0.48	2.43	13	1
1:A:115:PHE:CD1	1:A:115:PHE:C	0.48	2.87	5	12
1:A:86:LEU:HD12	1:A:86:LEU:C	0.48	2.28	18	1
1:A:67:LEU:HD12	1:A:67:LEU:C	0.48	2.29	1	7
1:A:84:PHE:CD2	1:A:122:VAL:CG1	0.48	2.97	15	9
1:A:71:LEU:HD12	1:A:122:VAL:HG22	0.48	1.86	17	1
1:A:60:ILE:HG23	1:A:95:TRP:HE1	0.48	1.69	2	2
1:A:11:ILE:HD12	1:A:19:PHE:CD2	0.48	2.43	10	1
1:A:13:ASN:OD1	1:A:17:GLU:C	0.48	2.52	11	2
1:A:22:ARG:CD	1:A:33:LEU:HD12	0.48	2.39	5	1
1:A:107:LEU:HD22	1:A:110:LEU:HD13	0.47	1.86	7	1
1:A:8:VAL:CG1	1:A:84:PHE:CE1	0.47	2.97	9	1
1:A:11:ILE:O	1:A:18:ILE:HA	0.47	2.09	13	4
1:A:115:PHE:CZ	1:A:123:ILE:HG13	0.47	2.43	18	7
1:A:71:LEU:HD23	1:A:73:TYR:CE1	0.47	2.44	10	2
1:A:6:ILE:HD11	3:A:131:8OG:C4'	0.47	2.39	11	2
1:A:82:LEU:CD1	1:A:84:PHE:CE1	0.47	2.97	20	1
1:A:40:ILE:HG22	1:A:53:GLU:CB	0.47	2.39	9	1
1:A:13:ASN:N	1:A:90:TRP:CZ3	0.47	2.83	3	8
1:A:65:PHE:O	1:A:66:SER:CB	0.47	2.62	14	4
1:A:123:ILE:O	1:A:127:LYS:N	0.47	2.45	17	6
1:A:80:ILE:HD11	1:A:82:LEU:CD2	0.47	2.38	10	2
1:A:59:GLY:C	1:A:95:TRP:CZ2	0.47	2.88	11	13
1:A:67:LEU:HD23	1:A:67:LEU:C	0.47	2.30	10	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:33:LEU:O	1:A:33:LEU:HG	0.47	2.09	15	2
1:A:33:LEU:HD13	1:A:114:ASP:HB3	0.47	1.85	13	1
1:A:66:SER:CB	1:A:86:LEU:HD21	0.47	2.40	17	1
1:A:110:LEU:HD22	1:A:123:ILE:CG2	0.47	2.39	4	2
1:A:13:ASN:CG	1:A:14:GLU:H	0.47	2.13	6	2
1:A:115:PHE:CE2	1:A:123:ILE:CG1	0.47	2.98	13	1
1:A:108:VAL:HG23	1:A:129:LEU:HD22	0.47	1.86	9	1
1:A:71:LEU:HD21	1:A:73:TYR:CE1	0.47	2.43	20	1
1:A:38:GLY:O	1:A:39:LYS:HB3	0.47	2.10	13	19
1:A:6:ILE:CD1	3:A:131:8OG:O4'	0.47	2.63	11	3
1:A:7:ALA:HB1	1:A:85:TRP:HE1	0.47	1.70	10	3
1:A:13:ASN:CG	1:A:90:TRP:CH2	0.47	2.89	2	6
1:A:6:ILE:HG12	3:A:131:8OG:H5"	0.46	1.87	3	2
1:A:19:PHE:O	1:A:19:PHE:CG	0.46	2.67	4	5
1:A:63:GLN:O	1:A:63:GLN:HG3	0.46	2.10	16	1
1:A:13:ASN:CA	1:A:90:TRP:CZ3	0.46	2.98	15	10
1:A:6:ILE:CD1	3:A:131:8OG:H4'	0.46	2.40	13	4
1:A:54:LEU:O	1:A:58:VAL:N	0.46	2.49	18	8
