



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 28, 2024 – 03:06 am BST

PDB ID : 5O5L  
Title : X-ray structure of a bacterial adenyl cyclase soluble domain, solved at cryogenic temperature  
Authors : Vercellino, I.; Korkhov, V.M.  
Deposited on : 2017-06-02  
Resolution : 2.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ 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 ⓘ](#)) were used in the production of this report:

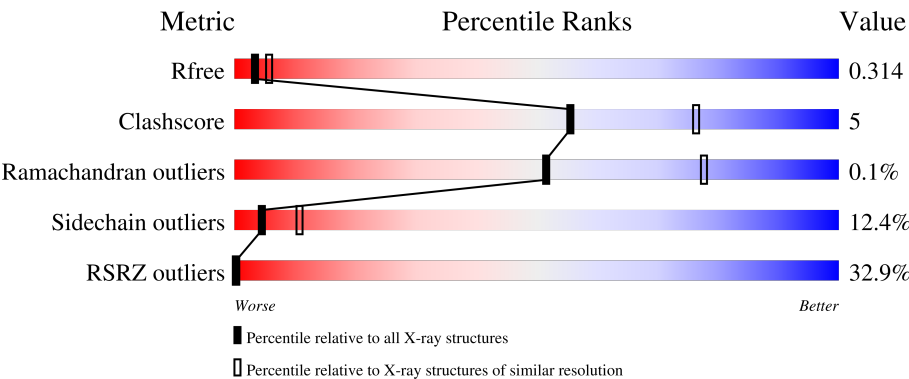
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
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:  
*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 Å.

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)	Similar resolution (#Entries, resolution range(Å))
R <sub>free</sub>	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	254	<div><div>70%17%12%</div></div>
1	B	254	<div><div>68%16%12%</div></div>
1	C	254	<div><div>3%72%14%12%</div></div>
1	D	254	<div><div>4%73%13%12%</div></div>
1	E	254	<div><div>22%70%16%12%</div></div>

Continued on next page...

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
1	F	254	
1	G	254	
1	H	254	
1	I	254	
1	J	254	
1	K	254	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	MN	C	504	-	-	-	X
3	MN	I	502	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 19781 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Adenylate cyclase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	224	Total	C	N	O	S	0	0	0
			1720	1079	306	325	10			
1	B	224	Total	C	N	O	S	0	0	0
			1733	1089	307	327	10			
1	C	224	Total	C	N	O	S	0	0	0
			1733	1089	307	327	10			
1	D	224	Total	C	N	O	S	0	0	0
			1733	1089	307	327	10			
1	E	224	Total	C	N	O	S	0	0	0
			1733	1089	307	327	10			
1	F	224	Total	C	N	O	S	0	0	0
			1733	1089	307	327	10			
1	G	224	Total	C	N	O	S	0	0	0
			1733	1089	307	327	10			
1	H	224	Total	C	N	O	S	0	0	0
			1733	1089	307	327	10			
1	I	224	Total	C	N	O	S	0	0	0
			1733	1089	307	327	10			
1	J	224	Total	C	N	O	S	0	0	0
			1733	1089	307	327	10			
1	K	224	Total	C	N	O	S	0	0	0
			1733	1089	307	327	10			

There are 308 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	176	MET	-	initiating methionine	UNP X8CHM4
A	177	GLY	-	expression tag	UNP X8CHM4
A	178	HIS	-	expression tag	UNP X8CHM4
A	179	HIS	-	expression tag	UNP X8CHM4
A	180	HIS	-	expression tag	UNP X8CHM4
A	181	HIS	-	expression tag	UNP X8CHM4
A	182	HIS	-	expression tag	UNP X8CHM4

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
A	183	HIS	-	expression tag	UNP X8CHM4
A	184	HIS	-	expression tag	UNP X8CHM4
A	185	HIS	-	expression tag	UNP X8CHM4
A	186	HIS	-	expression tag	UNP X8CHM4
A	187	HIS	-	expression tag	UNP X8CHM4
A	188	SER	-	expression tag	UNP X8CHM4
A	189	SER	-	expression tag	UNP X8CHM4
A	190	GLY	-	expression tag	UNP X8CHM4
A	191	LEU	-	expression tag	UNP X8CHM4
A	192	GLU	-	expression tag	UNP X8CHM4
A	193	VAL	-	expression tag	UNP X8CHM4
A	194	LEU	-	expression tag	UNP X8CHM4
A	195	PHE	-	expression tag	UNP X8CHM4
A	196	GLN	-	expression tag	UNP X8CHM4
A	197	GLY	-	expression tag	UNP X8CHM4
A	198	PRO	-	expression tag	UNP X8CHM4
A	199	SER	-	expression tag	UNP X8CHM4
A	200	GLY	-	expression tag	UNP X8CHM4
A	201	HIS	-	expression tag	UNP X8CHM4
A	202	MET	-	expression tag	UNP X8CHM4
A	342	PRO	ALA	conflict	UNP X8CHM4
B	176	MET	-	initiating methionine	UNP X8CHM4
B	177	GLY	-	expression tag	UNP X8CHM4
B	178	HIS	-	expression tag	UNP X8CHM4
B	179	HIS	-	expression tag	UNP X8CHM4
B	180	HIS	-	expression tag	UNP X8CHM4
B	181	HIS	-	expression tag	UNP X8CHM4
B	182	HIS	-	expression tag	UNP X8CHM4
B	183	HIS	-	expression tag	UNP X8CHM4
B	184	HIS	-	expression tag	UNP X8CHM4
B	185	HIS	-	expression tag	UNP X8CHM4
B	186	HIS	-	expression tag	UNP X8CHM4
B	187	HIS	-	expression tag	UNP X8CHM4
B	188	SER	-	expression tag	UNP X8CHM4
B	189	SER	-	expression tag	UNP X8CHM4
B	190	GLY	-	expression tag	UNP X8CHM4
B	191	LEU	-	expression tag	UNP X8CHM4
B	192	GLU	-	expression tag	UNP X8CHM4
B	193	VAL	-	expression tag	UNP X8CHM4
B	194	LEU	-	expression tag	UNP X8CHM4
B	195	PHE	-	expression tag	UNP X8CHM4
B	196	GLN	-	expression tag	UNP X8CHM4

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
B	197	GLY	-	expression tag	UNP X8CHM4
B	198	PRO	-	expression tag	UNP X8CHM4
B	199	SER	-	expression tag	UNP X8CHM4
B	200	GLY	-	expression tag	UNP X8CHM4
B	201	HIS	-	expression tag	UNP X8CHM4
B	202	MET	-	expression tag	UNP X8CHM4
B	342	PRO	ALA	conflict	UNP X8CHM4
C	176	MET	-	initiating methionine	UNP X8CHM4
C	177	GLY	-	expression tag	UNP X8CHM4
C	178	HIS	-	expression tag	UNP X8CHM4
C	179	HIS	-	expression tag	UNP X8CHM4
C	180	HIS	-	expression tag	UNP X8CHM4
C	181	HIS	-	expression tag	UNP X8CHM4
C	182	HIS	-	expression tag	UNP X8CHM4
C	183	HIS	-	expression tag	UNP X8CHM4
C	184	HIS	-	expression tag	UNP X8CHM4
C	185	HIS	-	expression tag	UNP X8CHM4
C	186	HIS	-	expression tag	UNP X8CHM4
C	187	HIS	-	expression tag	UNP X8CHM4
C	188	SER	-	expression tag	UNP X8CHM4
C	189	SER	-	expression tag	UNP X8CHM4
C	190	GLY	-	expression tag	UNP X8CHM4
C	191	LEU	-	expression tag	UNP X8CHM4
C	192	GLU	-	expression tag	UNP X8CHM4
C	193	VAL	-	expression tag	UNP X8CHM4
C	194	LEU	-	expression tag	UNP X8CHM4
C	195	PHE	-	expression tag	UNP X8CHM4
C	196	GLN	-	expression tag	UNP X8CHM4
C	197	GLY	-	expression tag	UNP X8CHM4
C	198	PRO	-	expression tag	UNP X8CHM4
C	199	SER	-	expression tag	UNP X8CHM4
C	200	GLY	-	expression tag	UNP X8CHM4
C	201	HIS	-	expression tag	UNP X8CHM4
C	202	MET	-	expression tag	UNP X8CHM4
C	342	PRO	ALA	conflict	UNP X8CHM4
D	176	MET	-	initiating methionine	UNP X8CHM4
D	177	GLY	-	expression tag	UNP X8CHM4
D	178	HIS	-	expression tag	UNP X8CHM4
D	179	HIS	-	expression tag	UNP X8CHM4
D	180	HIS	-	expression tag	UNP X8CHM4
D	181	HIS	-	expression tag	UNP X8CHM4
D	182	HIS	-	expression tag	UNP X8CHM4

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
D	183	HIS	-	expression tag	UNP X8CHM4
D	184	HIS	-	expression tag	UNP X8CHM4
D	185	HIS	-	expression tag	UNP X8CHM4
D	186	HIS	-	expression tag	UNP X8CHM4
D	187	HIS	-	expression tag	UNP X8CHM4
D	188	SER	-	expression tag	UNP X8CHM4
D	189	SER	-	expression tag	UNP X8CHM4
D	190	GLY	-	expression tag	UNP X8CHM4
D	191	LEU	-	expression tag	UNP X8CHM4
D	192	GLU	-	expression tag	UNP X8CHM4
D	193	VAL	-	expression tag	UNP X8CHM4
D	194	LEU	-	expression tag	UNP X8CHM4
D	195	PHE	-	expression tag	UNP X8CHM4
D	196	GLN	-	expression tag	UNP X8CHM4
D	197	GLY	-	expression tag	UNP X8CHM4
D	198	PRO	-	expression tag	UNP X8CHM4
D	199	SER	-	expression tag	UNP X8CHM4
D	200	GLY	-	expression tag	UNP X8CHM4
D	201	HIS	-	expression tag	UNP X8CHM4
D	202	MET	-	expression tag	UNP X8CHM4
D	342	PRO	ALA	conflict	UNP X8CHM4
E	176	MET	-	initiating methionine	UNP X8CHM4
E	177	GLY	-	expression tag	UNP X8CHM4
E	178	HIS	-	expression tag	UNP X8CHM4
E	179	HIS	-	expression tag	UNP X8CHM4
E	180	HIS	-	expression tag	UNP X8CHM4
E	181	HIS	-	expression tag	UNP X8CHM4
E	182	HIS	-	expression tag	UNP X8CHM4
E	183	HIS	-	expression tag	UNP X8CHM4
E	184	HIS	-	expression tag	UNP X8CHM4
E	185	HIS	-	expression tag	UNP X8CHM4
E	186	HIS	-	expression tag	UNP X8CHM4
E	187	HIS	-	expression tag	UNP X8CHM4
E	188	SER	-	expression tag	UNP X8CHM4
E	189	SER	-	expression tag	UNP X8CHM4
E	190	GLY	-	expression tag	UNP X8CHM4
E	191	LEU	-	expression tag	UNP X8CHM4
E	192	GLU	-	expression tag	UNP X8CHM4
E	193	VAL	-	expression tag	UNP X8CHM4
E	194	LEU	-	expression tag	UNP X8CHM4
E	195	PHE	-	expression tag	UNP X8CHM4
E	196	GLN	-	expression tag	UNP X8CHM4

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
E	197	GLY	-	expression tag	UNP X8CHM4
E	198	PRO	-	expression tag	UNP X8CHM4
E	199	SER	-	expression tag	UNP X8CHM4
E	200	GLY	-	expression tag	UNP X8CHM4
E	201	HIS	-	expression tag	UNP X8CHM4
E	202	MET	-	expression tag	UNP X8CHM4
E	342	PRO	ALA	conflict	UNP X8CHM4
F	176	MET	-	initiating methionine	UNP X8CHM4
F	177	GLY	-	expression tag	UNP X8CHM4
F	178	HIS	-	expression tag	UNP X8CHM4
F	179	HIS	-	expression tag	UNP X8CHM4
F	180	HIS	-	expression tag	UNP X8CHM4
F	181	HIS	-	expression tag	UNP X8CHM4
F	182	HIS	-	expression tag	UNP X8CHM4
F	183	HIS	-	expression tag	UNP X8CHM4
F	184	HIS	-	expression tag	UNP X8CHM4
F	185	HIS	-	expression tag	UNP X8CHM4
F	186	HIS	-	expression tag	UNP X8CHM4
F	187	HIS	-	expression tag	UNP X8CHM4
F	188	SER	-	expression tag	UNP X8CHM4
F	189	SER	-	expression tag	UNP X8CHM4
F	190	GLY	-	expression tag	UNP X8CHM4
F	191	LEU	-	expression tag	UNP X8CHM4
F	192	GLU	-	expression tag	UNP X8CHM4
F	193	VAL	-	expression tag	UNP X8CHM4
F	194	LEU	-	expression tag	UNP X8CHM4
F	195	PHE	-	expression tag	UNP X8CHM4
F	196	GLN	-	expression tag	UNP X8CHM4
F	197	GLY	-	expression tag	UNP X8CHM4
F	198	PRO	-	expression tag	UNP X8CHM4
F	199	SER	-	expression tag	UNP X8CHM4
F	200	GLY	-	expression tag	UNP X8CHM4
F	201	HIS	-	expression tag	UNP X8CHM4
F	202	MET	-	expression tag	UNP X8CHM4
F	342	PRO	ALA	conflict	UNP X8CHM4
G	176	MET	-	initiating methionine	UNP X8CHM4
G	177	GLY	-	expression tag	UNP X8CHM4
G	178	HIS	-	expression tag	UNP X8CHM4
G	179	HIS	-	expression tag	UNP X8CHM4
G	180	HIS	-	expression tag	UNP X8CHM4
G	181	HIS	-	expression tag	UNP X8CHM4
G	182	HIS	-	expression tag	UNP X8CHM4

*Continued on next page...*



*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
G	183	HIS	-	expression tag	UNP X8CHM4
G	184	HIS	-	expression tag	UNP X8CHM4
G	185	HIS	-	expression tag	UNP X8CHM4
G	186	HIS	-	expression tag	UNP X8CHM4
G	187	HIS	-	expression tag	UNP X8CHM4
G	188	SER	-	expression tag	UNP X8CHM4
G	189	SER	-	expression tag	UNP X8CHM4
G	190	GLY	-	expression tag	UNP X8CHM4
G	191	LEU	-	expression tag	UNP X8CHM4
G	192	GLU	-	expression tag	UNP X8CHM4
G	193	VAL	-	expression tag	UNP X8CHM4
G	194	LEU	-	expression tag	UNP X8CHM4
G	195	PHE	-	expression tag	UNP X8CHM4
G	196	GLN	-	expression tag	UNP X8CHM4
G	197	GLY	-	expression tag	UNP X8CHM4
G	198	PRO	-	expression tag	UNP X8CHM4
G	199	SER	-	expression tag	UNP X8CHM4
G	200	GLY	-	expression tag	UNP X8CHM4
G	201	HIS	-	expression tag	UNP X8CHM4
G	202	MET	-	expression tag	UNP X8CHM4
G	342	PRO	ALA	conflict	UNP X8CHM4
H	176	MET	-	initiating methionine	UNP X8CHM4
H	177	GLY	-	expression tag	UNP X8CHM4
H	178	HIS	-	expression tag	UNP X8CHM4
H	179	HIS	-	expression tag	UNP X8CHM4
H	180	HIS	-	expression tag	UNP X8CHM4
H	181	HIS	-	expression tag	UNP X8CHM4
H	182	HIS	-	expression tag	UNP X8CHM4
H	183	HIS	-	expression tag	UNP X8CHM4
H	184	HIS	-	expression tag	UNP X8CHM4
H	185	HIS	-	expression tag	UNP X8CHM4
H	186	HIS	-	expression tag	UNP X8CHM4
H	187	HIS	-	expression tag	UNP X8CHM4
H	188	SER	-	expression tag	UNP X8CHM4
H	189	SER	-	expression tag	UNP X8CHM4
H	190	GLY	-	expression tag	UNP X8CHM4
H	191	LEU	-	expression tag	UNP X8CHM4
H	192	GLU	-	expression tag	UNP X8CHM4
H	193	VAL	-	expression tag	UNP X8CHM4
H	194	LEU	-	expression tag	UNP X8CHM4
H	195	PHE	-	expression tag	UNP X8CHM4
H	196	GLN	-	expression tag	UNP X8CHM4

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
H	197	GLY	-	expression tag	UNP X8CHM4
H	198	PRO	-	expression tag	UNP X8CHM4
H	199	SER	-	expression tag	UNP X8CHM4
H	200	GLY	-	expression tag	UNP X8CHM4
H	201	HIS	-	expression tag	UNP X8CHM4
H	202	MET	-	expression tag	UNP X8CHM4
H	342	PRO	ALA	conflict	UNP X8CHM4
I	176	MET	-	initiating methionine	UNP X8CHM4
I	177	GLY	-	expression tag	UNP X8CHM4
I	178	HIS	-	expression tag	UNP X8CHM4
I	179	HIS	-	expression tag	UNP X8CHM4
I	180	HIS	-	expression tag	UNP X8CHM4
I	181	HIS	-	expression tag	UNP X8CHM4
I	182	HIS	-	expression tag	UNP X8CHM4
I	183	HIS	-	expression tag	UNP X8CHM4
I	184	HIS	-	expression tag	UNP X8CHM4
I	185	HIS	-	expression tag	UNP X8CHM4
I	186	HIS	-	expression tag	UNP X8CHM4
I	187	HIS	-	expression tag	UNP X8CHM4
I	188	SER	-	expression tag	UNP X8CHM4
I	189	SER	-	expression tag	UNP X8CHM4
I	190	GLY	-	expression tag	UNP X8CHM4
I	191	LEU	-	expression tag	UNP X8CHM4
I	192	GLU	-	expression tag	UNP X8CHM4
I	193	VAL	-	expression tag	UNP X8CHM4
I	194	LEU	-	expression tag	UNP X8CHM4
I	195	PHE	-	expression tag	UNP X8CHM4
I	196	GLN	-	expression tag	UNP X8CHM4
I	197	GLY	-	expression tag	UNP X8CHM4
I	198	PRO	-	expression tag	UNP X8CHM4
I	199	SER	-	expression tag	UNP X8CHM4
I	200	GLY	-	expression tag	UNP X8CHM4
I	201	HIS	-	expression tag	UNP X8CHM4
I	202	MET	-	expression tag	UNP X8CHM4
I	342	PRO	ALA	conflict	UNP X8CHM4
J	176	MET	-	initiating methionine	UNP X8CHM4
J	177	GLY	-	expression tag	UNP X8CHM4
J	178	HIS	-	expression tag	UNP X8CHM4
J	179	HIS	-	expression tag	UNP X8CHM4
J	180	HIS	-	expression tag	UNP X8CHM4
J	181	HIS	-	expression tag	UNP X8CHM4
J	182	HIS	-	expression tag	UNP X8CHM4

