Full wwPDB X-ray Structure Validation Report ⓘ

Jun 13, 2020 – 09:37 pm BST

PDB ID	:	5O5K
Title	:	X-ray structure of a bacterial adenylyl cyclase soluble domain
Authors	:	Vercellino, I.; Korkhov, V.M.
Deposited on	:	2017-06-02
Resolution	:	3.40 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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

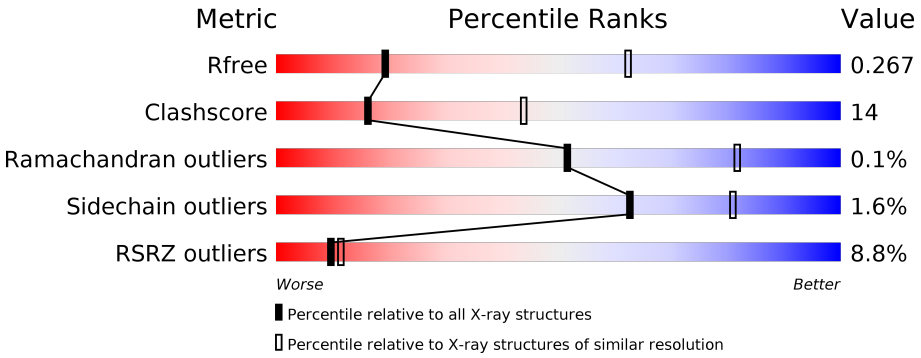
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 3.40 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_{free}	130704	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

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 on the lower bar indicate the fraction of residues that contain outliers for >=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 <=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	60% 24% • 15%
1	B	254	62% 22% • 15%
1	C	254	62% 22% • 15%
1	D	254	% 55% 28% • 15%
1	E	254	3% 62% 22% • 15%
1	F	254	8% 62% 22% • 15%

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Mol	Chain	Length	Quality of chain
1	G	254	19% 62% 22% 15%
1	H	254	16% 59% 25% 15%
1	I	254	7% 59% 26% 15%
1	J	254	7% 54% 30% 15%
1	K	254	19% 63% 22% 15%

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
2	ONM	I	504	-	-	X	-
4	SO4	C	503	-	-	-	X
4	SO4	E	504	-	-	X	-
4	SO4	F	502	-	-	-	X
4	SO4	H	501	-	-	-	X
4	SO4	I	503	-	-	-	X
4	SO4	J	505	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 18919 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	216	Total	C	N	O	S	0	0	0
			1670	1054	295	311	10			
1	B	216	Total	C	N	O	S	0	0	0
			1670	1054	295	311	10			
1	D	216	Total	C	N	O	S	0	0	0
			1670	1054	295	311	10			
1	C	216	Total	C	N	O	S	0	0	0
			1670	1054	295	311	10			
1	E	216	Total	C	N	O	S	0	0	0
			1670	1054	295	311	10			
1	F	216	Total	C	N	O	S	0	0	0
			1670	1054	295	311	10			
1	I	216	Total	C	N	O	S	0	0	0
			1670	1054	295	311	10			
1	J	216	Total	C	N	O	S	0	0	0
			1670	1054	295	311	10			
1	H	216	Total	C	N	O	S	0	0	0
			1670	1054	295	311	10			
1	G	216	Total	C	N	O	S	0	0	0
			1670	1054	295	311	10			
1	K	216	Total	C	N	O	S	0	0	0
			1670	1054	295	311	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

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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

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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
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
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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
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
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

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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
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

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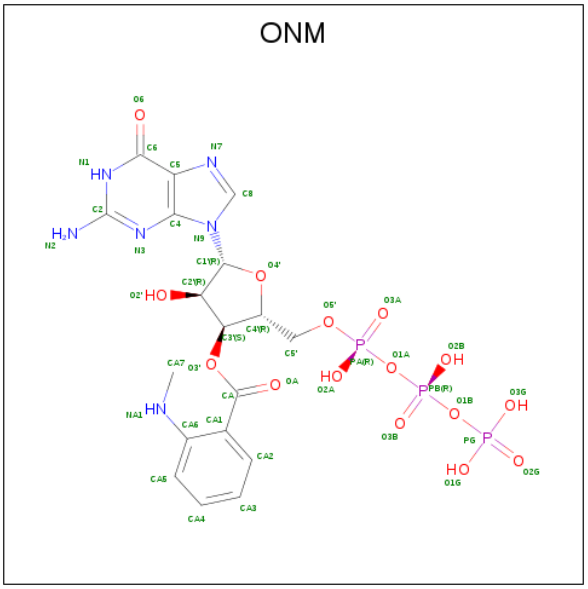
Chain	Residue	Modelled	Actual	Comment	Reference
K	197	GLY	-	expression tag	UNP X8CHM4
K	198	PRO	-	expression tag	UNP X8CHM4
K	199	SER	-	expression tag	UNP X8CHM4
K	200	GLY	-	expression tag	UNP X8CHM4
K	201	HIS	-	expression tag	UNP X8CHM4
K	202	MET	-	expression tag	UNP X8CHM4
K	342	PRO	ALA	conflict	UNP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

- Molecule 2 is 3'-O-(N-METHYLANTHRANILOYL)-GUANOSINE-5'-TRIPHOSPHATE (three-letter code: ONM) (formula: $C_{18}H_{23}N_6O_{15}P_3$).



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	D	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	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	I	1	Total	C	N	O	P	0	0
			42	18	6	15	3		

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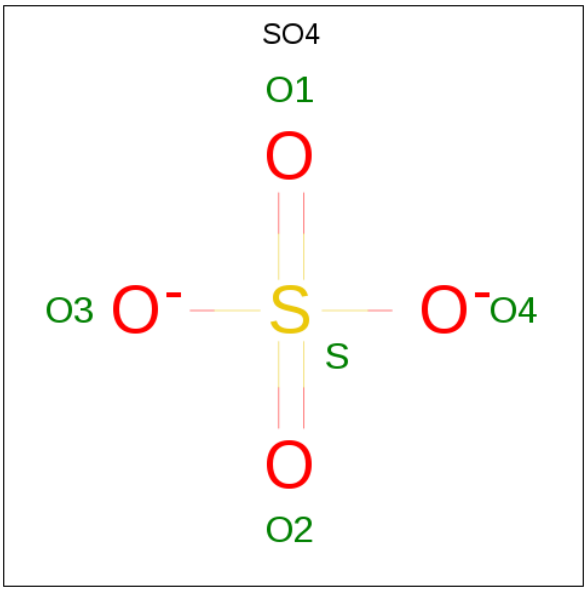
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	J	1	Total	C	N	O	P	0	0
			42	18	6	15	3		
2	H	1	Total	C	N	O	P	0	0
			42	18	6	15	3		
2	G	1	Total	C	N	O	P	0	0
			42	18	6	15	3		
2	K	1	Total	C	N	O	P	0	0
			42	18	6	15	3		

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

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

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



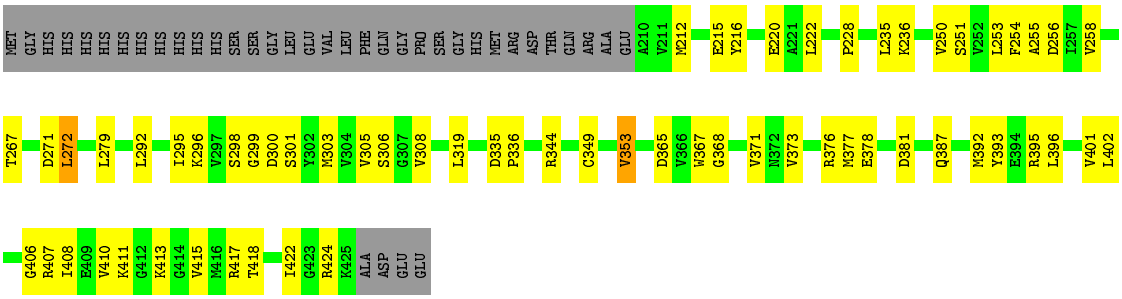
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	D	1	Total O S 5 4 1	0	0
4	C	1	Total O S 5 4 1	0	0
4	C	1	Total O S 5 4 1	0	0
4	E	1	Total O S 5 4 1	0	0
4	E	1	Total O S 5 4 1	0	0
4	F	1	Total O S 5 4 1	0	0
4	I	1	Total O S 5 4 1	0	0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

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

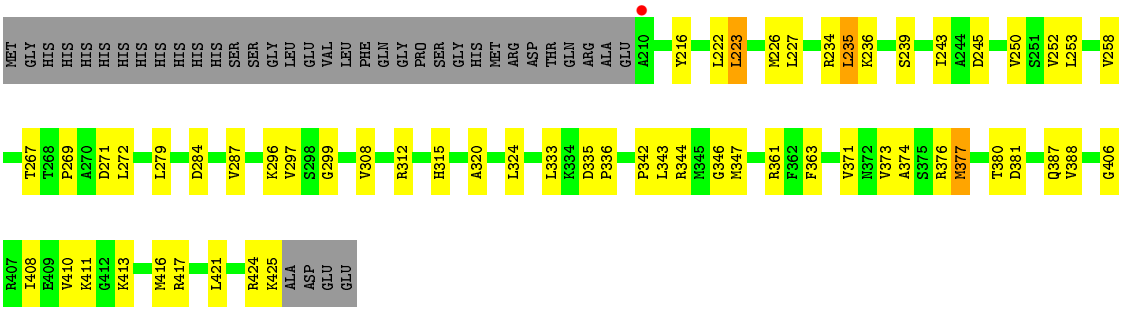
- Molecule 1: Adenylate cyclase

Chain A:



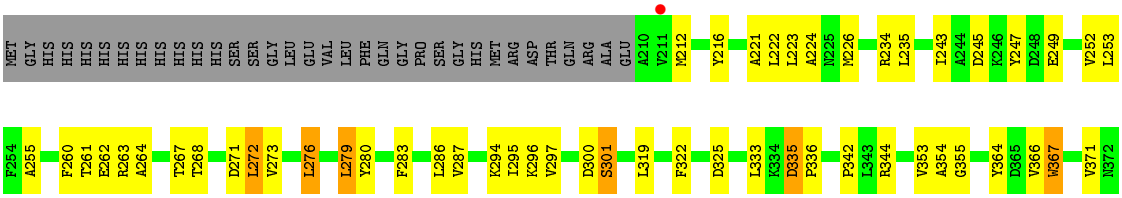
- Molecule 1: Adenylate cyclase

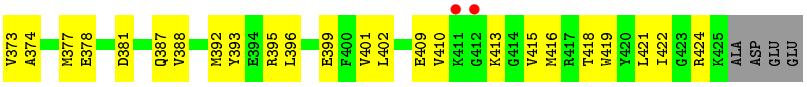
Chain B:



- Molecule 1: Adenylate cyclase

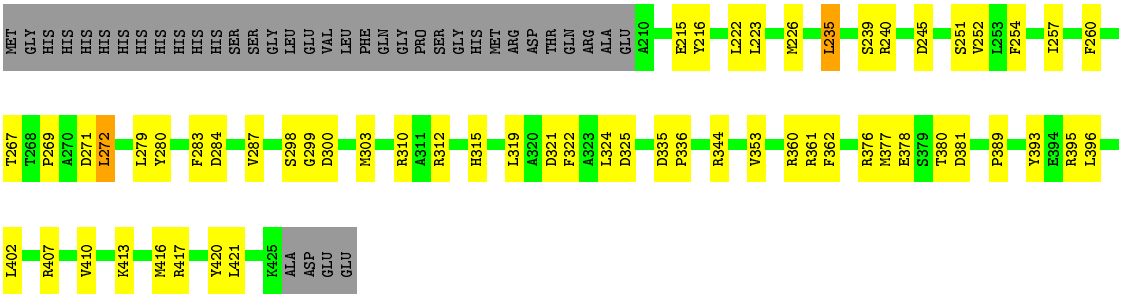
Chain D:





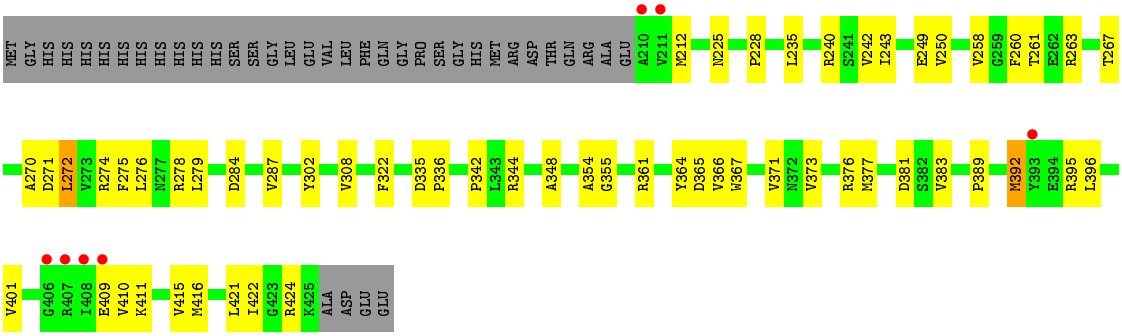
- Molecule 1: Adenylate cyclase

Chain C:



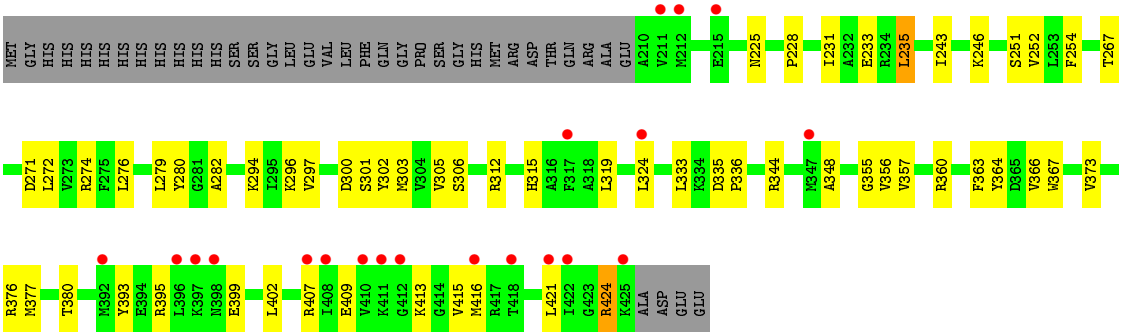
- Molecule 1: Adenylate cyclase

Chain E:



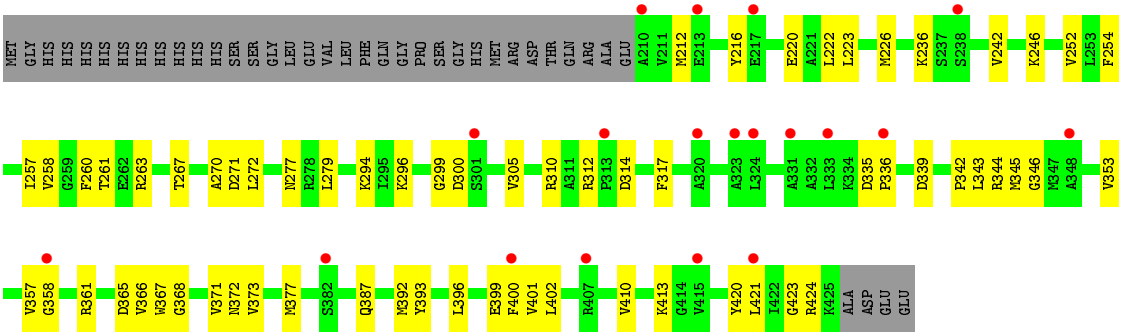
- Molecule 1: Adenylate cyclase

Chain F:



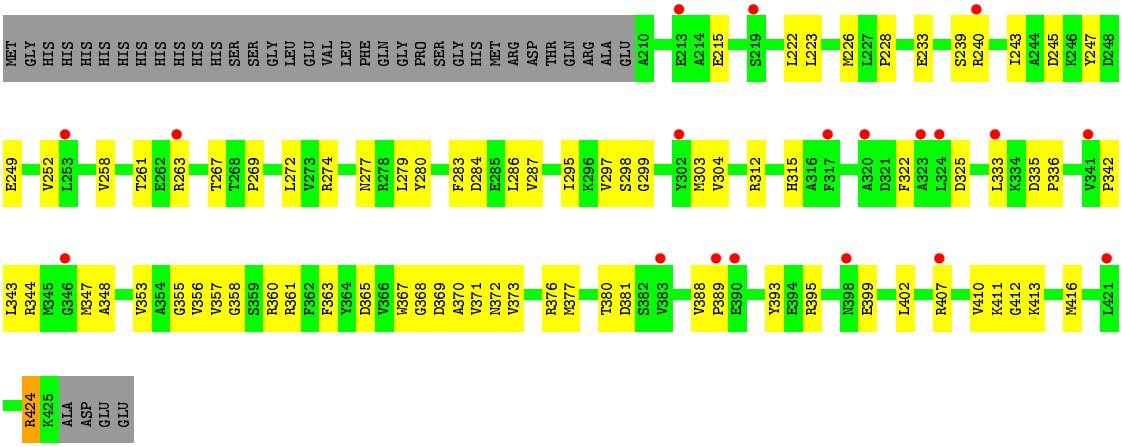
- Molecule 1: Adenylate cyclase

Chain I:



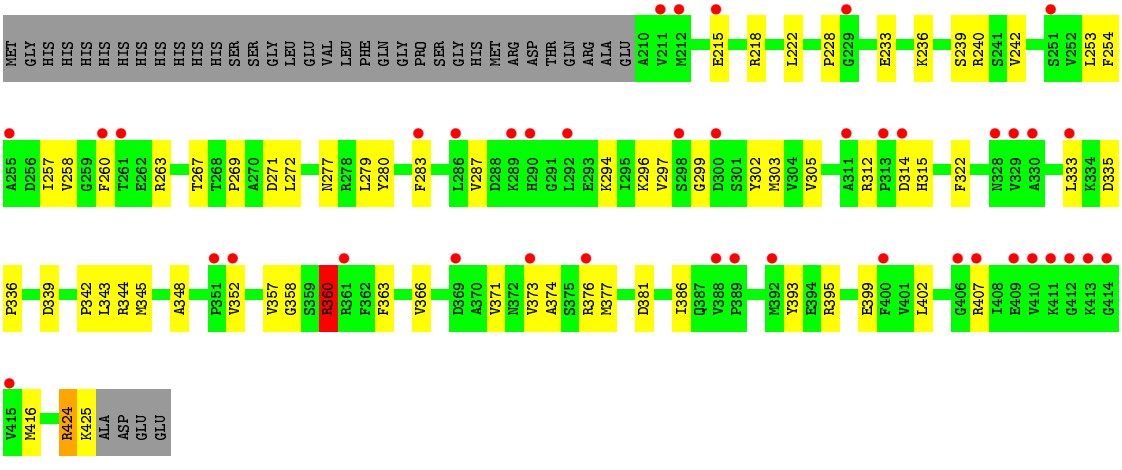
• Molecule 1: Adenylate cyclase

Chain J:



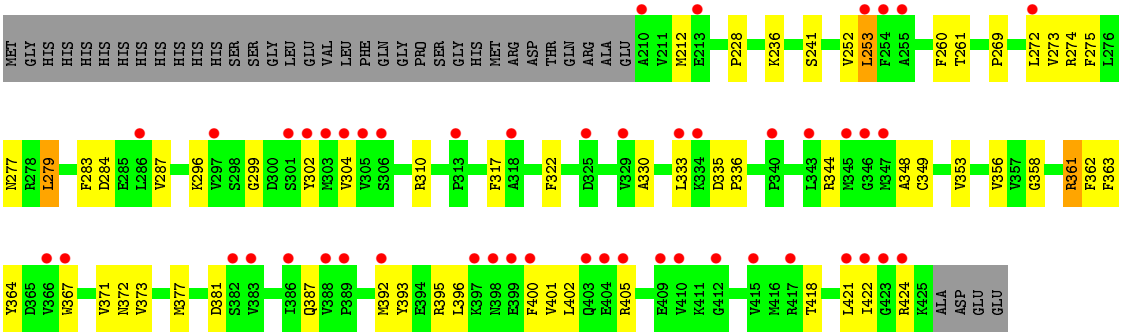
• Molecule 1: Adenylate cyclase

Chain H:



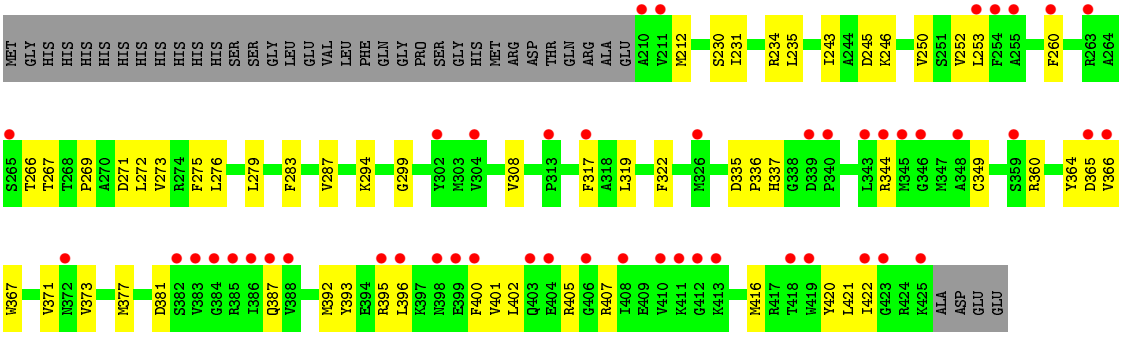
• Molecule 1: Adenylate cyclase

Chain G:



- Molecule 1: Adenylate cyclase

Chain K:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	145.42Å 85.69Å 318.01Å 90.00° 103.77° 90.00°	Depositor
Resolution (Å)	47.30 – 3.40 47.30 – 3.40	Depositor EDS
% Data completeness (in resolution range)	98.3 (47.30-3.40) 98.4 (47.30-3.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.15 (at 3.40Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.245 , 0.266 0.245 , 0.267	Depositor DCC
R_{free} test set	2002 reflections (3.86%)	wwPDB-VP
Wilson B-factor (Å^2)	106.7	Xtriage
Anisotropy	0.131	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 109.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	0.036 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	18919	wwPDB-VP
Average B, all atoms (Å^2)	149.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.32% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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, SO4, ONM

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	0.80	1/1701 (0.1%)	1.02	6/2297 (0.3%)
1	B	0.76	0/1701	0.97	7/2297 (0.3%)
1	C	0.77	1/1701 (0.1%)	1.00	5/2297 (0.2%)
1	D	0.69	0/1701	0.93	10/2297 (0.4%)
1	E	0.51	0/1701	0.72	2/2297 (0.1%)
1	F	0.48	0/1701	0.74	1/2297 (0.0%)
1	G	0.42	0/1701	0.64	2/2297 (0.1%)
1	H	0.46	0/1701	0.70	1/2297 (0.0%)
1	I	0.45	0/1701	0.70	1/2297 (0.0%)
1	J	0.46	0/1701	0.70	1/2297 (0.0%)
1	K	0.38	0/1701	0.60	0/2297
All	All	0.58	2/18711 (0.0%)	0.81	36/25267 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	252	VAL	CB-CG1	-6.61	1.39	1.52
1	A	353	VAL	CB-CG2	-5.42	1.41	1.52

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	360	ARG	NE-CZ-NH1	-11.26	114.67	120.30
1	J	360	ARG	NE-CZ-NH1	-10.59	115.00	120.30
1	A	272	LEU	CB-CG-CD2	-10.52	93.11	111.00
1	D	279	LEU	CA-CB-CG	8.80	135.54	115.30
1	D	279	LEU	CB-CG-CD2	-8.60	96.38	111.00
1	C	272	LEU	CB-CG-CD2	-7.60	98.08	111.00
1	C	235	LEU	CB-CG-CD2	7.50	123.74	111.00
1	C	279	LEU	CB-CG-CD2	-7.23	98.72	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	235	LEU	CB-CG-CD2	6.91	122.74	111.00
1	A	279	LEU	CA-CB-CG	6.85	131.05	115.30
1	I	279	LEU	CA-CB-CG	6.76	130.86	115.30
1	D	300	ASP	CB-CG-OD1	-6.53	112.42	118.30
1	A	272	LEU	CB-CG-CD1	6.50	122.04	111.00
1	E	235	LEU	CB-CG-CD2	6.12	121.41	111.00
1	C	396	LEU	CB-CG-CD2	-6.08	100.66	111.00
1	A	235	LEU	CB-CG-CD2	-6.01	100.79	111.00
1	D	276	LEU	CB-CG-CD1	-5.86	101.03	111.00
1	G	279	LEU	CA-CB-CG	5.86	128.77	115.30
1	D	272	LEU	CB-CG-CD2	-5.81	101.13	111.00
1	A	253	LEU	CB-CG-CD2	5.71	120.70	111.00
1	B	377	MET	CG-SD-CE	5.70	109.33	100.20
1	B	234	ARG	NE-CZ-NH2	-5.64	117.48	120.30
1	B	235	LEU	CB-CG-CD2	-5.63	101.42	111.00
1	D	335	ASP	CB-CG-OD1	-5.59	113.27	118.30
1	G	253	LEU	CA-CB-CG	5.47	127.88	115.30
1	D	234	ARG	NE-CZ-NH1	-5.45	117.57	120.30
1	A	256	ASP	CB-CG-OD2	-5.33	113.50	118.30
1	B	227	LEU	O-C-N	5.24	131.05	121.10
1	D	335	ASP	CB-CG-OD2	5.23	123.01	118.30
1	B	253	LEU	CB-CG-CD2	5.20	119.84	111.00
1	C	279	LEU	CB-CG-CD1	5.20	119.84	111.00
1	E	272	LEU	CA-CB-CG	5.20	127.26	115.30
1	B	297	VAL	CG1-CB-CG2	-5.17	102.62	110.90
1	B	223	LEU	CB-CG-CD1	-5.12	102.30	111.00
1	D	235	LEU	CB-CG-CD2	5.05	119.58	111.00
1	D	367	TRP	CA-CB-CG	5.05	123.29	113.70

There are no chirality outliers.