1:A:108:VAL:HG22	1:A:108:VAL:O	0.46	2.11	12	1
1:A:108:VAL:CG2	1:A:129:LEU:HD21	0.46	2.41	14	1
1:A:68:PHE:CD1	1:A:84:PHE:HB3	0.46	2.46	3	3
1:A:54:LEU:CD1	1:A:64:HIS:CE1	0.46	2.98	2	2
1:A:66:SER:HB3	1:A:86:LEU:HD23	0.46	1.86	7	1
1:A:65:PHE:O	1:A:66:SER:HB2	0.46	2.10	17	1
1:A:21:THR:HG22	1:A:98:GLU:CD	0.46	2.31	8	3
1:A:59:GLY:O	1:A:95:TRP:CZ2	0.46	2.68	3	2
1:A:4:LEU:HD11	3:A:131:8OG:O4'	0.46	2.11	4	1
1:A:80:ILE:CG1	1:A:82:LEU:HD13	0.46	2.39	18	1
1:A:108:VAL:HG23	1:A:129:LEU:CD2	0.46	2.39	14	1
1:A:22:ARG:HB3	1:A:33:LEU:HD13	0.46	1.88	15	1
1:A:4:LEU:HD12	1:A:80:ILE:HA	0.46	1.88	18	1
1:A:112:ALA:HB2	1:A:127:LYS:HD3	0.46	1.87	19	1
1:A:84:PHE:CE2	1:A:122:VAL:CG1	0.46	2.98	3	5
1:A:71:LEU:CD2	1:A:73:TYR:CD1	0.46	2.98	16	4
1:A:7:ALA:HB1	1:A:50:VAL:CG1	0.46	2.39	6	3
1:A:60:ILE:HG21	1:A:94:PRO:HA	0.46	1.87	1	1
3:A:131:8OG:OP1	3:A:131:8OG:C3'	0.46	2.63	19	7
1:A:4:LEU:HD13	1:A:6:ILE:HD11	0.46	1.88	18	5
1:A:33:LEU:HD23	1:A:111:ASN:CB	0.46	2.41	14	1
1:A:68:PHE:CE2	1:A:126:LEU:CD1	0.46	2.98	17	1
1:A:13:ASN:CB	1:A:17:GLU:O	0.46	2.64	16	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:120:GLU:N	1:A:121:PRO:HD2	0.46	2.25	15	16
1:A:73:TYR:CE1	1:A:80:ILE:CG2	0.46	2.99	4	1
1:A:53:GLU:O	1:A:57:GLU:N	0.46	2.49	7	3
1:A:67:LEU:HD11	1:A:70:LYS:CD	0.46	2.41	15	1
1:A:6:ILE:N	1:A:81:THR:O	0.46	2.49	20	10
1:A:35:PHE:CE1	1:A:84:PHE:CE2	0.46	3.04	17	3
1:A:50:VAL:O	1:A:54:LEU:HD13	0.46	2.10	4	1
1:A:71:LEU:CD2	1:A:73:TYR:CE1	0.46	2.99	16	2
1:A:11:ILE:HA	1:A:87:VAL:CB	0.45	2.41	19	7
1:A:89:ARG:CG	1:A:90:TRP:N	0.45	2.78	5	3
1:A:35:PHE:CE2	1:A:110:LEU:CD1	0.45	3.00	6	1
1:A:13:ASN:HB2	1:A:90:TRP:CH2	0.45	2.47	20	6
1:A:7:ALA:O	1:A:37:GLY:CA	0.45	2.64	4	2
1:A:11:ILE:CG2	1:A:87:VAL:HG11	0.45	2.41	10	2
1:A:13:ASN:ND2	1:A:104:TRP:CG	0.45	2.83	13	1
1:A:67:LEU:C	1:A:67:LEU:HD12	0.45	2.31	17	1
1:A:73:TYR:CD1	1:A:73:TYR:N	0.45	2.84	2	3
1:A:20:ILE:CG2	1:A:35:PHE:CE2	0.45	2.99	9	1