*Continued on next page...*

*Continued from previous page...*

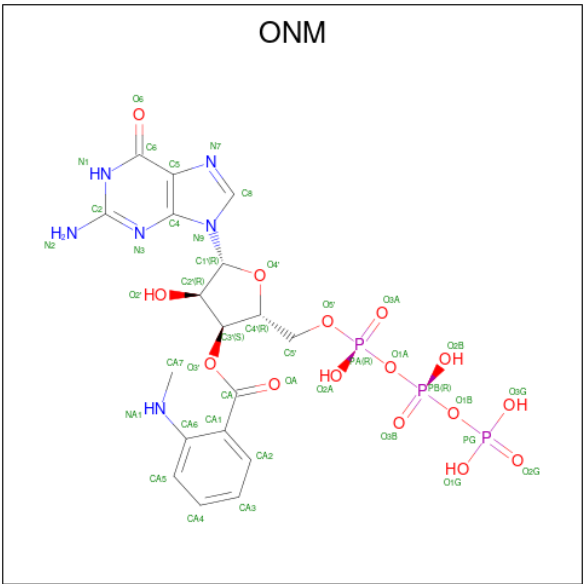
Chain	Residue	Modelled	Actual	Comment	Reference
J	183	HIS	-	expression tag	UNP X8CHM4
J	184	HIS	-	expression tag	UNP X8CHM4
J	185	HIS	-	expression tag	UNP X8CHM4
J	186	HIS	-	expression tag	UNP X8CHM4
J	187	HIS	-	expression tag	UNP X8CHM4
J	188	SER	-	expression tag	UNP X8CHM4
J	189	SER	-	expression tag	UNP X8CHM4
J	190	GLY	-	expression tag	UNP X8CHM4
J	191	LEU	-	expression tag	UNP X8CHM4
J	192	GLU	-	expression tag	UNP X8CHM4
J	193	VAL	-	expression tag	UNP X8CHM4
J	194	LEU	-	expression tag	UNP X8CHM4
J	195	PHE	-	expression tag	UNP X8CHM4
J	196	GLN	-	expression tag	UNP X8CHM4
J	197	GLY	-	expression tag	UNP X8CHM4
J	198	PRO	-	expression tag	UNP X8CHM4
J	199	SER	-	expression tag	UNP X8CHM4
J	200	GLY	-	expression tag	UNP X8CHM4
J	201	HIS	-	expression tag	UNP X8CHM4
J	202	MET	-	expression tag	UNP X8CHM4
J	342	PRO	ALA	conflict	UNP X8CHM4
K	176	MET	-	initiating methionine	UNP X8CHM4
K	177	GLY	-	expression tag	UNP X8CHM4
K	178	HIS	-	expression tag	UNP X8CHM4
K	179	HIS	-	expression tag	UNP X8CHM4
K	180	HIS	-	expression tag	UNP X8CHM4
K	181	HIS	-	expression tag	UNP X8CHM4
K	182	HIS	-	expression tag	UNP X8CHM4
K	183	HIS	-	expression tag	UNP X8CHM4
K	184	HIS	-	expression tag	UNP X8CHM4
K	185	HIS	-	expression tag	UNP X8CHM4
K	186	HIS	-	expression tag	UNP X8CHM4
K	187	HIS	-	expression tag	UNP X8CHM4
K	188	SER	-	expression tag	UNP X8CHM4
K	189	SER	-	expression tag	UNP X8CHM4
K	190	GLY	-	expression tag	UNP X8CHM4
K	191	LEU	-	expression tag	UNP X8CHM4
K	192	GLU	-	expression tag	UNP X8CHM4
K	193	VAL	-	expression tag	UNP X8CHM4
K	194	LEU	-	expression tag	UNP X8CHM4
K	195	PHE	-	expression tag	UNP X8CHM4
K	196	GLN	-	expression tag	UNP X8CHM4

*Continued on next page...*

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
K	197	GLY	-	expression tag	UNP X8CHM4
K	198	PRO	-	expression tag	UNP X8CHM4
K	199	SER	-	expression tag	UNP X8CHM4
K	200	GLY	-	expression tag	UNP X8CHM4
K	201	HIS	-	expression tag	UNP X8CHM4
K	202	MET	-	expression tag	UNP X8CHM4
K	342	PRO	ALA	conflict	UNP X8CHM4

- Molecule 2 is 3'-O-(N-METHYLANTHRANILOYL)-GUANOSINE-5'-TRIPHOSPHATE (three-letter code: ONM) (formula: C<sub>18</sub>H<sub>23</sub>N<sub>6</sub>O<sub>15</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			42	18	6	15	3		
2	B	1	Total	C	N	O	P	0	0
			42	18	6	15	3		
2	C	1	Total	C	N	O	P	0	0
			42	18	6	15	3		
2	D	1	Total	C	N	O	P	0	0
			42	18	6	15	3		
2	E	1	Total	C	N	O	P	0	0
			42	18	6	15	3		
2	F	1	Total	C	N	O	P	0	0
			42	18	6	15	3		
2	G	1	Total	C	N	O	P	0	0
			42	18	6	15	3		

Continued on next page...

*Continued from previous page...*

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	H	1	Total	C	N	O	P	0	0
			42	18	6	15	3		
2	I	1	Total	C	N	O	P	0	0
			42	18	6	15	3		
2	J	1	Total	C	N	O	P	0	0
			42	18	6	15	3		
2	K	1	Total	C	N	O	P	0	0
			42	18	6	15	3		

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Mn	0	0
			2	2		
3	B	2	Total	Mn	0	0
			2	2		
3	C	2	Total	Mn	0	0
			2	2		
3	D	2	Total	Mn	0	0
			2	2		
3	E	2	Total	Mn	0	0
			2	2		
3	F	2	Total	Mn	0	0
			2	2		
3	G	2	Total	Mn	0	0
			2	2		
3	H	2	Total	Mn	0	0
			2	2		
3	I	2	Total	Mn	0	0
			2	2		
3	J	2	Total	Mn	0	0
			2	2		
3	K	2	Total	Mn	0	0
			2	2		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	E	1	Total	O	S	0	0
			5	4	1		

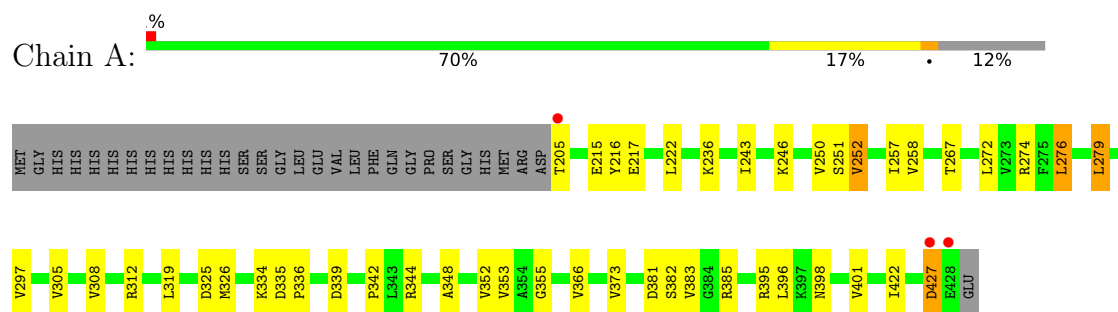
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	53	Total	O	0	0
			53	53		
5	B	60	Total	O	0	0
			60	60		
5	C	66	Total	O	0	0
			66	66		
5	D	37	Total	O	0	0
			37	37		
5	E	1	Total	O	0	0
			1	1		

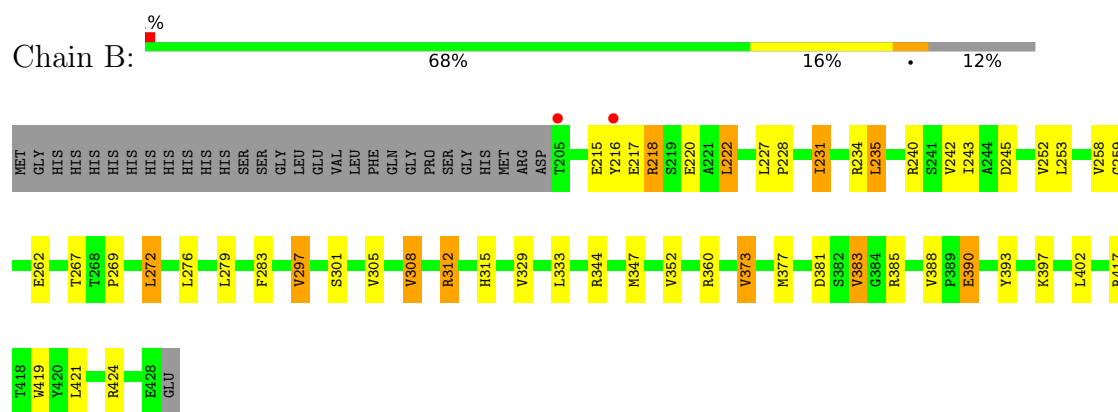
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-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. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

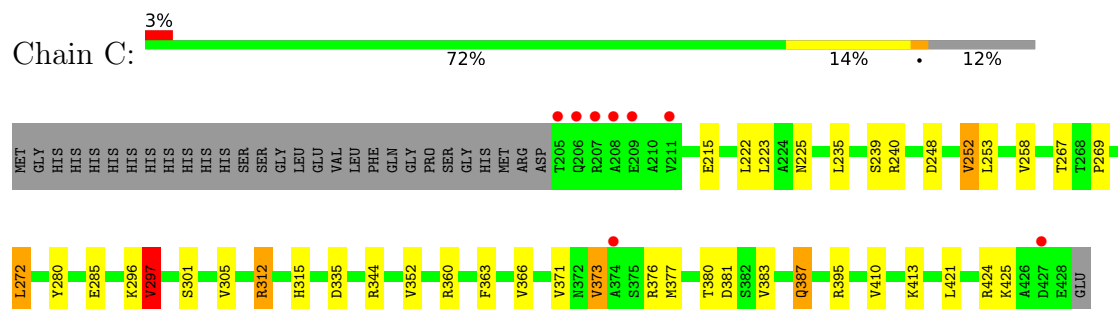
- Molecule 1: Adenylate cyclase



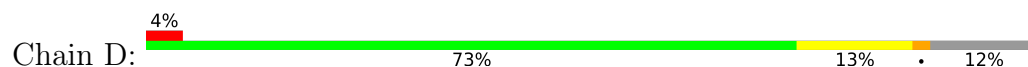
- Molecule 1: Adenylate cyclase

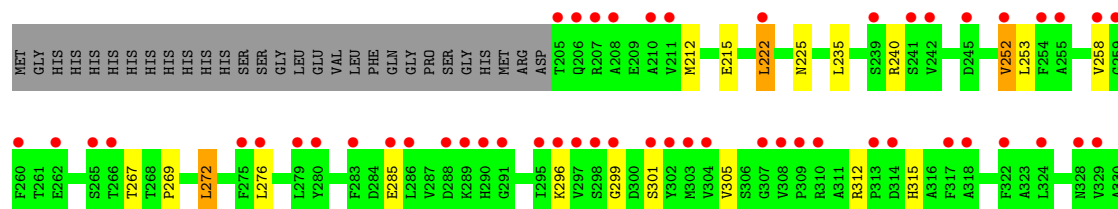


- Molecule 1: Adenylate cyclase

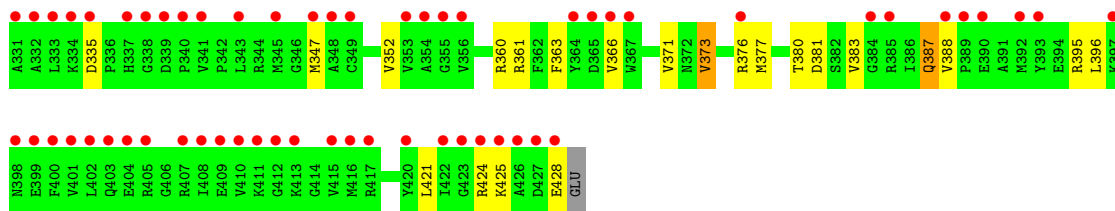


- Molecule 1: Adenylate cyclase

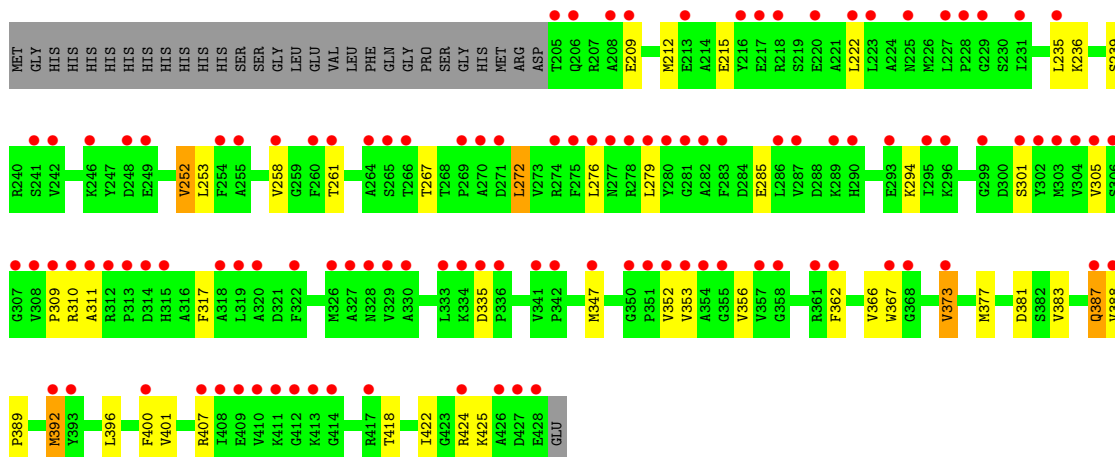
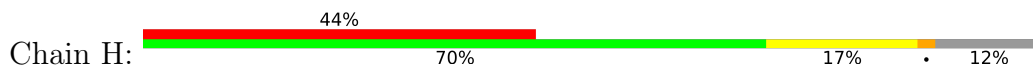




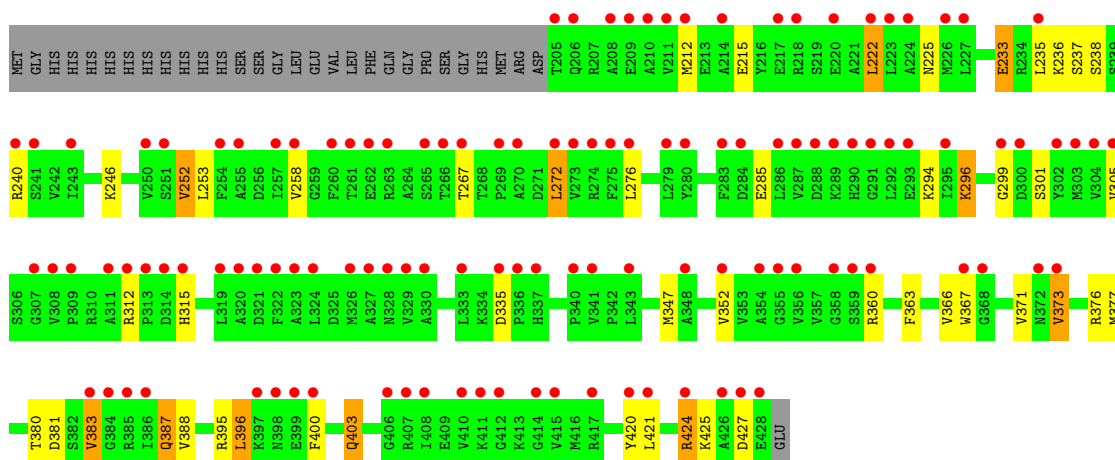




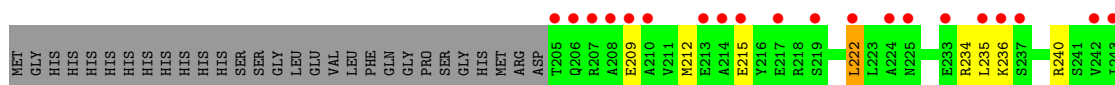
• Molecule 1: Adenylate cyclase

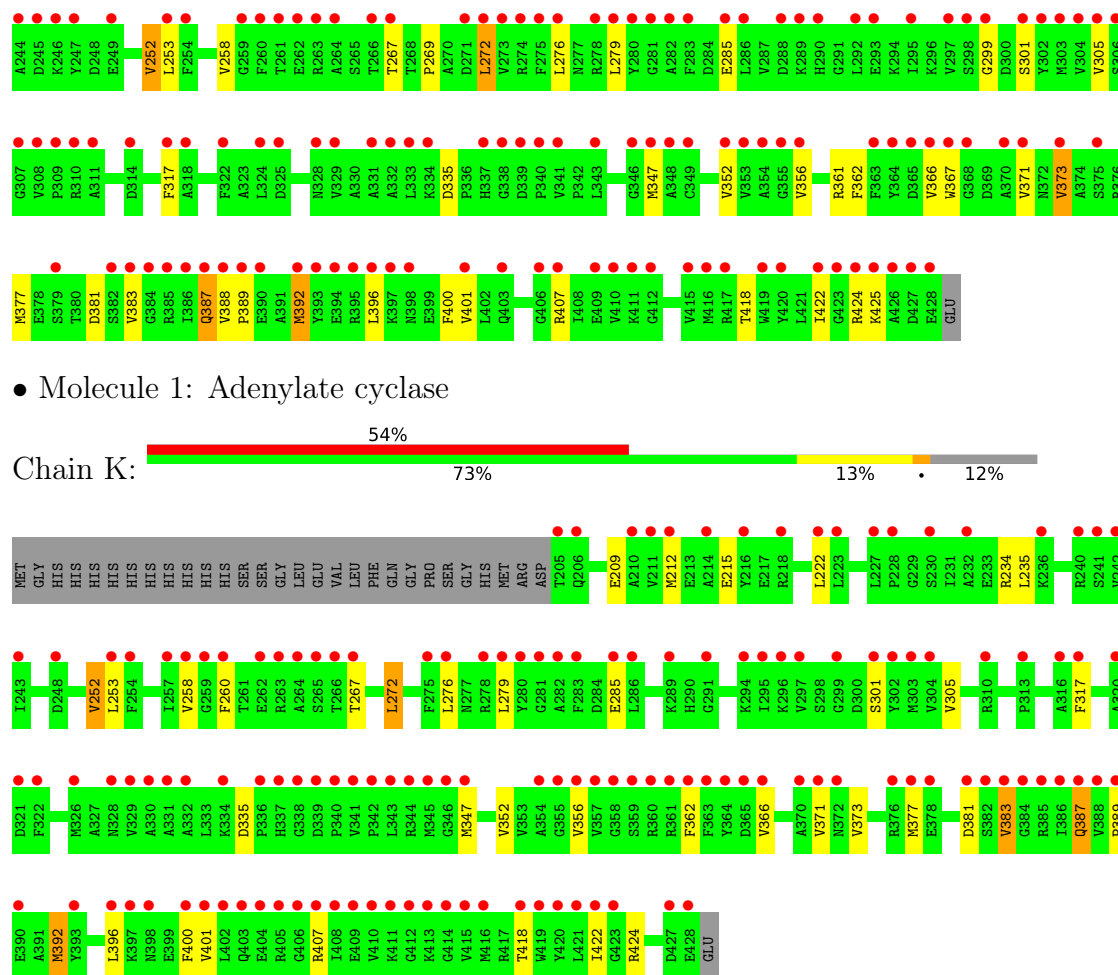


• Molecule 1: Adenylate cyclase



• Molecule 1: Adenylate cyclase





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	144.48Å 84.12Å 310.75Å 90.00° 103.87° 90.00°	Depositor
Resolution (Å)	49.38 – 2.70 49.38 – 2.70	Depositor EDS
% Data completeness (in resolution range)	98.5 (49.38-2.70) 98.6 (49.38-2.70)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.70 (at 2.69Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, $R_{free}$	0.265 , 0.289 0.285 , 0.314	Depositor DCC
$R_{free}$ test set	4920 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	76.9	Xtriage
Anisotropy	0.126	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 83.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.014 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	19781	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	135.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.99% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MN, ONM, SO4

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.51	0/1751	0.76	0/2366
1	B	0.49	0/1764	0.78	1/2382 (0.0%)
1	C	0.48	0/1764	0.70	1/2382 (0.0%)
1	D	0.44	0/1764	0.65	0/2382
1	E	0.40	0/1764	0.63	0/2382
1	F	0.40	0/1764	0.62	0/2382
1	G	0.41	0/1764	0.64	0/2382
1	H	0.41	0/1764	0.63	0/2382
1	I	0.41	0/1764	0.64	0/2382
1	J	0.39	0/1764	0.62	0/2382
1	K	0.38	0/1764	0.62	0/2382
All	All	0.43	0/19391	0.66	2/26186 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	297	VAL	N-CA-CB	6.59	126.01	111.50
1	B	297	VAL	N-CA-CB	5.25	123.04	111.50

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the 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 within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1720	0	1693	24	0
1	B	1733	0	1724	28	0
1	C	1733	0	1724	24	0
1	D	1733	0	1724	16	0
1	E	1733	0	1724	20	0
1	F	1733	0	1724	18	0
1	G	1733	0	1724	19	0
1	H	1733	0	1724	24	0
1	I	1733	0	1724	28	0
1	J	1733	0	1724	22	0
1	K	1733	0	1724	13	0
2	A	42	0	19	0	0
2	B	42	0	19	0	0
2	C	42	0	19	1	0
2	D	42	0	19	0	0
2	E	42	0	19	1	0
2	F	42	0	19	2	0
2	G	42	0	19	2	0
2	H	42	0	19	1	0
2	I	42	0	19	2	0
2	J	42	0	19	1	0
2	K	42	0	19	1	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
3	E	2	0	0	0	0
3	F	2	0	0	0	0
3	G	2	0	0	0	0
3	H	2	0	0	0	0
3	I	2	0	0	0	0
3	J	2	0	0	0	0
3	K	2	0	0	0	0
4	A	5	0	0	0	0
4	B	10	0	0	0	0
4	C	5	0	0	0	0
4	D	5	0	0	0	0
4	E	5	0	0	0	0
5	A	53	0	0	0	0
5	B	60	0	0	0	0
5	C	66	0	0	0	0
5	D	37	0	0	0	0
5	E	1	0	0	0	0

Continued on next page...

