



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2020 – 05:13 PM BST

PDB ID : 5CB5  
Title : Structural Insights into the Mechanism of Escherichia coli Ymdb  
Authors : Zhang, W.; Wang, C.; Song, Y.; Shao, C.; Zhang, X.; Zang, J.  
Deposited on : 2015-06-30  
Resolution : 2.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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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 : 2.13.1  
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) : 2.13.1

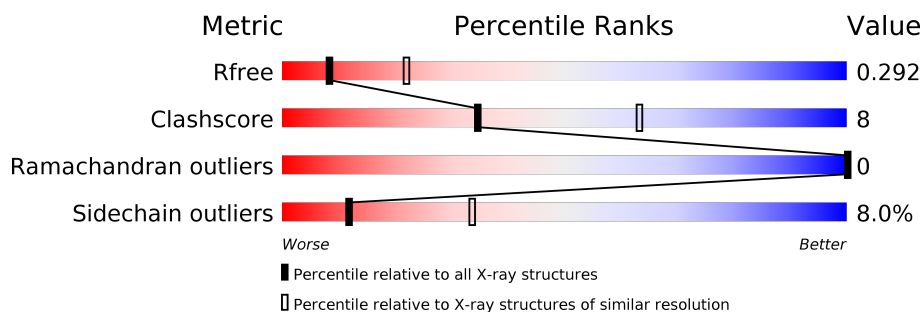
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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.













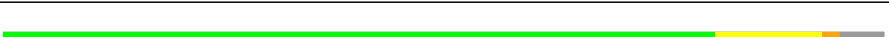
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	183	77% 15% • 5%
1	B	183	78% 10% 5% • 6%
1	C	183	81% 11% •• 5%
1	D	183	73% 16% •• 7%
1	E	183	80% 12% • 5%
1	F	183	76% 13% 5% 5%
1	G	183	83% 9% •• 5%

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Mol	Chain	Length	Quality of chain
1	H	183	
1	I	183	
1	J	183	
1	K	183	
1	L	183	
1	M	183	
1	N	183	
1	O	183	
1	P	183	
1	Q	183	
1	R	183	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SO4	C	202	-	-	X	-
3	SO4	D	202	-	-	X	-
3	SO4	J	202	-	-	X	-
3	SO4	K	202	-	-	X	-
3	SO4	M	202	-	-	X	-
3	SO4	O	202	-	-	X	-
3	SO4	Q	403	-	-	X	-

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 23896 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 O-acetyl-ADP-ribose deacetylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	R	173	Total	C	N	O	S	0	0	0
			1281	810	229	238	4			
1	A	173	Total	C	N	O	S	0	0	0
			1259	798	222	235	4			
1	B	172	Total	C	N	O	S	0	0	0
			1280	809	228	239	4			
1	C	173	Total	C	N	O	S	0	0	0
			1283	811	226	242	4			
1	D	170	Total	C	N	O	S	0	0	0
			1236	781	220	231	4			
1	E	173	Total	C	N	O	S	0	0	0
			1293	816	230	243	4			
1	F	173	Total	C	N	O	S	0	0	0
			1283	810	226	243	4			
1	G	173	Total	C	N	O	S	0	0	0
			1280	810	226	240	4			
1	H	173	Total	C	N	O	S	0	0	0
			1293	816	230	243	4			
1	I	173	Total	C	N	O	S	0	0	0
			1272	805	226	237	4			
1	J	172	Total	C	N	O	S	0	0	0
			1280	808	228	240	4			
1	K	172	Total	C	N	O	S	0	0	0
			1256	796	219	237	4			
1	L	172	Total	C	N	O	S	0	0	0
			1259	797	222	236	4			
1	M	173	Total	C	N	O	S	0	0	0
			1279	809	226	240	4			
1	N	173	Total	C	N	O	S	0	0	0
			1255	794	221	236	4			
1	O	171	Total	C	N	O	S	0	0	0
			1271	803	226	238	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	P	173	Total	C	N	O	S	0	0	0
			1277	807	227	239	4			
1	Q	173	Total	C	N	O	S	0	0	0
			1289	814	229	242	4			