1:A:35:PHE:HZ	1:A:123:ILE:HD11	0.45	1.72	16	3
1:A:126:LEU:HD22	1:A:129:LEU:HD13	0.45	1.88	13	3
1:A:73:TYR:CE2	1:A:80:ILE:CG2	0.45	2.98	9	1
1:A:18:ILE:HD12	1:A:18:ILE:N	0.45	2.26	15	1
1:A:8:VAL:CG2	1:A:35:PHE:CD2	0.45	3.00	13	1
1:A:11:ILE:CG2	1:A:90:TRP:CE3	0.45	3.00	15	7
1:A:6:ILE:HD12	1:A:6:ILE:N	0.45	2.27	3	2
1:A:98:GLU:CD	1:A:98:GLU:N	0.45	2.70	17	1
1:A:62:PRO:HB3	1:A:90:TRP:HB2	0.45	1.89	8	8
1:A:4:LEU:CD1	3:A:131:8OG:O4'	0.45	2.63	20	2
1:A:4:LEU:HD21	3:A:131:8OG:N3	0.45	2.27	15	2
1:A:6:ILE:CD1	3:A:131:8OG:O5'	0.45	2.64	10	2
1:A:20:ILE:HG21	1:A:35:PHE:CE2	0.45	2.47	9	1
1:A:59:GLY:HA3	1:A:95:TRP:CH2	0.45	2.46	1	10
1:A:89:ARG:HG3	1:A:90:TRP:N	0.45	2.26	13	8
1:A:71:LEU:CD2	1:A:73:TYR:CD2	0.45	3.00	18	1
1:A:10:ILE:HG21	1:A:107:LEU:HG	0.45	1.87	15	2
1:A:72:GLU:CG	1:A:81:THR:HG23	0.45	2.42	9	1
1:A:53:GLU:CG	1:A:57:GLU:OE2	0.45	2.65	15	1
1:A:55:GLN:O	1:A:59:GLY:N	0.45	2.49	16	1
1:A:21:THR:O	1:A:33:LEU:HA	0.44	2.11	1	1
1:A:75:PHE:N	1:A:78:ARG:O	0.44	2.50	15	3
1:A:18:ILE:N	1:A:105:MET:O	0.44	2.49	14	7

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:90:TRP:NE1	1:A:94:PRO:HD3	0.44	2.27	20	2
1:A:35:PHE:CE1	1:A:84:PHE:CZ	0.44	3.04	3	1
1:A:70:LYS:NZ	1:A:83:TRP:CZ3	0.44	2.85	4	1
1:A:33:LEU:HD23	1:A:111:ASN:HB3	0.44	1.89	14	2
1:A:58:VAL:HG13	1:A:60:ILE:CG1	0.44	2.42	15	2
1:A:19:PHE:CE2	1:A:94:PRO:CB	0.44	3.01	8	1
1:A:107:LEU:HD11	1:A:126:LEU:HD21	0.44	1.88	12	1
1:A:6:ILE:HG12	3:A:131:8OG:H4'	0.44	1.90	12	2
1:A:13:ASN:OD1	1:A:90:TRP:CZ2	0.44	2.71	18	7
1:A:19:PHE:HB3	1:A:90:TRP:CH2	0.44	2.48	10	1
1:A:4:LEU:HD11	1:A:80:ILE:HG13	0.44	1.88	15	1
1:A:71:LEU:HD11	1:A:122:VAL:HG23	0.44	1.90	1	1
1:A:8:VAL:CG2	1:A:35:PHE:HB2	0.44	2.43	3	7
1:A:64:HIS:HD2	1:A:65:PHE:N	0.44	2.10	6	1
1:A:67:LEU:HD22	1:A:70:LYS:CE	0.44	2.43	17	1
1:A:60:ILE:HG13	1:A:61:THR:N	0.44	2.28	1	1
1:A:6:ILE:HD13	1:A:80:ILE:CD1	0.44	2.43	6	2
1:A:45:THR:O	1:A:49:ALA:N	0.44	2.48	16	6
1:A:126:LEU:HD21	1:A:129:LEU:HD13	0.44	1.90	2	2