There are no planarity outliers.

5.2 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 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	1670	0	1670	53	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1670	0	1670	44	0
1	C	1670	0	1670	48	0
1	D	1670	0	1670	58	0
1	E	1670	0	1670	40	0
1	F	1670	0	1670	47	0
1	G	1670	0	1670	52	0
1	H	1670	0	1670	54	0
1	I	1670	0	1670	74	0
1	J	1670	0	1670	87	0
1	K	1670	0	1670	42	1
2	A	42	0	19	2	0
2	B	42	0	19	1	0
2	C	42	0	19	1	0
2	D	42	0	19	2	0
2	E	42	0	19	3	0
2	F	42	0	19	6	0
2	G	42	0	19	5	0
2	H	42	0	19	6	0
2	I	42	0	19	21	0
2	J	42	0	19	13	0
2	K	42	0	19	5	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	1	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	10	0	0	0	0
4	B	5	0	0	0	0
4	C	10	0	0	0	0
4	D	5	0	0	1	0
4	E	10	0	0	3	0
4	F	5	0	0	0	0
4	H	5	0	0	1	0
4	I	5	0	0	0	0
4	J	10	0	0	0	0
All	All	18919	0	18579	540	1

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 14.

All (540) 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)
2:H:504:ONM:C4'	2:H:504:ONM:O4'	1.65	1.22
2:K:501:ONM:C4'	2:K:501:ONM:O4'	1.65	1.21
2:I:504:ONM:C4'	2:I:504:ONM:O4'	1.64	1.18
2:A:501:ONM:O4'	2:A:501:ONM:C4'	1.63	1.16
2:J:501:ONM:O4'	2:J:501:ONM:C4'	1.64	1.15
1:A:267:THR:HB	1:A:272:LEU:CD1	1.76	1.14
1:I:216:TYR:CE1	1:J:215:GLU:OE1	2.06	1.09
2:G:501:ONM:C4'	2:G:501:ONM:O4'	1.64	1.07
1:D:223:LEU:HD21	1:C:222:LEU:HD13	1.32	1.05
1:A:267:THR:HB	1:A:272:LEU:HD13	1.38	1.01
1:C:267:THR:HB	1:C:272:LEU:CD1	1.95	0.97
1:J:344:ARG:NH2	2:J:501:ONM:O3G	1.99	0.95
1:K:267:THR:HB	1:K:272:LEU:CD1	1.98	0.94
1:F:267:THR:HB	1:F:272:LEU:CD1	1.98	0.93
1:D:267:THR:HB	1:D:272:LEU:CD1	2.03	0.88
2:I:504:ONM:HN22	1:J:303:MET:HE1	1.37	0.87
1:I:216:TYR:HE1	1:J:215:GLU:OE1	1.56	0.86
2:I:504:ONM:OA	1:J:372:ASN:HB2	1.76	0.85
1:I:353:VAL:HG21	1:J:269:PRO:HB2	1.59	0.84
1:D:401:VAL:HG13	1:D:422:ILE:HB	1.57	0.84
1:I:216:TYR:CZ	1:J:215:GLU:OE1	2.31	0.84
1:I:258:VAL:HB	1:I:342:PRO:HB2	1.60	0.84
1:E:401:VAL:HG13	1:E:422:ILE:HB	1.61	0.83
1:A:296:LYS:NZ	1:A:365:ASP:OD1	2.12	0.82
2:I:504:ONM:O1A	1:J:376:ARG:NH2	2.12	0.82
1:A:215:GLU:OE1	1:C:310:ARG:NH1	2.13	0.82
1:J:243:ILE:O	1:J:355:GLY:HA3	1.80	0.81
1:A:220:GLU:OE2	1:A:236:LYS:NZ	2.14	0.80
1:A:401:VAL:HG13	1:A:422:ILE:HB	1.61	0.80
1:G:296:LYS:HB3	1:G:363:PHE:HE2	1.46	0.79
1:F:233:GLU:HG2	1:G:310:ARG:HH12	1.47	0.78
1:A:267:THR:CB	1:A:272:LEU:CD1	2.59	0.78
1:I:277:ASN:OD1	1:J:358:GLY:N	2.16	0.78
1:G:373:VAL:O	1:G:377:MET:HG2	1.85	0.77
1:F:243:ILE:O	1:F:355:GLY:HA3	1.85	0.77
1:F:296:LYS:HB3	1:F:363:PHE:HE1	1.50	0.76
1:D:223:LEU:HD11	1:C:222:LEU:HD22	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:373:VAL:O	1:E:377:MET:HG2	1.86	0.76
1:K:267:THR:HB	1:K:272:LEU:HD13	1.67	0.76
1:G:284:ASP:OD1	1:G:302:TYR:OH	2.01	0.76
1:J:344:ARG:HG2	1:J:381:ASP:HB3	1.67	0.75
1:F:296:LYS:HB3	1:F:363:PHE:CE1	2.22	0.75
1:D:267:THR:HB	1:D:272:LEU:HD12	1.68	0.75
1:G:252:VAL:HG21	1:G:371:VAL:HG12	1.69	0.75
1:J:267:THR:HB	1:J:272:LEU:HD13	1.68	0.75
1:E:249:GLU:OE2	1:E:395:ARG:NH2	2.20	0.74
1:H:344:ARG:NH2	2:H:504:ONM:O3G	2.19	0.73
1:I:373:VAL:O	1:I:377:MET:HG2	1.89	0.73
1:C:267:THR:HB	1:C:272:LEU:HD11	1.71	0.72
2:H:504:ONM:OA	1:G:372:ASN:ND2	2.22	0.72
1:K:344:ARG:HG2	1:K:381:ASP:HB3	1.72	0.72
1:J:393:TYR:HD1	1:J:402:LEU:HD13	1.55	0.71
1:G:296:LYS:HB3	1:G:363:PHE:CE2	2.26	0.70
1:A:387:GLN:OE1	1:A:418:THR:HG21	1.92	0.70
1:H:258:VAL:HB	1:H:342:PRO:HB2	1.73	0.70
1:H:269:PRO:HB2	1:G:353:VAL:HG21	1.72	0.70
1:F:312:ARG:HD2	1:F:315:HIS:HA	1.74	0.69
1:I:216:TYR:OH	1:J:215:GLU:OE1	2.09	0.69
1:C:410:VAL:HG23	1:C:413:LYS:HB2	1.73	0.69
1:K:387:GLN:OE1	1:K:405:ARG:NH1	2.26	0.69
1:A:387:GLN:HG2	1:A:418:THR:HG23	1.75	0.69
1:B:324:LEU:HD21	1:B:421:LEU:HD22	1.76	0.68
1:A:267:THR:HB	1:A:272:LEU:HD11	1.74	0.68
1:A:349:CYS:SG	1:A:395:ARG:NH2	2.67	0.68
1:I:296:LYS:HE3	1:J:298:SER:OG	1.93	0.68
1:J:267:THR:HB	1:J:272:LEU:CD1	2.23	0.68
1:A:393:TYR:HD1	1:A:402:LEU:HD13	1.59	0.68
1:E:270:ALA:HB1	1:E:274:ARG:NH2	2.09	0.67
1:J:373:VAL:O	1:J:377:MET:HG2	1.94	0.67
1:K:373:VAL:O	1:K:377:MET:HG2	1.95	0.67
1:D:267:THR:HG22	1:D:271:ASP:HB2	1.77	0.66
1:K:401:VAL:HG13	1:K:422:ILE:HB	1.76	0.66
1:G:393:TYR:HD1	1:G:402:LEU:HD13	1.59	0.66
1:H:253:LEU:HD22	1:H:322:PHE:HE2	1.59	0.66
1:I:223:LEU:HD21	1:J:222:LEU:HD13	1.78	0.66
2:I:504:ONM:N2	1:J:303:MET:HE1	2.09	0.66
1:I:361:ARG:NH2	1:J:228:PRO:HG3	2.09	0.66
1:G:275:PHE:CG	1:G:336:PRO:HD3	2.32	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:233:GLU:HG2	1:G:310:ARG:NH1	2.11	0.65
1:J:279:LEU:HD12	1:J:333:LEU:HD13	1.79	0.64
1:E:344:ARG:HG2	1:E:381:ASP:HB3	1.78	0.64
1:F:324:LEU:HD21	1:F:421:LEU:HD22	1.78	0.64
1:I:317:PHE:HD2	1:I:400:PHE:HE2	1.44	0.64
1:I:372:ASN:OD1	1:J:261:THR:OG1	2.14	0.64
1:J:356:VAL:HG22	1:J:363:PHE:O	1.97	0.64
1:F:235:LEU:HD21	1:F:356:VAL:HG21	1.80	0.64
1:I:358:GLY:N	1:J:277:ASN:OD1	2.26	0.64
1:D:243:ILE:O	1:D:355:GLY:HA3	1.97	0.63
1:E:267:THR:HB	1:E:272:LEU:HD13	1.80	0.63
2:A:501:ONM:O1G	1:B:411:LYS:NZ	2.22	0.63
1:G:260:PHE:CZ	1:G:272:LEU:HG	2.34	0.63
1:I:372:ASN:HD21	2:J:501:ONM:H5'2	1.64	0.62
2:H:504:ONM:H3'	1:G:372:ASN:OD1	1.99	0.62
1:A:353:VAL:HG21	1:B:269:PRO:HB2	1.82	0.62
1:E:366:VAL:HG23	1:E:371:VAL:HG11	1.81	0.62
1:J:299:GLY:HA3	2:J:501:ONM:C8	2.28	0.62
1:J:393:TYR:CD1	1:J:402:LEU:HD13	2.34	0.62
1:H:358:GLY:N	1:G:277:ASN:OD1	2.32	0.62
1:B:245:ASP:HB3	1:C:239:SER:OG	1.99	0.62
1:C:324:LEU:HD21	1:C:421:LEU:HD22	1.81	0.62
1:K:260:PHE:HE2	2:K:501:ONM:CA2	2.13	0.62
1:B:410:VAL:HG23	1:B:413:LYS:HB2	1.83	0.61
1:G:317:PHE:HD2	1:G:400:PHE:HE2	1.47	0.61
1:I:246:LYS:HA	1:I:353:VAL:HG22	1.82	0.61
1:F:254:PHE:CZ	1:F:303:MET:HG3	2.35	0.61
1:I:226:MET:HE1	1:J:226:MET:HB3	1.82	0.61
1:B:235:LEU:CD1	1:B:243:ILE:HD12	2.31	0.61
1:B:267:THR:HB	1:B:272:LEU:HD13	1.81	0.61
1:G:377:MET:O	1:G:387:GLN:NE2	2.33	0.61
1:C:300:ASP:OD2	3:C:504:MN:MN	1.58	0.60
1:I:353:VAL:CG2	1:J:269:PRO:HB2	2.30	0.60
1:E:267:THR:HG22	1:E:271:ASP:HB2	1.83	0.60
1:G:228:PRO:HG2	1:G:364:TYR:CD2	2.36	0.60
1:D:353:VAL:HG21	1:C:269:PRO:HB2	1.84	0.60
1:D:387:GLN:OE1	1:D:418:THR:HG21	2.01	0.60
2:I:504:ONM:HA71	1:J:369:ASP:HB2	1.84	0.60
2:I:504:ONM:O2'	1:J:371:VAL:HG23	2.01	0.60
1:H:277:ASN:OD1	1:G:358:GLY:N	2.31	0.59
1:D:267:THR:HB	1:D:272:LEU:HD11	1.82	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:267:THR:HB	1:F:272:LEU:HD11	1.82	0.59
1:I:312:ARG:NH1	1:I:314:ASP:OD2	2.26	0.59
2:H:504:ONM:OA	2:H:504:ONM:NA1	2.30	0.59
1:I:258:VAL:CB	1:I:342:PRO:HB2	2.32	0.59
1:I:257:ILE:HB	1:I:300:ASP:OD1	2.02	0.59
1:K:260:PHE:HE2	2:K:501:ONM:HA2	1.68	0.59
1:C:257:ILE:HB	1:C:300:ASP:OD1	2.02	0.59
1:I:310:ARG:HH22	1:H:236:LYS:HB2	1.66	0.59
1:I:377:MET:O	1:I:387:GLN:NE2	2.33	0.59
1:C:393:TYR:HD1	1:C:402:LEU:HD13	1.68	0.59
1:H:399:GLU:HB3	1:H:424:ARG:HH11	1.68	0.59
1:C:280:TYR:CD1	1:C:283:PHE:HD2	2.21	0.58
1:E:242:VAL:HG21	1:F:274:ARG:HG2	1.85	0.58
1:F:267:THR:HB	1:F:272:LEU:HD12	1.83	0.58
1:H:260:PHE:CZ	1:H:272:LEU:HG	2.38	0.58
1:J:365:ASP:HB3	1:J:367:TRP:CZ2	2.38	0.58
1:H:376:ARG:NH2	2:G:501:ONM:O3A	2.37	0.58
1:I:294:LYS:HD3	1:J:361:ARG:HB2	1.85	0.58
1:A:367:TRP:NE1	1:B:299:GLY:HA2	2.19	0.58
1:C:280:TYR:HD1	1:C:283:PHE:HD2	1.51	0.58
1:I:252:VAL:HG21	1:I:371:VAL:HG12	1.84	0.58
1:K:377:MET:O	1:K:387:GLN:NE2	2.37	0.58
1:H:296:LYS:HB3	1:H:363:PHE:CE1	2.38	0.58
1:I:300:ASP:HB2	2:I:504:ONM:O4'	2.04	0.58
1:I:299:GLY:HA3	2:I:504:ONM:C4	2.34	0.58
1:I:261:THR:OG1	1:J:412:GLY:HA3	2.04	0.57
1:I:258:VAL:HA	2:I:504:ONM:O2G	2.04	0.57
1:A:344:ARG:HG2	1:A:381:ASP:HB3	1.85	0.57
1:J:258:VAL:HB	1:J:342:PRO:HB2	1.86	0.57
1:C:344:ARG:HG2	1:C:381:ASP:HB3	1.86	0.57
1:F:246:LYS:HD2	1:G:241:SER:OG	2.04	0.57
1:F:294:LYS:HE3	1:F:302:TYR:HE1	1.70	0.57
1:A:216:TYR:HD1	1:B:216:TYR:HD1	1.53	0.57
1:J:348:ALA:HB3	1:J:370:ALA:O	2.05	0.57
1:I:367:TRP:HB3	2:J:501:ONM:CA3	2.35	0.57
1:A:258:VAL:HG13	1:A:344:ARG:NH1	2.19	0.56
1:H:279:LEU:HD12	1:H:333:LEU:HD13	1.85	0.56
1:A:296:LYS:HE2	1:A:303:MET:HE3	1.87	0.56
1:C:402:LEU:HA	1:C:420:TYR:O	2.05	0.56
1:G:299:GLY:HA3	2:G:501:ONM:N3	2.20	0.56
1:E:267:THR:HB	1:E:272:LEU:CD1	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:335:ASP:OD2	1:I:339:ASP:N	2.38	0.56
1:G:304:VAL:HG21	1:G:322:PHE:CZ	2.40	0.56
1:A:296:LYS:HE2	1:A:303:MET:CE	2.35	0.56
1:F:407:ARG:HA	1:F:416:MET:O	2.05	0.56
1:H:287:VAL:HG12	1:H:322:PHE:CE1	2.41	0.56
1:I:393:TYR:HD1	1:I:402:LEU:HD13	1.70	0.56
4:D:504:SO4:O1	1:F:274:ARG:NH2	2.38	0.56
1:F:306:SER:HB2	1:F:319:LEU:HD13	1.88	0.56
1:I:270:ALA:HA	1:J:353:VAL:HG21	1.88	0.56
1:B:258:VAL:HB	1:B:342:PRO:HB2	1.89	0.56
1:I:368:GLY:HA2	2:J:501:ONM:CA5	2.37	0.55
1:B:296:LYS:HB3	1:B:363:PHE:CE1	2.41	0.55
1:D:262:GLU:OE2	1:D:262:GLU:N	2.38	0.55
1:E:250:VAL:HG11	1:E:308:VAL:HG13	1.87	0.55
1:I:261:THR:HG21	1:J:372:ASN:OD1	2.06	0.55
1:D:268:THR:O	1:D:272:LEU:HD13	2.06	0.55
1:G:396:LEU:HD23	1:G:421:LEU:HD13	1.88	0.55
1:H:335:ASP:HB2	1:H:336:PRO:HD2	1.89	0.55
1:K:267:THR:HB	1:K:272:LEU:HD11	1.83	0.55
1:I:361:ARG:HH21	1:J:228:PRO:HG3	1.71	0.55
1:B:235:LEU:CD1	1:B:243:ILE:CD1	2.85	0.55
1:D:335:ASP:HB2	1:D:336:PRO:HD2	1.88	0.55
1:A:228:PRO:HG3	1:B:361:ARG:NH2	2.22	0.55
1:G:344:ARG:HG2	1:G:381:ASP:HB3	1.89	0.55
1:I:220:GLU:OE2	1:I:236:LYS:NZ	2.40	0.55
1:D:373:VAL:O	1:D:377:MET:HG2	2.07	0.54
2:F:501:ONM:N3	2:F:501:ONM:H5'2	2.22	0.54
1:C:222:LEU:CD2	1:C:226:MET:SD	2.95	0.54
1:D:387:GLN:HG2	1:D:418:THR:HG23	1.89	0.54
1:K:234:ARG:NH2	1:K:243:ILE:HG23	2.23	0.54
1:I:267:THR:HG22	1:I:271:ASP:HB2	1.90	0.54
1:J:245:ASP:HB2	1:J:247:TYR:CE2	2.43	0.54
1:F:344:ARG:HH22	2:F:501:ONM:PG	2.31	0.54
1:B:373:VAL:O	1:B:377:MET:HG2	2.08	0.54
1:H:393:TYR:HD1	1:H:402:LEU:HD13	1.72	0.54
1:I:372:ASN:ND2	2:J:501:ONM:H5'2	2.22	0.53
1:E:274:ARG:HD3	4:E:504:SO4:S	2.48	0.53
1:F:409:GLU:HG2	1:F:415:VAL:HG22	1.91	0.53
1:D:396:LEU:HD23	1:D:421:LEU:HD13	1.91	0.53
1:H:269:PRO:HB2	1:G:353:VAL:CG2	2.37	0.53
1:K:396:LEU:HD23	1:K:421:LEU:HD13	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:335:ASP:HB2	1:C:336:PRO:HD2	1.90	0.53
1:I:299:GLY:HA3	2:I:504:ONM:N9	2.24	0.53
1:H:312:ARG:HD3	1:H:314:ASP:OD1	2.09	0.53
1:K:299:GLY:HA3	2:K:501:ONM:C4	2.39	0.53
1:B:250:VAL:HG11	1:B:308:VAL:HG13	1.90	0.53
1:C:312:ARG:HG3	1:C:315:HIS:HB3	1.90	0.53
1:F:344:ARG:NH2	2:F:501:ONM:O3G	2.42	0.53
1:J:263:ARG:HH12	1:J:342:PRO:HD2	1.74	0.52
1:B:296:LYS:HB3	1:B:363:PHE:HE1	1.75	0.52
1:H:344:ARG:HG2	1:H:381:ASP:HB3	1.91	0.52
2:H:504:ONM:N3	2:H:504:ONM:H5'1	2.25	0.52
1:D:252:VAL:HG13	1:D:374:ALA:HB2	1.91	0.52
1:E:365:ASP:HB3	1:E:367:TRP:CH2	2.44	0.52
1:G:349:CYS:SG	1:G:395:ARG:NH2	2.82	0.52
1:F:279:LEU:HD12	1:F:333:LEU:HD13	1.91	0.52
1:F:376:ARG:O	1:F:380:THR:HG22	2.09	0.52
1:J:356:VAL:HG13	1:J:363:PHE:H	1.75	0.52
1:I:246:LYS:O	1:H:239:SER:HA	2.10	0.52
1:J:344:ARG:HH22	2:J:501:ONM:PG	2.32	0.52
1:A:373:VAL:O	1:A:377:MET:HG2	2.10	0.52
1:C:267:THR:HG22	1:C:271:ASP:HB2	1.91	0.52
1:A:393:TYR:CD1	1:A:402:LEU:HD13	2.42	0.51
1:K:234:ARG:NH2	1:K:245:ASP:OD2	2.44	0.51
1:A:335:ASP:HB2	1:A:336:PRO:HD2	1.92	0.51
1:K:335:ASP:HB2	1:K:336:PRO:HD2	1.91	0.51
1:E:361:ARG:NH2	1:F:228:PRO:HG3	2.26	0.51
2:G:501:ONM:H5'2	2:G:501:ONM:O3B	2.10	0.51
1:J:377:MET:HG3	1:J:389:PRO:HD3	1.92	0.51
1:D:296:LYS:HE3	1:C:298:SER:OG	2.10	0.51
1:H:294:LYS:O	1:G:361:ARG:HG3	2.11	0.51
1:K:275:PHE:CG	1:K:336:PRO:HD3	2.46	0.51
1:D:226:MET:HB3	1:C:226:MET:HE1	1.93	0.51
1:E:243:ILE:O	1:E:355:GLY:HA3	2.11	0.51
1:I:372:ASN:HD21	2:J:501:ONM:C5'	2.24	0.51
1:C:257:ILE:HG21	1:C:260:PHE:HD1	1.76	0.50
1:I:344:ARG:NH1	2:I:504:ONM:O1G	2.45	0.50
1:I:365:ASP:HB3	1:I:367:TRP:CH2	2.46	0.50
1:J:377:MET:O	1:J:381:ASP:HB2	2.10	0.50
1:D:409:GLU:HG2	1:D:415:VAL:HG22	1.93	0.50
1:G:261:THR:HG23	2:G:501:ONM:O5'	2.12	0.50
1:A:408:ILE:O	1:A:415:VAL:HA	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:376:ARG:O	1:C:380:THR:HG22	2.11	0.50
1:D:245:ASP:HB2	1:D:247:TYR:HE2	1.77	0.50
1:K:275:PHE:CD1	1:K:336:PRO:HD3	2.47	0.50
1:D:353:VAL:HG21	1:C:269:PRO:CB	2.40	0.50
1:J:239:SER:HA	1:K:246:LYS:O	2.12	0.50
1:D:216:TYR:HD1	1:C:216:TYR:HD1	1.58	0.50
1:D:253:LEU:HB2	1:D:319:LEU:HD21	1.93	0.50
1:F:393:TYR:HD1	1:F:402:LEU:HD13	1.76	0.50
1:I:260:PHE:HE2	2:I:504:ONM:CA2	2.24	0.50
1:D:344:ARG:HG2	1:D:381:ASP:HB3	1.93	0.50
2:I:504:ONM:NA1	1:J:368:GLY:C	2.65	0.50
1:D:294:LYS:NZ	1:C:360:ARG:O	2.31	0.50
1:K:349:CYS:SG	1:K:395:ARG:NH2	2.85	0.50
1:G:356:VAL:HG22	1:G:363:PHE:O	2.12	0.49
1:K:267:THR:HG22	1:K:271:ASP:HB2	1.93	0.49
1:C:222:LEU:O	1:C:226:MET:HG3	2.11	0.49
1:F:254:PHE:CE1	1:F:303:MET:HG3	2.48	0.49
1:F:231:ILE:HG13	1:F:364:TYR:CD1	2.47	0.49
1:G:287:VAL:HG12	1:G:322:PHE:CE1	2.47	0.49
1:H:312:ARG:HD2	1:H:315:HIS:HA	1.94	0.49
1:I:277:ASN:HB2	1:J:357:VAL:HG12	1.94	0.49
1:J:347:MET:HB2	1:J:388:VAL:HG12	1.94	0.49
1:B:410:VAL:HG21	1:B:416:MET:SD	2.53	0.49
1:E:284:ASP:OD1	1:E:302:TYR:OH	2.27	0.49
1:K:407:ARG:HA	1:K:416:MET:O	2.12	0.49
1:A:222:LEU:HD12	1:B:236:LYS:HG3	1.94	0.49
1:E:348:ALA:HA	1:E:392:MET:HG3	1.94	0.49
1:D:388:VAL:HG23	1:D:419:TRP:HB2	1.94	0.49
1:F:373:VAL:O	1:F:377:MET:HG2	2.12	0.49
1:G:393:TYR:CD1	1:G:402:LEU:HD13	2.45	0.49
1:H:257:ILE:HA	1:H:343:LEU:HD23	1.94	0.49
1:J:376:ARG:O	1:J:380:THR:HG22	2.13	0.49
2:I:504:ONM:O1B	1:J:411:LYS:HD3	2.12	0.49
1:D:261:THR:O	1:D:264:ALA:N	2.32	0.49