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	19781	0	19142	199	0

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 5.

All (199) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:269:PRO:HB2	1:D:353:VAL:HG21	1.48	0.93
1:B:227:LEU:HD22	1:B:231:ILE:HD11	1.54	0.90
1:G:299:GLY:HA2	1:H:367:TRP:HE1	1.42	0.83
1:A:353:VAL:HG21	1:B:269:PRO:HB2	1.65	0.77
1:C:269:PRO:HB2	1:D:353:VAL:CG2	2.14	0.76
1:I:299:GLY:HA2	1:J:367:TRP:HE1	1.51	0.75
1:D:387:GLN:OE1	1:D:418:THR:HG21	1.88	0.73
1:E:387:GLN:OE1	1:E:418:THR:HG21	1.90	0.71
1:H:387:GLN:OE1	1:H:418:THR:HG21	1.91	0.71
1:K:387:GLN:OE1	1:K:418:THR:HG21	1.92	0.70
1:F:380:THR:HG23	1:F:387:GLN:HE22	1.57	0.69
1:J:387:GLN:OE1	1:J:418:THR:HG21	1.91	0.69
1:C:269:PRO:CB	1:D:353:VAL:HG21	2.20	0.69
1:I:380:THR:HG23	1:I:387:GLN:HE22	1.58	0.69
1:G:380:THR:HG23	1:G:387:GLN:HE22	1.58	0.68
1:C:344:ARG:HH22	2:C:501:ONM:PG	2.16	0.68
1:A:353:VAL:HG21	1:B:269:PRO:CB	2.23	0.67
1:E:367:TRP:HE1	1:F:299:GLY:HA2	1.59	0.67
1:I:376:ARG:O	1:I:380:THR:HG22	1.94	0.67
1:I:296:LYS:HB3	1:I:363:PHE:CE1	2.30	0.67
1:C:376:ARG:O	1:C:380:THR:HG22	1.95	0.67
1:H:261:THR:HG23	2:H:501:ONM:H5'1	1.76	0.66
1:F:376:ARG:O	1:F:380:THR:HG22	1.97	0.64
1:C:380:THR:HG23	1:C:387:GLN:HE22	1.63	0.64
1:G:376:ARG:O	1:G:380:THR:HG22	1.99	0.63
1:I:236:LYS:HG3	1:J:222:LEU:HD12	1.80	0.63
1:A:258:VAL:HG21	1:A:383:VAL:HB	1.79	0.63
1:I:403:GLN:HG2	1:I:420:TYR:HB2	1.80	0.63
1:F:269:PRO:HB3	2:F:501:ONM:HA4	1.80	0.62
1:G:361:ARG:HB2	1:H:294:LYS:HD3	1.81	0.62
1:B:228:PRO:HD2	1:B:231:ILE:HG12	1.80	0.61
1:B:312:ARG:HD2	1:B:315:HIS:HA	1.81	0.61
1:B:347:MET:HB2	1:B:388:VAL:HG12	1.83	0.61

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:367:TRP:HE1	1:J:299:GLY:HA2	1.65	0.61
1:A:353:VAL:CG2	1:B:269:PRO:HB2	2.29	0.60
1:B:344:ARG:HG2	1:B:381:ASP:HB3	1.83	0.60
1:C:305:VAL:HG21	1:C:366:VAL:HG21	1.83	0.60
1:E:236:LYS:HG3	1:F:222:LEU:HD12	1.84	0.60
1:E:401:VAL:HG13	1:E:422:ILE:HB	1.85	0.59
1:D:401:VAL:HG13	1:D:422:ILE:HB	1.84	0.58
1:K:401:VAL:HG13	1:K:422:ILE:HB	1.85	0.58
1:E:399:GLU:HA	1:E:425:LYS:HD2	1.85	0.58
1:H:401:VAL:HG13	1:H:422:ILE:HB	1.85	0.58
1:I:296:LYS:HB3	1:I:363:PHE:HE1	1.67	0.58
1:G:296:LYS:HB3	1:G:363:PHE:CE1	2.39	0.57
1:G:305:VAL:HG21	1:G:366:VAL:HG21	1.86	0.57
1:F:305:VAL:HG21	1:F:366:VAL:HG21	1.87	0.57
1:J:401:VAL:HG13	1:J:422:ILE:HB	1.85	0.56
1:C:223:LEU:HD11	1:D:222:LEU:HD13	1.88	0.55
1:I:400:PHE:CE2	1:I:424:ARG:HD3	2.42	0.55
1:J:305:VAL:HG21	1:J:366:VAL:HG21	1.89	0.55
1:B:390:GLU:HG2	1:B:419:TRP:HE1	1.71	0.55
1:D:258:VAL:HG21	1:D:383:VAL:HB	1.89	0.55
1:A:348:ALA:HB2	1:A:373:VAL:HG22	1.90	0.54
1:B:258:VAL:HG21	1:B:383:VAL:HB	1.90	0.54
1:B:283:PHE:HE1	1:B:329:VAL:HG23	1.73	0.54
1:I:258:VAL:HG21	1:I:383:VAL:HB	1.90	0.54
1:H:252:VAL:HB	1:H:305:VAL:HG22	1.90	0.53
1:B:377:MET:O	1:B:381:ASP:HB2	2.09	0.53
1:E:261:THR:HG23	2:E:501:ONM:H5'1	1.91	0.53
1:C:258:VAL:HG21	1:C:383:VAL:HB	1.91	0.53
1:G:269:PRO:HB2	1:H:353:VAL:HG21	1.91	0.53
1:I:305:VAL:HG21	1:I:366:VAL:HG21	1.89	0.53
1:E:305:VAL:HG21	1:E:366:VAL:HG21	1.89	0.53
1:A:252:VAL:HB	1:A:305:VAL:HG22	1.92	0.52
1:B:245:ASP:HB3	1:C:239:SER:OG	2.09	0.52
1:B:305:VAL:CG1	1:B:308:VAL:HG13	2.39	0.52
1:K:305:VAL:HG21	1:K:366:VAL:HG21	1.92	0.52
1:K:252:VAL:HB	1:K:305:VAL:HG22	1.92	0.52
1:E:258:VAL:HG21	1:E:383:VAL:HB	1.91	0.52
1:G:252:VAL:HB	1:G:305:VAL:HG22	1.92	0.52
1:K:258:VAL:HG21	1:K:383:VAL:HB	1.92	0.52
1:H:258:VAL:HG21	1:H:383:VAL:HB	1.92	0.51
1:G:258:VAL:HG21	1:G:383:VAL:HB	1.92	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:305:VAL:HG21	1:H:366:VAL:HG21	1.92	0.51
1:J:258:VAL:HG21	1:J:383:VAL:HB	1.91	0.51
1:F:252:VAL:HB	1:F:305:VAL:HG22	1.92	0.51
1:E:294:LYS:HD3	1:F:361:ARG:HB2	1.92	0.51
1:F:258:VAL:HG21	1:F:383:VAL:HB	1.92	0.51
1:G:222:LEU:HD12	1:H:236:LYS:HG3	1.93	0.51
1:H:239:SER:HA	1:I:246:LYS:O	2.11	0.51
1:C:252:VAL:HB	1:C:305:VAL:HG22	1.92	0.51
1:J:252:VAL:HB	1:J:305:VAL:HG22	1.93	0.51
1:E:252:VAL:HB	1:E:305:VAL:HG22	1.92	0.50
1:K:260:PHE:HE2	2:K:501:ONM:HA2	1.76	0.50
1:I:252:VAL:HB	1:I:305:VAL:HG22	1.93	0.50
1:D:252:VAL:HB	1:D:305:VAL:HG22	1.94	0.50
1:F:296:LYS:HB3	1:F:363:PHE:CE1	2.45	0.50
1:A:348:ALA:CB	1:A:373:VAL:HG22	2.42	0.49
1:B:234:ARG:CZ	1:B:243:ILE:HG23	2.42	0.49
1:C:252:VAL:HG11	1:C:371:VAL:HG12	1.95	0.49
1:G:299:GLY:HA2	1:H:367:TRP:NE1	2.20	0.49
1:E:356:VAL:HG13	1:E:362:PHE:HB2	1.96	0.48
1:J:269:PRO:HA	2:J:501:ONM:HA4	1.95	0.48
1:E:277:ASN:HB2	1:F:357:VAL:HG12	1.96	0.48
1:C:380:THR:CG2	1:C:387:GLN:HE22	2.28	0.47
1:E:389:PRO:HD2	1:E:392:MET:HB2	1.96	0.47
1:A:258:VAL:HB	1:A:342:PRO:HB2	1.97	0.47
1:D:305:VAL:HG21	1:D:366:VAL:HG21	1.96	0.47
1:C:296:LYS:HB3	1:C:363:PHE:CE1	2.50	0.47
1:J:356:VAL:HG13	1:J:362:PHE:HB2	1.96	0.47
1:C:373:VAL:O	1:C:377:MET:HG2	2.15	0.47
1:A:216:TYR:HB2	1:B:216:TYR:HD1	1.80	0.46
1:A:250:VAL:HG11	1:A:308:VAL:HG13	1.97	0.46
1:D:389:PRO:HD2	1:D:392:MET:HB2	1.97	0.46
1:A:401:VAL:HG12	1:A:422:ILE:HD11	1.96	0.46
1:A:258:VAL:HG22	1:A:344:ARG:HE	1.81	0.46
1:B:393:TYR:HD1	1:B:402:LEU:HG	1.80	0.46
1:C:280:TYR:CD2	1:C:297:VAL:HG21	2.49	0.46
1:H:389:PRO:HD2	1:H:392:MET:HB2	1.98	0.46
1:A:274:ARG:HG2	1:B:242:VAL:HG21	1.96	0.46
1:K:389:PRO:HD2	1:K:392:MET:HB2	1.96	0.46
1:G:252:VAL:HG11	1:G:371:VAL:HG12	1.96	0.45
1:A:335:ASP:OD1	1:A:339:ASP:HB2	2.16	0.45
1:F:252:VAL:HG11	1:F:371:VAL:HG12	1.99	0.45

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:503:ONM:N3	2:G:503:ONM:H1	2.30	0.45
1:B:267:THR:HB	1:B:272:LEU:HD13	1.99	0.45
1:C:269:PRO:CB	1:D:353:VAL:CG2	2.88	0.45
1:D:317:PHE:HD2	1:D:400:PHE:HE2	1.65	0.45
1:J:252:VAL:HG11	1:J:371:VAL:HG12	1.99	0.45
2:I:503:ONM:O2'	1:J:371:VAL:HG22	2.17	0.45
1:G:373:VAL:O	1:G:377:MET:HG2	2.16	0.45
1:F:300:ASP:HB2	2:F:501:ONM:H5'1	1.99	0.45
1:H:310:ARG:HH11	1:I:233:GLU:HG2	1.82	0.44
1:I:252:VAL:HG11	1:I:371:VAL:HG12	1.99	0.44
1:H:311:ALA:HB2	1:I:238:SER:HB2	1.99	0.44
1:H:317:PHE:HD2	1:H:400:PHE:HE2	1.66	0.44
1:G:380:THR:CG2	1:G:387:GLN:HE22	2.29	0.44
1:I:373:VAL:O	1:I:377:MET:HG2	2.18	0.44
1:E:267:THR:HB	1:E:272:LEU:HD13	1.99	0.44
1:C:312:ARG:HD2	1:C:315:HIS:HA	1.99	0.44
1:I:312:ARG:HD2	1:I:315:HIS:HA	2.00	0.44
1:A:353:VAL:CG2	1:B:269:PRO:CB	2.91	0.44
1:F:373:VAL:O	1:F:377:MET:HG2	2.18	0.44
1:H:309:PRO:O	1:I:237:SER:HB2	2.17	0.44
1:J:317:PHE:HD2	1:J:400:PHE:HE2	1.65	0.44
1:K:317:PHE:HD2	1:K:400:PHE:HE2	1.66	0.44
1:A:257:ILE:HD11	1:A:279:LEU:HD22	2.00	0.43
1:A:335:ASP:HB2	1:A:336:PRO:CD	2.48	0.43
1:B:235:LEU:HD12	1:B:235:LEU:HA	1.93	0.43
1:B:373:VAL:O	1:B:377:MET:HG2	2.18	0.43
1:E:347:MET:HB2	1:E:388:VAL:HG12	1.99	0.43
1:C:377:MET:O	1:C:381:ASP:HB2	2.18	0.43
1:B:240:ARG:HE	1:C:248:ASP:CG	2.22	0.43
1:D:295:ILE:HG22	1:D:296:LYS:HG2	2.00	0.43
1:E:252:VAL:HG11	1:E:371:VAL:HG12	2.00	0.43
1:F:380:THR:CG2	1:F:387:GLN:HE22	2.29	0.43
1:K:356:VAL:HG13	1:K:362:PHE:HB2	1.99	0.43
1:A:246:LYS:HE2	1:B:269:PRO:HD2	2.01	0.43
1:I:377:MET:O	1:I:381:ASP:HB2	2.19	0.43
1:A:236:LYS:CG	1:B:222:LEU:HD12	2.49	0.43
1:A:276:LEU:HD12	1:A:276:LEU:HA	1.87	0.43
1:G:312:ARG:HD2	1:G:315:HIS:HA	2.01	0.43
1:H:347:MET:HB2	1:H:388:VAL:HG12	2.00	0.43
1:I:396:LEU:HG	1:I:400:PHE:CD1	2.54	0.42
1:B:259:GLY:O	1:B:262:GLU:HG2	2.18	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:272:LEU:HD12	1:C:272:LEU:HA	1.92	0.42
1:H:311:ALA:CB	1:I:238:SER:HB2	2.49	0.42
1:E:317:PHE:HD2	1:E:400:PHE:HE2	1.67	0.42
1:F:312:ARG:HD2	1:F:315:HIS:HA	2.01	0.42
1:I:267:THR:HB	1:I:272:LEU:HD13	2.01	0.42
1:A:236:LYS:HG3	1:B:222:LEU:HD12	2.00	0.42
1:C:267:THR:HB	1:C:272:LEU:HD13	2.02	0.42
1:E:377:MET:O	1:E:381:ASP:HB2	2.20	0.42
1:I:222:LEU:HD12	1:J:236:LYS:HG3	2.02	0.42
1:I:347:MET:HB2	1:I:388:VAL:HG12	2.00	0.42
1:A:344:ARG:HG2	1:A:381:ASP:HB3	2.02	0.42
1:D:373:VAL:O	1:D:377:MET:HG2	2.20	0.42
1:H:356:VAL:HG13	1:H:362:PHE:HB2	2.01	0.42
1:H:267:THR:HB	1:H:272:LEU:HD13	2.02	0.42
1:G:347:MET:HB2	1:G:388:VAL:HG12	2.01	0.42
1:H:377:MET:O	1:H:381:ASP:HB2	2.20	0.42
1:B:215:GLU:HA	1:B:218:ARG:HG3	2.02	0.42
1:H:310:ARG:NH2	1:I:236:LYS:HB3	2.35	0.42
1:J:267:THR:HB	1:J:272:LEU:HD13	2.02	0.42
1:I:299:GLY:HA2	1:J:367:TRP:NE1	2.29	0.41
1:J:377:MET:O	1:J:381:ASP:HB2	2.20	0.41
1:F:377:MET:O	1:F:381:ASP:HB2	2.20	0.41
1:K:377:MET:O	1:K:381:ASP:HB2	2.20	0.41
1:H:373:VAL:O	1:H:377:MET:HG2	2.21	0.41
1:J:234:ARG:CZ	1:K:234:ARG:HD3	2.51	0.41
1:C:410:VAL:HG23	1:C:413:LYS:HB2	2.03	0.41
1:G:267:THR:HB	1:G:272:LEU:HD13	2.02	0.41
1:G:377:MET:O	1:G:381:ASP:HB2	2.20	0.41
1:J:347:MET:HB2	1:J:388:VAL:HG12	2.01	0.41
1:K:252:VAL:HG11	1:K:371:VAL:HG12	2.02	0.41
1:C:344:ARG:HG2	1:C:381:ASP:HB3	2.02	0.41
1:I:294:LYS:HD3	1:J:361:ARG:HB2	2.03	0.41
1:J:389:PRO:HD2	1:J:392:MET:HB2	2.03	0.41
1:K:267:THR:HB	1:K:272:LEU:HD13	2.02	0.41
1:E:218:ARG:HD2	1:F:236:LYS:O	2.21	0.40
1:J:373:VAL:O	1:J:377:MET:HG2	2.21	0.40
1:A:243:ILE:O	1:A:355:GLY:HA3	2.20	0.40
1:A:251:SER:HB3	1:A:319:LEU:HD22	2.03	0.40
1:D:344:ARG:HG2	1:D:381:ASP:HB3	2.04	0.40
1:G:269:PRO:HA	2:G:503:ONM:HA4	2.03	0.40
2:I:503:ONM:H5'2	2:I:503:ONM:N3	2.36	0.40

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:356:VAL:HG13	1:D:362:PHE:HB2	2.04	0.40
1:E:373:VAL:O	1:E:377:MET:HG2	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 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 X-ray entries followed by that with respect to entries of similar resolution.