1:A:7:ALA:HB1	1:A:50:VAL:HB	0.44	1.89	11	1
1:A:35:PHE:CZ	1:A:110:LEU:HD21	0.44	2.47	14	1
1:A:67:LEU:HD12	1:A:85:TRP:CZ3	0.44	2.47	10	1
1:A:90:TRP:CE2	1:A:94:PRO:HG3	0.44	2.48	11	1
1:A:60:ILE:HD13	1:A:94:PRO:CA	0.44	2.43	18	1
1:A:32:LYS:O	1:A:34:GLU:N	0.43	2.51	7	9
1:A:69:GLU:O	1:A:84:PHE:O	0.43	2.35	7	1
1:A:110:LEU:CD2	1:A:123:ILE:HG23	0.43	2.40	9	1
1:A:8:VAL:HG23	1:A:35:PHE:CD2	0.43	2.48	13	1
1:A:58:VAL:CG1	1:A:60:ILE:HG13	0.43	2.43	15	2
1:A:73:TYR:N	1:A:73:TYR:CD1	0.43	2.86	15	1
1:A:68:PHE:CE1	1:A:69:GLU:HB2	0.43	2.48	17	3
1:A:11:ILE:O	1:A:19:PHE:N	0.43	2.49	12	3
1:A:13:ASN:CG	1:A:17:GLU:O	0.43	2.56	8	1
1:A:58:VAL:HG12	1:A:60:ILE:HD12	0.43	1.84	9	1
1:A:68:PHE:CG	1:A:126:LEU:HD13	0.43	2.48	14	1
1:A:18:ILE:N	1:A:18:ILE:CD1	0.43	2.82	15	1
1:A:58:VAL:C	1:A:60:ILE:H	0.43	2.17	1	1
1:A:65:PHE:O	1:A:66:SER:O	0.43	2.36	20	1
1:A:112:ALA:O	1:A:115:PHE:CD1	0.43	2.72	19	7
1:A:75:PHE:HB2	1:A:78:ARG:O	0.43	2.14	8	3
1:A:18:ILE:HG22	1:A:20:ILE:HD13	0.43	1.89	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:62:PRO:HB3	1:A:90:TRP:HA	0.43	1.91	19	3
1:A:110:LEU:C	1:A:110:LEU:HD23	0.43	2.34	15	1
1:A:115:PHE:CE1	1:A:116:PRO:O	0.43	2.72	3	9
1:A:108:VAL:CG1	1:A:129:LEU:HD21	0.43	2.44	6	1
1:A:10:ILE:HG22	1:A:35:PHE:CD2	0.43	2.48	7	1
1:A:58:VAL:CG1	1:A:60:ILE:CD1	0.43	2.94	16	1
1:A:18:ILE:HB	1:A:107:LEU:HB2	0.43	1.90	17	1
1:A:5:GLN:O	1:A:6:ILE:HD12	0.43	2.14	4	1
1:A:85:TRP:CD1	1:A:85:TRP:N	0.43	2.86	9	2
1:A:13:ASN:OD1	1:A:17:GLU:HB2	0.43	2.14	8	1
1:A:19:PHE:O	1:A:19:PHE:CD2	0.43	2.72	16	2
1:A:8:VAL:HG22	1:A:84:PHE:CD1	0.43	2.49	15	1
3:A:131:8OG:OP2	3:A:131:8OG:C3'	0.43	2.67	15	2
1:A:90:TRP:CD1	1:A:90:TRP:C	0.43	2.92	20	1
1:A:17:GLU:HB3	1:A:105:MET:O	0.43	2.14	8	1
1:A:20:ILE:HD11	1:A:105:MET:HB2	0.43	1.91	14	1
1:A:107:LEU:CD1	1:A:110:LEU:HD22	0.43	2.44	14	2
1:A:60:ILE:HD11	1:A:94:PRO:CB	0.43	2.43	20	1
1:A:71:LEU:HD22	1:A:122:VAL:CG2	0.43	2.44	13	2