There are 144 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	-5	HIS	-	expression tag	UNP P0A8D6
R	-4	HIS	-	expression tag	UNP P0A8D6
R	-3	HIS	-	expression tag	UNP P0A8D6
R	-2	HIS	-	expression tag	UNP P0A8D6
R	-1	HIS	-	expression tag	UNP P0A8D6
R	0	HIS	-	expression tag	UNP P0A8D6
R	25	ALA	ASN	engineered mutation	UNP P0A8D6
R	35	ALA	ASP	engineered mutation	UNP P0A8D6
A	-5	HIS	-	expression tag	UNP P0A8D6
A	-4	HIS	-	expression tag	UNP P0A8D6
A	-3	HIS	-	expression tag	UNP P0A8D6
A	-2	HIS	-	expression tag	UNP P0A8D6
A	-1	HIS	-	expression tag	UNP P0A8D6
A	0	HIS	-	expression tag	UNP P0A8D6
A	25	ALA	ASN	engineered mutation	UNP P0A8D6
A	35	ALA	ASP	engineered mutation	UNP P0A8D6
B	-5	HIS	-	expression tag	UNP P0A8D6
B	-4	HIS	-	expression tag	UNP P0A8D6
B	-3	HIS	-	expression tag	UNP P0A8D6
B	-2	HIS	-	expression tag	UNP P0A8D6
B	-1	HIS	-	expression tag	UNP P0A8D6
B	0	HIS	-	expression tag	UNP P0A8D6
B	25	ALA	ASN	engineered mutation	UNP P0A8D6
B	35	ALA	ASP	engineered mutation	UNP P0A8D6
C	-5	HIS	-	expression tag	UNP P0A8D6
C	-4	HIS	-	expression tag	UNP P0A8D6
C	-3	HIS	-	expression tag	UNP P0A8D6
C	-2	HIS	-	expression tag	UNP P0A8D6
C	-1	HIS	-	expression tag	UNP P0A8D6
C	0	HIS	-	expression tag	UNP P0A8D6
C	25	ALA	ASN	engineered mutation	UNP P0A8D6
C	35	ALA	ASP	engineered mutation	UNP P0A8D6
D	-5	HIS	-	expression tag	UNP P0A8D6
D	-4	HIS	-	expression tag	UNP P0A8D6

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-3	HIS	-	expression tag	UNP P0A8D6
D	-2	HIS	-	expression tag	UNP P0A8D6
D	-1	HIS	-	expression tag	UNP P0A8D6
D	0	HIS	-	expression tag	UNP P0A8D6
D	25	ALA	ASN	engineered mutation	UNP P0A8D6
D	35	ALA	ASP	engineered mutation	UNP P0A8D6
E	-5	HIS	-	expression tag	UNP P0A8D6
E	-4	HIS	-	expression tag	UNP P0A8D6
E	-3	HIS	-	expression tag	UNP P0A8D6
E	-2	HIS	-	expression tag	UNP P0A8D6
E	-1	HIS	-	expression tag	UNP P0A8D6
E	0	HIS	-	expression tag	UNP P0A8D6
E	25	ALA	ASN	engineered mutation	UNP P0A8D6
E	35	ALA	ASP	engineered mutation	UNP P0A8D6
F	-5	HIS	-	expression tag	UNP P0A8D6
F	-4	HIS	-	expression tag	UNP P0A8D6
F	-3	HIS	-	expression tag	UNP P0A8D6
F	-2	HIS	-	expression tag	UNP P0A8D6
F	-1	HIS	-	expression tag	UNP P0A8D6
F	0	HIS	-	expression tag	UNP P0A8D6
F	25	ALA	ASN	engineered mutation	UNP P0A8D6
F	35	ALA	ASP	engineered mutation	UNP P0A8D6
G	-5	HIS	-	expression tag	UNP P0A8D6
G	-4	HIS	-	expression tag	UNP P0A8D6
G	-3	HIS	-	expression tag	UNP P0A8D6
G	-2	HIS	-	expression tag	UNP P0A8D6
G	-1	HIS	-	expression tag	UNP P0A8D6
G	0	HIS	-	expression tag	UNP P0A8D6
G	25	ALA	ASN	engineered mutation	UNP P0A8D6
G	35	ALA	ASP	engineered mutation	UNP P0A8D6
H	-5	HIS	-	expression tag	UNP P0A8D6
H	-4	HIS	-	expression tag	UNP P0A8D6
H	-3	HIS	-	expression tag	UNP P0A8D6
H	-2	HIS	-	expression tag	UNP P0A8D6
H	-1	HIS	-	expression tag	UNP P0A8D6
H	0	HIS	-	expression tag	UNP P0A8D6
H	25	ALA	ASN	engineered mutation	UNP P0A8D6
H	35	ALA	ASP	engineered mutation	UNP P0A8D6
I	-5	HIS	-	expression tag	UNP P0A8D6
I	-4	HIS	-	expression tag	UNP P0A8D6
I	-3	HIS	-	expression tag	UNP P0A8D6
I	-2	HIS	-	expression tag	UNP P0A8D6