1:G:287:VAL:HG12	1:G:322:PHE:CZ	2.47	0.49
1:H:296:LYS:HB3	1:H:363:PHE:HE1	1.76	0.49
1:D:283:PHE:O	1:D:287:VAL:HG13	2.13	0.49
1:H:263:ARG:HH12	1:H:342:PRO:HD2	1.77	0.49
1:H:399:GLU:HB3	1:H:424:ARG:NH1	2.28	0.49
1:K:253:LEU:HB2	1:K:319:LEU:HD21	1.95	0.49
2:K:501:ONM:H5'2	2:K:501:ONM:O3B	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:377:MET:O	1:D:387:GLN:NE2	2.46	0.48
1:J:410:VAL:HG23	1:J:413:LYS:HB2	1.95	0.48
1:A:387:GLN:HG2	1:A:418:THR:CG2	2.42	0.48
1:E:396:LEU:HD23	1:E:421:LEU:HD13	1.96	0.48
1:I:257:ILE:HA	1:I:343:LEU:HD23	1.96	0.48
1:B:344:ARG:HG2	1:B:381:ASP:HB3	1.95	0.48
1:I:357:VAL:HG12	1:J:277:ASN:HB2	1.94	0.48
1:B:239:SER:OG	1:C:245:ASP:HB3	2.13	0.48
1:B:406:GLY:O	1:B:417:ARG:HA	2.13	0.48
1:I:310:ARG:NH1	1:H:233:GLU:O	2.27	0.48
1:B:342:PRO:O	1:B:343:LEU:HD23	2.13	0.48
1:E:335:ASP:HB2	1:E:336:PRO:HD2	1.96	0.48
1:K:250:VAL:HG11	1:K:308:VAL:HG13	1.94	0.48
1:B:235:LEU:HD12	1:B:243:ILE:CD1	2.44	0.48
1:D:260:PHE:O	1:D:263:ARG:HB2	2.14	0.48
1:H:258:VAL:HG13	1:H:344:ARG:HH21	1.77	0.48
1:I:367:TRP:NE1	1:J:299:GLY:HA2	2.29	0.48
1:H:360:ARG:HG3	1:G:284:ASP:HB3	1.95	0.48
1:I:368:GLY:HA2	2:J:501:ONM:CA6	2.43	0.48
1:A:267:THR:HG22	1:A:271:ASP:HB2	1.95	0.48
1:D:263:ARG:HH12	1:D:342:PRO:CD	2.27	0.48
1:H:299:GLY:HA2	1:G:367:TRP:HE1	1.78	0.48
1:J:280:TYR:CD2	1:J:297:VAL:HG21	2.48	0.48
1:H:254:PHE:CE1	1:H:303:MET:HG3	2.49	0.48
1:I:410:VAL:HG23	1:I:413:LYS:HB2	1.95	0.48
1:K:266:THR:HB	1:K:337:HIS:ND1	2.29	0.47
1:E:258:VAL:HB	1:E:342:PRO:HB2	1.97	0.47
1:I:242:VAL:HG21	1:J:274:ARG:HG2	1.95	0.47
1:K:234:ARG:NH1	1:K:243:ILE:HG12	2.29	0.47
1:K:287:VAL:HG12	1:K:322:PHE:CZ	2.49	0.47
1:A:377:MET:O	1:A:387:GLN:NE2	2.48	0.47
1:C:287:VAL:HG12	1:C:322:PHE:CZ	2.49	0.47
1:H:242:VAL:HG21	1:G:274:ARG:HG2	1.94	0.47
1:J:252:VAL:HG11	1:J:371:VAL:HA	1.95	0.47
1:J:399:GLU:HB3	1:J:424:ARG:HH11	1.80	0.47
1:A:368:GLY:O	1:A:371:VAL:HG22	2.14	0.47
1:C:410:VAL:HG21	1:C:416:MET:SD	2.54	0.47
1:I:242:VAL:HB	1:J:274:ARG:HG2	1.97	0.47
1:B:279:LEU:HD12	1:B:333:LEU:HD13	1.97	0.47
1:G:279:LEU:HD22	1:G:333:LEU:HD13	1.97	0.47
1:H:263:ARG:HH12	1:H:342:PRO:CD	2.27	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:242:VAL:CB	1:J:274:ARG:HG2	2.45	0.46
1:B:425:LYS:HB3	1:B:425:LYS:HE2	1.77	0.46
1:C:267:THR:HB	1:C:272:LEU:HD13	1.88	0.46
1:F:294:LYS:HE3	1:F:302:TYR:CE1	2.49	0.46
1:F:399:GLU:HB3	1:F:424:ARG:HH11	1.80	0.46
1:K:317:PHE:HD2	1:K:400:PHE:HE2	1.63	0.46
1:F:297:VAL:HG13	1:F:297:VAL:O	2.15	0.46
1:F:251:SER:HA	1:F:348:ALA:O	2.15	0.46
1:H:348:ALA:HB3	1:H:374:ALA:HB2	1.98	0.46
1:J:410:VAL:HG21	1:J:416:MET:SD	2.55	0.46
1:A:407:ARG:HG3	1:A:407:ARG:NH1	2.31	0.46
1:F:267:THR:HG22	1:F:271:ASP:HB2	1.97	0.46
1:H:335:ASP:OD2	1:H:339:ASP:N	2.45	0.46
1:B:376:ARG:O	1:B:380:THR:HG22	2.15	0.46
1:H:215:GLU:HA	1:H:218:ARG:HD2	1.96	0.46
1:H:267:THR:HG22	1:H:271:ASP:HB2	1.97	0.46
1:H:360:ARG:NH2	4:H:501:SO4:O1	2.49	0.46
1:B:335:ASP:HB2	1:B:336:PRO:HD2	1.97	0.46
1:B:252:VAL:HG11	1:B:371:VAL:HA	1.96	0.46
1:E:275:PHE:HD1	1:E:278:ARG:NH2	2.12	0.46
1:B:223:LEU:HD12	1:B:223:LEU:HA	1.59	0.46
1:D:221:ALA:O	1:D:224:ALA:HB3	2.16	0.46
1:J:295:ILE:HA	1:J:295:ILE:HD13	1.73	0.46
1:I:367:TRP:HB3	2:J:501:ONM:CA2	2.45	0.46
1:K:287:VAL:HG12	1:K:322:PHE:CE1	2.51	0.46
1:A:406:GLY:O	1:A:417:ARG:HA	2.16	0.46
1:G:405:ARG:HB3	1:G:418:THR:HG22	1.97	0.46
1:I:396:LEU:HD23	1:I:421:LEU:HD13	1.97	0.46
1:K:393:TYR:HD1	1:K:402:LEU:HD13	1.80	0.46
1:A:298:SER:O	1:A:300:ASP:N	2.48	0.46
1:A:292:LEU:HD22	1:A:306:SER:HB2	1.97	0.46
1:A:408:ILE:HD12	1:A:410:VAL:HG13	1.96	0.46
1:D:273:VAL:HG21	1:C:353:VAL:HG11	1.98	0.46
1:I:270:ALA:CA	1:J:353:VAL:HG21	2.45	0.46
1:H:373:VAL:O	1:H:377:MET:HG2	2.16	0.45
1:A:250:VAL:HG11	1:A:308:VAL:HG13	1.97	0.45
1:C:251:SER:HB3	1:C:319:LEU:HD22	1.97	0.45
1:D:279:LEU:HD23	1:D:333:LEU:HD13	1.97	0.45
1:D:263:ARG:NH1	1:D:342:PRO:HD2	2.31	0.45
1:D:399:GLU:HB3	1:D:424:ARG:HH11	1.81	0.45
2:E:501:ONM:H5'2	2:E:501:ONM:O3B	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:269:PRO:O	1:K:273:VAL:HG23	2.16	0.45
1:B:267:THR:HB	1:B:272:LEU:CD1	2.46	0.45
1:D:276:LEU:HA	1:D:276:LEU:HD12	1.63	0.45
1:D:280:TYR:CE2	1:D:297:VAL:HG11	2.51	0.45
4:E:505:SO4:O2	1:F:274:ARG:HD3	2.16	0.45
1:F:280:TYR:CD2	1:F:297:VAL:HG21	2.51	0.45
1:G:356:VAL:HG13	1:G:363:PHE:O	2.17	0.45
1:I:346:GLY:HA3	1:I:377:MET:C	2.37	0.45
1:A:353:VAL:HG21	1:B:269:PRO:CB	2.46	0.45
2:B:501:ONM:CA	2:B:501:ONM:H2'	2.29	0.45
1:C:272:LEU:HD23	2:C:501:ONM:CA4	2.47	0.45
1:F:279:LEU:O	1:F:282:ALA:HB3	2.17	0.45
1:J:280:TYR:HD1	1:J:283:PHE:HD2	1.64	0.45
1:G:335:ASP:HB2	1:G:336:PRO:HD2	1.98	0.45
1:H:366:VAL:HG23	1:H:371:VAL:HG11	1.99	0.45
1:I:335:ASP:HB2	1:I:336:PRO:HD2	1.98	0.45
1:A:377:MET:O	1:A:381:ASP:HB2	2.16	0.45
1:D:245:ASP:HB2	1:D:247:TYR:CE2	2.51	0.45
1:J:261:THR:OG1	2:J:501:ONM:OA	2.34	0.45
1:A:254:PHE:CE1	1:A:303:MET:HG3	2.53	0.44
1:C:377:MET:HG3	1:C:389:PRO:HD3	1.98	0.44
1:G:283:PHE:HZ	1:G:330:ALA:HB2	1.81	0.44
1:K:276:LEU:HA	1:K:276:LEU:HD12	1.75	0.44
1:A:410:VAL:HG23	1:A:413:LYS:HB2	1.99	0.44
1:B:320:ALA:HB1	1:B:421:LEU:HD11	1.98	0.44
1:G:344:ARG:HD3	1:G:381:ASP:O	2.17	0.44
1:H:407:ARG:HA	1:H:416:MET:O	2.18	0.44
2:I:504:ONM:NA1	1:J:369:ASP:N	2.65	0.44
1:D:295:ILE:HD13	1:D:295:ILE:HA	1.83	0.44
1:D:410:VAL:HG23	1:D:413:LYS:HB2	1.99	0.44
1:H:377:MET:O	1:H:381:ASP:HB2	2.18	0.44
1:H:352:VAL:CG1	1:H:366:VAL:HB	2.47	0.44
1:J:284:ASP:O	1:J:287:VAL:HG22	2.18	0.44
1:A:251:SER:HB3	1:A:319:LEU:HD23	2.00	0.44
1:A:387:GLN:CG	1:A:418:THR:CG2	2.95	0.44
1:G:275:PHE:CD1	1:G:336:PRO:HD3	2.53	0.44
1:D:354:ALA:HB1	1:D:364:TYR:CZ	2.53	0.44
1:E:261:THR:HG23	2:E:501:ONM:H5'1	2.00	0.44
1:E:367:TRP:HB3	2:F:501:ONM:CA2	2.48	0.44
1:G:401:VAL:HG13	1:G:422:ILE:HB	2.00	0.44
1:H:283:PHE:HB3	1:H:302:TYR:CZ	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:343:LEU:HD23	1:B:343:LEU:HA	1.76	0.44
1:G:356:VAL:CG1	1:G:362:PHE:HB2	2.48	0.44
1:I:368:GLY:H	2:J:501:ONM:H2'	1.64	0.44
1:A:255:ALA:O	1:A:301:SER:HA	2.18	0.44
1:A:296:LYS:CE	1:A:303:MET:HE3	2.48	0.44
1:A:376:ARG:CZ	1:A:411:LYS:HB3	2.48	0.44
1:B:408:ILE:HD12	1:B:410:VAL:HG13	2.00	0.44
1:D:366:VAL:HG23	1:D:371:VAL:HG11	2.00	0.44
1:H:352:VAL:HG11	1:H:366:VAL:HB	1.99	0.44
1:F:393:TYR:CD1	1:F:402:LEU:HD13	2.53	0.44
1:K:231:ILE:HG13	1:K:364:TYR:CD1	2.53	0.44
1:D:344:ARG:HB3	1:D:378:GLU:HG2	2.00	0.43
2:F:501:ONM:OA	2:F:501:ONM:NA1	2.50	0.43
1:J:368:GLY:O	1:J:371:VAL:HG22	2.18	0.43
1:D:249:GLU:OE2	1:D:395:ARG:NH2	2.52	0.43
1:J:407:ARG:HA	1:J:416:MET:O	2.18	0.43
1:B:347:MET:HB2	1:B:388:VAL:HG12	2.00	0.43
1:F:252:VAL:HG12	1:F:305:VAL:HG22	2.01	0.43
1:B:284:ASP:O	1:B:287:VAL:HG22	2.18	0.43
1:C:235:LEU:HD12	1:C:362:PHE:CE2	2.53	0.43
1:C:254:PHE:CZ	1:C:303:MET:HG3	2.54	0.43
1:K:365:ASP:HB3	1:K:367:TRP:CH2	2.54	0.43
1:B:222:LEU:O	1:B:226:MET:HG3	2.18	0.43
1:E:276:LEU:HA	1:E:276:LEU:HD12	1.70	0.43
1:H:305:VAL:HG21	1:H:366:VAL:HG21	2.00	0.43
1:H:222:LEU:HD12	1:G:236:LYS:HG3	2.00	0.43
1:C:223:LEU:HA	1:C:223:LEU:HD12	1.73	0.43
1:C:222:LEU:HD22	1:C:226:MET:SD	2.59	0.43
1:E:376:ARG:NH2	1:E:411:LYS:HD2	2.33	0.43
1:G:228:PRO:HG2	1:G:364:TYR:CE2	2.53	0.43
1:J:343:LEU:HA	1:J:343:LEU:HD23	1.83	0.43
1:E:258:VAL:HG21	1:E:383:VAL:HG12	2.00	0.43
1:E:377:MET:HG3	1:E:389:PRO:HD3	2.01	0.43
1:J:335:ASP:HB2	1:J:336:PRO:HD2	1.99	0.43
1:K:366:VAL:HG23	1:K:371:VAL:HG11	2.01	0.43
1:A:267:THR:CB	1:A:272:LEU:HD13	2.28	0.43
1:A:344:ARG:HD2	1:A:378:GLU:O	2.18	0.43
1:D:377:MET:HE3	1:D:387:GLN:HG2	2.00	0.43
1:E:287:VAL:HG12	1:E:322:PHE:CZ	2.54	0.43
1:G:304:VAL:HG21	1:G:322:PHE:CE2	2.54	0.43
2:I:504:ONM:N2	1:J:365:ASP:OD1	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:348:ALA:HB2	1:J:373:VAL:HG23	2.01	0.43
1:K:231:ILE:HG22	1:K:235:LEU:HD23	2.00	0.43
1:K:234:ARG:CZ	1:K:243:ILE:HG23	2.49	0.42
1:D:255:ALA:O	1:D:301:SER:HA	2.19	0.42
1:D:410:VAL:HG21	1:D:416:MET:SD	2.59	0.42
1:I:260:PHE:HE2	2:I:504:ONM:HA2	1.84	0.42
2:I:504:ONM:CA6	1:J:368:GLY:HA2	2.49	0.42
1:A:392:MET:HG2	1:A:396:LEU:HD13	2.01	0.42
1:I:367:TRP:HE1	1:J:299:GLY:HA2	1.83	0.42
1:B:312:ARG:HD2	1:B:315:HIS:HA	2.02	0.42
1:G:348:ALA:CB	1:G:373:VAL:HG23	2.49	0.42
1:H:263:ARG:NH1	1:H:342:PRO:HD2	2.35	0.42
1:J:286:LEU:HD21	1:J:325:ASP:HB3	2.02	0.42
1:E:258:VAL:HG11	1:E:383:VAL:HG11	2.01	0.42
2:I:504:ONM:CA5	1:J:368:GLY:HA2	2.49	0.42
1:D:367:TRP:NE1	1:C:299:GLY:HA2	2.34	0.42
1:H:228:PRO:HG3	1:G:361:ARG:NH2	2.35	0.42
1:E:409:GLU:HG2	1:E:415:VAL:HG22	2.01	0.42
1:H:345:MET:HB3	1:H:386:ILE:HG23	2.02	0.42
1:A:407:ARG:HG3	1:A:407:ARG:HH11	1.84	0.42
1:E:260:PHE:HE1	1:E:275:PHE:HE2	1.67	0.42
1:E:263:ARG:NH1	1:E:342:PRO:HD2	2.35	0.42
1:H:280:TYR:CD2	1:H:297:VAL:HG21	2.55	0.42
1:H:393:TYR:CD1	1:H:402:LEU:HD13	2.55	0.42
1:B:377:MET:O	1:B:381:ASP:HB2	2.20	0.42
1:E:225:ASN:HD21	1:F:360:ARG:HA	1.85	0.42
2:E:501:ONM:N2	1:F:366:VAL:O	2.53	0.42
1:I:272:LEU:HD23	2:I:504:ONM:CA3	2.50	0.42
1:J:376:ARG:NH2	1:J:411:LYS:HD2	2.35	0.42
1:E:274:ARG:HD3	4:E:504:SO4:O2	2.19	0.42
1:G:269:PRO:O	1:G:273:VAL:HG23	2.20	0.42
1:G:279:LEU:HD11	1:G:283:PHE:CE2	2.54	0.42
1:A:295:ILE:HG23	1:A:295:ILE:HD12	1.79	0.41
1:A:367:TRP:HE1	1:B:299:GLY:HA2	1.83	0.41
1:C:344:ARG:NH1	1:C:378:GLU:OE2	2.53	0.41
1:J:249:GLU:HB3	1:J:315:HIS:NE2	2.35	0.41
1:J:399:GLU:HB3	1:J:424:ARG:NH1	2.36	0.41
1:F:335:ASP:HB2	1:F:336:PRO:HD2	2.02	0.41
1:A:228:PRO:HG3	1:B:361:ARG:HH21	1.85	0.41
1:C:407:ARG:HG3	1:C:417:ARG:HG2	2.02	0.41
1:E:275:PHE:CZ	1:E:279:LEU:HD12	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:276:LEU:HA	1:F:276:LEU:HD12	1.78	0.41
1:F:300:ASP:OD2	2:F:501:ONM:O2A	2.38	0.41
1:H:297:VAL:O	1:H:297:VAL:HG13	2.20	0.41
1:K:279:LEU:HD11	1:K:283:PHE:CE2	2.55	0.41
1:J:233:GLU:CD	1:K:230:SER:HB3	2.41	0.41
1:B:252:VAL:HG13	1:B:374:ALA:HB2	2.03	0.41
1:D:393:TYR:HD1	1:D:402:LEU:HD13	1.86	0.41
1:F:373:VAL:HG12	1:F:413:LYS:HG3	2.02	0.41
1:I:401:VAL:HG12	1:I:423:GLY:O	2.20	0.41
1:J:304:VAL:HG21	1:J:322:PHE:CE2	2.56	0.41
1:K:252:VAL:HG11	1:K:371:VAL:HG12	2.03	0.41
1:K:402:LEU:HA	1:K:420:TYR:O	2.21	0.41
1:A:305:VAL:HG12	1:A:308:VAL:HG22	2.03	0.41
1:C:284:ASP:O	1:C:287:VAL:HG22	2.21	0.41
1:D:286:LEU:HD21	1:D:325:ASP:HB3	2.02	0.41
1:H:357:VAL:HG12	1:G:277:ASN:HB2	2.03	0.41
1:I:242:VAL:CG2	1:J:274:ARG:HG2	2.50	0.41
1:B:346:GLY:HA2	1:B:387:GLN:O	2.20	0.41
1:D:263:ARG:HH12	1:D:342:PRO:HD2	1.85	0.41
1:E:354:ALA:HB1	1:E:364:TYR:CZ	2.56	0.41
1:I:222:LEU:HD13	1:J:223:LEU:HD11	2.03	0.41
1:C:321:ASP:O	1:C:325:ASP:HB2	2.21	0.41
1:H:425:LYS:HB3	1:H:425:LYS:HE2	1.92	0.41
1:I:216:TYR:HH	1:J:215:GLU:CD	2.24	0.41
1:J:356:VAL:HG22	1:J:363:PHE:C	2.41	0.41
1:B:267:THR:HG22	1:B:271:ASP:HB2	2.02	0.41
1:D:216:TYR:CD1	1:C:216:TYR:HB2	2.56	0.41
1:F:312:ARG:HG3	1:F:315:HIS:HB3	2.03	0.41
1:G:253:LEU:HD22	1:G:322:PHE:HE2	1.85	0.41
1:I:258:VAL:HB	1:I:342:PRO:CB	2.39	0.41
1:J:312:ARG:HD2	1:J:315:HIS:HA	2.03	0.41
1:K:349:CYS:SG	1:K:395:ARG:CZ	3.09	0.41
1:D:287:VAL:HG12	1:D:322:PHE:CZ	2.56	0.41
1:E:260:PHE:HE1	1:E:275:PHE:CE2	2.39	0.41
1:I:305:VAL:HG21	1:I:366:VAL:HG21	2.03	0.41
1:I:399:GLU:HB3	1:I:424:ARG:HH11	1.86	0.41
1:C:251:SER:HB3	1:C:319:LEU:CD2	2.51	0.41
1:J:245:ASP:HB2	1:J:247:TYR:HE2	1.84	0.41
1:D:260:PHE:CD2	2:D:501:ONM:H4'	2.56	0.40
1:D:260:PHE:N	2:D:501:ONM:O2B	2.54	0.40
1:E:263:ARG:HH12	1:E:342:PRO:HD2	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:297:VAL:HA	1:F:301:SER:O	2.20	0.40
1:E:410:VAL:HG21	1:E:416:MET:SD	2.62	0.40
1:I:263:ARG:HH12	1:I:342:PRO:CD	2.35	0.40
1:A:349:CYS:SG	1:A:395:ARG:CZ	3.10	0.40
1:C:360:ARG:O	1:C:361:ARG:HB2	2.22	0.40
1:D:268:THR:HG23	1:D:268:THR:H	1.59	0.40
1:E:228:PRO:HG2	1:E:364:TYR:CD2	2.57	0.40
1:F:357:VAL:HG13	1:F:367:TRP:CH2	2.57	0.40
1:I:254:PHE:O	1:I:345:MET:HA	2.22	0.40
1:I:402:LEU:HD23	1:I:420:TYR:O	2.21	0.40
1:K:252:VAL:HG11	1:K:371:VAL:HA	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:294:LYS:NZ	1:K:360:ARG:O[2_759]	2.16	0.04

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	214/254 (84%)	211 (99%)	2 (1%)	1 (0%)	29 61
1	B	214/254 (84%)	211 (99%)	3 (1%)	0	100 100
1	C	214/254 (84%)	211 (99%)	3 (1%)	0	100 100
1	D	214/254 (84%)	213 (100%)	1 (0%)	0	100 100
1	E	214/254 (84%)	211 (99%)	3 (1%)	0	100 100
1	F	214/254 (84%)	208 (97%)	6 (3%)	0	100 100
1	G	214/254 (84%)	209 (98%)	4 (2%)	1 (0%)	29 61

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	214/254 (84%)	210 (98%)	4 (2%)	0	100	100
1	I	214/254 (84%)	212 (99%)	2 (1%)	0	100	100
1	J	214/254 (84%)	206 (96%)	8 (4%)	0	100	100
1	K	214/254 (84%)	210 (98%)	4 (2%)	0	100	100
All	All	2354/2794 (84%)	2312 (98%)	40 (2%)	2 (0%)	51	82

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	361	ARG
1	A	299	GLY

5.3.2 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 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	175/207 (84%)	173 (99%)	2 (1%)	73	86
1	B	175/207 (84%)	174 (99%)	1 (1%)	86	94
1	C	175/207 (84%)	172 (98%)	3 (2%)	60	80
1	D	175/207 (84%)	171 (98%)	4 (2%)	50	74
1	E	175/207 (84%)	171 (98%)	4 (2%)	50	74
1	F	175/207 (84%)	172 (98%)	3 (2%)	60	80
1	G	175/207 (84%)	172 (98%)	3 (2%)	60	80
1	H	175/207 (84%)	171 (98%)	4 (2%)	50	74
1	I	175/207 (84%)	173 (99%)	2 (1%)	73	86
1	J	175/207 (84%)	172 (98%)	3 (2%)	60	80
1	K	175/207 (84%)	173 (99%)	2 (1%)	73	86
All	All	1925/2277 (84%)	1894 (98%)	31 (2%)	62	81