1:A:80:ILE:HD11	1:A:82:LEU:HD23	0.43	1.91	7	1
1:A:14:GLU:O	1:A:14:GLU:CG	0.42	2.66	11	6
1:A:19:PHE:CE2	1:A:94:PRO:HB2	0.42	2.49	4	2
1:A:19:PHE:HB2	1:A:90:TRP:CH2	0.42	2.49	17	2
1:A:71:LEU:CD1	1:A:71:LEU:N	0.42	2.81	9	1
1:A:60:ILE:HD12	1:A:91:GLU:O	0.42	2.13	1	1
1:A:115:PHE:CB	1:A:116:PRO:HD2	0.42	2.44	9	15
1:A:8:VAL:HG21	1:A:35:PHE:CD1	0.42	2.50	12	3
1:A:70:LYS:CE	1:A:83:TRP:CZ3	0.42	3.02	4	1
1:A:13:ASN:HB2	1:A:17:GLU:O	0.42	2.14	13	2
1:A:31:ASN:HA	1:A:114:ASP:O	0.42	2.14	20	2
1:A:60:ILE:HG23	1:A:95:TRP:NE1	0.42	2.29	6	1
1:A:13:ASN:N	1:A:17:GLU:O	0.42	2.50	12	1
1:A:2:LYS:HE2	1:A:4:LEU:HD23	0.42	1.87	11	1
1:A:11:ILE:O	1:A:18:ILE:CG1	0.42	2.67	12	1
1:A:78:ARG:CZ	3:A:131:8OG:C2	0.42	2.97	18	1
1:A:11:ILE:HA	1:A:87:VAL:CG1	0.42	2.44	19	1
1:A:50:VAL:CG1	1:A:85:TRP:CZ2	0.42	3.00	2	2
1:A:33:LEU:O	1:A:115:PHE:HB2	0.42	2.14	20	2
1:A:50:VAL:HG22	1:A:51:VAL:N	0.42	2.30	5	2
1:A:14:GLU:CG	1:A:14:GLU:O	0.42	2.68	8	2
1:A:59:GLY:CA	1:A:95:TRP:CH2	0.42	3.02	14	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:64:HIS:ND1	1:A:87:VAL:CG2	0.42	2.81	14	4
1:A:83:TRP:N	1:A:83:TRP:CD1	0.42	2.87	11	5
1:A:60:ILE:HD12	1:A:93:GLU:C	0.42	2.34	19	1
1:A:35:PHE:HB3	1:A:36:PRO:HD2	0.42	1.91	6	3
1:A:118:ALA:O	3:A:131:8OG:O6	0.42	2.37	20	2
1:A:84:PHE:CE1	1:A:122:VAL:CG2	0.42	2.98	10	1
1:A:60:ILE:CG1	1:A:61:THR:N	0.42	2.83	1	1
1:A:60:ILE:CD1	1:A:94:PRO:HA	0.42	2.44	4	2
1:A:78:ARG:HG2	3:A:131:8OG:N2	0.42	2.29	8	3
1:A:53:GLU:CG	1:A:57:GLU:OE1	0.42	2.67	12	1
1:A:62:PRO:CA	1:A:89:ARG:O	0.42	2.68	3	1
1:A:54:LEU:CD2	1:A:64:HIS:CE1	0.42	3.01	5	1
1:A:68:PHE:CE2	1:A:126:LEU:HD23	0.42	2.49	6	1
1:A:19:PHE:CE2	1:A:102:GLY:O	0.42	2.72	12	1
1:A:64:HIS:O	1:A:65:PHE:HB2	0.42	2.15	14	1
3:A:131:8OG:OP2	3:A:131:8OG:H2"	0.42	2.15	15	1
1:A:58:VAL:HG12	1:A:60:ILE:CG2	0.42	2.26	19	1
3:A:131:8OG:P	3:A:131:8OG:C3'	0.41	3.05	5	1
1:A:82:LEU:HD23	1:A:84:PHE:CZ	0.41	2.50	11	1
1:A:33:LEU:HD13	1:A:114:ASP:CB	0.41	2.45	13	1