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Chain	Residue	Modelled	Actual	Comment	Reference
I	-1	HIS	-	expression tag	UNP P0A8D6
I	0	HIS	-	expression tag	UNP P0A8D6
I	25	ALA	ASN	engineered mutation	UNP P0A8D6
I	35	ALA	ASP	engineered mutation	UNP P0A8D6
J	-5	HIS	-	expression tag	UNP P0A8D6
J	-4	HIS	-	expression tag	UNP P0A8D6
J	-3	HIS	-	expression tag	UNP P0A8D6
J	-2	HIS	-	expression tag	UNP P0A8D6
J	-1	HIS	-	expression tag	UNP P0A8D6
J	0	HIS	-	expression tag	UNP P0A8D6
J	25	ALA	ASN	engineered mutation	UNP P0A8D6
J	35	ALA	ASP	engineered mutation	UNP P0A8D6
K	-5	HIS	-	expression tag	UNP P0A8D6
K	-4	HIS	-	expression tag	UNP P0A8D6
K	-3	HIS	-	expression tag	UNP P0A8D6
K	-2	HIS	-	expression tag	UNP P0A8D6
K	-1	HIS	-	expression tag	UNP P0A8D6
K	0	HIS	-	expression tag	UNP P0A8D6
K	25	ALA	ASN	engineered mutation	UNP P0A8D6
K	35	ALA	ASP	engineered mutation	UNP P0A8D6
L	-5	HIS	-	expression tag	UNP P0A8D6
L	-4	HIS	-	expression tag	UNP P0A8D6
L	-3	HIS	-	expression tag	UNP P0A8D6
L	-2	HIS	-	expression tag	UNP P0A8D6
L	-1	HIS	-	expression tag	UNP P0A8D6
L	0	HIS	-	expression tag	UNP P0A8D6
L	25	ALA	ASN	engineered mutation	UNP P0A8D6
L	35	ALA	ASP	engineered mutation	UNP P0A8D6
M	-5	HIS	-	expression tag	UNP P0A8D6
M	-4	HIS	-	expression tag	UNP P0A8D6
M	-3	HIS	-	expression tag	UNP P0A8D6
M	-2	HIS	-	expression tag	UNP P0A8D6
M	-1	HIS	-	expression tag	UNP P0A8D6
M	0	HIS	-	expression tag	UNP P0A8D6
M	25	ALA	ASN	engineered mutation	UNP P0A8D6
M	35	ALA	ASP	engineered mutation	UNP P0A8D6
N	-5	HIS	-	expression tag	UNP P0A8D6
N	-4	HIS	-	expression tag	UNP P0A8D6
N	-3	HIS	-	expression tag	UNP P0A8D6
N	-2	HIS	-	expression tag	UNP P0A8D6
N	-1	HIS	-	expression tag	UNP P0A8D6
N	0	HIS	-	expression tag	UNP P0A8D6

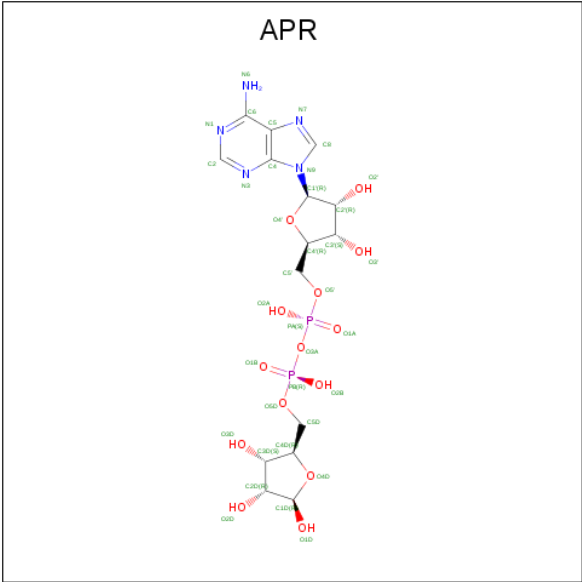
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Chain	Residue	Modelled	Actual	Comment	Reference
N	25	ALA	ASN	engineered mutation	UNP P0A8D6
N	35	ALA	ASP	engineered mutation	UNP P0A8D6
O	-5	HIS	-	expression tag	UNP P0A8D6
O	-4	HIS	-	expression tag	UNP P0A8D6
O	-3	HIS	-	expression tag	UNP P0A8D6
O	-2	HIS	-	expression tag	UNP P0A8D6
O	-1	HIS	-	expression tag	UNP P0A8D6
O	0	HIS	-	expression tag	UNP P0A8D6
O	25	ALA	ASN	engineered mutation	UNP P0A8D6
O	35	ALA	ASP	engineered mutation	UNP P0A8D6
P	-5	HIS	-	expression tag	UNP P0A8D6
P	-4	HIS	-	expression tag	UNP P0A8D6
P	-3	HIS	-	expression tag	UNP P0A8D6
P	-2	HIS	-	expression tag	UNP P0A8D6
P	-1	HIS	-	expression tag	UNP P0A8D6
P	0	HIS	-	expression tag	UNP P0A8D6
P	25	ALA	ASN	engineered mutation	UNP P0A8D6
P	35	ALA	ASP	engineered mutation	UNP P0A8D6
Q	-5	HIS	-	expression tag	UNP P0A8D6
Q	-4	HIS	-	expression tag	UNP P0A8D6
Q	-3	HIS	-	expression tag	UNP P0A8D6
Q	-2	HIS	-	expression tag	UNP P0A8D6
Q	-1	HIS	-	expression tag	UNP P0A8D6
Q	0	HIS	-	expression tag	UNP P0A8D6
Q	25	ALA	ASN	engineered mutation	UNP P0A8D6
Q	35	ALA	ASP	engineered mutation	UNP P0A8D6