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	222/254 (87%)	215 (97%)	6 (3%)	1 (0%)	29	54
1	B	222/254 (87%)	218 (98%)	3 (1%)	1 (0%)	29	54
1	C	222/254 (87%)	218 (98%)	4 (2%)	0	100	100
1	D	222/254 (87%)	218 (98%)	4 (2%)	0	100	100
1	E	222/254 (87%)	219 (99%)	3 (1%)	0	100	100
1	F	222/254 (87%)	219 (99%)	3 (1%)	0	100	100
1	G	222/254 (87%)	218 (98%)	4 (2%)	0	100	100
1	H	222/254 (87%)	218 (98%)	4 (2%)	0	100	100
1	I	222/254 (87%)	216 (97%)	6 (3%)	0	100	100
1	J	222/254 (87%)	219 (99%)	3 (1%)	0	100	100
1	K	222/254 (87%)	219 (99%)	3 (1%)	0	100	100
All	All	2442/2794 (87%)	2397 (98%)	43 (2%)	2 (0%)	51	78

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	397	LYS
1	A	427	ASP

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	177/207 (86%)	155 (88%)	22 (12%)	4	11
1	B	181/207 (87%)	156 (86%)	25 (14%)	3	8
1	C	181/207 (87%)	160 (88%)	21 (12%)	5	12
1	D	181/207 (87%)	160 (88%)	21 (12%)	5	12
1	E	181/207 (87%)	160 (88%)	21 (12%)	5	12
1	F	181/207 (87%)	159 (88%)	22 (12%)	5	11
1	G	181/207 (87%)	158 (87%)	23 (13%)	4	10
1	H	181/207 (87%)	160 (88%)	21 (12%)	5	12
1	I	181/207 (87%)	154 (85%)	27 (15%)	3	7
1	J	181/207 (87%)	159 (88%)	22 (12%)	5	11
1	K	181/207 (87%)	159 (88%)	22 (12%)	5	11
All	All	1987/2277 (87%)	1740 (88%)	247 (12%)	4	11

All (247) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	205	THR
1	A	215	GLU
1	A	217	GLU
1	A	222	LEU
1	A	252	VAL
1	A	267	THR
1	A	272	LEU
1	A	276	LEU
1	A	279	LEU
1	A	297	VAL
1	A	312	ARG
1	A	325	ASP
1	A	326	MET
1	A	334	LYS
1	A	352	VAL

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	366	VAL
1	A	382	SER
1	A	385	ARG
1	A	395	ARG
1	A	396	LEU
1	A	398	ASN
1	A	427	ASP
1	B	217	GLU
1	B	218	ARG
1	B	220	GLU
1	B	222	LEU
1	B	231	ILE
1	B	235	LEU
1	B	252	VAL
1	B	253	LEU
1	B	272	LEU
1	B	276	LEU
1	B	279	LEU
1	B	297	VAL
1	B	301	SER
1	B	308	VAL
1	B	312	ARG
1	B	333	LEU
1	B	352	VAL
1	B	360	ARG
1	B	373	VAL
1	B	383	VAL
1	B	385	ARG
1	B	390	GLU
1	B	417	ARG
1	B	421	LEU
1	B	424	ARG
1	C	215	GLU
1	C	222	LEU
1	C	225	ASN
1	C	235	LEU
1	C	240	ARG
1	C	252	VAL
1	C	253	LEU
1	C	272	LEU
1	C	285	GLU
1	C	297	VAL

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	301	SER
1	C	312	ARG
1	C	335	ASP
1	C	352	VAL
1	C	360	ARG
1	C	373	VAL
1	C	387	GLN
1	C	395	ARG
1	C	421	LEU
1	C	424	ARG
1	C	425	LYS
1	D	209	GLU
1	D	212	MET
1	D	215	GLU
1	D	222	LEU
1	D	235	LEU
1	D	252	VAL
1	D	253	LEU
1	D	272	LEU
1	D	276	LEU
1	D	279	LEU
1	D	285	GLU
1	D	301	SER
1	D	335	ASP
1	D	352	VAL
1	D	373	VAL
1	D	387	GLN
1	D	392	MET
1	D	396	LEU
1	D	407	ARG
1	D	424	ARG
1	D	425	LYS
1	E	209	GLU
1	E	212	MET
1	E	215	GLU
1	E	222	LEU
1	E	235	LEU
1	E	252	VAL
1	E	253	LEU
1	E	272	LEU
1	E	276	LEU
1	E	279	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	E	285	GLU
1	E	301	SER
1	E	335	ASP
1	E	352	VAL
1	E	373	VAL
1	E	387	GLN
1	E	392	MET
1	E	396	LEU
1	E	407	ARG
1	E	424	ARG
1	E	425	LYS
1	F	215	GLU
1	F	222	LEU
1	F	225	ASN
1	F	235	LEU
1	F	240	ARG
1	F	252	VAL
1	F	253	LEU
1	F	272	LEU
1	F	276	LEU
1	F	285	GLU
1	F	301	SER
1	F	335	ASP
1	F	352	VAL
1	F	360	ARG
1	F	373	VAL
1	F	387	GLN
1	F	392	MET
1	F	395	ARG
1	F	403	GLN
1	F	421	LEU
1	F	424	ARG
1	F	425	LYS
1	G	212	MET
1	G	215	GLU
1	G	222	LEU
1	G	225	ASN
1	G	235	LEU
1	G	240	ARG
1	G	252	VAL
1	G	253	LEU
1	G	272	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	G	276	LEU
1	G	285	GLU
1	G	301	SER
1	G	335	ASP
1	G	352	VAL
1	G	360	ARG
1	G	373	VAL
1	G	387	GLN
1	G	395	ARG
1	G	396	LEU
1	G	421	LEU
1	G	424	ARG
1	G	425	LYS
1	G	428	GLU
1	H	209	GLU
1	H	212	MET
1	H	215	GLU
1	H	222	LEU
1	H	235	LEU
1	H	252	VAL
1	H	253	LEU
1	H	272	LEU
1	H	276	LEU
1	H	279	LEU
1	H	285	GLU
1	H	301	SER
1	H	335	ASP
1	H	352	VAL
1	H	373	VAL
1	H	387	GLN
1	H	392	MET
1	H	396	LEU
1	H	407	ARG
1	H	424	ARG
1	H	425	LYS
1	I	212	MET
1	I	215	GLU
1	I	222	LEU
1	I	225	ASN
1	I	233	GLU
1	I	235	LEU
1	I	240	ARG

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	I	252	VAL
1	I	253	LEU
1	I	272	LEU
1	I	276	LEU
1	I	285	GLU
1	I	296	LYS
1	I	301	SER
1	I	335	ASP
1	I	352	VAL
1	I	360	ARG
1	I	373	VAL
1	I	383	VAL
1	I	387	GLN
1	I	395	ARG
1	I	396	LEU
1	I	403	GLN
1	I	421	LEU
1	I	424	ARG
1	I	425	LYS
1	I	427	ASP
1	J	209	GLU
1	J	212	MET
1	J	215	GLU
1	J	222	LEU
1	J	235	LEU
1	J	240	ARG
1	J	252	VAL
1	J	253	LEU
1	J	272	LEU
1	J	276	LEU
1	J	279	LEU
1	J	285	GLU
1	J	301	SER
1	J	335	ASP
1	J	352	VAL
1	J	373	VAL
1	J	387	GLN
1	J	392	MET
1	J	396	LEU
1	J	407	ARG
1	J	424	ARG
1	J	425	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	K	209	GLU
1	K	212	MET
1	K	215	GLU
1	K	222	LEU
1	K	235	LEU
1	K	252	VAL
1	K	253	LEU
1	K	272	LEU
1	K	276	LEU
1	K	279	LEU
1	K	285	GLU
1	K	301	SER
1	K	335	ASP
1	K	347	MET
1	K	352	VAL
1	K	373	VAL
1	K	383	VAL
1	K	387	GLN
1	K	392	MET
1	K	396	LEU
1	K	407	ARG
1	K	424	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	387	GLN
1	F	225	ASN
1	F	387	GLN
1	F	403	GLN
1	G	387	GLN
1	I	225	ASN
1	I	387	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 39 ligands modelled in this entry, 22 are monoatomic - leaving 17 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or 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 length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	ONM	H	501	3	37,45,45	0.52	0	47,69,69	0.68	0
2	ONM	K	501	3	37,45,45	0.59	0	47,69,69	0.56	0
4	SO4	B	503	-	4,4,4	0.16	0	6,6,6	0.10	0
4	SO4	C	502	-	4,4,4	0.18	0	6,6,6	0.31	0
2	ONM	C	501	3	37,45,45	0.68	0	47,69,69	0.67	0
2	ONM	D	502	3	37,45,45	0.72	1 (2%)	47,69,69	0.98	3 (6%)
2	ONM	J	501	3	37,45,45	0.60	0	47,69,69	0.61	0
2	ONM	B	502	3	37,45,45	0.67	1 (2%)	47,69,69	0.81	1 (2%)
4	SO4	A	504	-	4,4,4	0.28	0	6,6,6	0.20	0
2	ONM	F	501	3	37,45,45	0.63	0	47,69,69	0.54	0
4	SO4	B	501	-	4,4,4	0.21	0	6,6,6	0.17	0
4	SO4	D	501	-	4,4,4	0.17	0	6,6,6	0.15	0
2	ONM	A	501	3	37,45,45	0.60	1 (2%)	47,69,69	0.82	1 (2%)
2	ONM	G	503	3	37,45,45	0.59	0	47,69,69	0.55	0
2	ONM	E	501	3	37,45,45	0.57	0	47,69,69	0.78	1 (2%)
4	SO4	E	502	-	4,4,4	0.18	0	6,6,6	0.09	0
2	ONM	I	503	3	37,45,45	0.57	0	47,69,69	0.67	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ONM	H	501	3	-	0/28/48/48	0/4/4/4
2	ONM	K	501	3	-	8/28/48/48	0/4/4/4
2	ONM	C	501	3	-	4/28/48/48	0/4/4/4
2	ONM	D	502	3	-	2/28/48/48	0/4/4/4
2	ONM	J	501	3	-	1/28/48/48	0/4/4/4
2	ONM	B	502	3	-	5/28/48/48	0/4/4/4
2	ONM	F	501	3	-	4/28/48/48	0/4/4/4
2	ONM	A	501	3	-	3/28/48/48	0/4/4/4
2	ONM	G	503	3	-	2/28/48/48	0/4/4/4
2	ONM	E	501	3	-	3/28/48/48	0/4/4/4
2	ONM	I	503	3	-	5/28/48/48	0/4/4/4

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	502	ONM	C8-N7	-2.29	1.31	1.35
2	A	501	ONM	C8-N7	-2.09	1.31	1.35
2	B	502	ONM	C8-N7	-2.06	1.31	1.35

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	501	ONM	PB-O1A-PA	3.14	143.59	132.83
2	D	502	ONM	PB-O1B-PG	-3.01	122.48	132.83
2	D	502	ONM	O5'-PA-O3A	-2.87	97.87	109.07
2	D	502	ONM	PB-O1A-PA	2.40	141.08	132.83
2	A	501	ONM	PB-O1B-PG	-2.32	124.85	132.83
2	B	502	ONM	O3'-C3'-C4'	-2.12	104.28	109.56

There are no chirality outliers.

All (37) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	ONM	PB-O1B-PG-O3G
2	B	502	ONM	C5'-O5'-PA-O1A
2	D	502	ONM	PB-O1B-PG-O3G
2	D	502	ONM	PB-O1B-PG-O1G
2	I	503	ONM	PB-O1B-PG-O1G

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
2	K	501	ONM	PB-O1B-PG-O3G
2	C	501	ONM	PB-O1A-PA-O3A
2	F	501	ONM	PB-O1A-PA-O3A
2	K	501	ONM	O3'-CA-CA1-CA6
2	F	501	ONM	OA-CA-O3'-C3'
2	K	501	ONM	PB-O1B-PG-O1G
2	B	502	ONM	PA-O1A-PB-O2B
2	E	501	ONM	PB-O1A-PA-O3A
2	G	503	ONM	PA-O1A-PB-O3B
2	B	502	ONM	C5'-O5'-PA-O2A
2	F	501	ONM	CA1-CA-O3'-C3'
2	E	501	ONM	O4'-C4'-C5'-O5'
2	I	503	ONM	PG-O1B-PB-O3B
2	K	501	ONM	PB-O1A-PA-O3A
2	E	501	ONM	C3'-C4'-C5'-O5'
2	F	501	ONM	O4'-C4'-C5'-O5'
2	K	501	ONM	O3'-CA-CA1-CA2
2	K	501	ONM	OA-CA-CA1-CA6
2	J	501	ONM	PB-O1A-PA-O5'
2	A	501	ONM	PB-O1B-PG-O2G
2	I	503	ONM	PB-O1B-PG-O2G
2	A	501	ONM	PB-O1B-PG-O1G
2	I	503	ONM	PB-O1B-PG-O3G
2	C	501	ONM	C5'-O5'-PA-O1A
2	G	503	ONM	O4'-C4'-C5'-O5'
2	I	503	ONM	O4'-C4'-C5'-O5'
2	B	502	ONM	PB-O1A-PA-O2A
2	K	501	ONM	PB-O1A-PA-O2A
2	B	502	ONM	C5'-O5'-PA-O3A
2	C	501	ONM	C5'-O5'-PA-O2A
2	C	501	ONM	O4'-C4'-C5'-O5'
2	K	501	ONM	PB-O1B-PG-O2G

There are no ring outliers.

8 monomers are involved in 11 short contacts:

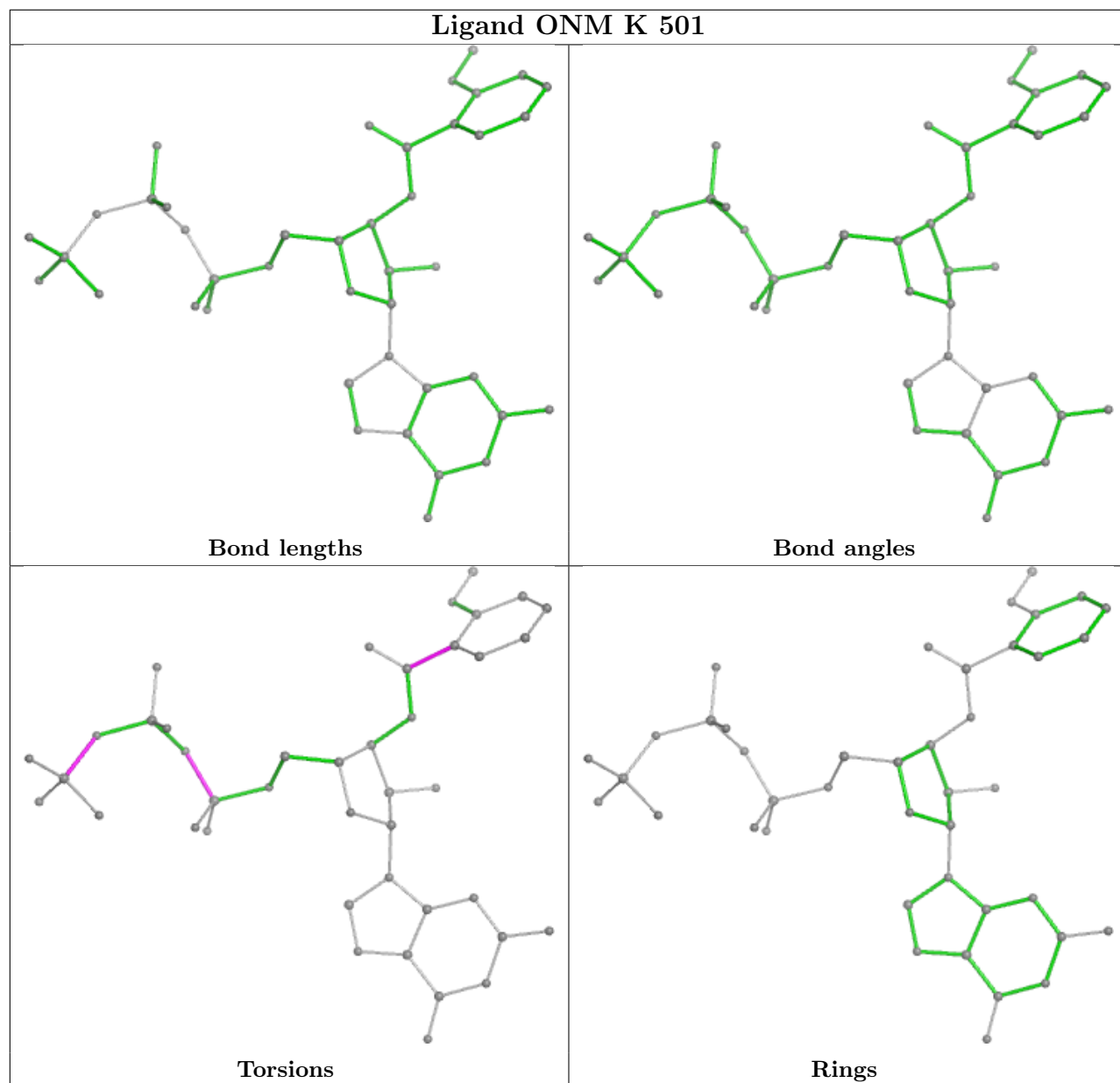
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	501	ONM	1	0
2	K	501	ONM	1	0
2	C	501	ONM	1	0
2	J	501	ONM	1	0
2	F	501	ONM	2	0

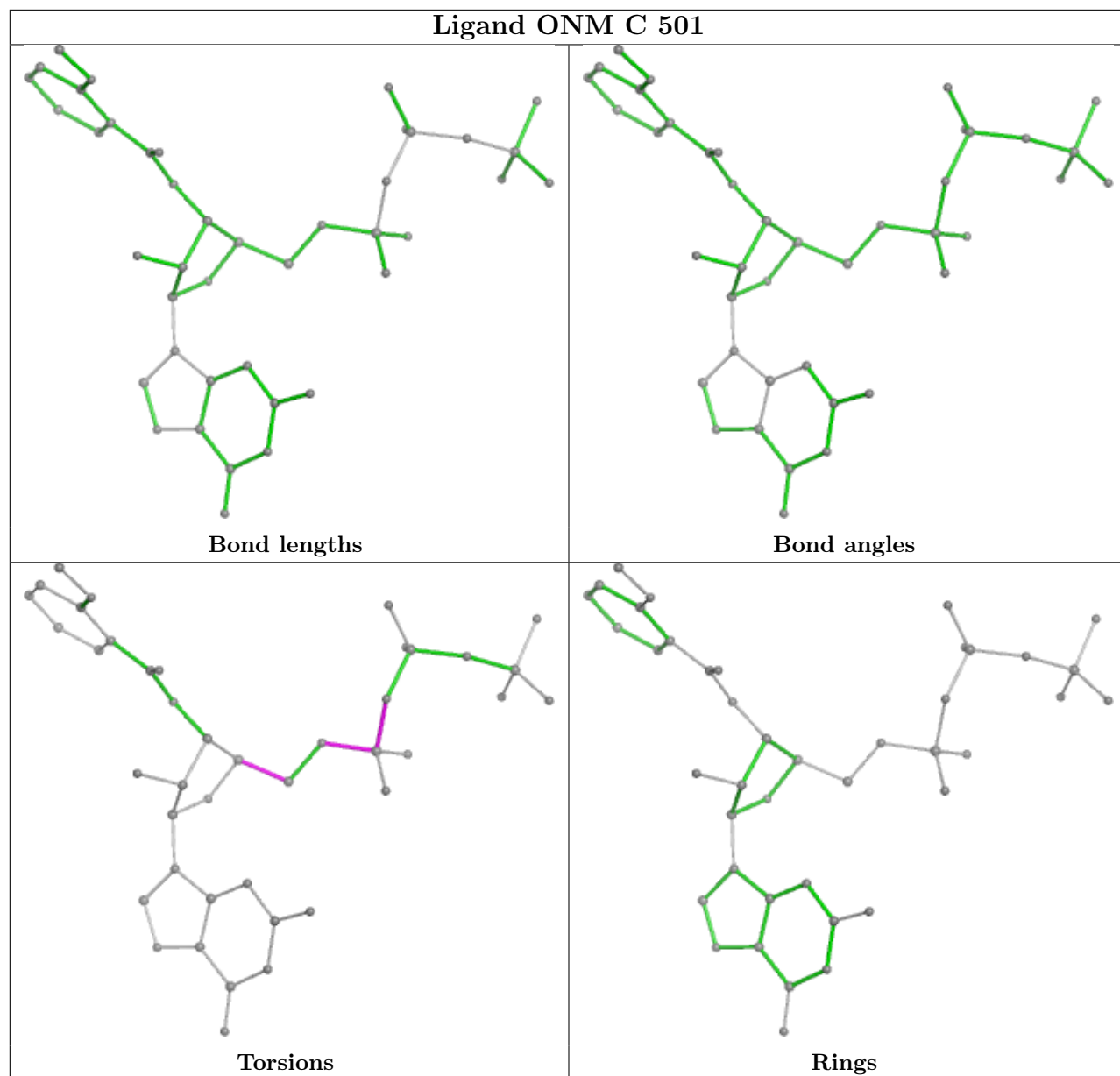
*Continued on next page...*

*Continued from previous page...*

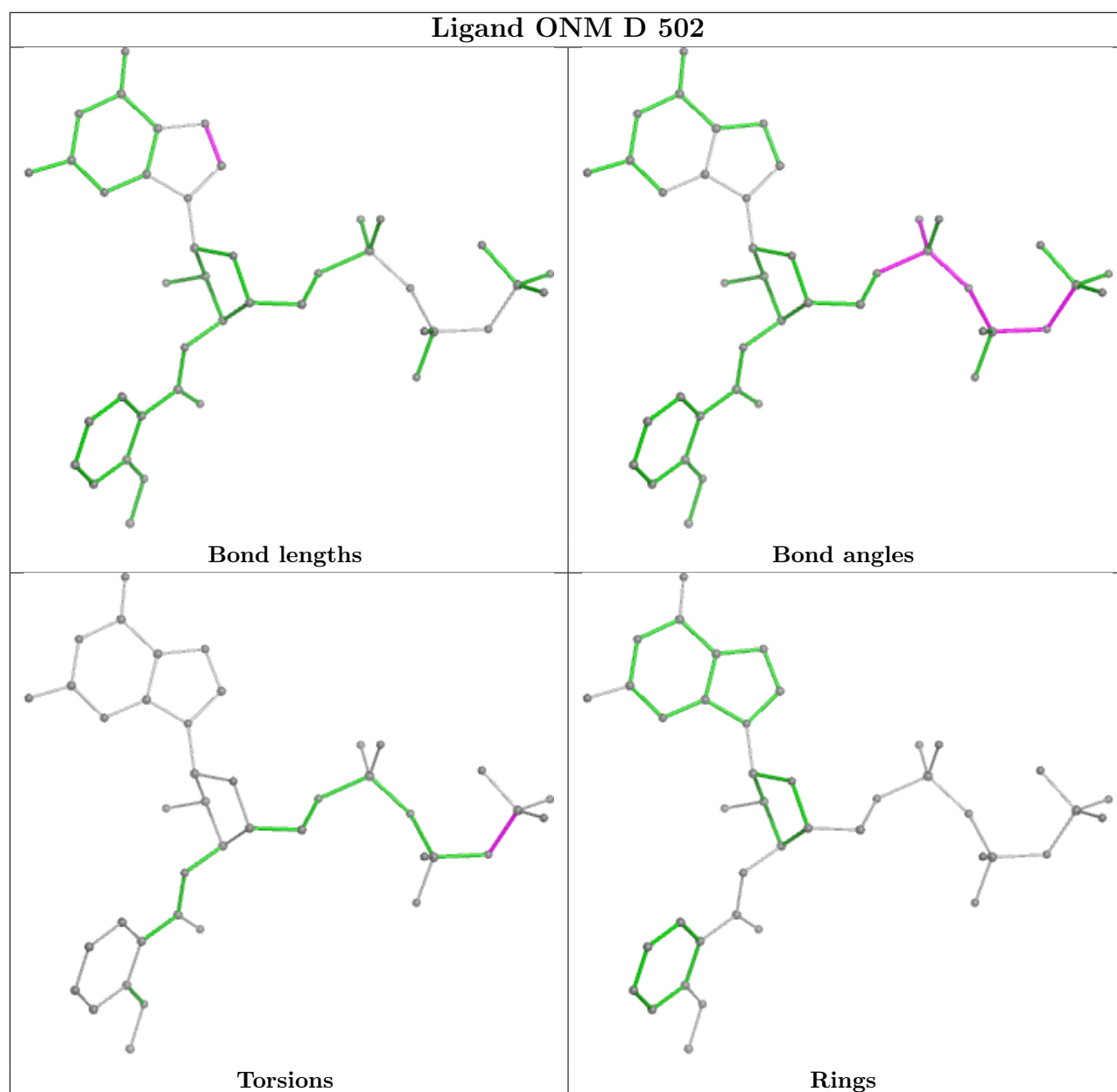
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	503	ONM	2	0
2	E	501	ONM	1	0
2	I	503	ONM	2	0