1:A:21:THR:HG22	1:A:100:GLN:O	0.41	2.15	2	1
1:A:69:GLU:O	1:A:84:PHE:N	0.41	2.52	2	2
1:A:64:HIS:HA	1:A:87:VAL:HG13	0.41	1.92	3	1
1:A:95:TRP:O	1:A:97:LYS:N	0.41	2.53	3	1
1:A:6:ILE:CD1	3:A:131:8OG:C4'	0.41	2.98	13	3
1:A:33:LEU:C	1:A:33:LEU:HD23	0.41	2.36	19	1
1:A:19:PHE:CE1	1:A:94:PRO:HB2	0.41	2.50	5	1
1:A:8:VAL:HG23	1:A:9:GLY:N	0.41	2.30	16	4
1:A:68:PHE:CE1	1:A:69:GLU:CB	0.41	3.04	11	1
1:A:123:ILE:HD13	1:A:123:ILE:O	0.41	2.14	15	1
1:A:37:GLY:HA2	1:A:57:GLU:HG3	0.41	1.92	17	1
1:A:84:PHE:HE1	1:A:122:VAL:HG21	0.41	1.67	10	1
1:A:8:VAL:HG23	1:A:35:PHE:HB2	0.41	1.92	13	1
1:A:83:TRP:CD1	1:A:83:TRP:N	0.41	2.89	3	2
1:A:13:ASN:ND2	1:A:104:TRP:CB	0.41	2.84	9	1
1:A:68:PHE:CG	1:A:126:LEU:HD23	0.41	2.49	18	1
1:A:115:PHE:HZ	1:A:120:GLU:HA	0.41	1.74	15	2
1:A:119:ASN:C	1:A:121:PRO:HD2	0.41	2.36	13	1
1:A:68:PHE:CD1	1:A:84:PHE:CB	0.41	3.04	12	1
1:A:63:GLN:N	1:A:89:ARG:O	0.41	2.54	18	1
1:A:33:LEU:CD1	1:A:111:ASN:CB	0.41	2.99	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:62:PRO:O	1:A:64:HIS:N	0.41	2.53	20	2
1:A:11:ILE:O	1:A:18:ILE:HG13	0.41	2.16	10	2
1:A:66:SER:O	1:A:85:TRP:CE3	0.41	2.74	14	3
1:A:54:LEU:O	1:A:58:VAL:CB	0.41	2.69	13	1
1:A:8:VAL:CG2	1:A:35:PHE:CB	0.41	2.99	15	1
1:A:112:ALA:CB	1:A:127:LYS:CD	0.41	2.98	15	1
1:A:15:ASN:O	1:A:17:GLU:HG2	0.41	2.15	17	1
1:A:68:PHE:CE2	1:A:69:GLU:OE1	0.41	2.74	17	1
1:A:71:LEU:N	1:A:82:LEU:O	0.41	2.54	20	1
1:A:82:LEU:HD22	1:A:122:VAL:HG21	0.41	1.93	8	1
1:A:48:GLN:O	1:A:52:ARG:CB	0.41	2.69	15	1
1:A:11:ILE:CG2	1:A:90:TRP:HB3	0.40	2.46	4	1
1:A:67:LEU:C	1:A:67:LEU:CD2	0.40	2.89	7	2
1:A:64:HIS:CD2	1:A:65:PHE:N	0.40	2.88	6	1
1:A:68:PHE:CD1	1:A:68:PHE:C	0.40	2.94	9	2
1:A:58:VAL:O	1:A:96:GLY:N	0.40	2.54	10	1
1:A:45:THR:O	1:A:49:ALA:HB2	0.40	2.16	18	1
1:A:126:LEU:O	1:A:129:LEU:HB3	0.40	2.16	2	1
1:A:6:ILE:CG2	1:A:82:LEU:CD1	0.40	3.00	3	2
1:A:68:PHE:CZ	1:A:126:LEU:HG	0.40	2.51	4	1
1:A:10:ILE:CD1	1:A:18:ILE:HD13	0.40	2.38	7	1