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	212	MET
1	A	424	ARG
1	B	424	ARG
1	D	212	MET
1	D	222	LEU
1	D	301	SER
1	D	392	MET
1	C	215	GLU
1	C	240	ARG
1	C	395	ARG
1	E	212	MET
1	E	240	ARG
1	E	392	MET
1	E	424	ARG
1	F	225	ASN
1	F	395	ARG
1	F	424	ARG
1	I	212	MET
1	I	392	MET
1	J	240	ARG
1	J	395	ARG
1	J	424	ARG
1	H	240	ARG
1	H	360	ARG
1	H	395	ARG
1	H	424	ARG
1	G	212	MET
1	G	392	MET
1	G	424	ARG
1	K	212	MET
1	K	392	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 46 ligands modelled in this entry, 22 are monoatomic - leaving 24 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	C	501	3	37,45,45	4.03	17 (45%)	48,69,69	2.53	14 (29%)
4	SO4	E	505	-	4,4,4	1.15	0	6,6,6	0.47	0
2	ONM	H	504	3	37,45,45	4.64	17 (45%)	48,69,69	3.23	17 (35%)
2	ONM	J	501	3	37,45,45	4.71	17 (45%)	48,69,69	3.04	17 (35%)
4	SO4	J	502	-	4,4,4	0.28	0	6,6,6	0.52	0
2	ONM	I	504	3	37,45,45	4.73	19 (51%)	48,69,69	2.57	17 (35%)
2	ONM	A	501	3	37,45,45	4.23	15 (40%)	48,69,69	2.88	14 (29%)
2	ONM	F	501	3	37,45,45	4.38	19 (51%)	48,69,69	2.68	15 (31%)
2	ONM	K	501	3	37,45,45	4.98	19 (51%)	48,69,69	2.78	17 (35%)
4	SO4	A	504	-	4,4,4	0.23	0	6,6,6	0.16	0
4	SO4	H	501	-	4,4,4	0.21	0	6,6,6	0.14	0
4	SO4	I	503	-	4,4,4	0.20	0	6,6,6	0.22	0
2	ONM	D	501	3	37,45,45	4.09	18 (48%)	48,69,69	2.95	10 (20%)
4	SO4	F	502	-	4,4,4	0.22	0	6,6,6	0.26	0
4	SO4	J	505	-	4,4,4	0.43	0	6,6,6	0.19	0
4	SO4	C	503	-	4,4,4	0.16	0	6,6,6	0.18	0
4	SO4	C	502	-	4,4,4	0.17	0	6,6,6	0.23	0
4	SO4	D	504	-	4,4,4	1.33	0	6,6,6	0.73	0
4	SO4	A	505	-	4,4,4	1.19	0	6,6,6	1.30	1 (16%)
2	ONM	E	501	3	37,45,45	4.40	19 (51%)	48,69,69	2.30	12 (25%)
2	ONM	G	501	3	37,45,45	5.00	19 (51%)	48,69,69	2.73	18 (37%)
4	SO4	B	502	-	4,4,4	0.18	0	6,6,6	0.15	0
4	SO4	E	504	-	4,4,4	0.19	0	6,6,6	0.33	0
2	ONM	B	501	3	37,45,45	4.06	17 (45%)	48,69,69	2.62	9 (18%)

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	C	501	3	-	8/28/48/48	0/4/4/4
2	ONM	D	501	3	-	7/28/48/48	0/4/4/4
2	ONM	H	504	3	-	9/28/48/48	0/4/4/4
2	ONM	F	501	3	-	4/28/48/48	0/4/4/4
2	ONM	G	501	3	-	7/28/48/48	0/4/4/4
2	ONM	J	501	3	-	6/28/48/48	0/4/4/4
2	ONM	K	501	3	-	5/28/48/48	0/4/4/4
2	ONM	E	501	3	-	9/28/48/48	0/4/4/4
2	ONM	I	504	3	-	3/28/48/48	0/4/4/4
2	ONM	A	501	3	-	5/28/48/48	0/4/4/4
2	ONM	B	501	3	-	7/28/48/48	0/4/4/4

All (196) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	501	ONM	C2'-C1'	-13.23	1.33	1.53
2	D	501	ONM	C2'-C1'	-12.99	1.34	1.53
2	C	501	ONM	C2'-C1'	-11.44	1.36	1.53
2	K	501	ONM	C2'-C1'	-11.43	1.36	1.53
2	A	501	ONM	C2'-C1'	-11.27	1.36	1.53
2	B	501	ONM	C2'-C1'	-11.25	1.36	1.53
2	F	501	ONM	C2'-C1'	-11.18	1.36	1.53
2	I	504	ONM	C2'-C1'	-10.99	1.37	1.53
2	K	501	ONM	C4-N3	10.99	1.52	1.35
2	G	501	ONM	C4-N3	10.97	1.52	1.35
2	E	501	ONM	C2'-C1'	-10.61	1.37	1.53
2	H	504	ONM	C2'-C1'	-10.52	1.37	1.53
2	J	501	ONM	C2'-C1'	-10.09	1.38	1.53
2	A	501	ONM	C3'-C4'	-10.06	1.25	1.52
2	B	501	ONM	C3'-C4'	-10.05	1.25	1.52
2	I	504	ONM	C4-N3	10.02	1.51	1.35
2	C	501	ONM	C3'-C4'	-9.95	1.26	1.52
2	D	501	ONM	C3'-C4'	-9.56	1.27	1.52
2	K	501	ONM	C6-C5	9.42	1.57	1.41
2	G	501	ONM	C3'-C4'	-9.35	1.27	1.52
2	H	504	ONM	C3'-C4'	-9.34	1.27	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	501	ONM	C3'-C4'	-9.31	1.27	1.52
2	J	501	ONM	C6-C5	9.29	1.57	1.41
2	A	501	ONM	C6-C5	9.28	1.57	1.41
2	I	504	ONM	C3'-C4'	-9.28	1.28	1.52
2	H	504	ONM	O4'-C4'	9.25	1.65	1.45
2	K	501	ONM	O4'-C4'	9.08	1.65	1.45
2	H	504	ONM	C4-N3	9.03	1.49	1.35
2	J	501	ONM	C4-N3	8.89	1.49	1.35
2	K	501	ONM	C3'-C4'	-8.84	1.29	1.52
2	H	504	ONM	C6-N1	8.83	1.48	1.33
2	J	501	ONM	O4'-C4'	8.79	1.64	1.45
2	G	501	ONM	O4'-C4'	8.78	1.64	1.45
2	I	504	ONM	O4'-C4'	8.78	1.64	1.45
2	G	501	ONM	C6-C5	8.77	1.56	1.41
2	J	501	ONM	C3'-C4'	-8.74	1.29	1.52
2	E	501	ONM	C3'-C4'	-8.70	1.29	1.52
2	I	504	ONM	C6-C5	8.61	1.56	1.41
2	A	501	ONM	C4-N3	8.35	1.48	1.35
2	A	501	ONM	O4'-C4'	8.26	1.63	1.45
2	I	504	ONM	C6-N1	8.26	1.47	1.33
2	F	501	ONM	O4'-C4'	8.21	1.63	1.45
2	E	501	ONM	C4-N3	8.20	1.48	1.35
2	G	501	ONM	C6-N1	8.19	1.47	1.33
2	E	501	ONM	O4'-C4'	8.14	1.63	1.45
2	J	501	ONM	C6-N1	7.81	1.46	1.33
2	C	501	ONM	O4'-C4'	7.75	1.62	1.45
2	D	501	ONM	O4'-C4'	7.75	1.62	1.45
2	K	501	ONM	O3'-CA	7.71	1.50	1.34
2	J	501	ONM	O4'-C1'	7.68	1.51	1.41
2	G	501	ONM	C2'-C3'	7.63	1.70	1.52
2	F	501	ONM	C6-C5	7.60	1.54	1.41
2	H	504	ONM	O4'-C1'	7.59	1.51	1.41
2	E	501	ONM	O3'-CA	7.53	1.49	1.34
2	F	501	ONM	C4-N3	7.53	1.47	1.35
2	B	501	ONM	C6-C5	7.48	1.54	1.41
2	K	501	ONM	C2'-C3'	7.43	1.69	1.52
2	I	504	ONM	C2-N2	7.41	1.48	1.33
2	G	501	ONM	O4'-C1'	7.23	1.51	1.41
2	D	501	ONM	C4-N3	7.23	1.47	1.35
2	B	501	ONM	O4'-C4'	7.21	1.61	1.45
2	B	501	ONM	C4-N3	7.18	1.46	1.35
2	F	501	ONM	C2-N2	7.15	1.48	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	501	ONM	C2'-C3'	7.07	1.68	1.52
2	K	501	ONM	O4'-C1'	7.06	1.50	1.41
2	C	501	ONM	C4-N3	7.04	1.46	1.35
2	J	501	ONM	C2-N2	7.02	1.47	1.33
2	H	504	ONM	C2'-C3'	6.92	1.68	1.52
2	E	501	ONM	O4'-C1'	6.91	1.50	1.41
2	C	501	ONM	C6-C5	6.91	1.53	1.41
2	G	501	ONM	C2-N2	6.81	1.47	1.33
2	H	504	ONM	C2-N1	6.78	1.47	1.35
2	F	501	ONM	O4'-C1'	6.68	1.50	1.41
2	H	504	ONM	C6-C5	6.67	1.52	1.41
2	K	501	ONM	C6-N1	6.61	1.44	1.33
2	I	504	ONM	O3'-CA	6.58	1.48	1.34
2	K	501	ONM	C2-N2	6.35	1.46	1.33
2	E	501	ONM	C6-C5	6.32	1.52	1.41
2	D	501	ONM	C6-C5	6.30	1.52	1.41
2	F	501	ONM	C6-N1	6.28	1.44	1.33
2	J	501	ONM	O3'-CA	6.27	1.47	1.34
2	E	501	ONM	C6-N1	6.22	1.43	1.33
2	F	501	ONM	O3'-CA	6.16	1.47	1.34
2	J	501	ONM	C2-N1	6.15	1.46	1.35
2	H	504	ONM	C2-N2	6.13	1.46	1.33
2	I	504	ONM	C2-N1	6.11	1.46	1.35
2	H	504	ONM	O3'-CA	6.08	1.47	1.34
2	I	504	ONM	O4'-C1'	6.00	1.49	1.41
2	C	501	ONM	C2-N2	5.96	1.45	1.33
2	G	501	ONM	C2-N1	5.94	1.46	1.35
2	B	501	ONM	C2-N2	5.87	1.45	1.33
2	K	501	ONM	O3'-C3'	5.85	1.53	1.44
2	B	501	ONM	O4'-C1'	5.82	1.49	1.41
2	D	501	ONM	C6-N1	5.81	1.43	1.33
2	B	501	ONM	C6-N1	5.78	1.43	1.33
2	E	501	ONM	C2-N2	5.77	1.45	1.33
2	A	501	ONM	C2-N2	5.74	1.45	1.33
2	F	501	ONM	C2'-C3'	5.72	1.65	1.52
2	E	501	ONM	CA1-CA	5.62	1.62	1.50
2	C	501	ONM	C6-N1	5.60	1.42	1.33
2	K	501	ONM	CA7-NA1	5.59	1.54	1.45
2	A	501	ONM	O4'-C1'	5.58	1.48	1.41
2	F	501	ONM	C2-N1	5.54	1.45	1.35
2	J	501	ONM	O3'-C3'	5.39	1.53	1.44
2	A	501	ONM	C6-N1	5.36	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	ONM	O4'-C1'	5.29	1.48	1.41
2	I	504	ONM	C2'-C3'	5.28	1.64	1.52
2	G	501	ONM	O3'-CA	5.26	1.45	1.34
2	E	501	ONM	CA6-NA1	5.16	1.47	1.37
2	D	501	ONM	C2-N2	5.13	1.44	1.33
2	K	501	ONM	C2-N1	5.10	1.44	1.35
2	E	501	ONM	C2'-C3'	5.03	1.64	1.52
2	D	501	ONM	C2'-C3'	5.02	1.64	1.52
2	K	501	ONM	CA6-NA1	4.92	1.46	1.37
2	C	501	ONM	O4'-C1'	4.87	1.47	1.41
2	E	501	ONM	C2-N1	4.85	1.44	1.35
2	A	501	ONM	C2'-C3'	4.85	1.63	1.52
2	B	501	ONM	O3'-CA	4.83	1.44	1.34
2	I	504	ONM	CA6-NA1	4.80	1.46	1.37
2	G	501	ONM	CA6-NA1	4.78	1.46	1.37
2	C	501	ONM	C2'-C3'	4.74	1.63	1.52
2	A	501	ONM	C2-N1	4.68	1.43	1.35
2	E	501	ONM	O3'-C3'	4.51	1.51	1.44
2	I	504	ONM	CA1-CA	4.47	1.59	1.50
2	G	501	ONM	CA1-CA	4.44	1.59	1.50
2	J	501	ONM	CA1-CA	4.43	1.59	1.50
2	D	501	ONM	C2-N1	4.40	1.43	1.35
2	H	504	ONM	CA1-CA	4.37	1.59	1.50
2	J	501	ONM	CA6-NA1	4.32	1.45	1.37
2	C	501	ONM	O3'-CA	4.31	1.43	1.34
2	K	501	ONM	CA1-CA	4.28	1.59	1.50
2	C	501	ONM	C2-N1	4.28	1.43	1.35
2	B	501	ONM	C2'-C3'	4.18	1.62	1.52
2	B	501	ONM	C2-N1	4.18	1.42	1.35
2	B	501	ONM	CA6-NA1	3.99	1.45	1.37
2	F	501	ONM	CA1-CA	3.98	1.58	1.50
2	A	501	ONM	O3'-CA	3.88	1.42	1.34
2	H	504	ONM	CA6-NA1	3.88	1.44	1.37
2	I	504	ONM	O3'-C3'	3.86	1.50	1.44
2	E	501	ONM	CA7-NA1	3.82	1.51	1.45
2	A	501	ONM	CA1-CA	3.69	1.58	1.50
2	H	504	ONM	O3'-C3'	3.67	1.50	1.44
2	F	501	ONM	CA6-NA1	3.52	1.44	1.37
2	G	501	ONM	CA7-NA1	3.48	1.51	1.45
2	F	501	ONM	O3'-C3'	3.46	1.50	1.44
2	D	501	ONM	O3'-CA	3.44	1.41	1.34
2	C	501	ONM	CA1-CA	3.34	1.57	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	ONM	CA6-NA1	3.33	1.43	1.37
2	D	501	ONM	C5-C4	-3.27	1.32	1.40
2	B	501	ONM	CA1-CA	3.24	1.57	1.50
2	K	501	ONM	C2-N3	3.18	1.49	1.34
2	D	501	ONM	CA6-NA1	3.14	1.43	1.37
2	D	501	ONM	CA1-CA	3.13	1.56	1.50
2	I	504	ONM	CA7-NA1	3.03	1.50	1.45
2	H	504	ONM	PA-O5'	2.99	1.71	1.59
2	I	504	ONM	C2-N3	2.94	1.48	1.34
2	C	501	ONM	CA6-NA1	2.92	1.42	1.37
2	G	501	ONM	C2-N3	2.92	1.48	1.34
2	F	501	ONM	CA7-NA1	2.90	1.50	1.45
2	G	501	ONM	O3'-C3'	2.90	1.49	1.44
2	C	501	ONM	C5-C4	-2.71	1.33	1.40
2	E	501	ONM	C5-C4	-2.66	1.33	1.40
2	B	501	ONM	CA7-NA1	2.63	1.49	1.45
2	J	501	ONM	C2-N3	2.63	1.47	1.34
2	F	501	ONM	PA-O5'	2.55	1.69	1.59
2	J	501	ONM	CA7-NA1	2.54	1.49	1.45
2	A	501	ONM	C2-N3	2.51	1.46	1.34
2	C	501	ONM	CA7-NA1	2.48	1.49	1.45
2	H	504	ONM	CA7-NA1	2.46	1.49	1.45
2	B	501	ONM	C5-C4	-2.44	1.34	1.40
2	F	501	ONM	C5-C4	-2.42	1.34	1.40
2	J	501	ONM	PA-O5'	2.42	1.69	1.59
2	E	501	ONM	PA-O5'	2.38	1.68	1.59
2	K	501	ONM	PA-O5'	2.36	1.68	1.59
2	I	504	ONM	C8-N7	2.32	1.38	1.34
2	D	501	ONM	CA7-NA1	2.31	1.49	1.45
2	H	504	ONM	C2-N3	2.27	1.45	1.34
2	C	501	ONM	O3'-C3'	2.27	1.48	1.44
2	B	501	ONM	C2-N3	2.24	1.45	1.34
2	F	501	ONM	C2-N3	2.21	1.45	1.34
2	D	501	ONM	C2-N3	2.20	1.45	1.34
2	I	504	ONM	CA1-CA6	2.14	1.44	1.41
2	B	501	ONM	O3'-C3'	2.13	1.48	1.44
2	C	501	ONM	O6-C6	-2.13	1.19	1.24
2	K	501	ONM	C8-N7	2.12	1.38	1.34
2	E	501	ONM	C2-N3	2.10	1.44	1.34
2	E	501	ONM	O6-C6	-2.09	1.19	1.24
2	I	504	ONM	PA-O5'	2.08	1.67	1.59
2	D	501	ONM	O6-C6	-2.08	1.19	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	ONM	CA7-NA1	2.08	1.48	1.45
2	D	501	ONM	CA1-CA6	-2.07	1.37	1.41
2	F	501	ONM	O6-C6	-2.06	1.19	1.24
2	G	501	ONM	CA1-CA6	2.05	1.44	1.41
2	G	501	ONM	CA2-CA1	2.05	1.43	1.39
2	K	501	ONM	O6-C6	-2.03	1.19	1.24
2	G	501	ONM	PA-O5'	2.03	1.67	1.59

All (161) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	501	ONM	C1'-N9-C4	15.03	153.05	126.64
2	B	501	ONM	C1'-N9-C4	14.38	151.91	126.64
2	A	501	ONM	C1'-N9-C4	14.33	151.81	126.64
2	C	501	ONM	C1'-N9-C4	12.20	148.07	126.64
2	H	504	ONM	C1'-N9-C4	12.04	147.79	126.64
2	K	501	ONM	C1'-N9-C4	11.95	147.64	126.64
2	J	501	ONM	C1'-N9-C4	11.22	146.36	126.64
2	I	504	ONM	C1'-N9-C4	10.42	144.96	126.64
2	G	501	ONM	C1'-N9-C4	9.95	144.13	126.64
2	F	501	ONM	C1'-N9-C4	9.79	143.84	126.64
2	E	501	ONM	C1'-N9-C4	9.40	143.16	126.64
2	H	504	ONM	O3'-CA-CA1	8.81	125.42	111.69
2	D	501	ONM	PB-O1B-PG	-8.68	103.03	132.83
2	F	501	ONM	N3-C2-N1	-7.22	117.60	127.22
2	J	501	ONM	N3-C2-N1	-7.13	117.71	127.22
2	A	501	ONM	PB-O1B-PG	-6.81	109.47	132.83
2	I	504	ONM	N3-C2-N1	-6.63	118.38	127.22
2	G	501	ONM	N3-C2-N1	-6.42	118.66	127.22
2	G	501	ONM	C3'-O3'-CA	-6.13	107.40	117.21
2	J	501	ONM	PB-O1B-PG	-6.00	112.23	132.83
2	H	504	ONM	CA6-CA1-CA	-5.84	113.03	122.20
2	K	501	ONM	CA7-NA1-CA6	-5.79	113.37	122.44
2	E	501	ONM	N3-C2-N1	-5.56	119.80	127.22
2	J	501	ONM	PB-O1A-PA	-5.53	113.85	132.83
2	H	504	ONM	N3-C2-N1	-5.50	119.88	127.22
2	C	501	ONM	N3-C2-N1	-5.45	119.95	127.22
2	H	504	ONM	N2-C2-N1	5.31	125.52	117.25
2	I	504	ONM	C6-C5-C4	-5.28	115.75	120.80
2	F	501	ONM	C6-C5-C4	-5.27	115.77	120.80
2	J	501	ONM	C6-C5-C4	-5.21	115.83	120.80
2	J	501	ONM	O3'-CA-CA1	5.15	119.72	111.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	501	ONM	O4'-C1'-C2'	-4.86	99.83	106.93
2	B	501	ONM	N3-C2-N1	-4.82	120.79	127.22
2	J	501	ONM	N2-C2-N1	4.67	124.52	117.25
2	F	501	ONM	C3'-O3'-CA	4.59	124.57	117.21
2	K	501	ONM	N3-C2-N1	-4.58	121.12	127.22
2	J	501	ONM	C2-N3-C4	4.48	120.47	115.36
2	F	501	ONM	N2-C2-N1	4.42	124.12	117.25
2	A	501	ONM	O3'-CA-CA1	4.28	118.36	111.69
2	A	501	ONM	O4'-C1'-C2'	-4.26	100.69	106.93
2	F	501	ONM	PB-O1A-PA	-4.23	118.32	132.83
2	H	504	ONM	C3'-C2'-C1'	4.19	109.17	99.89
2	E	501	ONM	PB-O1B-PG	-4.18	118.49	132.83
2	K	501	ONM	O4'-C1'-C2'	-4.16	100.84	106.93
2	K	501	ONM	O3'-C3'-C2'	4.16	121.91	110.07
2	G	501	ONM	C6-N1-C2	4.12	122.48	115.93
2	K	501	ONM	O3G-PG-O1B	4.12	118.46	104.64
2	F	501	ONM	C6-N1-C2	3.98	122.25	115.93
2	C	501	ONM	N2-C2-N1	3.96	123.41	117.25
2	F	501	ONM	PB-O1B-PG	-3.92	119.37	132.83
2	H	504	ONM	CA1-CA6-NA1	-3.87	116.76	121.25
2	B	501	ONM	O3'-CA-CA1	3.81	117.62	111.69
2	G	501	ONM	C3'-C2'-C1'	-3.80	91.48	99.89
2	H	504	ONM	CA2-CA1-CA	3.77	126.40	118.66
2	A	501	ONM	C5-C6-N1	-3.77	118.28	123.43
2	G	501	ONM	C5-C6-N1	-3.73	118.33	123.43
2	H	504	ONM	PB-O1B-PG	-3.73	120.04	132.83
2	K	501	ONM	O3'-CA-CA1	3.69	117.44	111.69
2	I	504	ONM	O3'-CA-CA1	3.66	117.39	111.69
2	E	501	ONM	N2-C2-N1	3.63	122.90	117.25
2	B	501	ONM	C5-C6-N1	-3.59	118.52	123.43
2	H	504	ONM	C5-C6-N1	-3.55	118.58	123.43
2	G	501	ONM	O2'-C2'-C3'	3.55	121.24	111.17
2	E	501	ONM	C6-C5-C4	-3.54	117.42	120.80
2	J	501	ONM	C3'-C2'-C1'	3.53	107.70	99.89
2	J	501	ONM	O1G-PG-O1B	3.52	116.45	104.64
2	H	504	ONM	O5'-C5'-C4'	3.52	121.09	108.99
2	A	501	ONM	O3'-C3'-C4'	-3.51	100.82	109.56
2	C	501	ONM	C5-C6-N1	-3.51	118.63	123.43
2	K	501	ONM	C3'-O3'-CA	3.49	122.81	117.21
2	D	501	ONM	O3'-CA-CA1	3.49	117.12	111.69
2	E	501	ONM	C6-N1-C2	3.47	121.44	115.93
2	K	501	ONM	C2-N3-C4	3.39	119.23	115.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	501	ONM	O3'-CA-CA1	3.38	116.96	111.69
2	E	501	ONM	C5-C6-N1	-3.37	118.82	123.43
2	G	501	ONM	O3'-C3'-C2'	3.36	119.64	110.07
2	F	501	ONM	C3'-C2'-C1'	3.36	107.33	99.89
2	I	504	ONM	C6-N1-C2	3.34	121.23	115.93
2	H	504	ONM	C6-C5-C4	-3.32	117.63	120.80
2	J	501	ONM	C6-N1-C2	3.32	121.20	115.93
2	A	501	ONM	CA7-NA1-CA6	-3.26	117.33	122.44
2	K	501	ONM	C6-C5-C4	-3.26	117.69	120.80
2	H	504	ONM	O3'-C3'-C2'	3.19	119.14	110.07
2	H	504	ONM	C6-N1-C2	3.18	120.98	115.93
2	C	501	ONM	PB-O1A-PA	-3.17	121.93	132.83
2	I	504	ONM	CA1-CA6-NA1	3.16	124.92	121.25
2	A	501	ONM	C4-C5-N7	-3.16	106.11	109.40
2	B	501	ONM	O5'-C5'-C4'	-3.14	98.20	108.99
2	I	504	ONM	C2-N3-C4	3.13	118.93	115.36
2	G	501	ONM	C5'-C4'-C3'	-3.09	104.15	114.40
2	F	501	ONM	C2-N3-C4	3.09	118.88	115.36
2	C	501	ONM	C6-N1-C2	3.08	120.81	115.93
2	G	501	ONM	O3G-PG-O1B	3.07	114.94	104.64
2	D	501	ONM	N3-C2-N1	-3.07	123.12	127.22
2	F	501	ONM	O3'-CA-CA1	3.04	116.42	111.69
2	F	501	ONM	C5-C6-N1	-2.98	119.35	123.43
2	A	501	ONM	N3-C2-N1	-2.96	123.28	127.22
2	K	501	ONM	C5'-C4'-C3'	-2.94	104.67	114.40
2	B	501	ONM	C2-N3-C4	2.92	118.69	115.36
2	J	501	ONM	O5'-PA-O3A	-2.92	97.66	109.07
2	C	501	ONM	C2-N3-C4	2.92	118.69	115.36
2	H	504	ONM	C2'-C3'-C4'	2.90	108.36	103.22
2	D	501	ONM	C2-N3-C4	2.89	118.66	115.36
2	G	501	ONM	O3'-C3'-C4'	-2.89	102.36	109.56
2	J	501	ONM	C3'-O3'-CA	2.85	121.77	117.21
2	I	504	ONM	O5'-C5'-C4'	2.84	118.78	108.99
2	I	504	ONM	PB-O1A-PA	-2.82	123.15	132.83
2	K	501	ONM	CA5-CA6-NA1	-2.81	117.71	121.23
2	I	504	ONM	CA5-CA6-NA1	-2.78	117.75	121.23
2	G	501	ONM	C6-C5-C4	-2.76	118.17	120.80
2	E	501	ONM	C3'-C2'-C1'	-2.75	93.79	99.89
2	G	501	ONM	CA2-CA1-CA6	2.73	121.91	118.81
2	I	504	ONM	CA2-CA1-CA6	2.72	121.89	118.81
2	G	501	ONM	C2'-C3'-C4'	2.70	108.02	103.22
2	C	501	ONM	PB-O1B-PG	-2.69	123.58	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	501	ONM	C6-N1-C2	2.68	120.19	115.93
2	G	501	ONM	C2-N3-C4	2.66	118.39	115.36
2	C	501	ONM	C4-C5-N7	-2.63	106.66	109.40
2	D	501	ONM	C5-C6-N1	-2.62	119.85	123.43
2	G	501	ONM	O3'-CA-CA1	2.60	115.74	111.69
2	I	504	ONM	CA7-NA1-CA6	-2.60	118.36	122.44
2	H	504	ONM	O3'-CA-OA	-2.56	119.35	123.53
2	J	501	ONM	O3'-C3'-C2'	2.56	117.35	110.07
2	I	504	ONM	N2-C2-N1	2.51	121.16	117.25
2	A	501	ONM	O3'-C3'-C2'	-2.49	103.00	110.07
2	G	501	ONM	PB-O1A-PA	-2.47	124.35	132.83
2	I	504	ONM	CA2-CA1-CA	-2.47	113.59	118.66
2	D	501	ONM	C3'-C2'-C1'	-2.46	94.43	99.89
2	C	501	ONM	CA7-NA1-CA6	-2.46	118.59	122.44
2	C	501	ONM	C6-C5-C4	-2.44	118.47	120.80
2	E	501	ONM	C3'-O3'-CA	2.41	121.07	117.21
2	A	501	ONM	C2'-C3'-C4'	2.41	107.49	103.22
2	C	501	ONM	C3'-C2'-C1'	2.39	105.18	99.89
2	E	501	ONM	O4'-C4'-C5'	-2.37	101.58	109.37
2	J	501	ONM	C4-C5-N7	-2.37	106.93	109.40
2	C	501	ONM	O3G-PG-O1B	2.36	112.56	104.64
2	I	504	ONM	O4'-C4'-C3'	2.36	109.93	104.87
2	H	504	ONM	C3'-O3'-CA	2.36	121.00	117.21
2	K	501	ONM	O3'-CA-OA	2.35	127.36	123.53
2	A	501	ONM	O3'-CA-OA	-2.34	119.71	123.53
2	A	501	ONM	C6-N1-C2	2.34	119.65	115.93
2	J	501	ONM	C5-C6-N1	-2.31	120.27	123.43
2	C	501	ONM	C5'-C4'-C3'	-2.31	106.74	114.40
2	F	501	ONM	CA1-CA6-NA1	-2.31	118.57	121.25
2	K	501	ONM	PB-O1A-PA	-2.29	124.98	132.83
2	F	501	ONM	O1G-PG-O1B	2.27	112.26	104.64
4	A	505	SO4	O4-S-O1	-2.26	97.52	109.31
2	I	504	ONM	O3'-C3'-C2'	2.26	116.49	110.07
2	F	501	ONM	CA7-NA1-CA6	-2.25	118.92	122.44
2	B	501	ONM	C3'-C2'-C1'	2.24	104.85	99.89
2	K	501	ONM	O2B-PB-O3B	-2.23	101.20	112.24
2	E	501	ONM	O3G-PG-O1B	2.22	112.07	104.64
2	B	501	ONM	PB-O1B-PG	-2.16	125.42	132.83
2	K	501	ONM	O2'-C2'-C3'	2.14	117.25	111.17
2	K	501	ONM	N2-C2-N3	2.14	121.28	117.79
2	G	501	ONM	N2-C2-N3	2.10	121.22	117.79
2	D	501	ONM	O3'-CA-OA	-2.08	120.13	123.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	501	ONM	CA6-CA1-CA	-2.08	118.94	122.20
2	D	501	ONM	O3'-C3'-C2'	-2.08	104.16	110.07
2	I	504	ONM	C5-C6-N1	-2.07	120.61	123.43
2	J	501	ONM	CA2-CA1-CA6	2.04	121.12	118.81