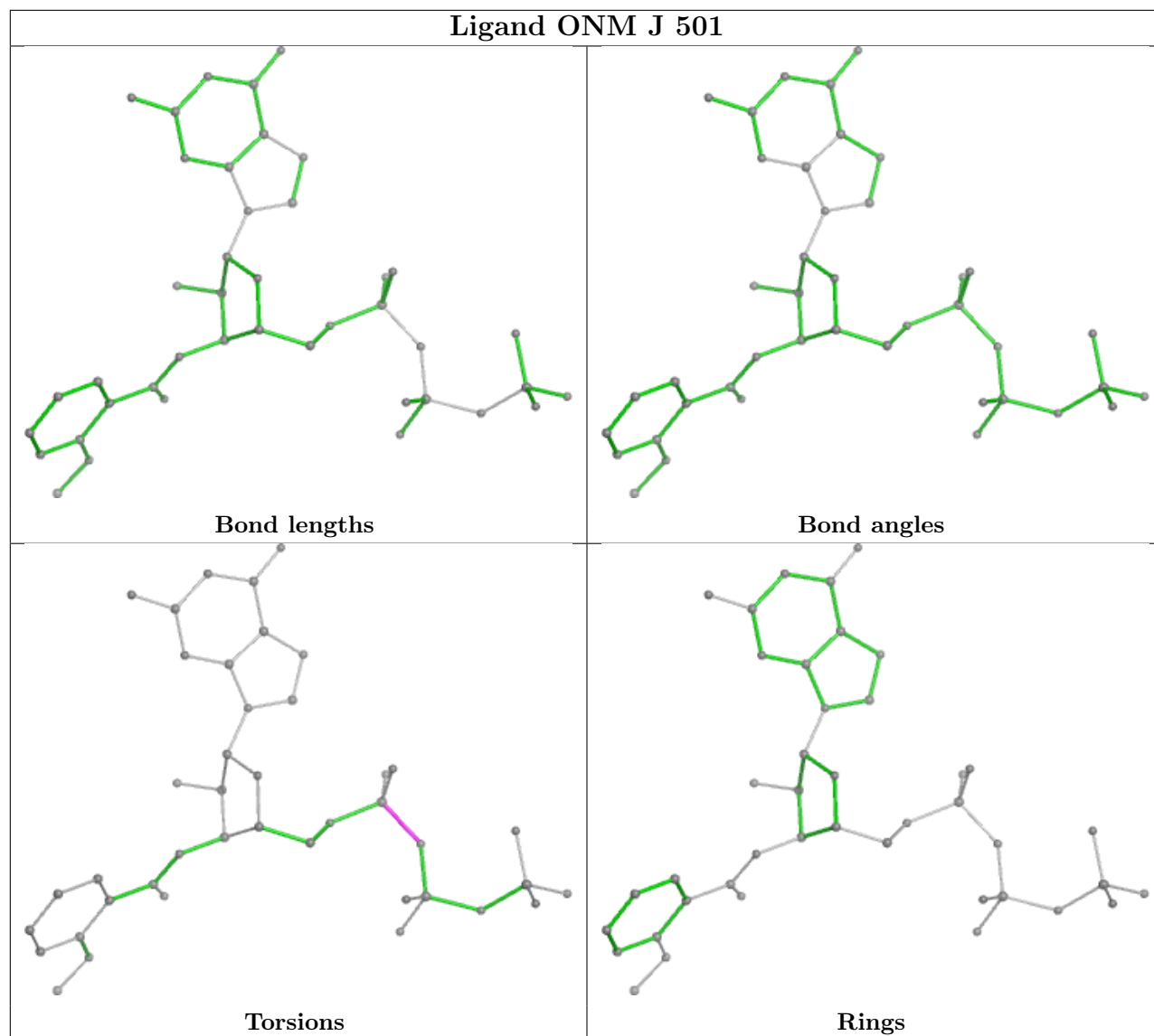
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