1:A:73:TYR:CE1	1:A:80:ILE:HG23	0.40	2.51	18	1
1:A:6:ILE:CG2	1:A:82:LEU:CD2	0.40	2.99	2	1
1:A:10:ILE:HG21	1:A:107:LEU:CG	0.40	2.47	2	1
1:A:6:ILE:HG22	1:A:82:LEU:HD12	0.40	1.94	4	1
1:A:67:LEU:HD13	1:A:70:LYS:HG2	0.40	1.93	9	1
1:A:90:TRP:NE1	1:A:92:GLY:O	0.40	2.55	19	1
1:A:58:VAL:HG12	1:A:60:ILE:H	0.40	1.76	1	1
1:A:13:ASN:OD1	1:A:17:GLU:O	0.40	2.39	7	1
1:A:84:PHE:CE1	1:A:122:VAL:CG1	0.40	2.98	10	1
1:A:10:ILE:HG13	1:A:35:PHE:CE2	0.40	2.52	13	1
1:A:10:ILE:O	1:A:87:VAL:CB	0.40	2.69	15	1
1:A:78:ARG:NE	3:A:131:8OG:C2	0.40	2.85	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	119/129 (92%)	95±2 (80±2%)	16±2 (13±2%)	8±1 (7±1%)	2 16
All	All	2380/2580 (92%)	1894 (80%)	316 (13%)	170 (7%)	2 16

All 13 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	42	MET	20
1	A	62	PRO	20
1	A	97	LYS	20
1	A	76	PRO	17
1	A	43	GLY	16
1	A	96	GLY	16
1	A	66	SER	15
1	A	77	ASP	14
1	A	65	PHE	14
1	A	33	LEU	9
1	A	39	LYS	5
1	A	41	GLU	3
1	A	59	GLY	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	105/110 (95%)	66±3 (63±3%)	39±3 (37±3%)	1 7
All	All	2100/2200 (95%)	1325 (63%)	775 (37%)	1 7

All 79 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	12	ARG	20
1	A	20	ILE	20
1	A	39	LYS	20
1	A	41	GLU	20

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Mol	Chain	Res	Type	Models (Total)
1	A	45	THR	20
1	A	81	THR	20
1	A	104	TRP	20
1	A	114	ASP	20
1	A	115	PHE	20
1	A	10	ILE	19
1	A	11	ILE	19
1	A	35	PHE	18
1	A	61	THR	18
1	A	70	LYS	18
1	A	107	LEU	18
1	A	64	HIS	17
1	A	68	PHE	17
1	A	120	GLU	17
1	A	34	GLU	16
1	A	60	ILE	15
1	A	90	TRP	15
1	A	3	LYS	15
1	A	19	PHE	15
1	A	32	LYS	15
1	A	97	LYS	15
1	A	50	VAL	14
1	A	89	ARG	14
1	A	129	LEU	14
1	A	55	GLN	13
1	A	98	GLU	13
1	A	16	ASN	13
1	A	31	ASN	11
1	A	66	SER	11
1	A	100	GLN	11
1	A	47	GLU	11
1	A	2	LYS	10
1	A	44	GLU	10
1	A	57	GLU	10
1	A	111	ASN	10
1	A	54	LEU	10
1	A	105	MET	8
1	A	42	MET	8
1	A	71	LEU	8
1	A	106	SER	8
1	A	75	PHE	8
1	A	67	LEU	8