There are no chirality outliers.

All (70) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	501	ONM	C5'-O5'-PA-O3A
2	C	501	ONM	C5'-O5'-PA-O2A
2	H	504	ONM	CA1-CA-O3'-C3'
2	H	504	ONM	OA-CA-O3'-C3'
2	H	504	ONM	C2'-C3'-O3'-CA
2	H	504	ONM	C3'-C4'-C5'-O5'
2	H	504	ONM	C5'-O5'-PA-O3A
2	J	501	ONM	CA1-CA-O3'-C3'
2	J	501	ONM	OA-CA-O3'-C3'
2	J	501	ONM	C5'-O5'-PA-O1A
2	A	501	ONM	PB-O1B-PG-O3G
2	F	501	ONM	PB-O1B-PG-O1G
2	K	501	ONM	CA5-CA6-NA1-CA7
2	K	501	ONM	CA1-CA6-NA1-CA7
2	K	501	ONM	PB-O1A-PA-O5'
2	D	501	ONM	C5'-O5'-PA-O2A
2	D	501	ONM	C5'-O5'-PA-O1A
2	E	501	ONM	O4'-C4'-C5'-O5'
2	E	501	ONM	C5'-O5'-PA-O2A
2	E	501	ONM	C5'-O5'-PA-O1A
2	E	501	ONM	PB-O1B-PG-O3G
2	G	501	ONM	PB-O1B-PG-O3G
2	C	501	ONM	O4'-C4'-C5'-O5'
2	J	501	ONM	C3'-C4'-C5'-O5'
2	J	501	ONM	O4'-C4'-C5'-O5'
2	D	501	ONM	O4'-C4'-C5'-O5'
2	C	501	ONM	C3'-C4'-C5'-O5'
2	D	501	ONM	C3'-C4'-C5'-O5'
2	E	501	ONM	C3'-C4'-C5'-O5'
2	G	501	ONM	CA5-CA6-NA1-CA7
2	E	501	ONM	OA-CA-O3'-C3'
2	E	501	ONM	CA1-CA-O3'-C3'
2	G	501	ONM	CA1-CA6-NA1-CA7

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Mol	Chain	Res	Type	Atoms
2	B	501	ONM	CA5-CA6-NA1-CA7
2	H	504	ONM	O4'-C4'-C5'-O5'
2	I	504	ONM	CA1-CA6-NA1-CA7
2	D	501	ONM	CA1-CA6-NA1-CA7
2	B	501	ONM	CA1-CA6-NA1-CA7
2	G	501	ONM	PB-O1A-PA-O5'
2	H	504	ONM	PB-O1B-PG-O1G
2	J	501	ONM	PB-O1B-PG-O1G
2	B	501	ONM	PB-O1B-PG-O1G
2	C	501	ONM	C5'-O5'-PA-O1A
2	I	504	ONM	PA-O1A-PB-O3B
2	F	501	ONM	PB-O1A-PA-O2A
2	E	501	ONM	PA-O1A-PB-O3B
2	G	501	ONM	C4'-C5'-O5'-PA
2	H	504	ONM	C5'-O5'-PA-O2A
2	D	501	ONM	C5'-O5'-PA-O3A
2	E	501	ONM	C5'-O5'-PA-O3A
2	G	501	ONM	C5'-O5'-PA-O3A
2	I	504	ONM	CA5-CA6-NA1-CA7
2	D	501	ONM	CA5-CA6-NA1-CA7
2	C	501	ONM	PB-O1B-PG-O2G
2	G	501	ONM	PB-O1B-PG-O2G
2	B	501	ONM	PB-O1B-PG-O2G
2	K	501	ONM	C4'-C5'-O5'-PA
2	A	501	ONM	PB-O1A-PA-O3A
2	F	501	ONM	OA-CA-O3'-C3'
2	A	501	ONM	PB-O1B-PG-O2G
2	C	501	ONM	PB-O1B-PG-O3G
2	C	501	ONM	PB-O1B-PG-O1G
2	A	501	ONM	PB-O1B-PG-O1G
2	B	501	ONM	PB-O1B-PG-O3G
2	H	504	ONM	C5'-O5'-PA-O1A
2	B	501	ONM	O4'-C4'-C5'-O5'
2	A	501	ONM	PA-O1A-PB-O2B
2	B	501	ONM	PA-O1A-PB-O2B
2	K	501	ONM	C5'-O5'-PA-O3A
2	F	501	ONM	O4'-C4'-C5'-O5'

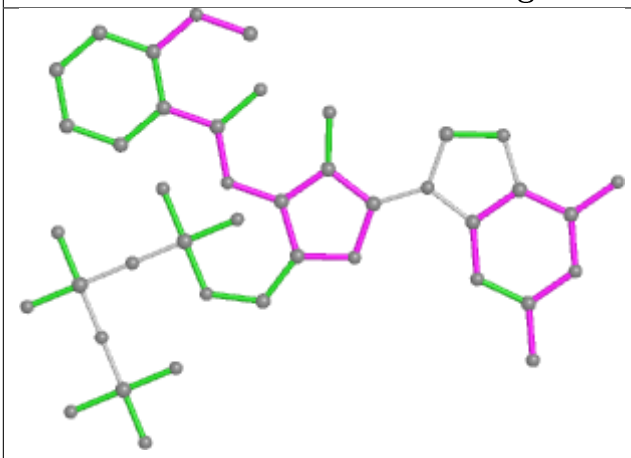
There are no ring outliers.

15 monomers are involved in 70 short contacts:

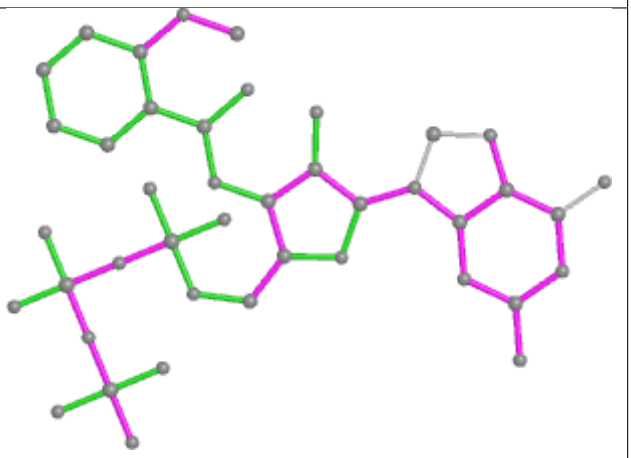
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	501	ONM	1	0
4	E	505	SO4	1	0
2	H	504	ONM	6	0
2	J	501	ONM	13	0
2	I	504	ONM	21	0
2	A	501	ONM	2	0
2	F	501	ONM	6	0
2	K	501	ONM	5	0
4	H	501	SO4	1	0
2	D	501	ONM	2	0
4	D	504	SO4	1	0
2	E	501	ONM	3	0
2	G	501	ONM	5	0
4	E	504	SO4	2	0
2	B	501	ONM	1	0