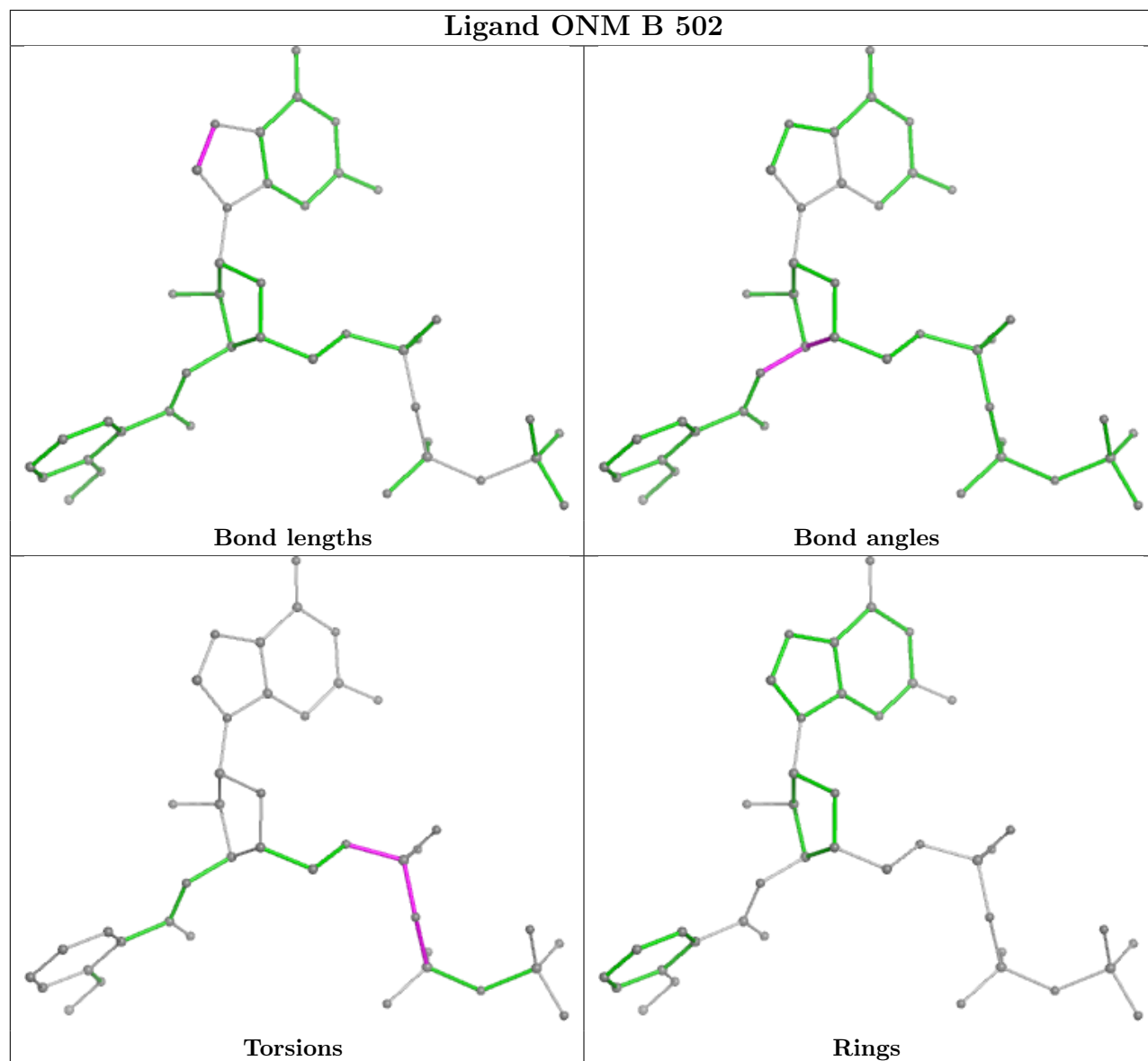


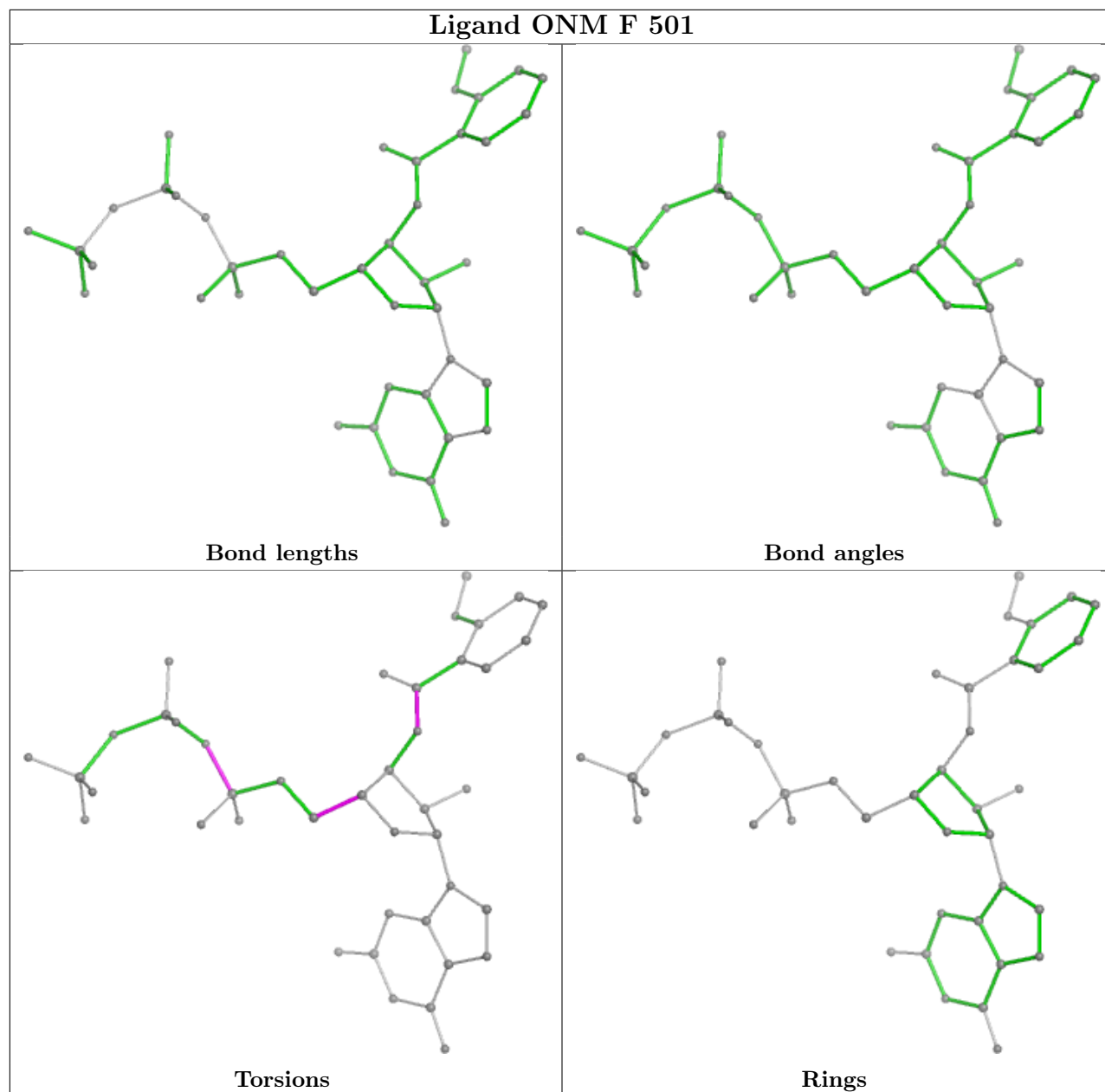


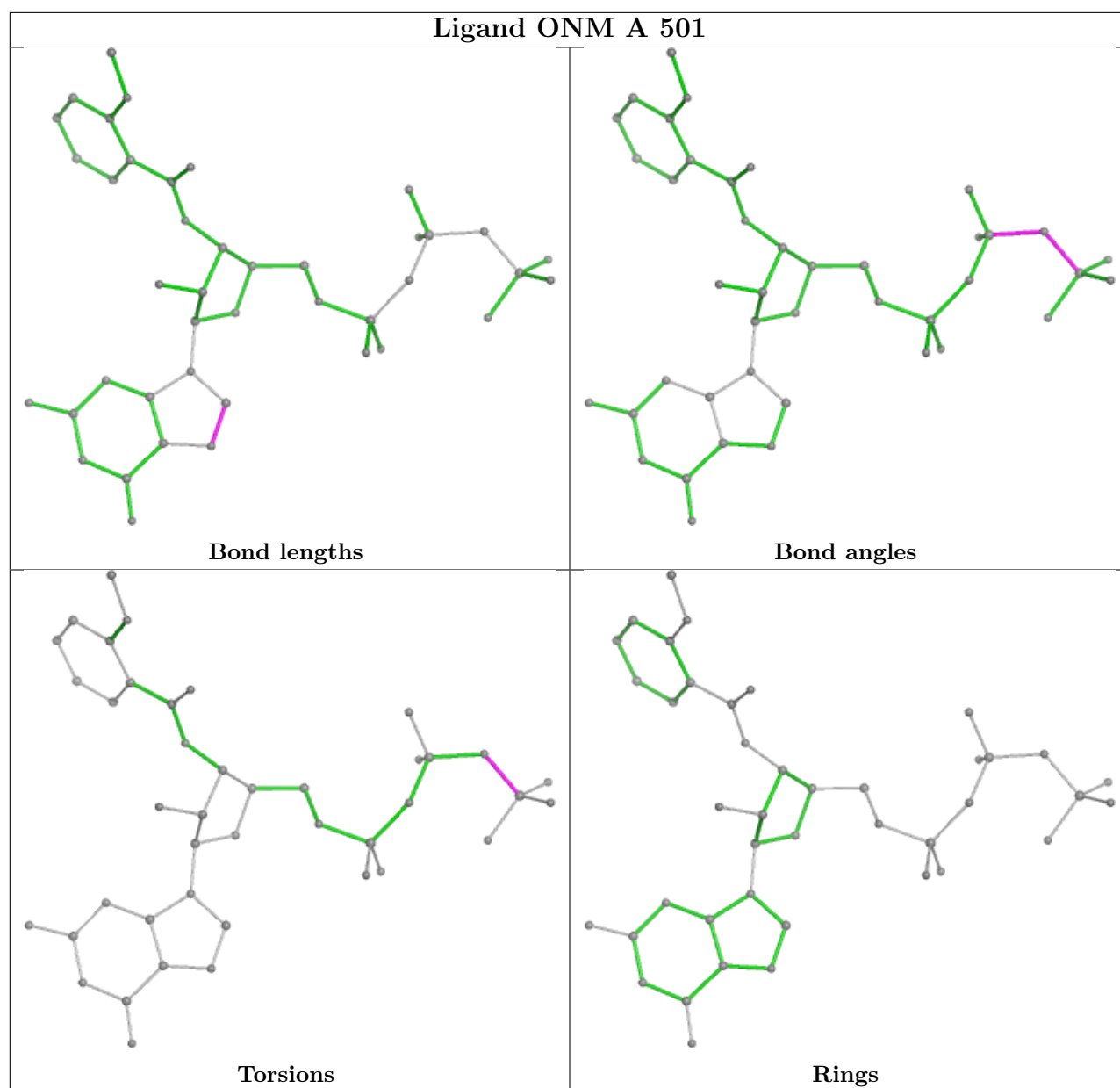


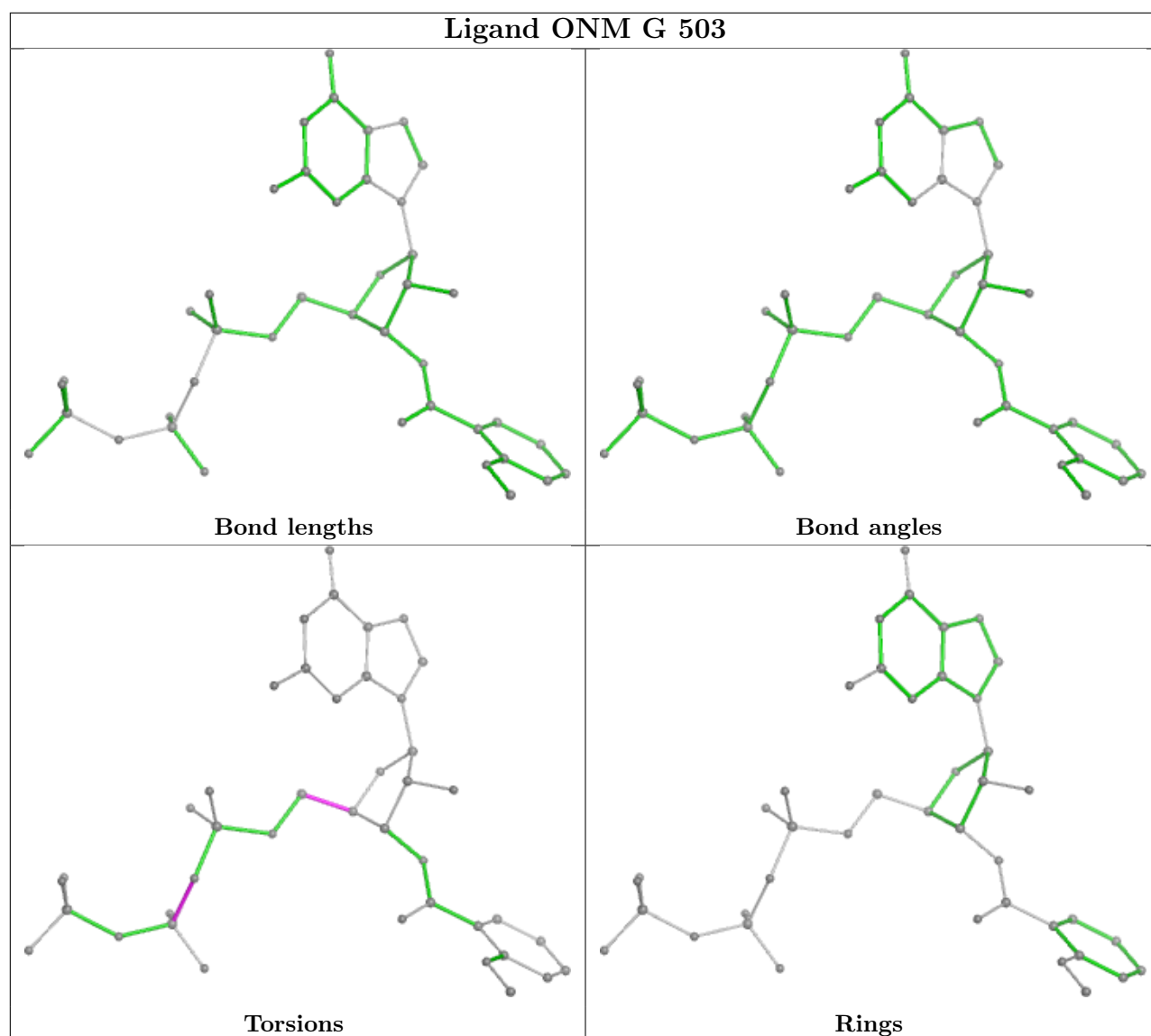


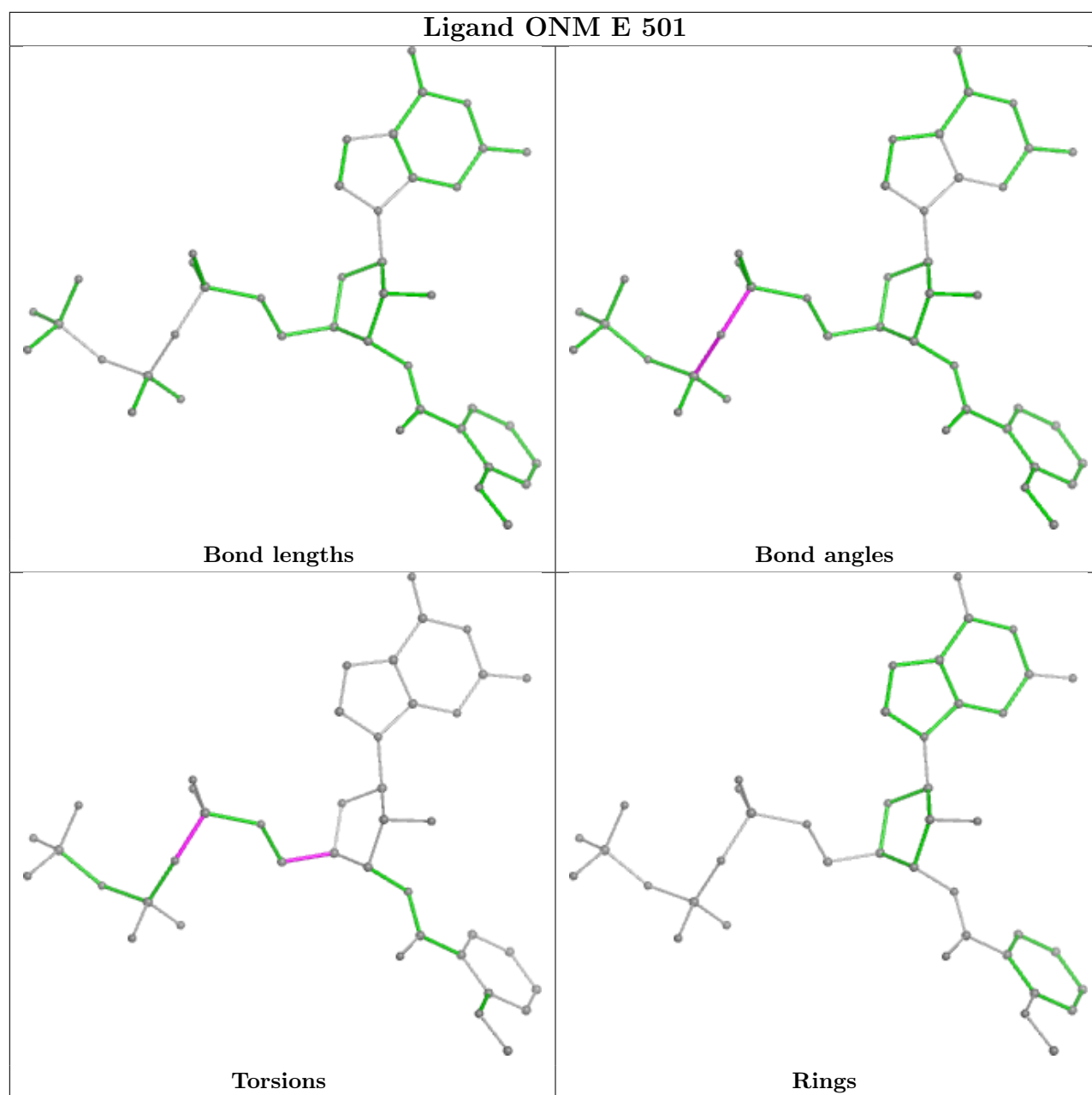


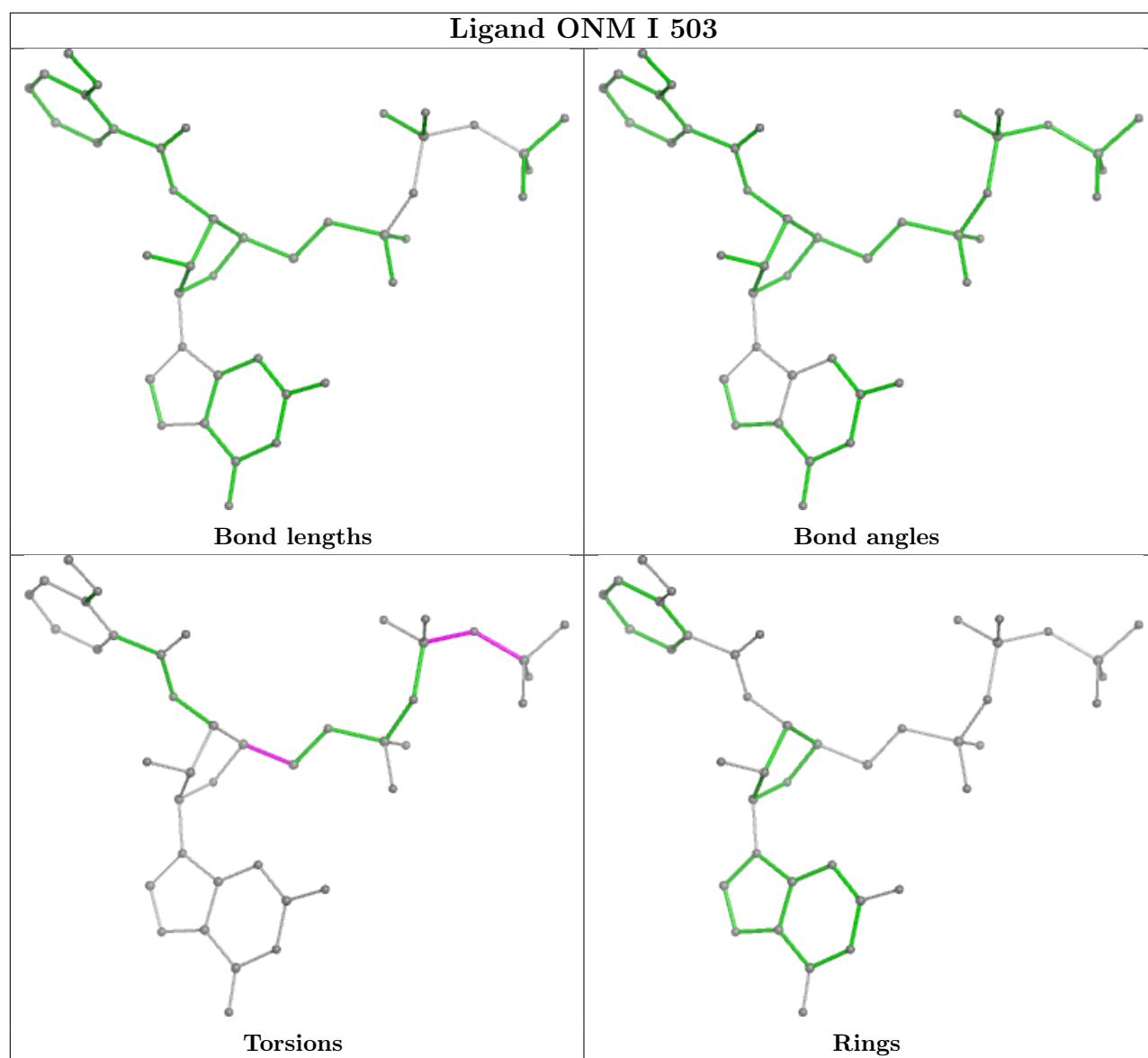












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	224/254 (88%)	-0.01	3 (1%) 77 78	40, 68, 113, 178	0
1	B	224/254 (88%)	0.09	2 (0%) 84 85	42, 69, 113, 184	0
1	C	224/254 (88%)	0.48	8 (3%) 42 42	45, 73, 138, 216	0
1	D	224/254 (88%)	0.39	10 (4%) 33 31	47, 86, 151, 209	0
1	E	224/254 (88%)	1.32	55 (24%) 0 0	73, 123, 223, 256	0
1	F	224/254 (88%)	2.63	110 (49%) 0 0	97, 163, 256, 272	0
1	G	224/254 (88%)	2.50	110 (49%) 0 0	105, 158, 215, 243	0
1	H	224/254 (88%)	2.65	113 (50%) 0 0	108, 149, 222, 249	0
1	I	224/254 (88%)	2.68	120 (53%) 0 0	104, 154, 209, 240	0
1	J	224/254 (88%)	3.31	143 (63%) 0 0	119, 186, 233, 256	0
1	K	224/254 (88%)	3.54	137 (61%) 0 0	153, 203, 242, 258	0
All	All	2464/2794 (88%)	1.78	811 (32%) 0 0	40, 135, 233, 272	0

All (811) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	383	VAL	17.5
1	K	265	SER	15.5
1	F	427	ASP	14.8
1	H	412	GLY	14.7
1	K	413	LYS	13.3
1	K	359	SER	13.2
1	J	422	ILE	12.7
1	F	398	ASN	12.7
1	F	412	GLY	12.4
1	K	302	TYR	12.1
1	K	410	VAL	11.9
1	I	333	LEU	11.8

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	H	290	HIS	11.6
1	K	343	LEU	11.5
1	J	347	MET	11.3
1	K	387	GLN	11.3
1	I	400	PHE	11.2
1	H	329	VAL	11.1
1	K	388	VAL	10.9
1	I	286	LEU	10.7
1	K	275	PHE	10.5
1	J	302	TYR	10.4
1	K	279	LEU	10.4
1	F	425	LYS	10.3
1	J	304	VAL	10.3
1	G	412	GLY	10.2
1	E	406	GLY	10.1
1	I	287	VAL	10.1
1	F	396	LEU	9.9
1	F	419	TRP	9.8
1	K	411	LYS	9.8
1	I	421	LEU	9.7
1	K	211	VAL	9.7
1	K	358	GLY	9.5
1	H	306	SER	9.3
1	G	354	ALA	9.3
1	H	248	ASP	9.3
1	J	281	GLY	9.1
1	I	411	LYS	9.0
1	I	341	VAL	9.0
1	I	359	SER	9.0
1	J	214	ALA	9.0
1	J	333	LEU	8.9
1	F	317	PHE	8.9
1	E	415	VAL	8.9
1	K	384	GLY	8.8
1	K	266	THR	8.8
1	G	422	ILE	8.8
1	H	302	TYR	8.7
1	I	329	VAL	8.7
1	J	260	PHE	8.7
1	J	353	VAL	8.7
1	I	320	ALA	8.6
1	J	266	THR	8.6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	F	421	LEU	8.6
1	H	286	LEU	8.5
1	J	428	GLU	8.5
1	F	208	ALA	8.4
1	H	313	PRO	8.2
1	J	282	ALA	8.2
1	I	324	LEU	8.2
1	J	343	LEU	8.2
1	E	205	THR	8.2
1	H	400	PHE	8.2
1	J	329	VAL	8.1
1	J	426	ALA	8.1
1	K	412	GLY	8.1
1	H	355	GLY	8.1
1	G	301	SER	8.0
1	G	332	ALA	7.9
1	G	291	GLY	7.9
1	K	263	ARG	7.9
1	F	408	ILE	7.8
1	J	324	LEU	7.7
1	K	403	GLN	7.7
1	K	360	ARG	7.7
1	H	276	LEU	7.5
1	F	211	VAL	7.5
1	K	253	LEU	7.5
1	E	210	ALA	7.4
1	K	404	GLU	7.4
1	K	401	VAL	7.4
1	I	265	SER	7.4
1	H	424	ARG	7.3
1	K	422	ILE	7.3
1	K	264	ALA	7.3
1	G	398	ASN	7.3
1	J	354	ALA	7.3
1	F	384	GLY	7.3
1	F	416	MET	7.3
1	K	345	MET	7.3
1	J	337	HIS	7.2
1	J	328	ASN	7.2
1	G	343	LEU	7.2
1	K	382	SER	7.1
1	K	355	GLY	7.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	G	318	ALA	7.1
1	J	289	LYS	7.1
1	F	324	LEU	7.1
1	F	420	TYR	7.0
1	K	340	PRO	7.0
1	J	388	VAL	7.0
1	H	409	GLU	7.0
1	F	397	LYS	7.0
1	F	205	THR	7.0
1	J	427	ASP	7.0
1	I	308	VAL	6.9
1	K	377	MET	6.9
1	K	407	ARG	6.9
1	I	426	ALA	6.8
1	H	308	VAL	6.7
1	J	334	LYS	6.7
1	K	248	ASP	6.7
1	K	408	ILE	6.7
1	K	366	VAL	6.7
1	E	336	PRO	6.7
1	G	310	ARG	6.7
1	J	206	GLN	6.7
1	K	386	ILE	6.7
1	K	297	VAL	6.6
1	J	341	VAL	6.6
1	F	418	THR	6.6
1	J	332	ALA	6.6
1	F	244	ALA	6.5
1	G	288	ASP	6.5
1	I	255	ALA	6.5
1	K	332	ALA	6.5
1	J	217	GLU	6.5
1	H	350	GLY	6.5
1	K	400	PHE	6.5
1	H	205	THR	6.5
1	H	206	GLN	6.5
1	J	261	THR	6.4
1	F	426	ALA	6.4
1	H	330	ALA	6.4
1	J	279	LEU	6.4
1	G	266	THR	6.3
1	F	390	GLU	6.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	G	426	ALA	6.3
1	G	328	ASN	6.3
1	H	216	TYR	6.2
1	J	415	VAL	6.2
1	K	218	ARG	6.2
1	G	302	TYR	6.2
1	K	236	LYS	6.2
1	K	378	GLU	6.2
1	K	338	GLY	6.2
1	G	353	VAL	6.1
1	H	353	VAL	6.1
1	I	211	VAL	6.1
1	K	283	PHE	6.1
1	I	270	ALA	6.1
1	J	407	ARG	6.1
1	G	403	GLN	6.0
1	H	410	VAL	6.0
1	I	276	LEU	6.0
1	H	407	ARG	6.0
1	K	406	GLY	6.0
1	K	409	GLU	6.0
1	E	341	VAL	6.0
1	K	257	ILE	6.0
1	I	291	GLY	6.0
1	J	272	LEU	6.0
1	H	426	ALA	5.9
1	J	285	GLU	5.9
1	J	275	PHE	5.9
1	I	315	HIS	5.9
1	J	278	ARG	5.9
1	K	356	VAL	5.9
1	H	223	LEU	5.8
1	J	367	TRP	5.8
1	G	280	TYR	5.7
1	J	310	ARG	5.7
1	K	415	VAL	5.7
1	F	411	LYS	5.7
1	G	409	GLU	5.7
1	K	280	TYR	5.7
1	J	424	ARG	5.7
1	G	347	MET	5.7
1	C	211	VAL	5.6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	F	394	GLU	5.6
1	E	211	VAL	5.6
1	J	306	SER	5.6
1	I	289	LYS	5.6
1	G	313	PRO	5.6
1	J	366	VAL	5.5
1	J	368	GLY	5.5
1	F	407	ARG	5.5
1	F	385	ARG	5.5
1	H	287	VAL	5.5
1	I	307	GLY	5.5
1	F	389	PRO	5.5
1	G	286	LEU	5.5
1	G	401	VAL	5.5
1	F	383	VAL	5.4
1	I	415	VAL	5.4
1	J	383	VAL	5.4
1	F	292	LEU	5.4
1	G	322	PHE	5.4
1	I	321	ASP	5.4
1	K	282	ALA	5.4
1	K	428	GLU	5.3
1	K	371	VAL	5.3
1	G	303	MET	5.3
1	I	208	ALA	5.3
1	K	372	ASN	5.3
1	K	337	HIS	5.3
1	H	413	LYS	5.3
1	I	279	LEU	5.3
1	E	409	GLU	5.3
1	K	342	PRO	5.3
1	K	354	ALA	5.3
1	I	424	ARG	5.2
1	F	410	VAL	5.2
1	G	285	GLU	5.2
1	J	339	ASP	5.2
1	J	365	ASP	5.2
1	E	299	GLY	5.2
1	E	223	LEU	5.2
1	G	400	PHE	5.2
1	E	408	ILE	5.2
1	J	398	ASN	5.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	F	364	TYR	5.2
1	G	331	ALA	5.2
1	J	325	ASP	5.2
1	I	241	SER	5.2
1	J	235	LEU	5.2
1	G	364	TYR	5.1
1	I	327	ALA	5.1
1	K	313	PRO	5.1
1	H	387	GLN	5.1
1	J	384	GLY	5.1
1	E	416	MET	5.1
1	K	296	LYS	5.1
1	G	349	CYS	5.1
1	F	253	LEU	5.0
1	K	414	GLY	5.0
1	H	411	LYS	5.0
1	H	227	LEU	5.0
1	J	318	ALA	5.0
1	K	304	VAL	5.0
1	E	261	THR	4.9
1	F	252	VAL	4.9
1	G	339	ASP	4.9
1	I	412	GLY	4.9
1	G	290	HIS	4.9
1	K	341	VAL	4.9
1	J	253	LEU	4.9
1	J	403	GLN	4.9
1	F	386	ILE	4.9
1	G	314	ASP	4.9
1	G	428	GLU	4.9
1	I	368	GLY	4.9
1	J	364	TYR	4.9
1	K	418	THR	4.9
1	F	400	PHE	4.8
1	E	413	LYS	4.8
1	J	314	ASP	4.8
1	J	417	ARG	4.8
1	H	283	PHE	4.8
1	I	336	PRO	4.8
1	I	398	ASN	4.8
1	I	290	HIS	4.8
1	I	407	ARG	4.8

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	G	309	PRO	4.7
1	H	333	LEU	4.7
1	F	366	VAL	4.7
1	K	276	LEU	4.7
1	K	346	GLY	4.7
1	H	322	PHE	4.7
1	G	366	VAL	4.7
1	I	254	PHE	4.7
1	G	365	ASP	4.7
1	F	267	THR	4.7
1	F	428	GLU	4.7
1	J	207	ARG	4.7
1	J	305	VAL	4.7
1	F	369	ASP	4.7
1	E	407	ARG	4.6
1	K	278	ARG	4.6
1	D	205	THR	4.6
1	G	425	LYS	4.6
1	H	312	ARG	4.6
1	K	363	PHE	4.6
1	J	346	GLY	4.6
1	F	212	MET	4.6
1	J	262	GLU	4.6
1	F	206	GLN	4.6
1	H	289	LYS	4.5
1	J	392	MET	4.5
1	I	260	PHE	4.5
1	J	356	VAL	4.5
1	G	208	ALA	4.5
1	F	242	VAL	4.5
1	G	413	LYS	4.5
1	H	326	MET	4.5
1	J	247	TYR	4.5
1	H	318	ALA	4.5
1	I	224	ALA	4.5
1	G	207	ARG	4.4
1	G	242	VAL	4.4
1	J	224	ALA	4.4
1	D	426	ALA	4.4
1	K	205	THR	4.4
1	J	352	VAL	4.4
1	F	319	LEU	4.4