- Molecule 2 is ADENOSINE-5-DIPHOSPHORIBOSE (three-letter code: APR) (formula:  $C_{15}H_{23}N_5O_{14}P_2$ ).





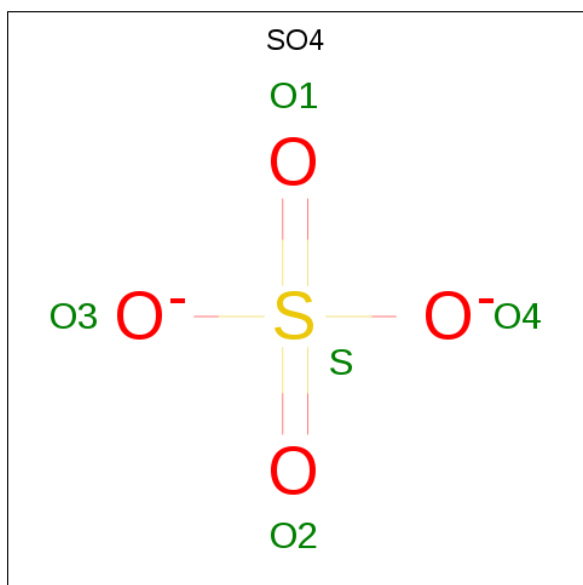
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	R	1	Total	C	N	O	P	0	0
			36	15	5	14	2		
2	A	1	Total	C	N	O	P	0	0
			36	15	5	14	2		
2	B	1	Total	C	N	O	P	0	0
			36	15	5	14	2		
2	C	1	Total	C	N	O	P	0	0
			36	15	5	14	2		
2	D	1	Total	C	N	O	P	0	0
			36	15	5	14	2		
2	E	1	Total	C	N	O	P	0	0
			36	15	5	14	2		
2	G	1	Total	C	N	O	P	0	0
			36	15	5	14	2		
2	H	1	Total	C	N	O	P	0	0
			36	15	5	14	2		
2	I	1	Total	C	N	O	P	0	0
			36	15	5	14	2		
2	J	1	Total	C	N	O	P	0	0
			36	15	5	14	2		
2	K	1	Total	C	N	O	P	0	0
			36	15	5	14	2		
2	L	1	Total	C	N	O	P	0	0
			36	15	5	14	2		
2	N	1	Total	C	N	O	P	0	0
			36	15	5	14	2		
2	O	1	Total	C	N	O	P	0	0
			36	15	5	14	2		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	P	1	Total	C	N	O	P	0	0
			36	15	5	14	2		
2	Q	1	Total	C	N	O	P	0	0
			36	15	5	14	2		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



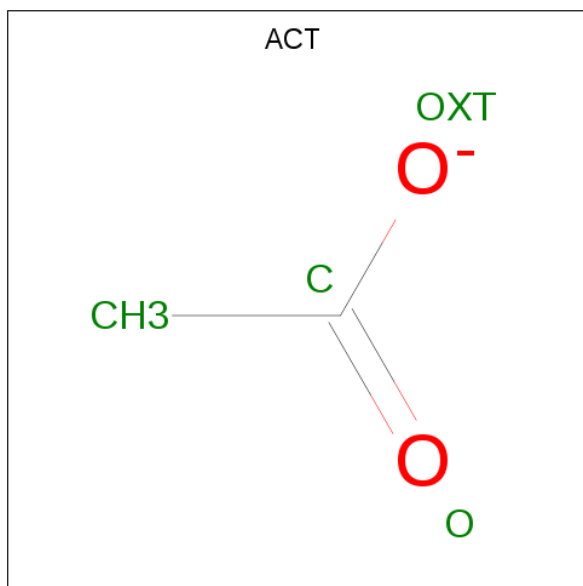
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	R	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		
3	G	1	Total	O	S	0	0
			5	4	1		
3	H	1	Total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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	I	1	Total O S 5 4 1	0	0
3	J	1	Total O S 5 4 1	0	0
3	K	1	Total O S 5 4 1	0	0
3	L	1	Total O S 5 4 1	0	0
3	M	1	Total O S 5 4 1	0	0
3	N	1	Total O S 5 4 1	0	0
3	O	1	Total O S 5 4 1	0	0
3	P	1	Total O S 5 4 1	0	0
3	Q	1	Total O S 5 4 1	0	0