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

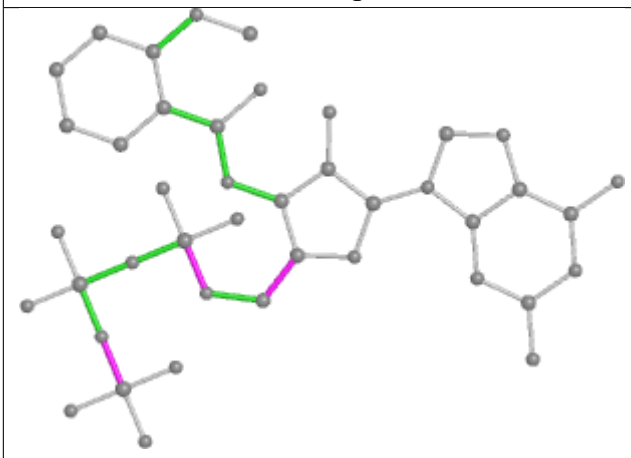
Ligand ONM C 501



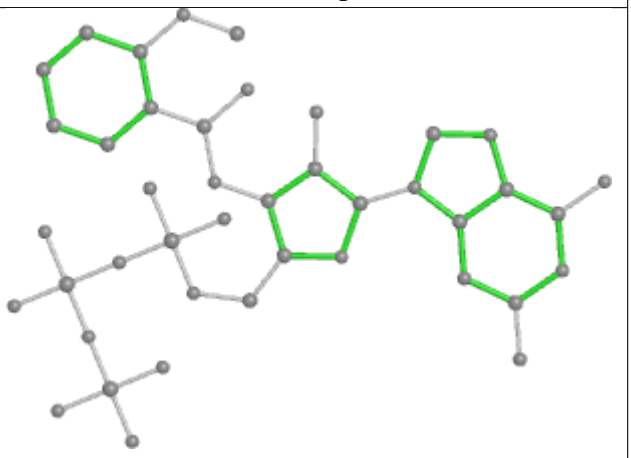
Bond lengths



Bond angles

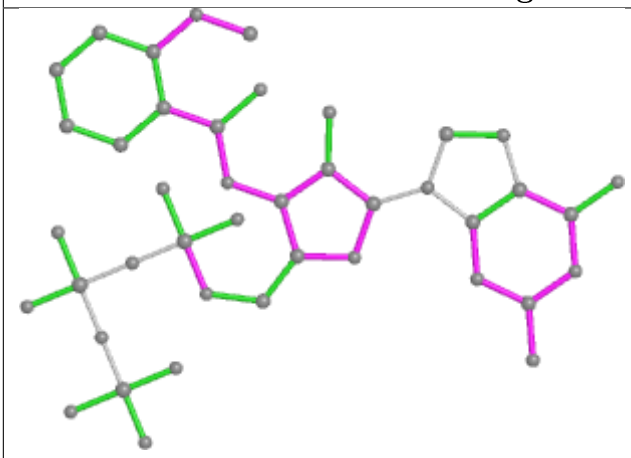


Torsions

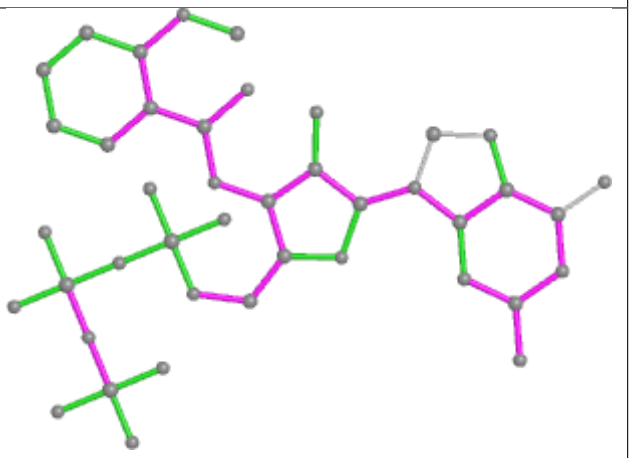


Rings

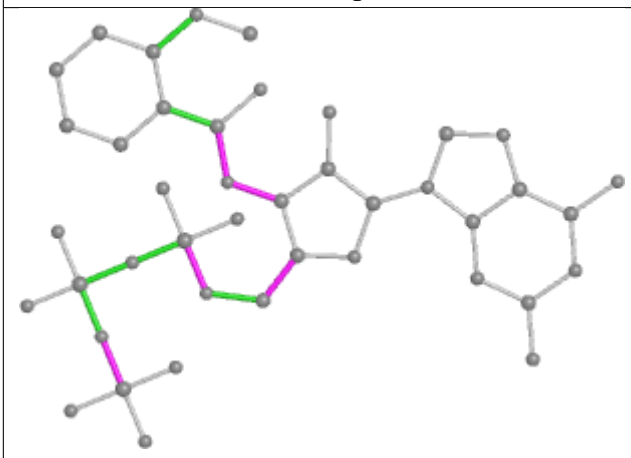
Ligand ONM H 504



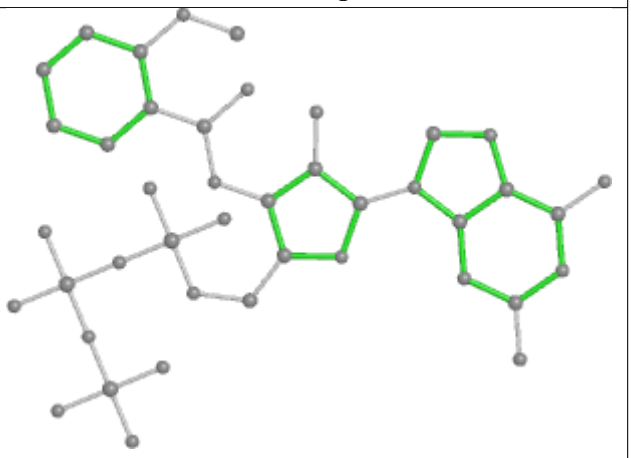
Bond lengths



Bond angles

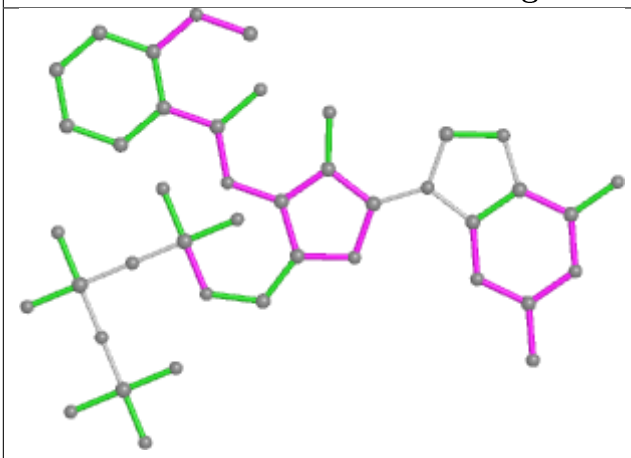


Torsions

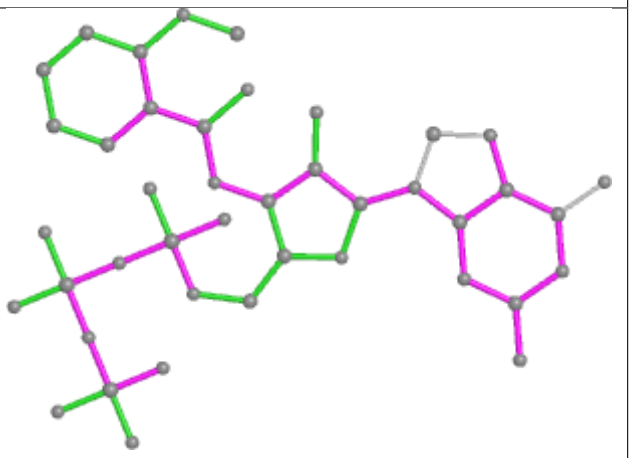


Rings

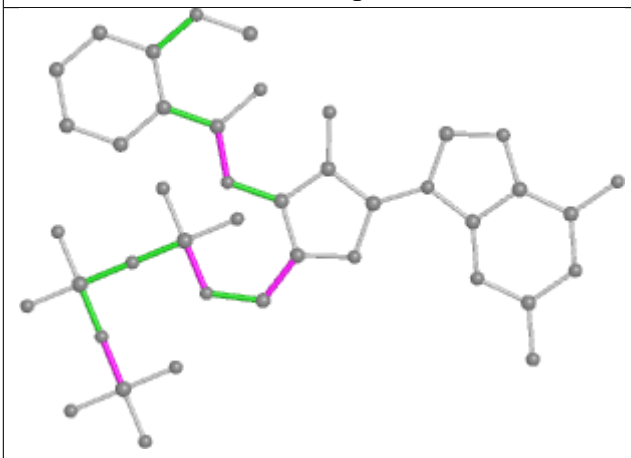
Ligand ONM J 501



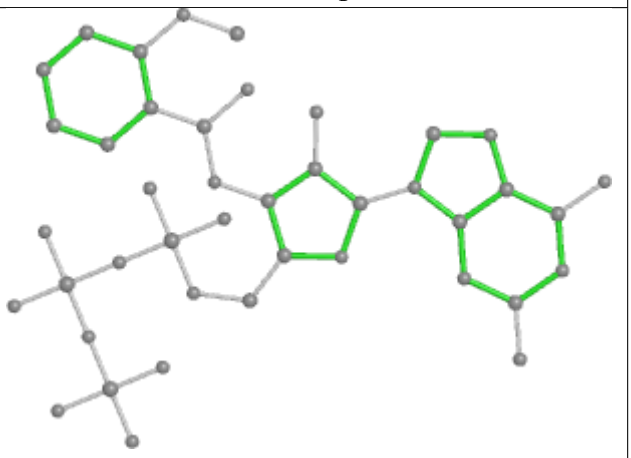
Bond lengths



Bond angles

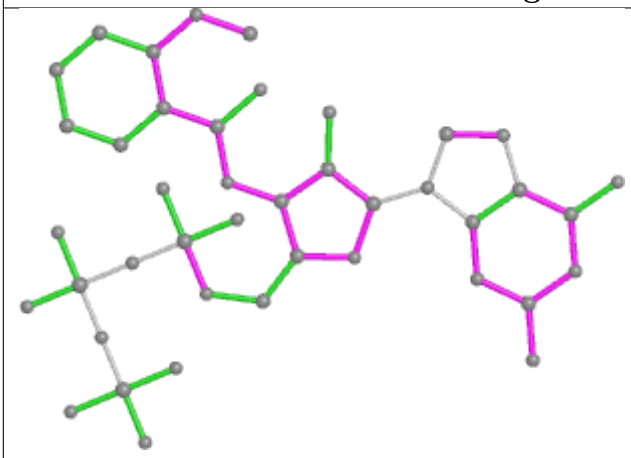


Torsions

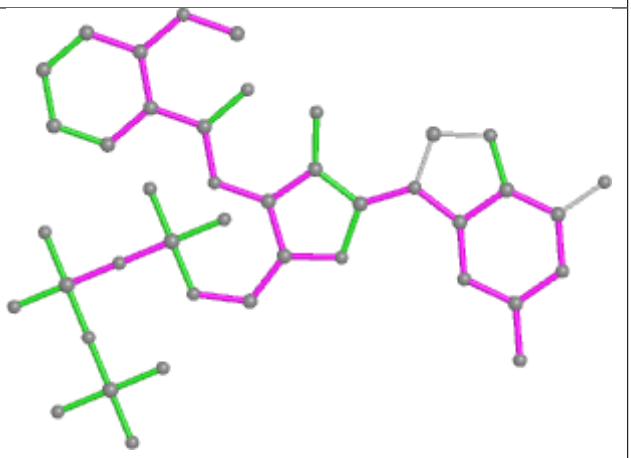


Rings

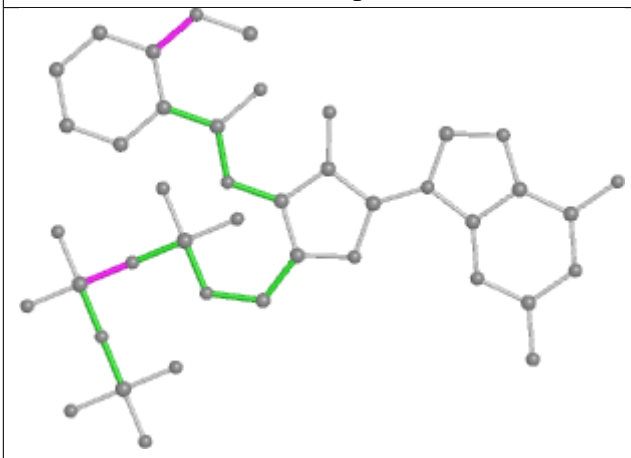
Ligand ONM I 504



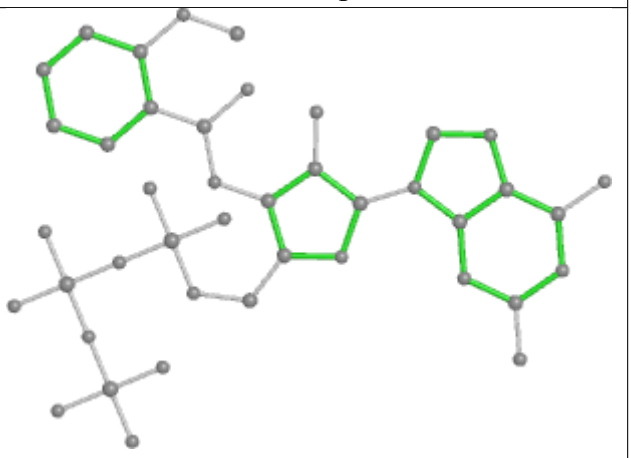
Bond lengths



Bond angles

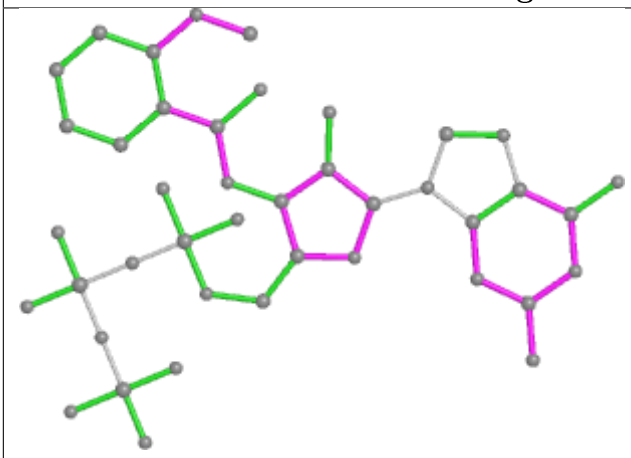


Torsions

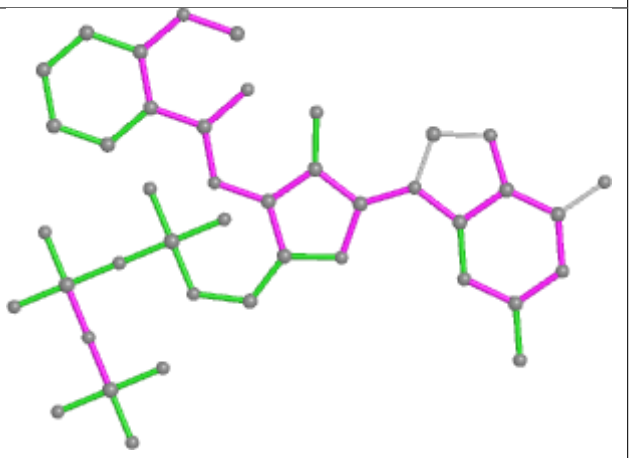


Rings

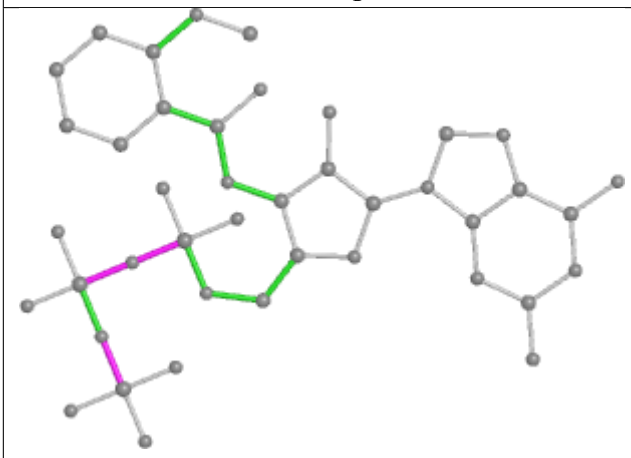
Ligand ONM A 501



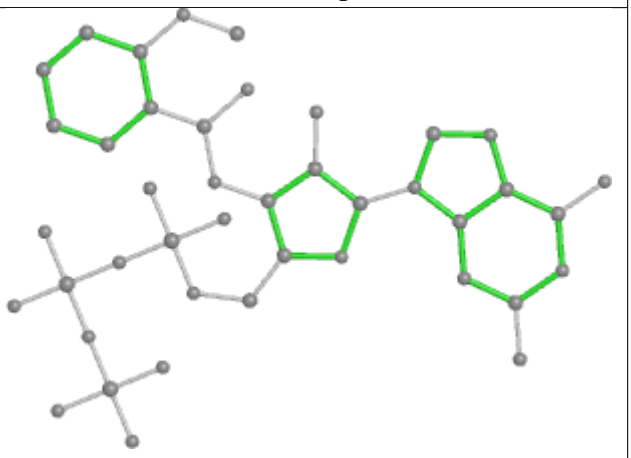
Bond lengths



Bond angles

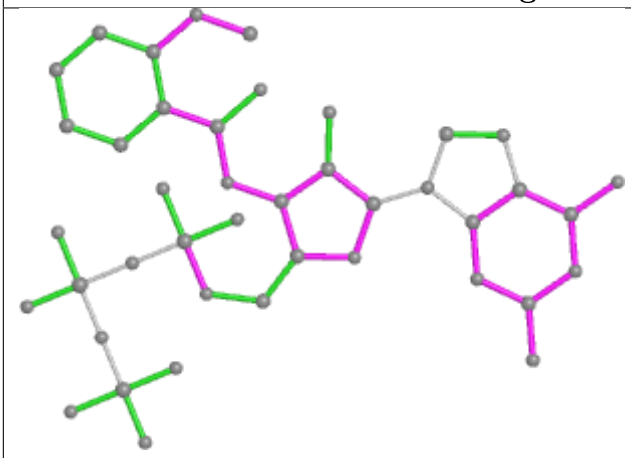


Torsions

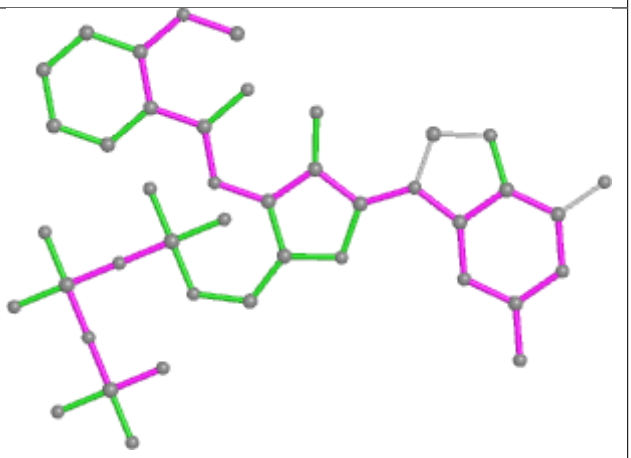


Rings

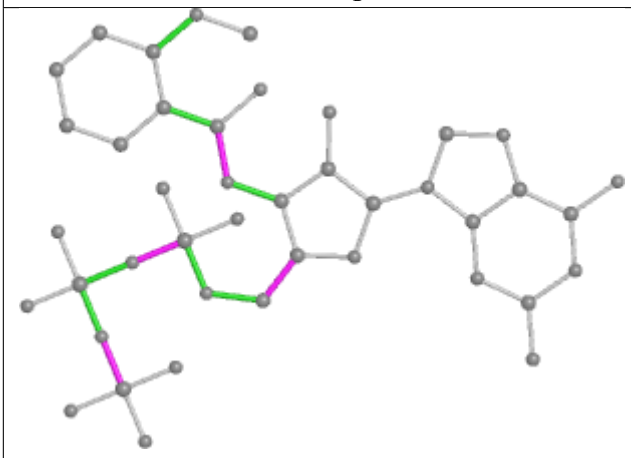
Ligand ONM F 501



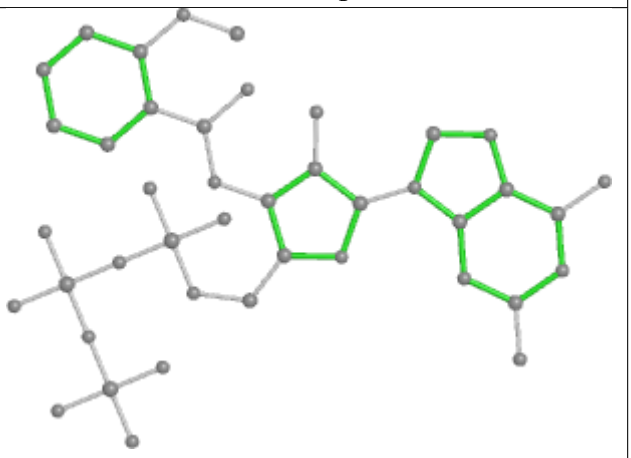
Bond lengths



Bond angles

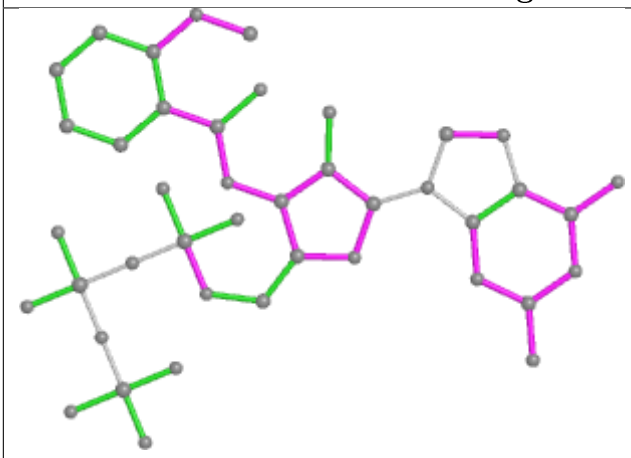


Torsions

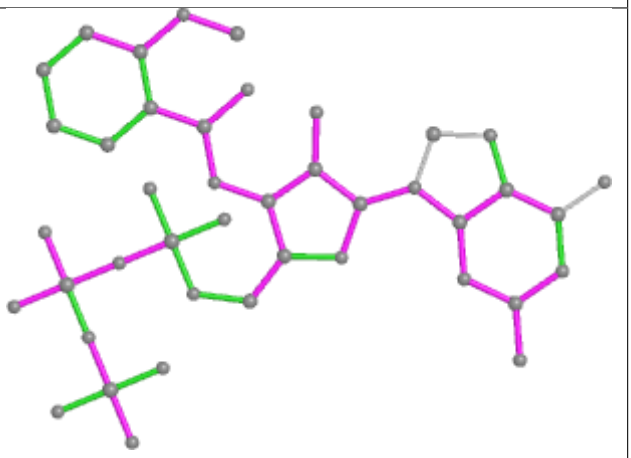


Rings

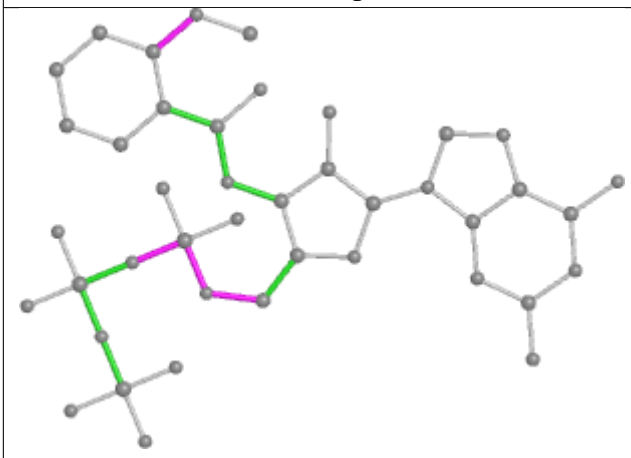
Ligand ONM K 501



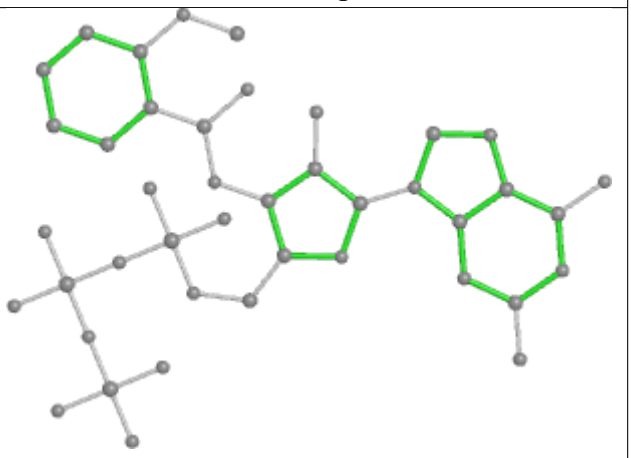
Bond lengths



Bond angles

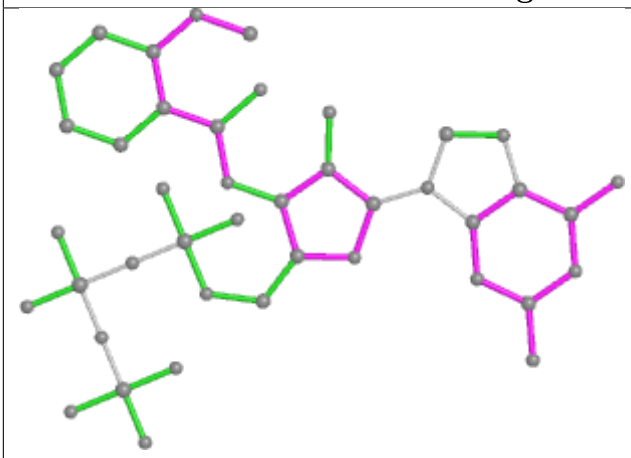


Torsions

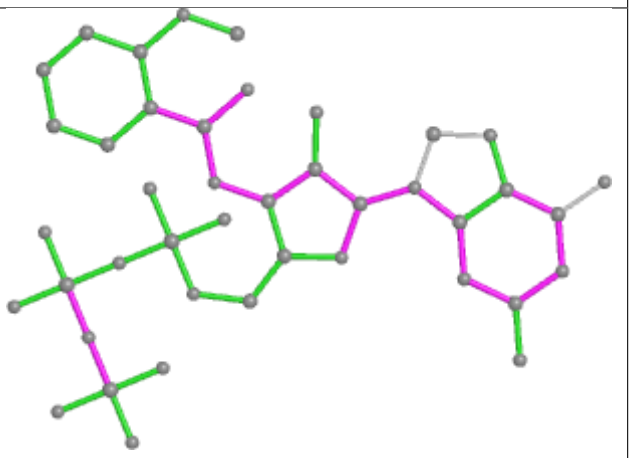


Rings

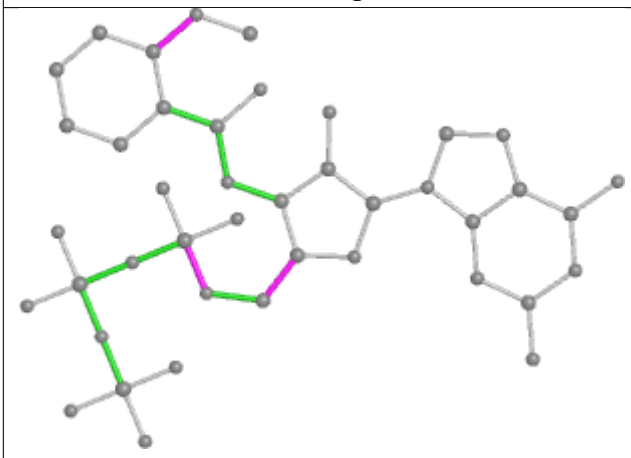
Ligand ONM D 501



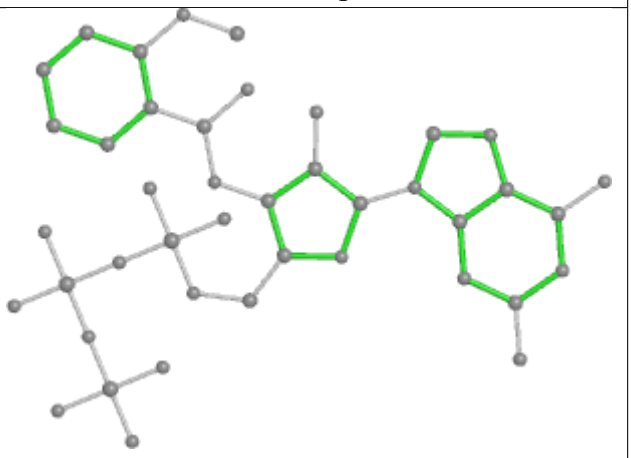
Bond lengths



Bond angles

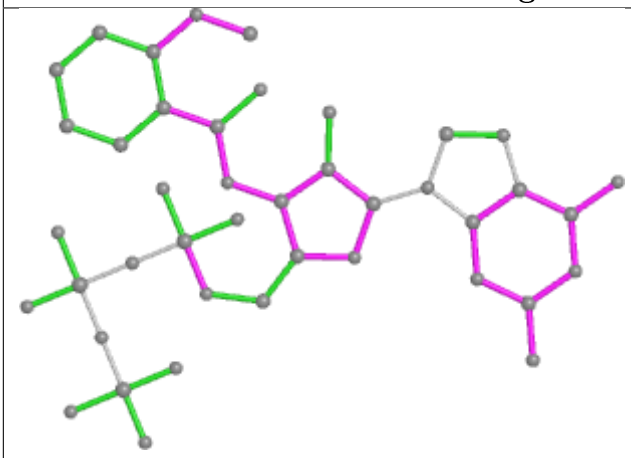


Torsions

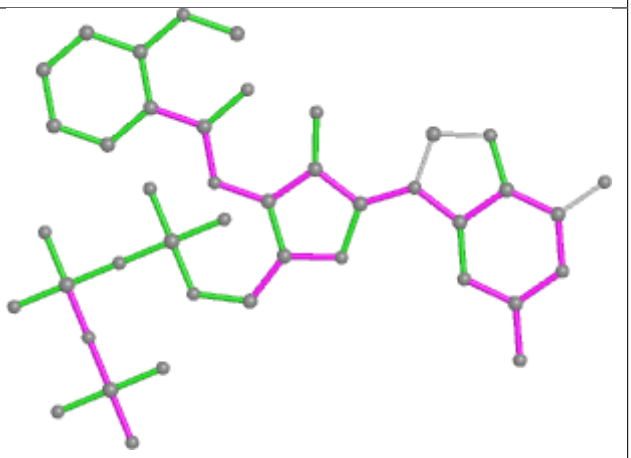


Rings

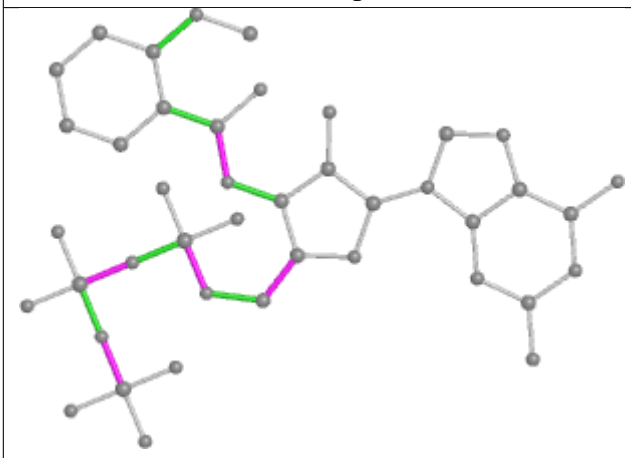
Ligand ONM E 501



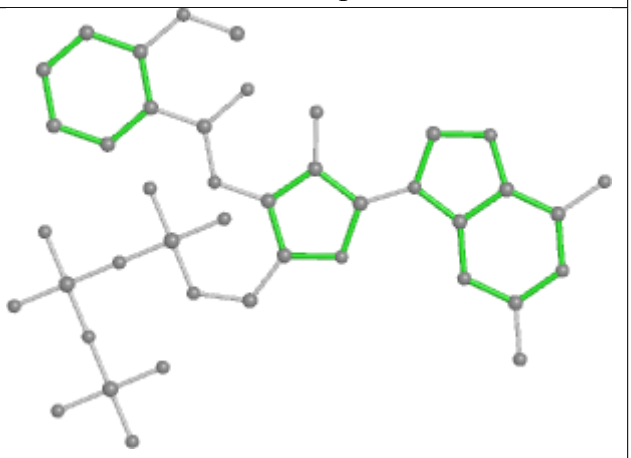
Bond lengths



Bond angles

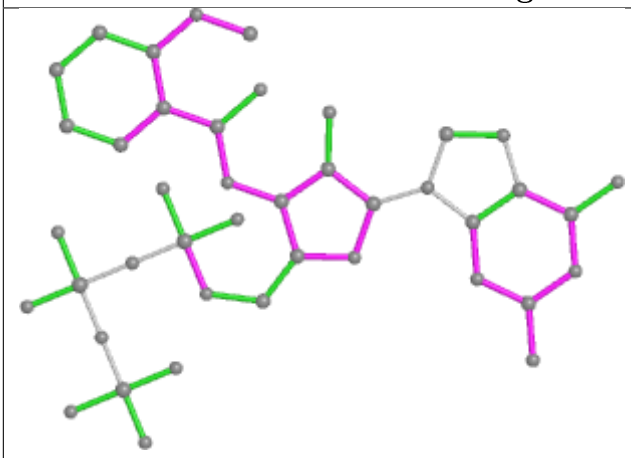


Torsions

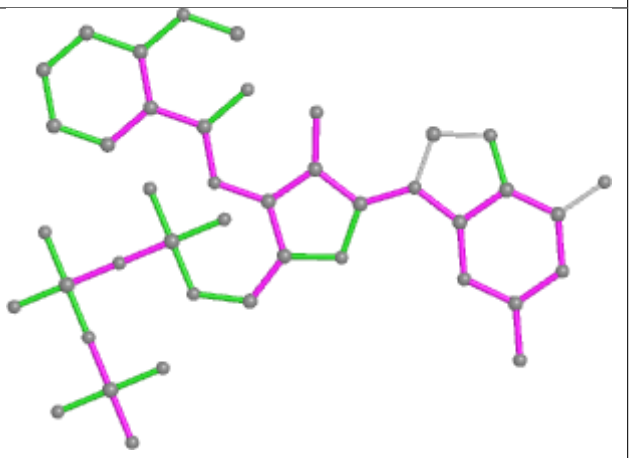


Rings

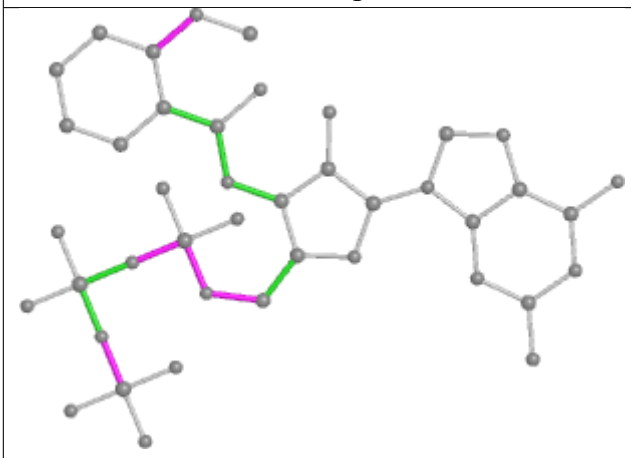
Ligand ONM G 501



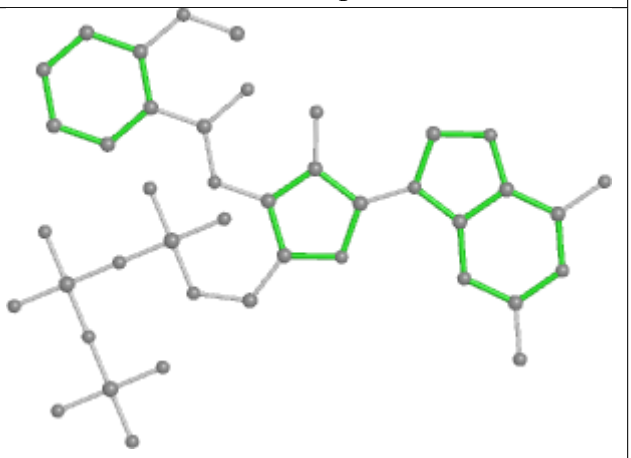
Bond lengths



Bond angles

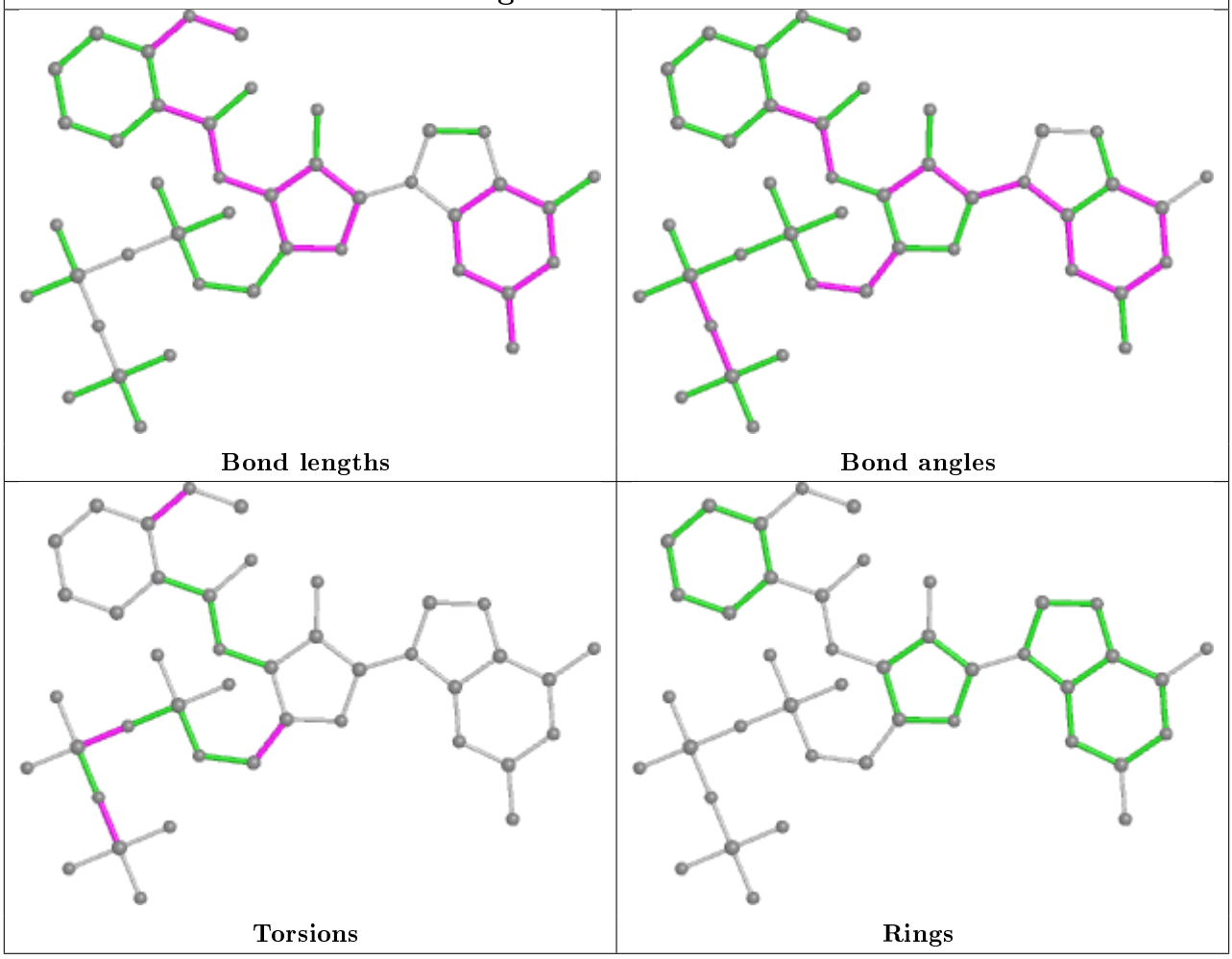


Torsions



Rings

Ligand ONM B 501



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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^{th} 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^2)	Q<0.9
1	A	216/254 (85%)	-0.34	0 100 100	40, 72, 142, 305	0
1	B	216/254 (85%)	-0.30	1 (0%) 91 90	37, 81, 156, 301	0
1	C	216/254 (85%)	-0.34	0 100 100	33, 73, 139, 263	0
1	D	216/254 (85%)	-0.21	3 (1%) 75 74	46, 88, 173, 318	0
1	E	216/254 (85%)	0.06	7 (3%) 47 46	60, 128, 229, 357	0
1	F	216/254 (85%)	0.42	20 (9%) 8 10	82, 151, 262, 417	0
1	G	216/254 (85%)	1.10	49 (22%) 0 1	91, 199, 305, 396	0
1	H	216/254 (85%)	1.17	41 (18%) 1 1	104, 186, 308, 402	0
1	I	216/254 (85%)	0.56	19 (8%) 10 11	101, 163, 268, 448	0
1	J	216/254 (85%)	0.54	19 (8%) 10 11	105, 187, 281, 372	0
1	K	216/254 (85%)	1.09	49 (22%) 0 1	131, 212, 317, 380	0
All	All	2376/2794 (85%)	0.34	208 (8%) 10 11	33, 143, 271, 448	0

All (208) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	412	GLY	8.5
1	K	412	GLY	7.1
1	K	313	PRO	6.6
1	H	407	ARG	6.5
1	I	213	GLU	6.4
1	G	347	MET	6.2
1	F	398	ASN	6.1
1	I	210	ALA	6.0
1	H	352	VAL	5.5
1	K	302	TYR	5.0
1	F	396	LEU	5.0
1	G	343	LEU	5.0

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Mol	Chain	Res	Type	RSRZ
1	H	413	LYS	4.9
1	G	301	SER	4.9
1	G	386	ILE	4.9
1	K	255	ALA	4.8
1	H	313	PRO	4.8
1	G	423	GLY	4.7
1	H	410	VAL	4.6
1	H	406	GLY	4.6
1	H	400	PHE	4.5
1	K	398	ASN	4.5
1	G	302	TYR	4.4
1	G	383	VAL	4.4
1	J	324	LEU	4.4
1	H	289	LYS	4.4
1	K	400	PHE	4.3
1	K	418	THR	4.3
1	G	422	ILE	4.3
1	H	286	LEU	4.2
1	K	388	VAL	4.2
1	K	343	LEU	4.1
1	G	255	ALA	4.1
1	J	389	PRO	4.0
1	H	414	GLY	4.0
1	K	404	GLU	4.0
1	H	328	ASN	3.9
1	H	255	ALA	3.9
1	K	345	MET	3.9
1	J	317	PHE	3.8
1	K	386	ILE	3.8
1	H	211	VAL	3.8
1	K	372	ASN	3.7
1	I	400	PHE	3.7
1	J	341	VAL	3.7
1	K	339	ASP	3.6
1	H	290	HIS	3.6
1	H	351	PRO	3.6
1	K	406	GLY	3.6
1	J	320	ALA	3.6
1	K	411	LYS	3.6
1	H	411	LYS	3.5
1	G	329	VAL	3.5
1	I	324	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
1	I	323	ALA	3.5
1	F	392	MET	3.5
1	H	212	MET	3.5
1	K	265	SER	3.4
1	J	263	ARG	3.4
1	G	340	PRO	3.4
1	K	263	ARG	3.4
1	F	422	ILE	3.4
1	K	425	LYS	3.4
1	F	412	GLY	3.4
1	K	385	ARG	3.4
1	K	383	VAL	3.4
1	F	215	GLU	3.4
1	H	215	GLU	3.4
1	G	421	LEU	3.3
1	K	396	LEU	3.3
1	K	253	LEU	3.2
1	G	303	MET	3.2
1	G	313	PRO	3.2
1	K	366	VAL	3.2
1	G	404	GLU	3.2
1	J	421	LEU	3.2
1	G	213	GLU	3.1
1	I	421	LEU	3.1
1	G	305	VAL	3.1
1	G	399	GLU	3.1
1	G	253	LEU	3.1
1	E	409	GLU	3.1
1	K	423	GLY	3.1
1	J	323	ALA	3.0