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	G	411	LYS	4.4
1	J	401	VAL	4.4
1	I	240	ARG	4.4
1	K	361	ARG	4.4
1	F	266	THR	4.4
1	K	232	ALA	4.4
1	J	416	MET	4.4
1	G	333	LEU	4.4
1	K	364	TYR	4.3
1	C	207	ARG	4.3
1	G	407	ARG	4.3
1	H	414	GLY	4.3
1	E	388	VAL	4.3
1	F	377	MET	4.3
1	K	267	THR	4.3
1	I	283	PHE	4.3
1	E	273	VAL	4.3
1	G	279	LEU	4.3
1	I	323	ALA	4.3
1	F	403	GLN	4.3
1	J	225	ASN	4.3
1	J	410	VAL	4.3
1	K	402	LEU	4.3
1	J	355	GLY	4.3
1	I	322	PHE	4.3
1	E	255	ALA	4.3
1	J	209	GLU	4.2
1	H	260	PHE	4.2
1	K	376	ARG	4.2
1	I	217	GLU	4.2
1	H	277	ASN	4.2
1	F	260	PHE	4.2
1	E	337	HIS	4.2
1	F	415	VAL	4.2
1	F	345	MET	4.2
1	K	397	LYS	4.2
1	G	408	ILE	4.2
1	G	427	ASP	4.2
1	J	208	ALA	4.2
1	I	335	ASP	4.2
1	H	305	VAL	4.1
1	K	326	MET	4.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	G	255	ALA	4.1
1	G	205	THR	4.1
1	K	421	LEU	4.1
1	I	273	VAL	4.1
1	I	269	PRO	4.1
1	E	411	LYS	4.1
1	F	424	ARG	4.1
1	I	299	GLY	4.1
1	I	428	GLU	4.1
1	J	297	VAL	4.1
1	G	367	TRP	4.1
1	J	299	GLY	4.1
1	K	381	ASP	4.1
1	G	388	VAL	4.1
1	I	305	VAL	4.1
1	C	209	GLU	4.1
1	J	298	SER	4.1
1	K	347	MET	4.1
1	I	227	LEU	4.1
1	F	216	TYR	4.1
1	D	208	ALA	4.1
1	K	259	GLY	4.0
1	I	274	ARG	4.0
1	G	222	LEU	4.0
1	E	206	GLN	4.0
1	J	283	PHE	4.0
1	I	267	THR	4.0
1	J	386	ILE	4.0
1	J	210	ALA	4.0
1	H	303	MET	4.0
1	E	414	GLY	4.0
1	K	281	GLY	4.0
1	H	427	ASP	4.0
1	H	351	PRO	4.0
1	G	348	ALA	4.0
1	I	408	ILE	4.0
1	F	401	VAL	3.9
1	I	223	LEU	3.9
1	K	303	MET	3.9
1	J	382	SER	3.9
1	H	293	GLU	3.9
1	E	410	VAL	3.9

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	I	314	ASP	3.9
1	G	385	ARG	3.9
1	F	370	ALA	3.9
1	D	206	GLN	3.9
1	H	222	LEU	3.9
1	H	320	ALA	3.9
1	H	209	GLU	3.9
1	H	354	ALA	3.9
1	H	281	GLY	3.9
1	G	402	LEU	3.8
1	I	272	LEU	3.8
1	C	206	GLN	3.8
1	I	284	ASP	3.8
1	G	210	ALA	3.8
1	K	317	PHE	3.8
1	F	232	ALA	3.8
1	G	404	GLU	3.8
1	I	313	PRO	3.8
1	F	402	LEU	3.8
1	H	311	ALA	3.8
1	J	286	LEU	3.8
1	G	211	VAL	3.8
1	I	383	VAL	3.8
1	F	241	SER	3.8
1	F	304	VAL	3.8
1	J	259	GLY	3.8
1	H	428	GLU	3.7
1	K	362	PHE	3.7
1	I	420	TYR	3.7
1	J	301	SER	3.7
1	J	280	TYR	3.7
1	H	341	VAL	3.7
1	H	254	PHE	3.7
1	J	271	ASP	3.7
1	K	365	ASP	3.7
1	H	231	ILE	3.7
1	K	262	GLU	3.7
1	I	355	GLY	3.7
1	K	423	GLY	3.7
1	J	213	GLU	3.7
1	H	328	ASN	3.7
1	F	373	VAL	3.7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	G	399	GLU	3.7
1	I	266	THR	3.6
1	I	226	MET	3.6
1	J	307	GLY	3.6
1	H	249	GLU	3.6
1	J	387	GLN	3.6
1	D	207	ARG	3.6
1	F	289	LYS	3.6
1	F	322	PHE	3.6
1	I	330	ALA	3.6
1	H	373	VAL	3.6
1	K	339	ASP	3.6
1	H	225	ASN	3.6
1	J	303	MET	3.6
1	G	299	GLY	3.6
1	K	294	LYS	3.6
1	F	207	ARG	3.6
1	J	395	ARG	3.6
1	H	314	ASP	3.6
1	E	213	GLU	3.6
1	J	236	LYS	3.6
1	J	317	PHE	3.5
1	J	245	ASP	3.5
1	K	328	ASN	3.5
1	K	385	ARG	3.5
1	H	242	VAL	3.5
1	H	352	VAL	3.5
1	K	260	PHE	3.5
1	H	307	GLY	3.5
1	K	420	TYR	3.5
1	G	262	GLU	3.5
1	K	357	VAL	3.5
1	F	343	LEU	3.5
1	G	245	ASP	3.5
1	E	334	LYS	3.5
1	K	240	ARG	3.5
1	H	393	TYR	3.4
1	H	269	PRO	3.4
1	I	275	PHE	3.4
1	G	265	SER	3.4
1	H	279	LEU	3.4
1	I	222	LEU	3.4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	E	335	ASP	3.4
1	H	388	VAL	3.4
1	E	376	ARG	3.4
1	I	328	ASN	3.4
1	B	205	THR	3.4
1	G	341	VAL	3.4
1	H	357	VAL	3.4
1	E	209	GLU	3.4
1	K	330	ALA	3.4
1	A	205	THR	3.4
1	G	276	LEU	3.4
1	I	410	VAL	3.4
1	G	239	SER	3.3
1	H	319	LEU	3.3
1	H	218	ARG	3.3
1	H	299	GLY	3.3
1	H	235	LEU	3.3
1	E	326	MET	3.3
1	G	340	PRO	3.3
1	C	427	ASP	3.3
1	G	307	GLY	3.3
1	J	264	ALA	3.3
1	I	340	PRO	3.3
1	E	383	VAL	3.3
1	H	309	PRO	3.3
1	E	276	LEU	3.3
1	J	292	LEU	3.3
1	K	427	ASP	3.3
1	K	243	ILE	3.3
1	G	423	GLY	3.3
1	F	417	ARG	3.3
1	J	274	ARG	3.3
1	F	341	VAL	3.2
1	I	406	GLY	3.2
1	F	404	GLU	3.2
1	I	319	LEU	3.2
1	I	367	TRP	3.2
1	J	338	GLY	3.2
1	I	302	TYR	3.2
1	F	248	ASP	3.2
1	H	358	GLY	3.2
1	J	242	VAL	3.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	H	310	ARG	3.2
1	F	409	GLU	3.2
1	J	249	GLU	3.2
1	H	417	ARG	3.2
1	F	330	ALA	3.2
1	H	367	TRP	3.2
1	I	205	THR	3.2
1	F	285	GLU	3.2
1	J	331	ALA	3.2
1	J	276	LEU	3.2
1	K	223	LEU	3.2
1	I	251	SER	3.2
1	E	275	PHE	3.1
1	G	317	PHE	3.1
1	I	295	ILE	3.1
1	J	322	PHE	3.1
1	G	355	GLY	3.1
1	I	280	TYR	3.1
1	J	244	ALA	3.1
1	G	283	PHE	3.1
1	H	275	PHE	3.1
1	K	286	LEU	3.1
1	F	303	MET	3.1
1	G	415	VAL	3.1
1	H	304	VAL	3.1
1	E	254	PHE	3.1
1	F	333	LEU	3.1
1	H	264	ALA	3.1
1	I	360	ARG	3.1
1	J	409	GLU	3.1
1	J	406	GLY	3.1
1	K	222	LEU	3.1
1	H	408	ILE	3.1
1	I	257	ILE	3.1
1	K	210	ALA	3.0
1	F	239	SER	3.0
1	K	301	SER	3.0
1	F	326	MET	3.0
1	D	427	ASP	3.0
1	K	390	GLU	3.0
1	I	417	ARG	3.0
1	C	205	THR	3.0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	F	320	ALA	3.0
1	G	295	ILE	3.0
1	E	217	GLU	3.0
1	H	274	ARG	3.0
1	H	280	TYR	3.0
1	E	421	LEU	3.0
1	G	337	HIS	2.9
1	K	299	GLY	2.9
1	F	399	GLU	2.9
1	J	412	GLY	2.9
1	I	212	MET	2.9
1	C	208	ALA	2.9
1	K	370	ALA	2.9
1	J	390	GLU	2.9
1	K	344	ARG	2.9
1	G	206	GLN	2.9
1	J	371	VAL	2.9
1	K	227	LEU	2.9
1	F	305	VAL	2.9
1	F	210	ALA	2.9
1	J	425	LYS	2.9
1	K	230	SER	2.9
1	E	283	PHE	2.9
1	G	390	GLU	2.9
1	J	215	GLU	2.9
1	K	242	VAL	2.9
1	K	416	MET	2.9
1	H	241	SER	2.9
1	F	321	ASP	2.9
1	F	263	ARG	2.9
1	F	328	ASN	2.9
1	J	389	PRO	2.9
1	I	235	LEU	2.9
1	H	334	LYS	2.8
1	F	287	VAL	2.8
1	J	420	TYR	2.8
1	I	293	GLU	2.8
1	F	332	ALA	2.8
1	J	397	LYS	2.8
1	K	334	LYS	2.8
1	G	297	VAL	2.8
1	F	280	TYR	2.8

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	I	243	ILE	2.8
1	G	304	VAL	2.8
1	G	416	MET	2.8
1	G	424	ARG	2.8
1	I	292	LEU	2.8
1	J	423	GLY	2.8
1	H	229	GLY	2.8
1	I	263	ARG	2.8
1	F	327	ALA	2.7
1	H	228	PRO	2.7
1	K	254	PHE	2.7
1	F	299	GLY	2.7
1	H	336	PRO	2.7
1	F	251	SER	2.7
1	F	243	ILE	2.7
1	G	397	LYS	2.7
1	I	427	ASP	2.7
1	K	228	PRO	2.7
1	H	392	MET	2.7
1	K	206	GLN	2.7
1	F	405	ARG	2.7
1	H	361	ARG	2.7
1	J	267	THR	2.7
1	G	389	PRO	2.6
1	I	358	GLY	2.6
1	G	384	GLY	2.6
1	K	216	TYR	2.6
1	E	264	ALA	2.6
1	F	413	LYS	2.6
1	K	331	ALA	2.6
1	J	311	ALA	2.6
1	J	385	ARG	2.6
1	E	310	ARG	2.6
1	H	266	THR	2.6
1	H	255	ALA	2.6
1	I	348	ALA	2.6
1	J	396	LEU	2.6
1	H	295	ILE	2.6
1	G	356	VAL	2.6
1	I	397	LYS	2.5
1	J	205	THR	2.5
1	A	428	GLU	2.5

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	E	219	SER	2.5
1	I	261	THR	2.5
1	G	260	PHE	2.5
1	G	345	MET	2.5
1	K	289	LYS	2.5
1	I	372	ASN	2.5
1	H	270	ALA	2.5
1	F	247	TYR	2.5
1	K	329	VAL	2.5
1	K	241	SER	2.5
1	H	220	GLU	2.5
1	I	309	PRO	2.5
1	G	298	SER	2.5
1	H	347	MET	2.5
1	I	262	GLU	2.5
1	E	208	ALA	2.5
1	J	243	ILE	2.5
1	J	295	ILE	2.5
1	E	207	ARG	2.5
1	G	338	GLY	2.5
1	F	209	GLU	2.5
1	F	254	PHE	2.5
1	F	347	MET	2.5
1	J	263	ARG	2.5
1	K	405	ARG	2.5
1	K	214	ALA	2.5
1	I	356	VAL	2.5
1	H	296	LYS	2.4
1	J	393	TYR	2.4
1	H	327	ALA	2.4
1	I	337	HIS	2.4
1	J	349	CYS	2.4
1	K	320	ALA	2.4
1	F	388	VAL	2.4
1	J	254	PHE	2.4
1	F	340	PRO	2.4
1	J	348	ALA	2.4
1	K	310	ARG	2.4
1	J	233	GLU	2.4
1	J	273	VAL	2.4
1	D	337	HIS	2.4
1	F	235	LEU	2.4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	H	261	THR	2.4
1	J	394	GLU	2.4
1	E	338	GLY	2.4
1	K	258	VAL	2.4
1	F	312	ARG	2.4
1	K	336	PRO	2.4
1	I	258	VAL	2.4
1	K	419	TRP	2.4
1	G	376	ARG	2.4
1	H	217	GLU	2.4
1	F	306	SER	2.4
1	H	271	ASP	2.4
1	K	321	ASP	2.4
1	I	209	GLU	2.4
1	J	340	PRO	2.3
1	J	222	LEU	2.3
1	G	296	LYS	2.3
1	K	295	ILE	2.3
1	F	337	HIS	2.3
1	I	384	GLY	2.3
1	F	297	VAL	2.3
1	F	246	LYS	2.3
1	G	420	TYR	2.3
1	J	290	HIS	2.3
1	F	355	GLY	2.3
1	I	210	ALA	2.3
1	K	398	ASN	2.3
1	H	265	SER	2.3
1	I	343	LEU	2.3
1	F	295	ILE	2.3
1	E	417	ARG	2.3
1	K	212	MET	2.3
1	G	334	LYS	2.3
1	E	286	LEU	2.3
1	E	343	LEU	2.3
1	I	303	MET	2.3
1	H	208	ALA	2.3
1	G	324	LEU	2.3
1	I	326	MET	2.3
1	I	385	ARG	2.3
1	J	363	PHE	2.3
1	J	308	VAL	2.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	I	220	GLU	2.2
1	E	297	VAL	2.2
1	E	412	GLY	2.2
1	F	422	ILE	2.2
1	I	288	ASP	2.2
1	H	258	VAL	2.2
1	I	414	GLY	2.2
1	H	342	PRO	2.2
1	K	396	LEU	2.2
1	E	218	ARG	2.2
1	I	354	ALA	2.2
1	K	316	ALA	2.2
1	E	380	THR	2.2
1	J	288	ASP	2.2
1	K	322	PHE	2.2
1	G	252	VAL	2.2
1	G	410	VAL	2.2
1	F	315	HIS	2.2
1	F	354	ALA	2.2
1	I	300	ASP	2.2
1	E	362	PHE	2.2
1	I	304	VAL	2.2
1	G	259	GLY	2.2
1	G	289	LYS	2.2
1	J	246	LYS	2.2
1	J	373	VAL	2.2
1	A	427	ASP	2.2
1	F	392	MET	2.2
1	H	282	ALA	2.2
1	D	355	GLY	2.2
1	J	219	SER	2.2
1	K	389	PRO	2.2
1	J	293	GLU	2.2
1	F	302	TYR	2.2
1	G	308	VAL	2.2
1	F	378	GLU	2.2
1	H	315	HIS	2.2
1	H	301	SER	2.1
1	K	393	TYR	2.1
1	H	213	GLU	2.1
1	H	368	GLY	2.1
1	E	311	ALA	2.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	I	218	ARG	2.1
1	H	335	ASP	2.1
1	G	417	ARG	2.1
1	I	214	ALA	2.1
1	F	226	MET	2.1
1	G	258	VAL	2.1
1	K	291	GLY	2.1
1	G	241	SER	2.1
1	J	379	SER	2.1
1	E	350	GLY	2.1
1	F	240	ARG	2.1
1	I	386	ILE	2.1
1	C	374	ALA	2.1
1	H	362	PHE	2.1
1	I	250	VAL	2.1
1	I	352	VAL	2.1
1	J	309	PRO	2.1
1	I	206	GLN	2.1
1	K	285	GLU	2.1
1	G	254	PHE	2.1
1	H	246	LYS	2.1
1	J	370	ALA	2.1
1	E	289	LYS	2.0
1	I	373	VAL	2.0
1	G	335	ASP	2.0
1	G	275	PHE	2.0
1	J	411	LYS	2.0
1	D	353	VAL	2.0
1	G	329	VAL	2.0
1	E	422	ILE	2.0
1	I	312	ARG	2.0
1	G	393	TYR	2.0
1	I	311	ALA	2.0
1	J	237	SER	2.0
1	J	419	TRP	2.0
1	D	428	GLU	2.0
1	H	278	ARG	2.0
1	I	399	GLU	2.0
1	B	216	TYR	2.0
1	J	375	SER	2.0
1	G	392	MET	2.0
1	E	344	ARG	2.0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	G	405	ARG	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	MN	I	502	1/1	0.30	1.52	96,96,96,96	1
3	MN	C	504	1/1	0.57	1.28	78,78,78,78	1
2	ONM	G	503	42/42	0.73	0.27	129,176,200,203	0
3	MN	E	504	1/1	0.73	0.12	162,162,162,162	0
2	ONM	K	501	42/42	0.73	0.26	193,216,224,226	1
3	MN	B	505	1/1	0.75	0.23	54,54,54,54	1
2	ONM	I	503	42/42	0.76	0.27	116,130,160,165	0
3	MN	E	503	1/1	0.79	0.04	134,134,134,134	0
4	SO4	E	502	5/5	0.81	0.34	170,171,172,177	0
3	MN	J	502	1/1	0.82	0.17	128,128,128,128	0
3	MN	G	502	1/1	0.82	0.08	161,161,161,161	0
2	ONM	E	501	42/42	0.83	0.20	120,139,150,155	1
2	ONM	H	501	42/42	0.83	0.24	117,129,163,169	1
3	MN	H	503	1/1	0.85	0.25	94,94,94,94	1
2	ONM	J	501	42/42	0.86	0.27	114,159,185,187	1
3	MN	J	503	1/1	0.88	0.09	118,118,118,118	0
3	MN	K	502	1/1	0.88	0.04	174,174,174,174	0
3	MN	K	503	1/1	0.88	0.16	103,103,103,103	1
3	MN	G	501	1/1	0.88	0.18	90,90,90,90	1
4	SO4	A	504	5/5	0.89	0.17	119,120,122,125	0
3	MN	F	503	1/1	0.89	0.12	128,128,128,128	0
2	ONM	F	501	42/42	0.90	0.19	101,112,157,166	0

*Continued on next page...*

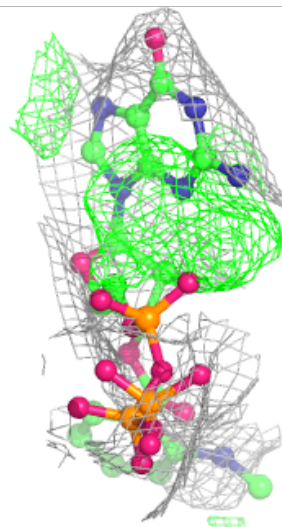
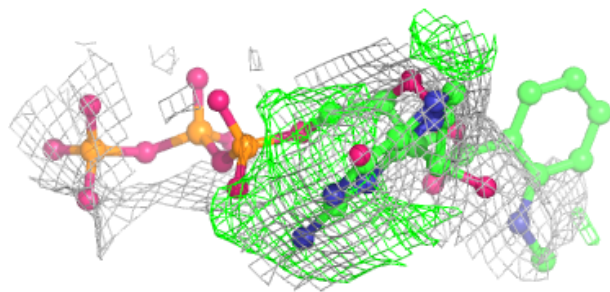
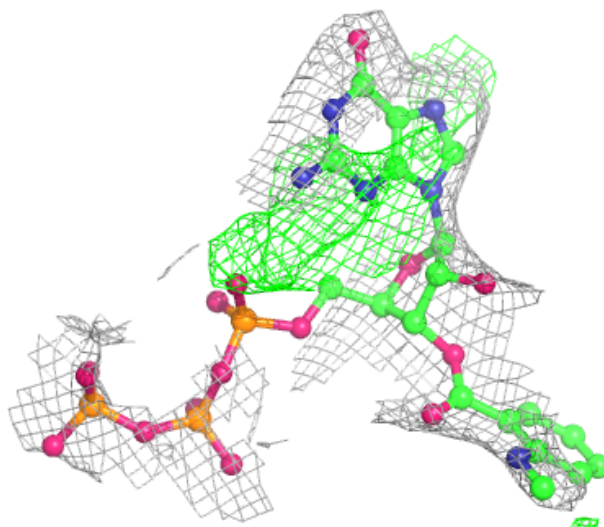
*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	SO4	B	503	5/5	0.94	0.34	123,128,130,131	0
3	MN	I	501	1/1	0.94	0.16	97,97,97,97	0
4	SO4	B	501	5/5	0.95	0.22	100,106,109,110	0
3	MN	A	503	1/1	0.95	0.08	82,82,82,82	0
2	ONM	A	501	42/42	0.95	0.18	40,55,72,80	1
3	MN	D	504	1/1	0.96	0.16	100,100,100,100	0
4	SO4	D	501	5/5	0.96	0.10	126,128,130,131	0
3	MN	F	502	1/1	0.96	0.56	93,93,93,93	1
2	ONM	C	501	42/42	0.97	0.22	53,61,72,75	0
3	MN	D	503	1/1	0.97	0.10	61,61,61,61	0
2	ONM	B	502	42/42	0.97	0.17	49,56,64,71	1
3	MN	C	503	1/1	0.98	0.16	53,53,53,53	0
4	SO4	C	502	5/5	0.98	0.23	94,99,103,104	0
2	ONM	D	502	42/42	0.98	0.19	42,53,73,79	1
3	MN	H	502	1/1	0.98	0.10	127,127,127,127	0
3	MN	B	504	1/1	0.99	0.06	58,58,58,58	0
3	MN	A	502	1/1	0.99	0.05	59,59,59,59	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