- Molecule 4 is ACETATE ION (three-letter code: ACT) (formula: C<sub>2</sub>H<sub>3</sub>O<sub>2</sub>).



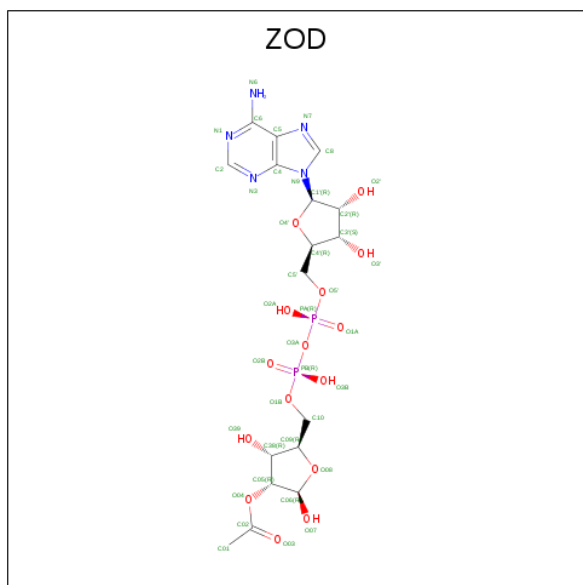
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total C O 4 2 2	0	0
4	J	1	Total C O 4 2 2	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	Q	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is [(2R,3R,4R,5R)-5-[[[(2R,3S,4R,5R)-5-(6-aminopurin-9-yl)-3,4-bis(oxidanyl)oxolan-2-yl]methoxy-oxidanyl-phosphoryl]oxy-oxidanyl-phosphoryl]oxymethyl]-2,4-bis(oxidanyl)oxolan-3-yl] ethanoate (three-letter code: ZOD) (formula: C<sub>17</sub>H<sub>25</sub>N<sub>5</sub>O<sub>15</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	F	1	Total 39	C 17	N 5	O 15	P 2	0	0
5	M	1	Total 39	C 17	N 5	O 15	P 2	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	R	17	Total O 17 17	0	0
6	A	11	Total O 11 11	0	0
6	B	16	Total O 16 16	0	0
6	C	10	Total O 10 10	0	0
6	D	12	Total O 12 12	0	0

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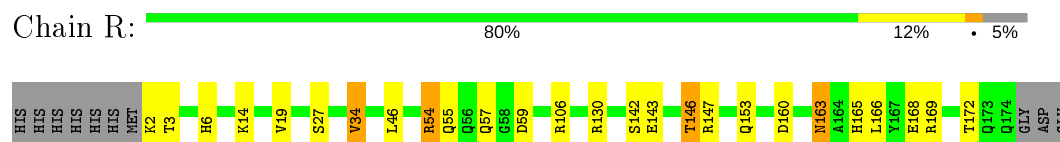
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	E	11	Total 11	O 11	0	0
6	F	10	Total 10	O 10	0	0
6	G	8	Total 8	O 8	0	0
6	H	12	Total 12	O 12	0	0
6	I	12	Total 12	O 12	0	0
6	J	12	Total 12	O 12	0	0
6	K	11	Total 11	O 11	0	0
6	L	11	Total 11	O 11	0	0
6	M	15	Total 15	O 15	0	0
6	N	12	Total 12	O 12	0	0
6	O	11	Total 11	O 11	0	0
6	P	14	Total 14	O 14	0	0
6	Q	9	Total 9	O 9	0	0

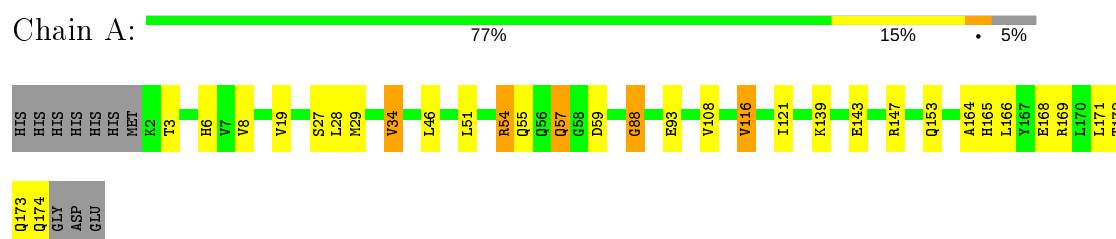
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