1	G	306	SER	3.0
1	K	304	VAL	3.0
1	K	384	GLY	3.0
1	F	397	LYS	3.0
1	G	297	VAL	3.0
1	G	325	ASP	3.0
1	G	412	GLY	3.0
1	F	416	MET	3.0
1	G	389	PRO	3.0
1	G	424	ARG	2.9
1	H	251	SER	2.9
1	G	392	MET	2.9

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Mol	Chain	Res	Type	RSRZ
1	G	409	GLU	2.9
1	G	210	ALA	2.9
1	G	398	ASN	2.9
1	J	302	TYR	2.9
1	E	408	ILE	2.8
1	G	367	TRP	2.8
1	K	403	GLN	2.8
1	J	398	ASN	2.8
1	F	324	LEU	2.8
1	B	210	ALA	2.8
1	G	304	VAL	2.8
1	H	388	VAL	2.7
1	G	346	GLY	2.7
1	G	388	VAL	2.7
1	G	397	LYS	2.7
1	D	412	GLY	2.7
1	K	348	ALA	2.7
1	F	411	LYS	2.7
1	I	217	GLU	2.7
1	I	336	PRO	2.7
1	G	333	LEU	2.6
1	K	340	PRO	2.6
1	K	410	VAL	2.6
1	G	272	LEU	2.6
1	E	210	ALA	2.6
1	J	240	ARG	2.6
1	E	407	ARG	2.6
1	H	292	LEU	2.6
1	K	408	ILE	2.6
1	H	330	ALA	2.6
1	G	417	ARG	2.6
1	G	318	ALA	2.5
1	E	406	GLY	2.5
1	F	425	LYS	2.5
1	K	260	PHE	2.5
1	K	326	MET	2.5
1	H	260	PHE	2.5
1	H	333	LEU	2.5
1	G	403	GLN	2.5
1	F	418	THR	2.4
1	I	382	SER	2.4
1	H	361	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	H	373	VAL	2.4
1	K	387	GLN	2.4
1	H	229	GLY	2.4
1	F	410	VAL	2.4
1	I	301	SER	2.4
1	H	311	ALA	2.4
1	G	366	VAL	2.4
1	K	317	PHE	2.4
1	K	382	SER	2.3
1	J	390	GLU	2.3
1	H	389	PRO	2.3
1	G	334	LYS	2.3
1	I	348	ALA	2.3
1	F	211	VAL	2.3
1	F	407	ARG	2.3
1	H	329	VAL	2.3
1	K	395	ARG	2.3
1	I	238	SER	2.3
1	J	383	VAL	2.3
1	K	346	GLY	2.3
1	H	409	GLU	2.3
1	E	211	VAL	2.2
1	G	415	VAL	2.2
1	K	422	ILE	2.2
1	I	407	ARG	2.2
1	H	261	THR	2.2
1	H	283	PHE	2.2
1	K	344	ARG	2.2
1	G	345	MET	2.2
1	H	392	MET	2.2
1	G	400	PHE	2.2
1	I	333	LEU	2.2
1	F	408	ILE	2.2
1	K	365	ASP	2.2
1	H	298	SER	2.2
1	G	286	LEU	2.2
1	F	212	MET	2.2
1	K	211	VAL	2.2
1	K	419	TRP	2.1
1	F	317	PHE	2.1
1	H	376	ARG	2.1
1	K	413	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	J	407	ARG	2.1
1	J	346	GLY	2.1
1	H	300	ASP	2.1
1	J	333	LEU	2.1
1	K	210	ALA	2.1
1	I	313	PRO	2.1
1	K	359	SER	2.1
1	H	369	ASP	2.1
1	H	314	ASP	2.1
1	K	399	GLU	2.1
1	G	405	ARG	2.1
1	J	219	SER	2.1
1	F	347	MET	2.1
1	J	253	LEU	2.1
1	J	213	GLU	2.1
1	I	415	VAL	2.1
1	H	415	VAL	2.1
1	G	254	PHE	2.0
1	I	320	ALA	2.0
1	I	331	ALA	2.0
1	I	358	GLY	2.0
1	D	211	VAL	2.0
1	D	411	LYS	2.0
1	G	382	SER	2.0
1	E	393	TYR	2.0
1	G	410	VAL	2.0
1	F	421	LEU	2.0
1	K	254	PHE	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 carbohydrates 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^{th} 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^2)	Q<0.9
4	SO4	H	501	5/5	0.52	0.49	263,265,267,267	0
4	SO4	J	505	5/5	0.53	0.47	253,258,261,262	0
4	SO4	I	503	5/5	0.55	0.52	258,260,262,263	0
4	SO4	C	503	5/5	0.65	0.49	216,219,220,220	0
4	SO4	F	502	5/5	0.70	0.41	236,238,238,240	0
2	ONM	K	501	42/42	0.80	0.28	164,174,200,206	0
4	SO4	J	502	5/5	0.83	0.28	179,184,188,188	0
4	SO4	E	504	5/5	0.83	0.42	203,209,213,215	0
2	ONM	G	501	42/42	0.86	0.27	167,175,200,207	0
3	MN	H	503	1/1	0.86	0.27	182,182,182,182	0
4	SO4	A	504	5/5	0.87	0.30	177,180,181,182	0
3	MN	G	503	1/1	0.88	0.27	213,213,213,213	0
4	SO4	A	505	5/5	0.88	0.21	135,135,136,137	0
3	MN	K	503	1/1	0.88	0.29	258,258,258,258	0
3	MN	H	502	1/1	0.88	0.19	146,146,146,146	0
2	ONM	H	504	42/42	0.88	0.28	140,149,160,163	0
3	MN	J	504	1/1	0.90	0.26	175,175,175,175	0
3	MN	E	503	1/1	0.90	0.18	146,146,146,146	0
2	ONM	J	501	42/42	0.91	0.29	148,156,169,172	0
3	MN	D	502	1/1	0.91	0.14	79,79,79,79	0
3	MN	F	503	1/1	0.91	0.17	136,136,136,136	0
3	MN	K	502	1/1	0.92	0.06	209,209,209,209	0
3	MN	C	505	1/1	0.92	0.31	146,146,146,146	0
2	ONM	E	501	42/42	0.92	0.22	123,130,153,159	0
2	ONM	I	504	42/42	0.93	0.29	163,168,193,200	0
3	MN	D	503	1/1	0.94	0.30	111,111,111,111	0
3	MN	F	504	1/1	0.94	0.33	164,164,164,164	0
2	ONM	F	501	42/42	0.94	0.22	127,135,141,142	0
4	SO4	E	505	5/5	0.95	0.20	123,123,123,124	0
4	SO4	C	502	5/5	0.95	0.25	119,125,129,129	0
3	MN	E	502	1/1	0.96	0.15	127,127,127,127	0
2	ONM	D	501	42/42	0.96	0.19	49,62,86,92	0
3	MN	I	501	1/1	0.96	0.23	126,126,126,126	0
2	ONM	A	501	42/42	0.96	0.18	59,68,91,97	0
4	SO4	D	504	5/5	0.96	0.20	121,121,121,122	0
3	MN	J	503	1/1	0.96	0.15	137,137,137,137	0
4	SO4	B	502	5/5	0.96	0.24	117,122,127,127	0
3	MN	G	502	1/1	0.97	0.10	157,157,157,157	0
2	ONM	C	501	42/42	0.97	0.21	67,76,88,91	0
3	MN	C	504	1/1	0.97	0.19	68,68,68,68	0
2	ONM	B	501	42/42	0.97	0.17	70,80,91,94	0

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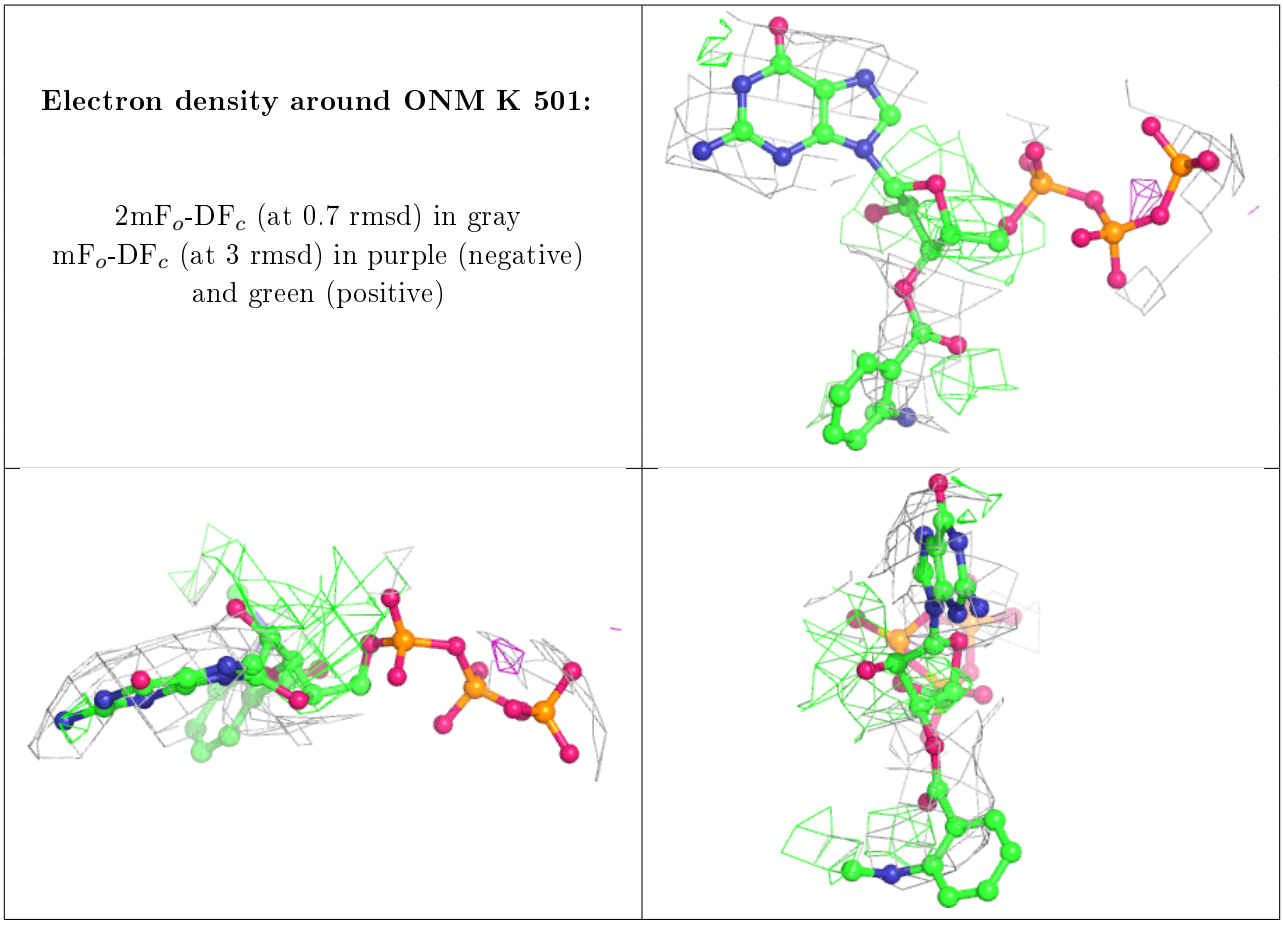
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	MN	A	503	1/1	0.98	0.17	101,101,101,101	0
3	MN	B	503	1/1	0.98	0.14	88,88,88,88	0
3	MN	I	502	1/1	0.98	0.36	236,236,236,236	0
3	MN	A	502	1/1	0.99	0.14	67,67,67,67	0
3	MN	B	504	1/1	0.99	0.19	150,150,150,150	0

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.

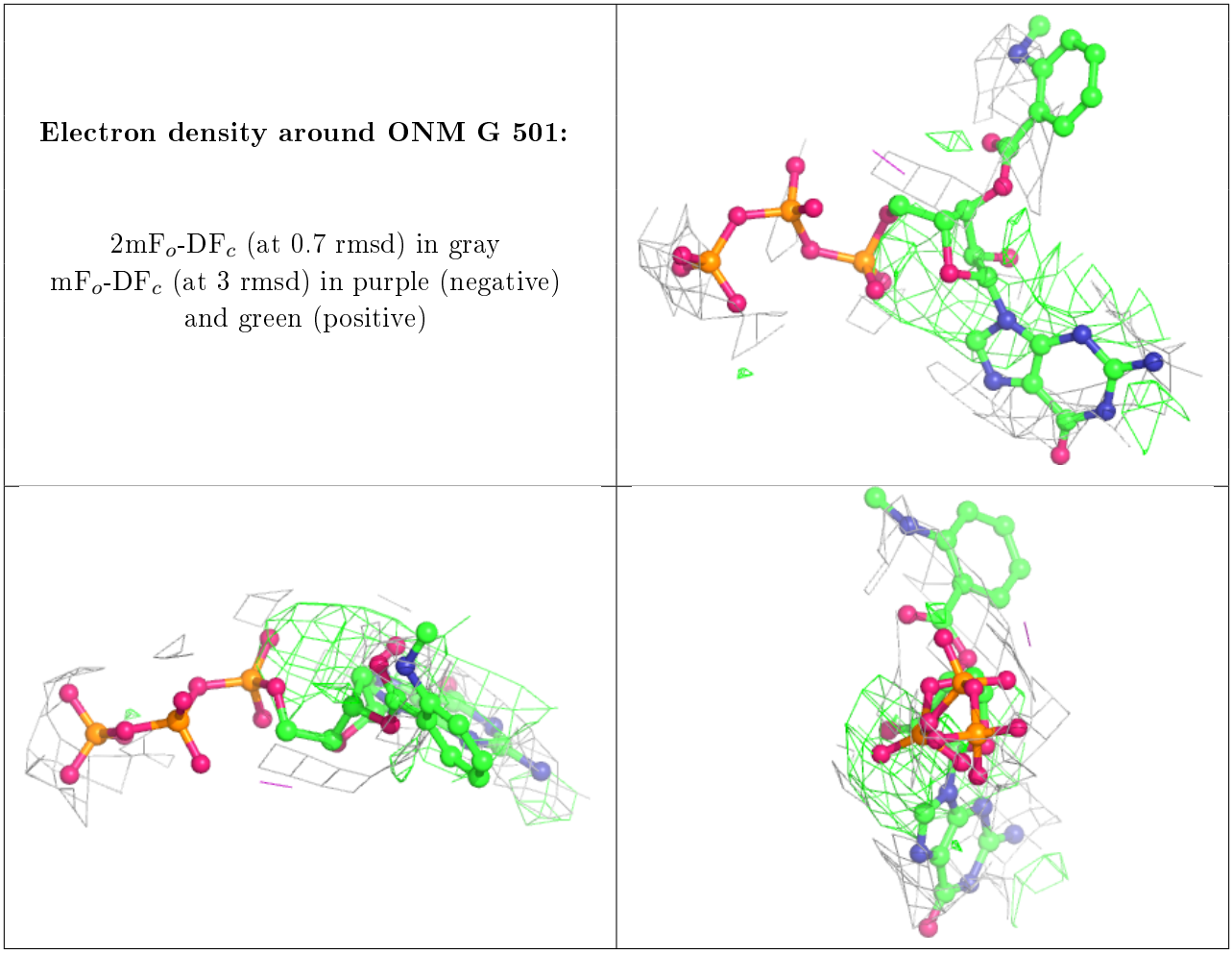
Electron density around ONM K 501:

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



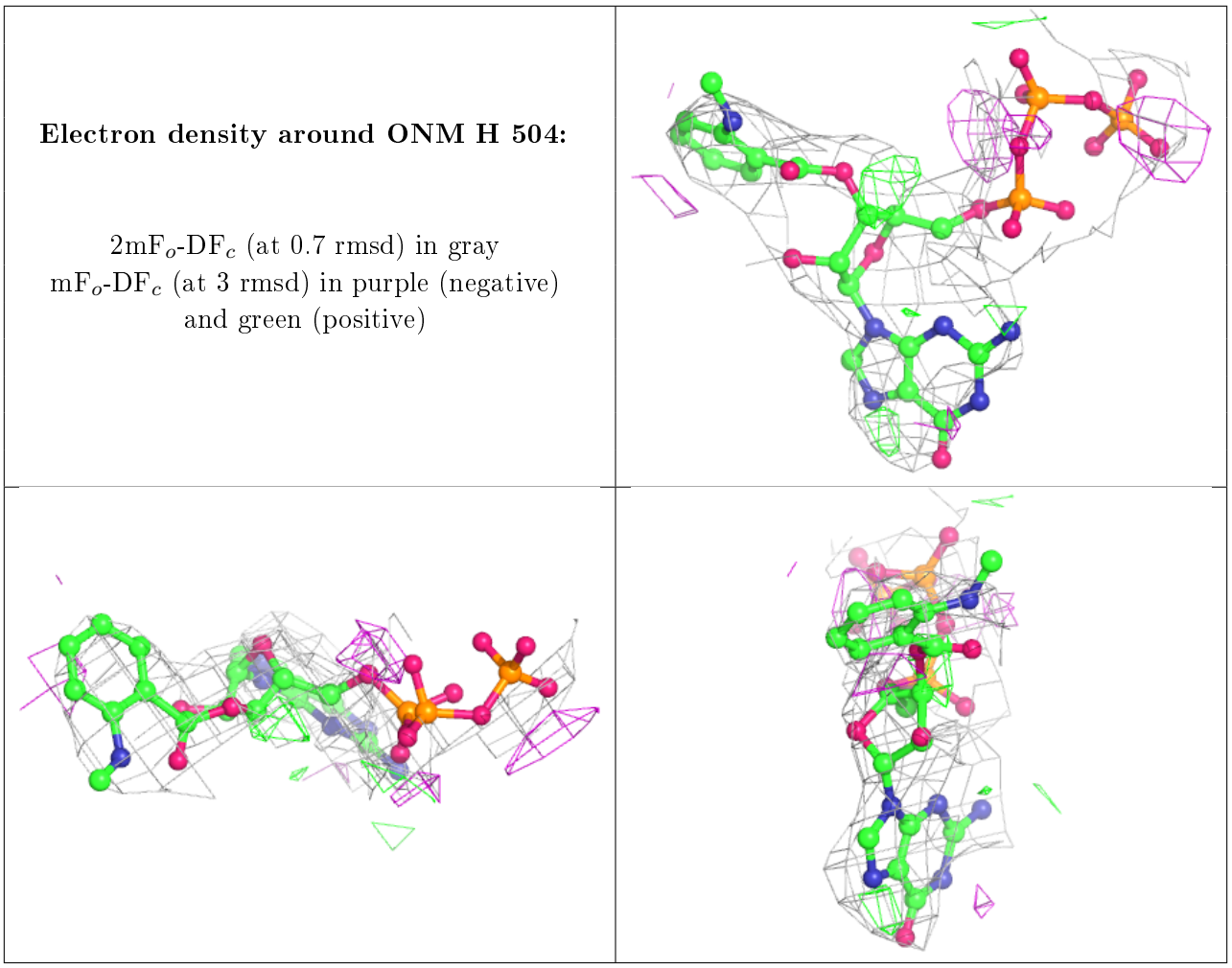
Electron density around ONM G 501:

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



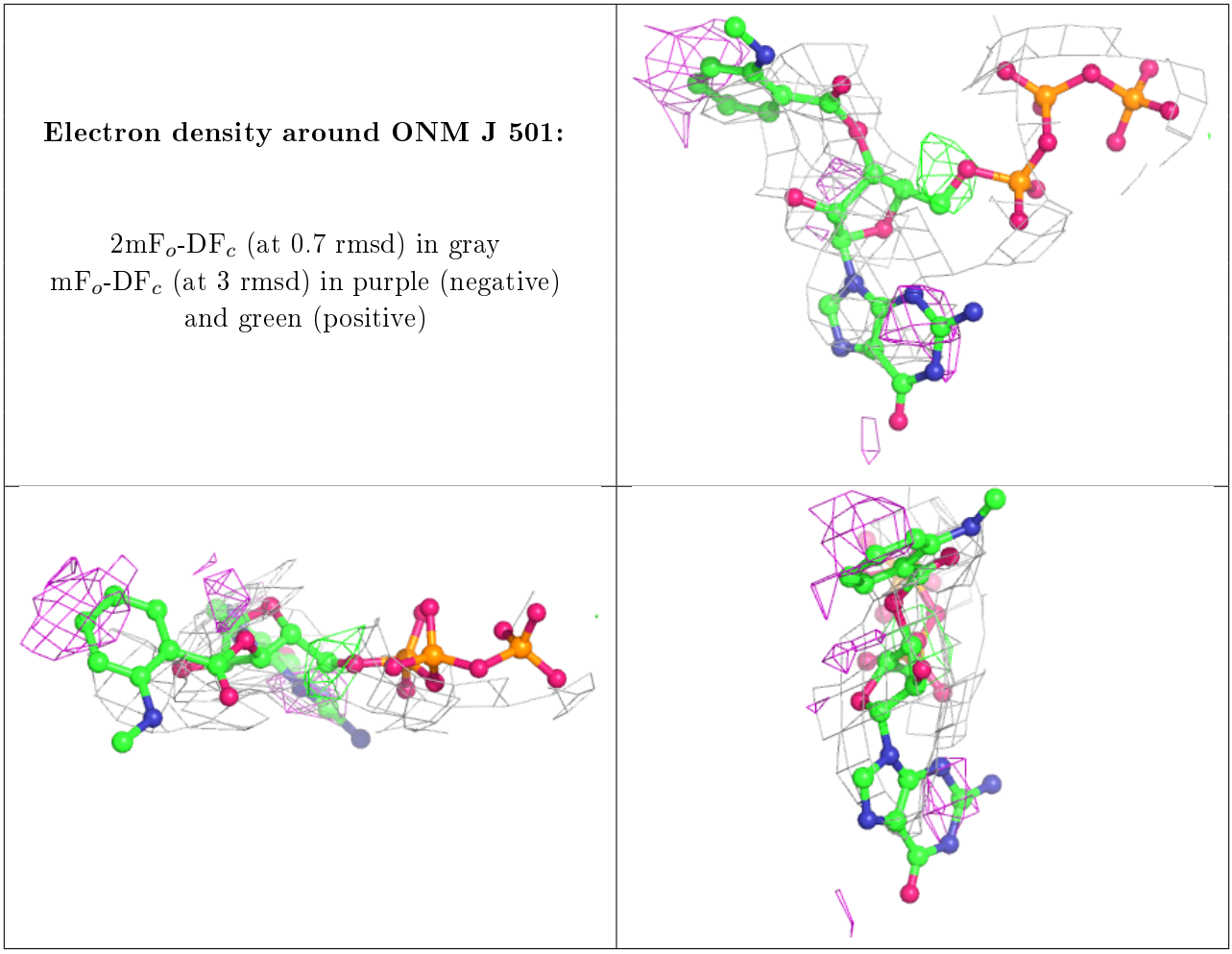
Electron density around ONM H 504:

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



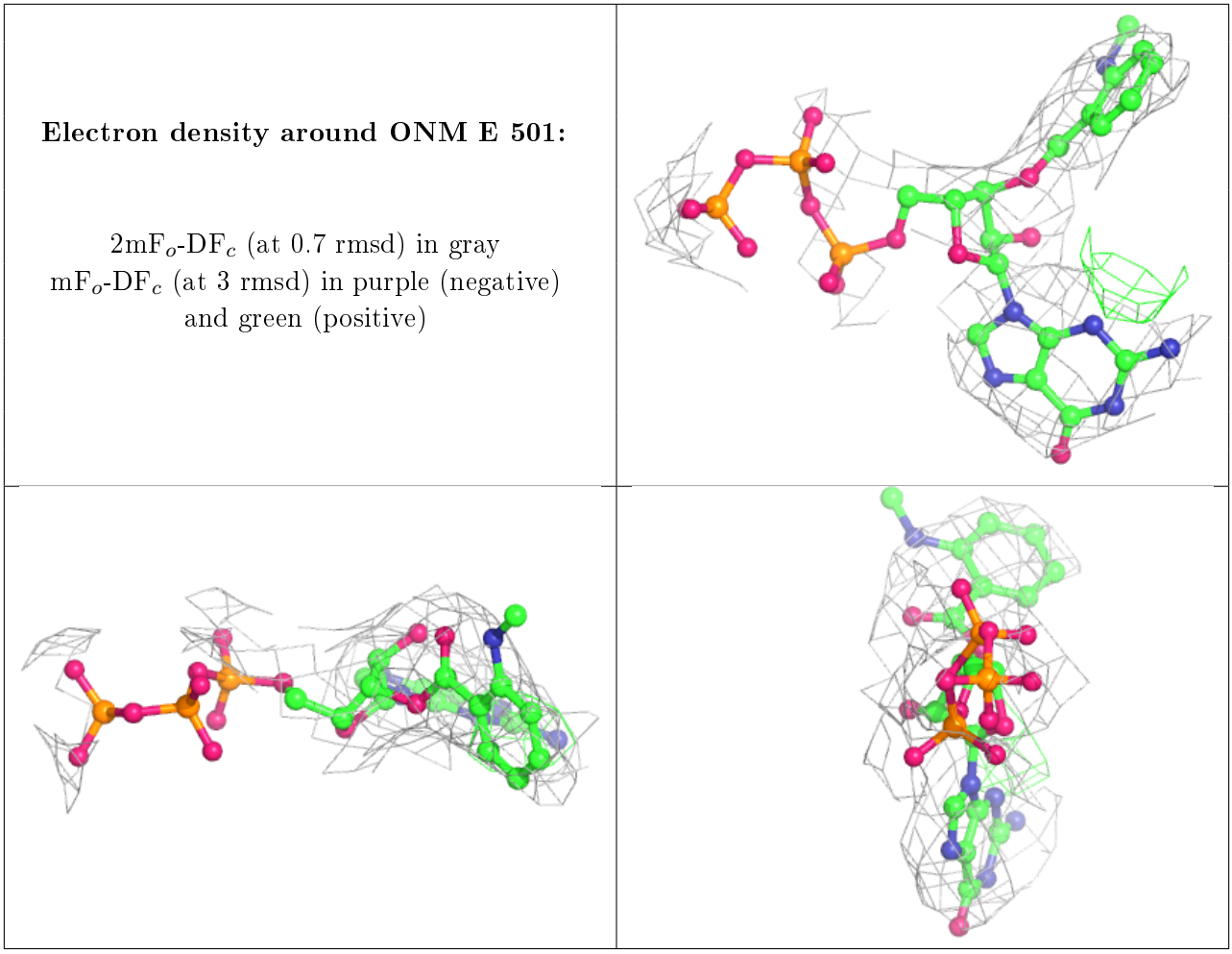
Electron density around ONM J 501:

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



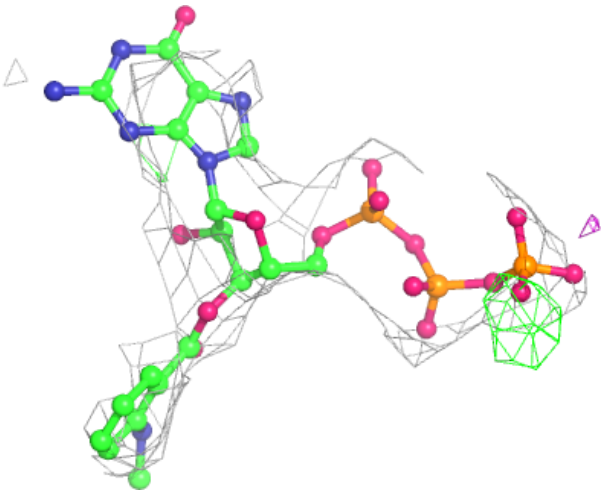
Electron density around ONM E 501:

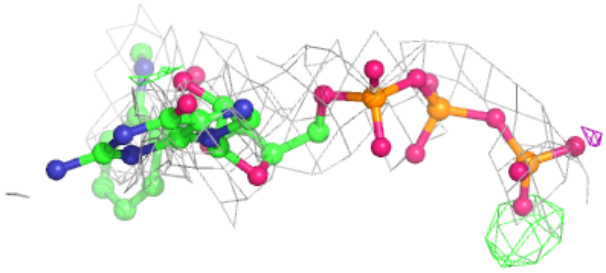
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

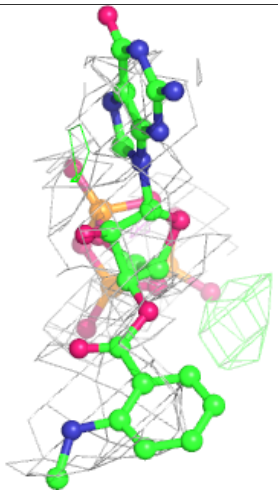


Electron density around ONM I 504:

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

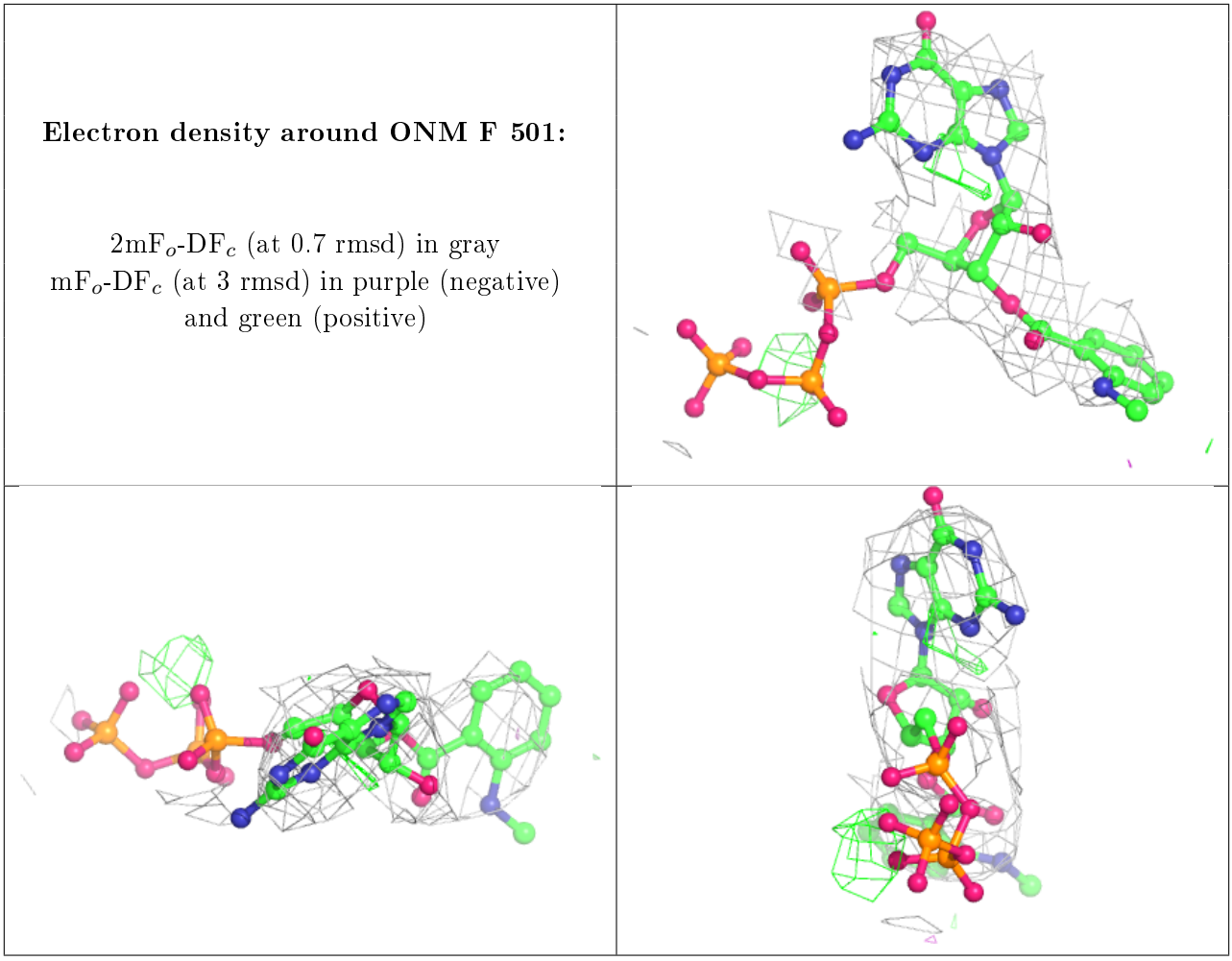






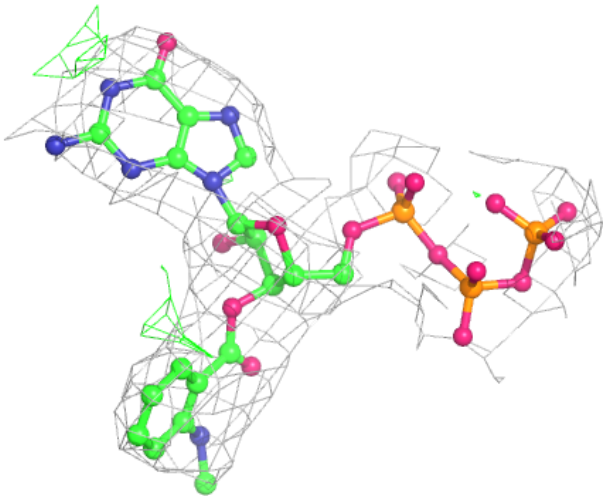
Electron density around ONM F 501:

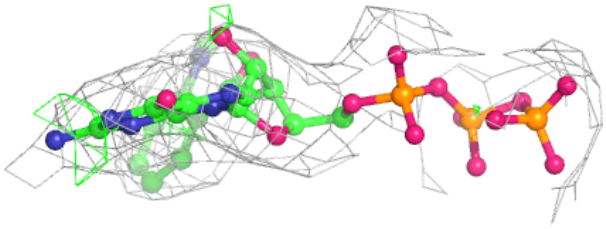
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

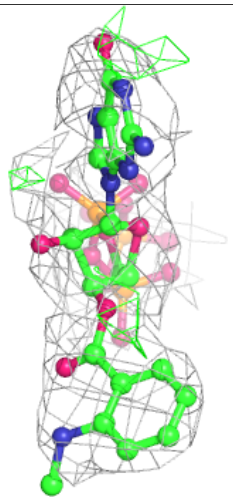


Electron density around ONM D 501:

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

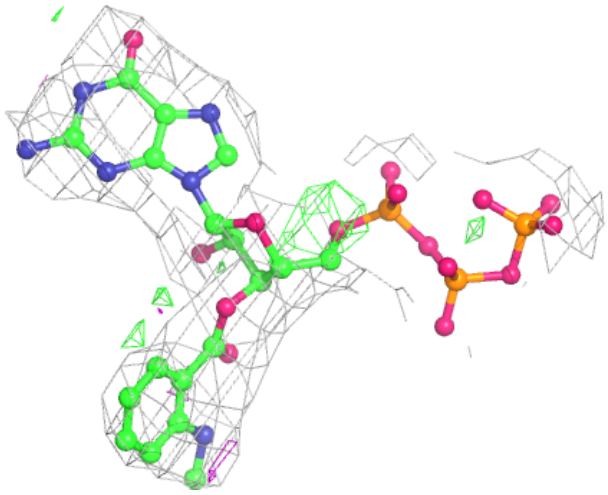


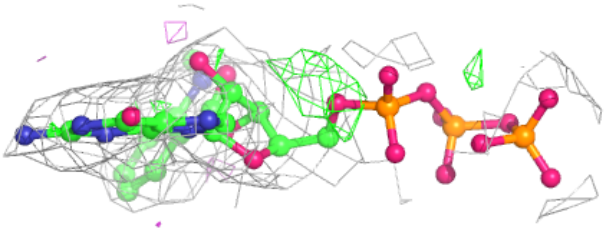


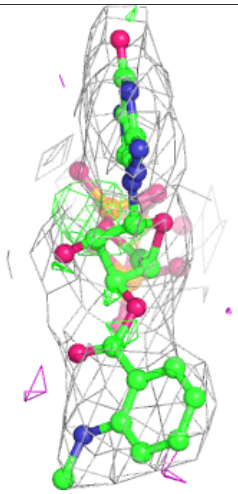


Electron density around ONM A 501:

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

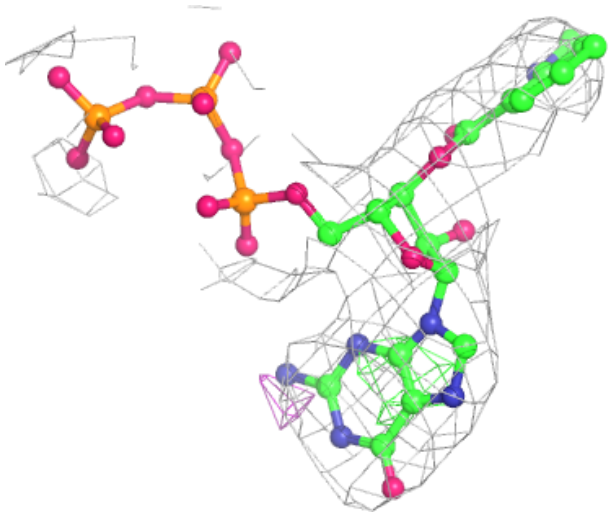


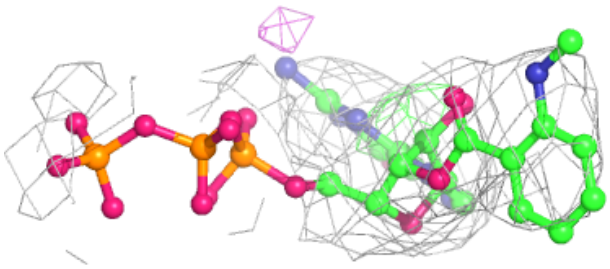


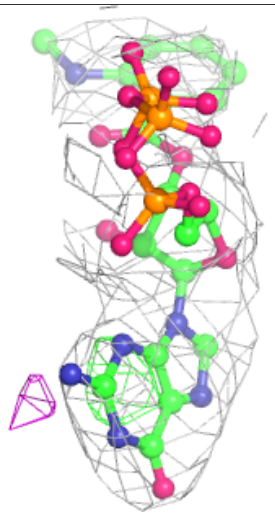


Electron density around ONM C 501:

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

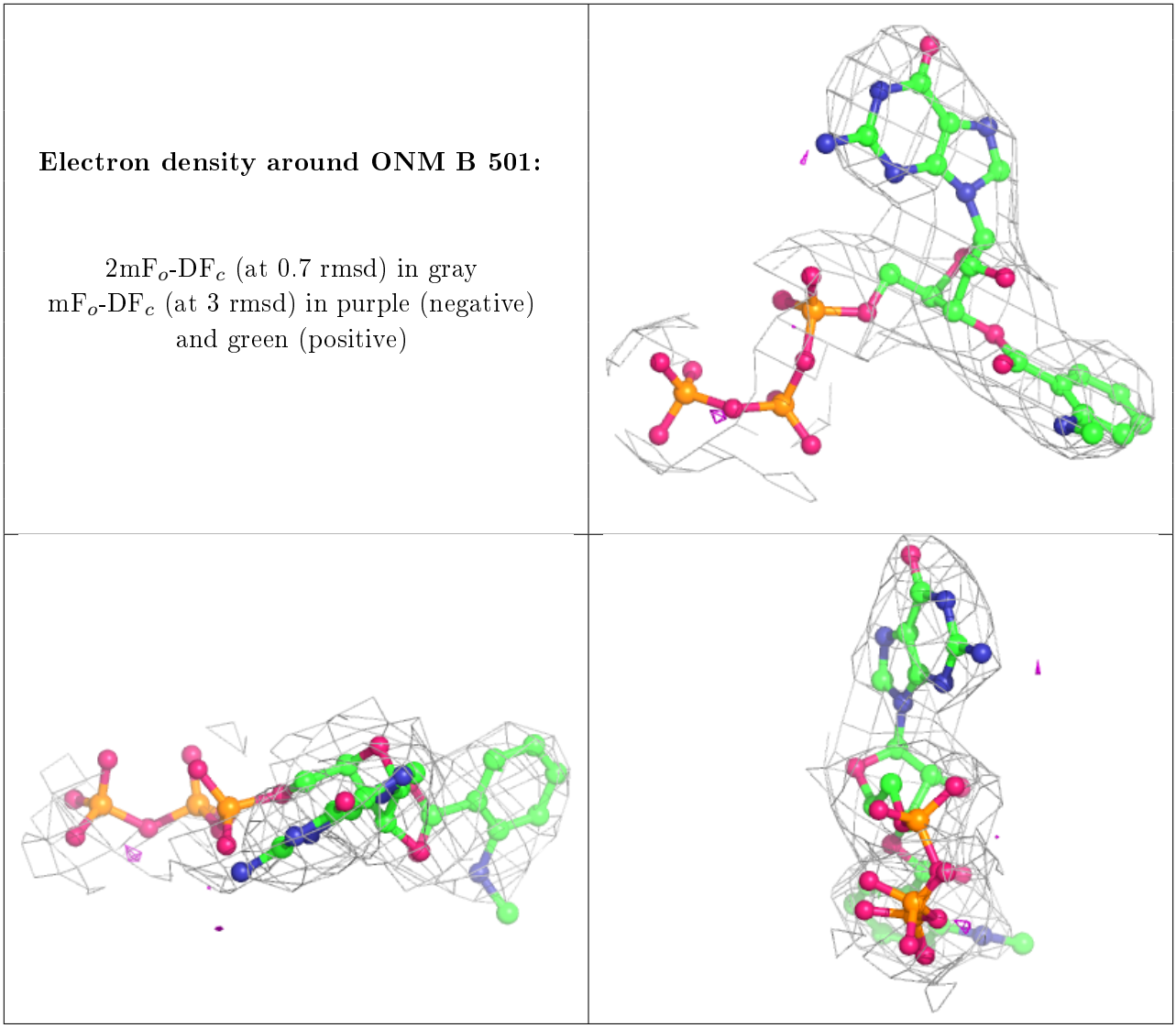






Electron density around ONM B 501:

$2mF_o$-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

There are no such residues in this entry.