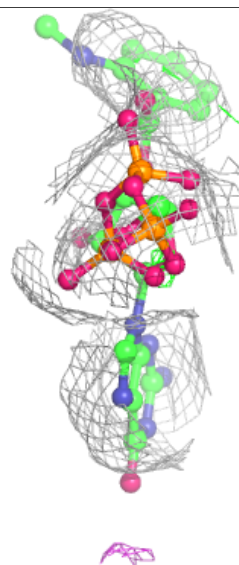
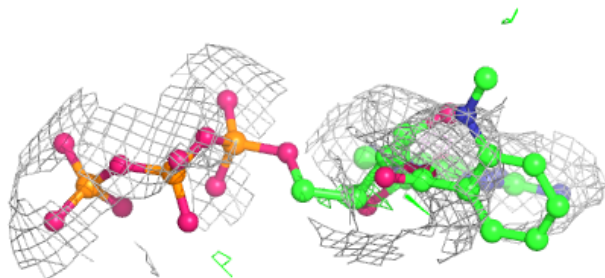
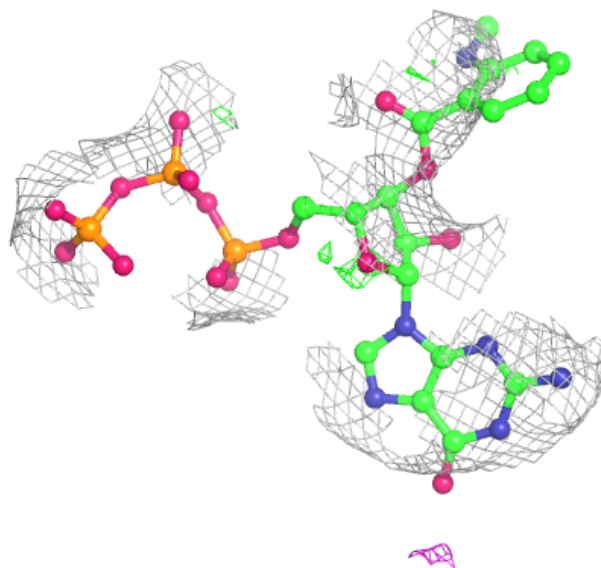
**Electron density around ONM G 503:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around ONM K 501:**

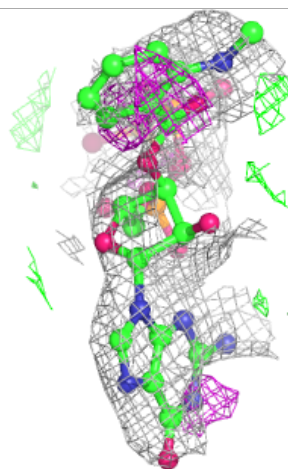
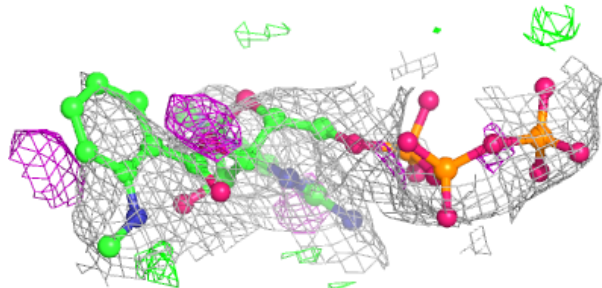
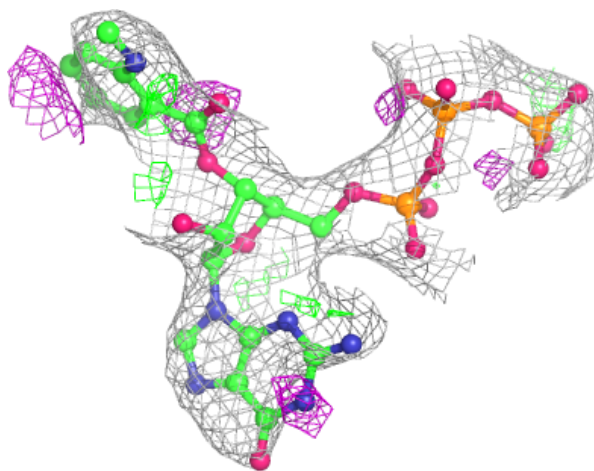
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





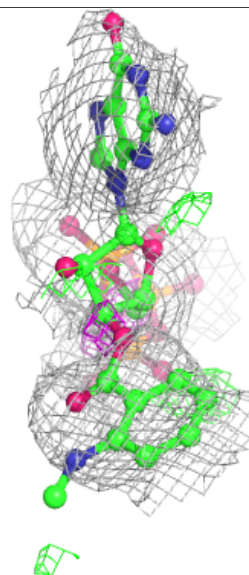
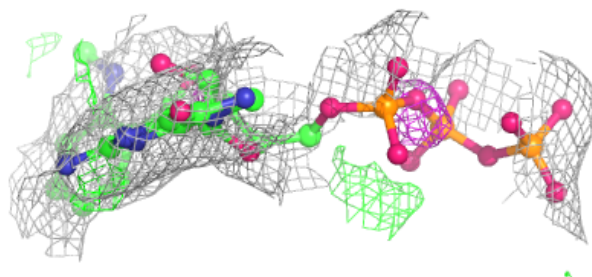
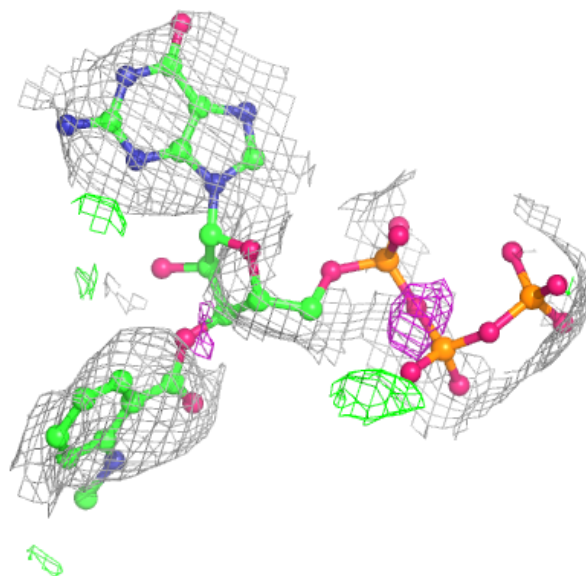
**Electron density around ONM I 503:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



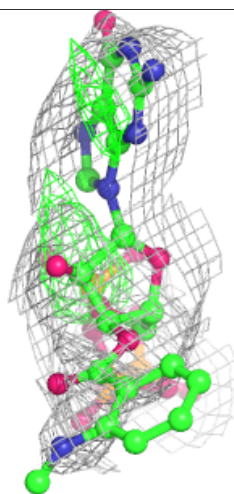
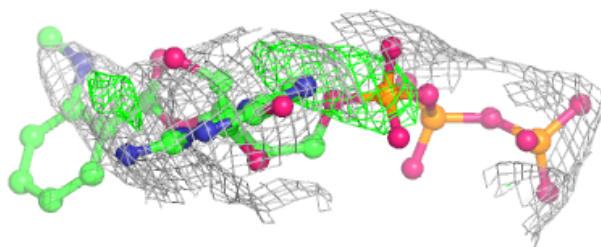
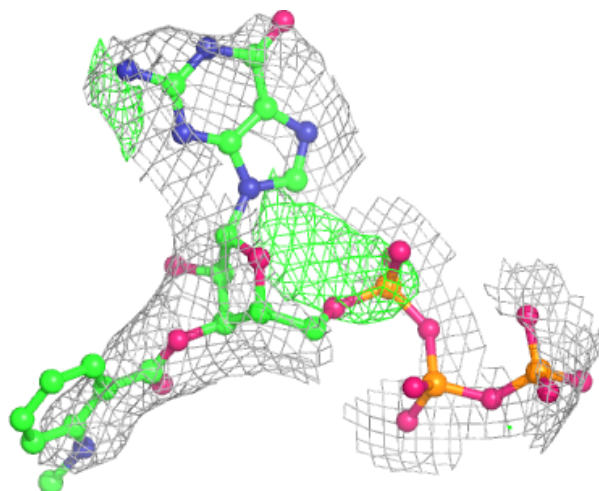
**Electron density around ONM E 501:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



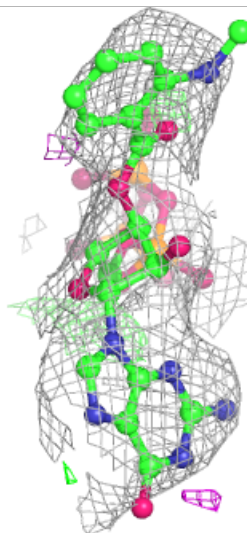
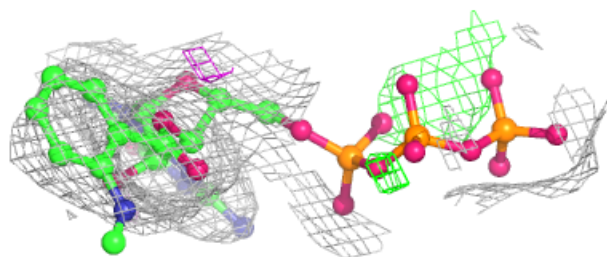
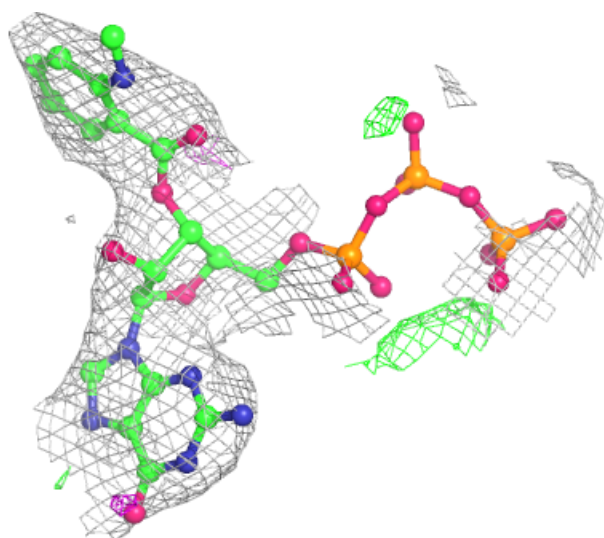
**Electron density around ONM J 501:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



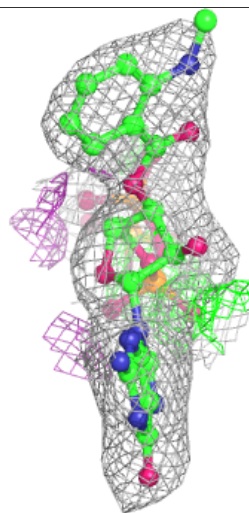
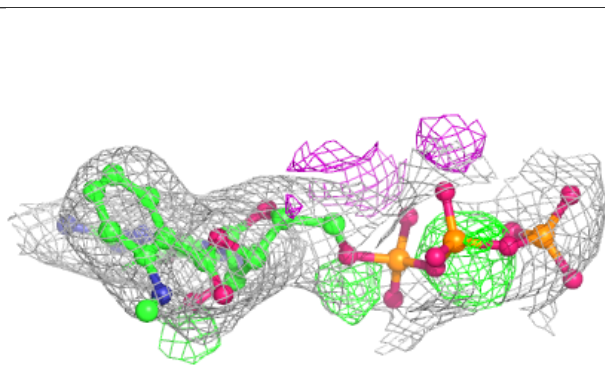
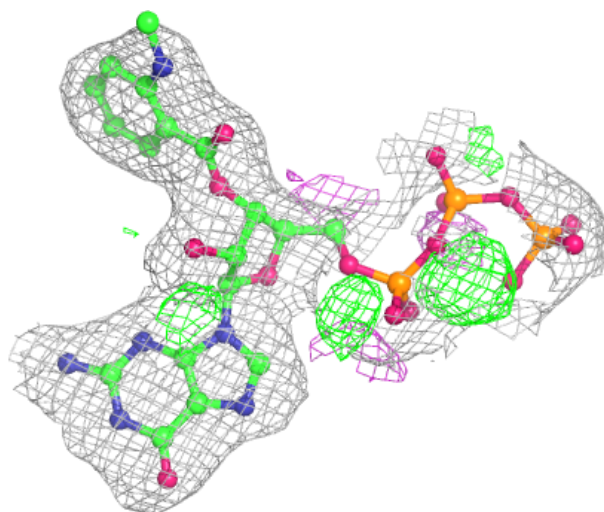
**Electron density around ONM F 501:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



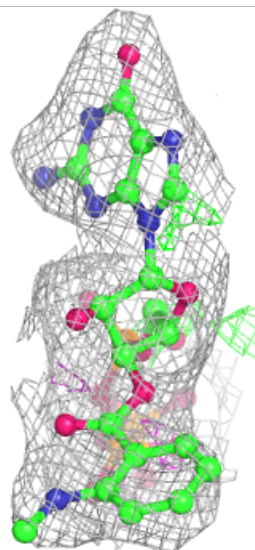
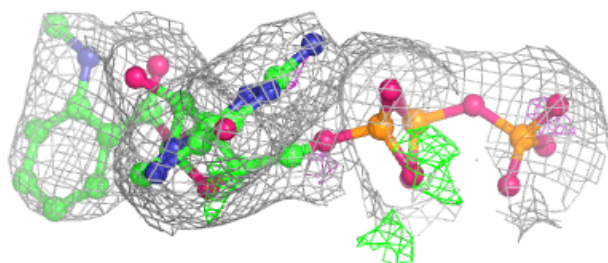
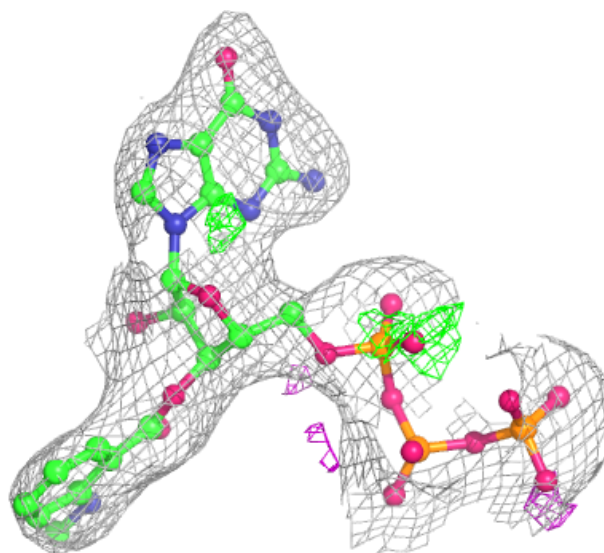
**Electron density around ONM A 501:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around ONM C 501:**

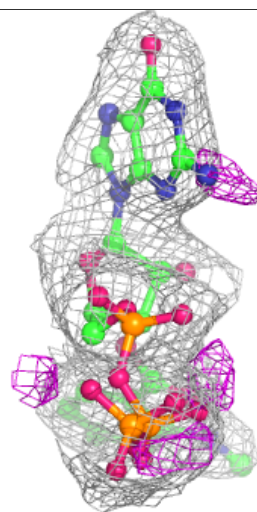
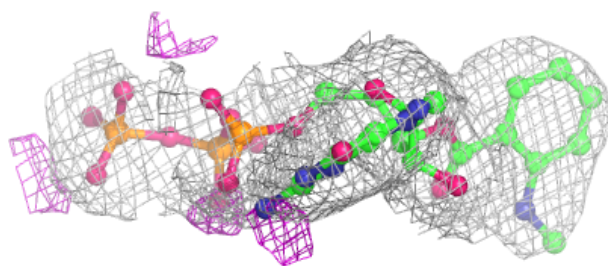
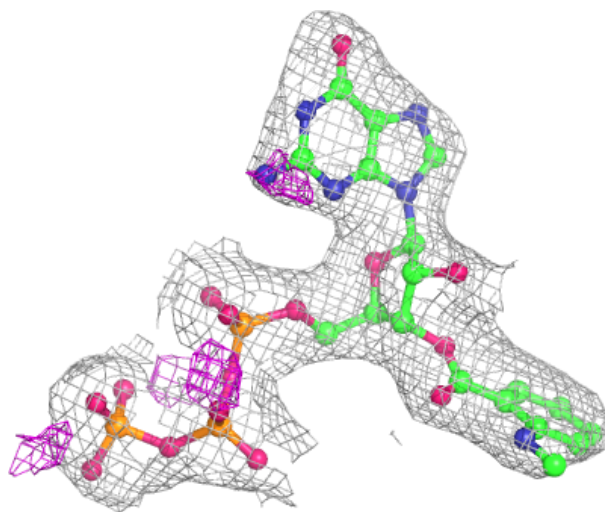
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





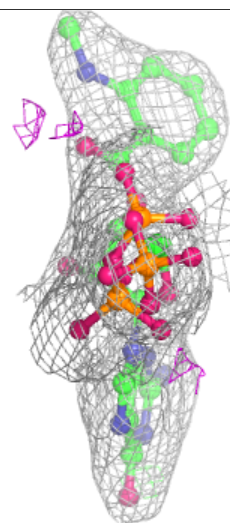
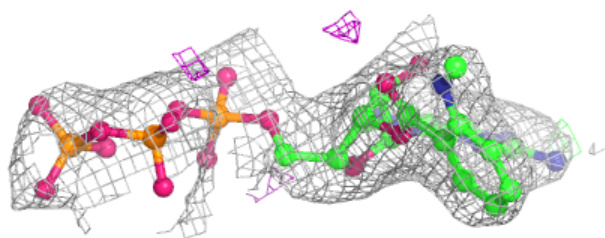
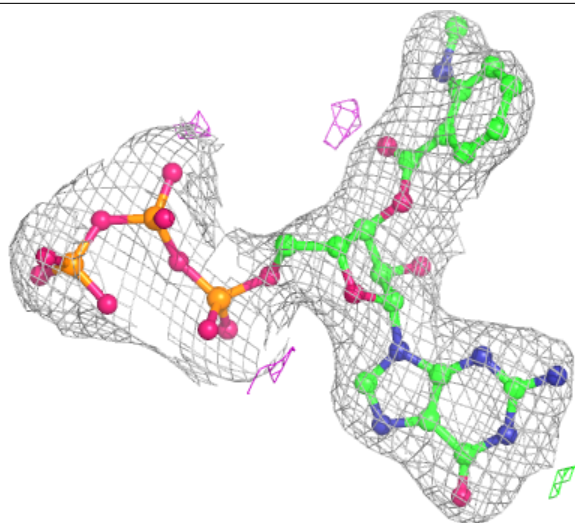
**Electron density around ONM B 502:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around ONM D 502:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.