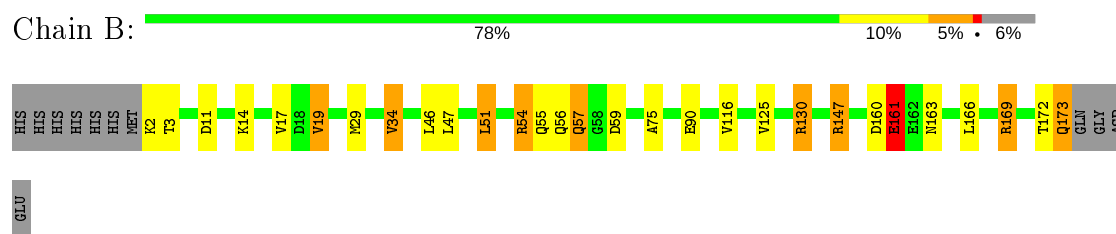
- Molecule 1: O-acetyl-ADP-ribose deacetylase



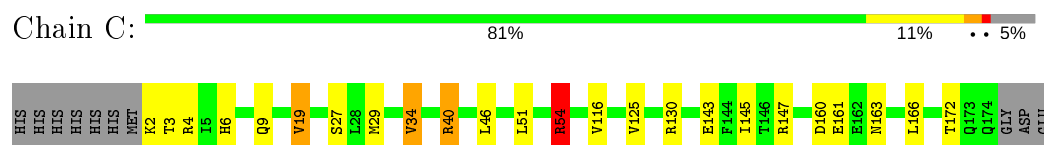
- Molecule 1: O-acetyl-ADP-ribose deacetylase



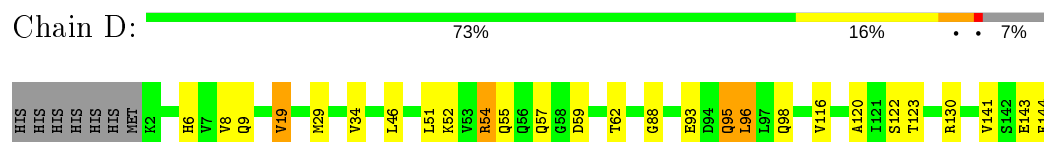
- Molecule 1: O-acetyl-ADP-ribose deacetylase



- Molecule 1: O-acetyl-ADP-ribose deacetylase



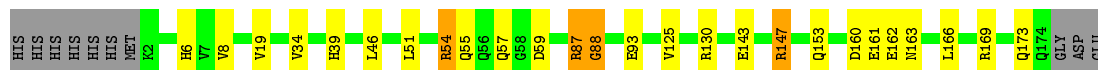
- Molecule 1: O-acetyl-ADP-ribose deacetylase





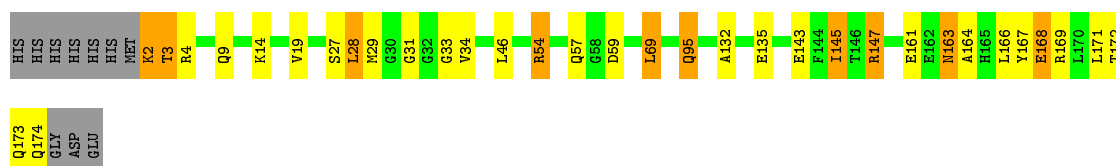
- Molecule 1: O-acetyl-ADP-ribose deacetylase

Chain E: 80% 12% 5%



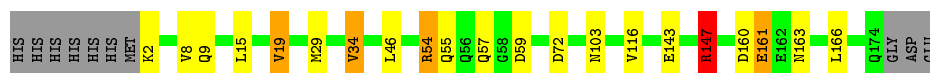
- Molecule 1: O-acetyl-ADP-ribose deacetylase

Chain F: 76% 13% 5% 5%



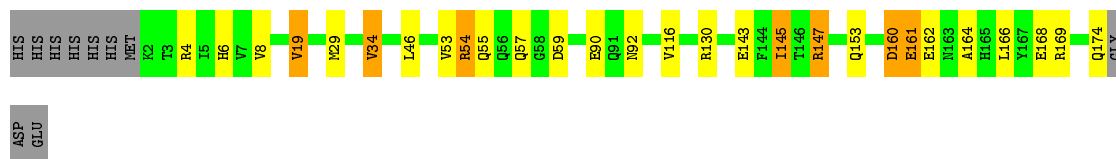
- Molecule 1: O-acetyl-ADP-ribose deacetylase