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Mol	Chain	Res	Type	Models (Total)
1	A	78	ARG	8
1	A	82	LEU	8
1	A	52	ARG	7
1	A	65	PHE	6
1	A	125	LYS	6
1	A	79	HIS	5
1	A	56	GLU	5
1	A	69	GLU	5
1	A	22	ARG	5
1	A	103	GLU	4
1	A	18	ILE	4
1	A	40	ILE	4
1	A	113	ASP	3
1	A	58	VAL	3
1	A	126	LEU	3
1	A	53	GLU	3
1	A	91	GLU	3
1	A	128	ARG	2
1	A	77	ASP	2
1	A	33	LEU	2
1	A	17	GLU	2
1	A	110	LEU	2
1	A	80	ILE	2
1	A	88	GLU	2
1	A	4	LEU	1
1	A	6	ILE	1
1	A	48	GLN	1
1	A	86	LEU	1
1	A	123	ILE	1
1	A	63	GLN	1
1	A	74	GLU	1
1	A	73	TYR	1
1	A	13	ASN	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 2 ligands modelled in this entry, 1 is 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	8OG	A	131	-	26,26,26	1.47±0.01	5±0 (19±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	8OG	A	131	-	33,40,40	2.01±0.01	10±0 (30±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	8OG	A	131	-	-	0±0,10,22,22	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	131	8OG	C4-N3	3.61	1.42	1.34	8	20
3	A	131	8OG	O8-C8	3.11	1.28	1.23	11	20
3	A	131	8OG	C2-N3	3.00	1.40	1.33	17	20
3	A	131	8OG	O6-C6	2.61	1.28	1.23	8	20
3	A	131	8OG	C5-C6	2.19	1.35	1.41	13	20

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

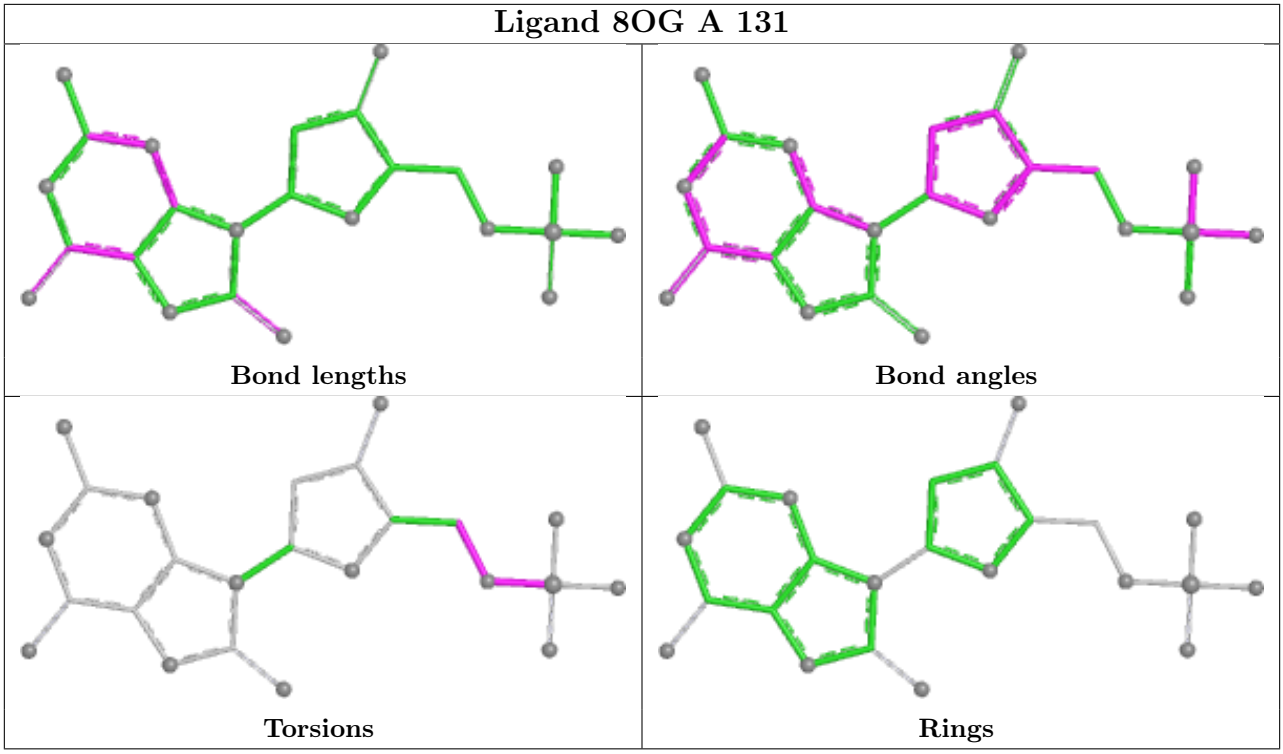
Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	A	131	8OG	C2-N1-C6	4.22	117.46	125.11	9	20
3	A	131	8OG	C4'-O4'-C1'	4.13	119.32	109.51	18	20
3	A	131	8OG	C5-C6-N1	4.01	123.13	112.13	5	20
3	A	131	8OG	O6-C6-C5	3.65	118.45	127.26	11	20
3	A	131	8OG	N9-C4-N3	3.57	130.60	126.13	19	20
3	A	131	8OG	O4'-C4'-C5'	3.55	120.70	109.33	18	20
3	A	131	8OG	O4'-C1'-C2'	2.71	101.19	106.25	12	20
3	A	131	8OG	C3'-C2'-C1'	2.51	108.74	102.60	6	20
3	A	131	8OG	OP2-P-OP1	2.19	119.35	110.83	11	20
3	A	131	8OG	C2'-C3'-C4'	2.17	107.21	102.80	18	20
3	A	131	8OG	N7-C8-N9	2.02	104.37	106.61	20	1

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.



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