Chain G: 83% 9% 5% 5%



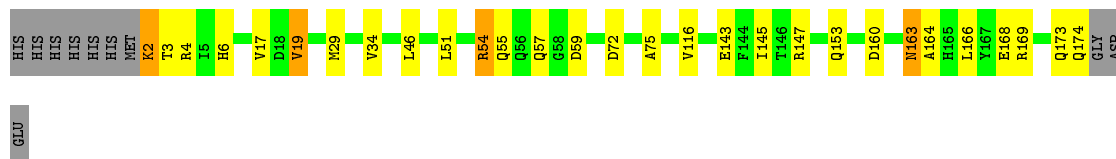
- Molecule 1: O-acetyl-ADP-ribose deacetylase

Chain H: 79% 11% 5% 5%



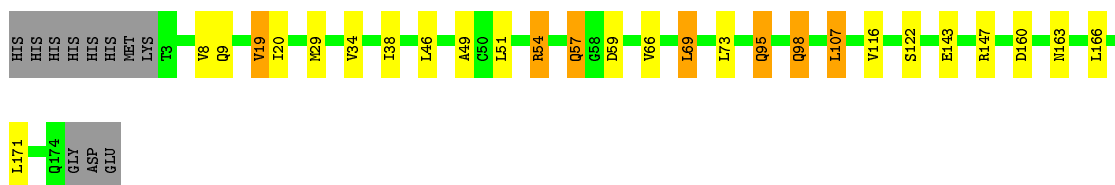
- Molecule 1: O-acetyl-ADP-ribose deacetylase

Chain I: 79% 14% 5% 5%



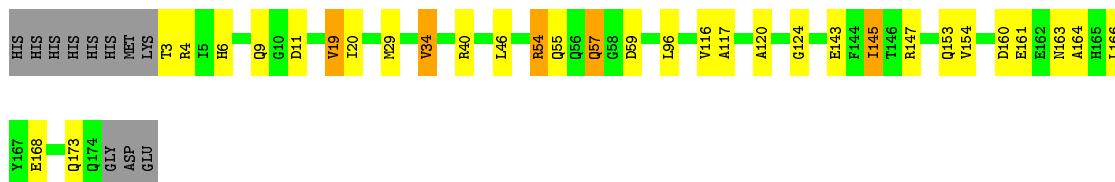
- Molecule 1: O-acetyl-ADP-ribose deacetylase

Chain J: 79% 11% 6% 6%



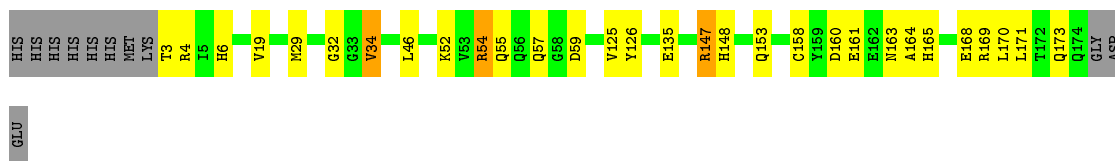
- Molecule 1: O-acetyl-ADP-ribose deacetylase

Chain K: 77% 15% 6%



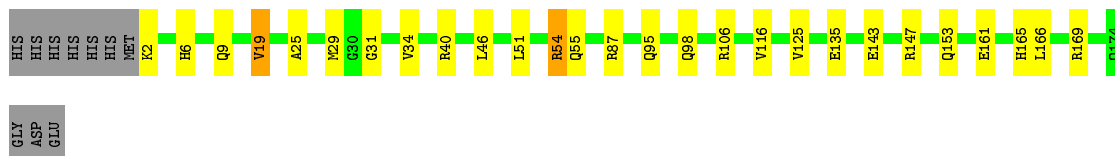
- Molecule 1: O-acetyl-ADP-ribose deacetylase

Chain L: 78% 15% 6%



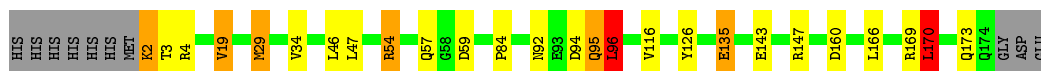
- Molecule 1: O-acetyl-ADP-ribose deacetylase

Chain M: 80% 14% 5%



- Molecule 1: O-acetyl-ADP-ribose deacetylase

Chain N: 80% 10% 5%



- Molecule 1: O-acetyl-ADP-ribose deacetylase

Chain O: 81% 10% 7%



- Molecule 1: O-acetyl-ADP-ribose deacetylase

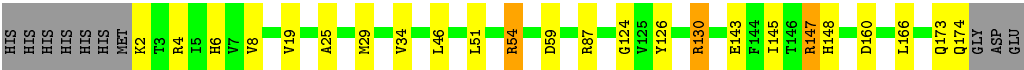


Chain P: 

81%

11%

5%



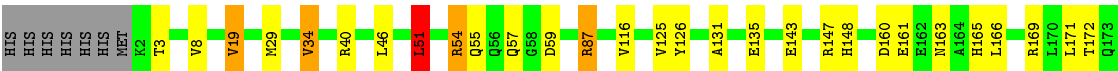
• Molecule 1: O-acetyl-ADP-ribose deacetylase

Chain Q: 

78%

14%

5%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	289.14Å 289.14Å 114.05Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	38.72 – 2.80 38.72 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.8 (38.72-2.80) 98.9 (38.72-2.80)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.58 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, $R_{free}$	0.262 , 0.290 0.263 , 0.292	Depositor DCC
$R_{free}$ test set	6667 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	37.0	Xtriage
Anisotropy	0.020	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 5.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.408 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	23896	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 19.99 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 9.5839e-03.*

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

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: APR, ZOD, SO4, ACT

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	0.76	0/1284	0.98	4/1757 (0.2%)
1	B	0.79	0/1305	1.01	3/1782 (0.2%)
1	C	0.77	0/1308	0.97	1/1787 (0.1%)
1	D	0.79	0/1261	1.03	6/1727 (0.3%)
1	E	0.78	2/1318 (0.2%)	1.00	5/1799 (0.3%)
1	F	0.77	0/1308	1.01	5/1788 (0.3%)
1	G	0.77	0/1305	0.97	2/1783 (0.1%)
1	H	0.76	0/1318	0.95	2/1799 (0.1%)
1	I	0.74	0/1296	0.94	0/1771
1	J	0.79	0/1305	0.96	1/1783 (0.1%)
1	K	0.76	0/1280	0.92	0/1752
1	L	0.75	1/1284 (0.1%)	0.93	2/1758 (0.1%)
1	M	0.76	0/1304	0.93	0/1782
1	N	0.76	0/1279	0.98	4/1751 (0.2%)
1	O	0.77	0/1296	0.97	2/1771 (0.1%)
1	P	0.72	0/1302	0.94	2/1780 (0.1%)
1	Q	0.77	0/1314	0.97	2/1794 (0.1%)
1	R	0.78	0/1306	0.93	1/1784 (0.1%)
All	All	0.77	3/23373 (0.0%)	0.97	42/31948 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	162	GLU	CD-OE2	-5.87	1.19	1.25
1	E	161	GLU	CD-OE2	-5.22	1.20	1.25
1	L	161	GLU	CD-OE2	-5.13	1.20	1.25

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	69	LEU	CA-CB-CG	9.31	136.72	115.30
1	E	87	ARG	N-CA-C	-8.98	86.76	111.00
1	F	69	LEU	CB-CG-CD2	-8.64	96.31	111.00
1	B	147	ARG	NE-CZ-NH1	8.62	124.61	120.30
1	C	54	ARG	CG-CD-NE	8.17	128.96	111.80
1	G	147	ARG	NE-CZ-NH1	8.09	124.34	120.30
1	P	147	ARG	NE-CZ-NH1	7.75	124.17	120.30
1	N	96	LEU	CA-CB-CG	7.26	132.00	115.30
1	D	96	LEU	CB-CG-CD1	-6.97	99.15	111.00
1	E	147	ARG	NE-CZ-NH1	6.79	123.70	120.30
1	D	96	LEU	CB-CG-CD2	6.66	122.32	111.00
1	H	147	ARG	NE-CZ-NH1	6.64	123.62	120.30
1	D	147	ARG	NE-CZ-NH1	6.64	123.62	120.30
1	F	28	LEU	CA-CB-CG	6.43	130.09	115.30
1	H	29	MET	N-CA-C	-6.30	93.98	111.00
1	O	147	ARG	NE-CZ-NH2	6.29	123.44	120.30
1	L	52	LYS	CD-CE-NZ	6.03	125.57	111.70
1	E	162	GLU	CG-CD-OE1	5.99	130.29	118.30
1	F	147	ARG	NE-CZ-NH2	5.96	123.28	120.30
1	D	51	LEU	CB-CA-C	-5.85	99.09	110.20
1	F	19	VAL	CB-CA-C	-5.81	100.36	111.40
1	E	19	VAL	CB-CA-C	-5.64	100.68	111.40
1	O	54	ARG	CG-CD-NE	5.56	123.47	111.80
1	A	116	VAL	CA-CB-CG2	-5.54	102.59	110.90
1	J	107	LEU	CB-CG-CD1	-5.53	101.60	111.00
1	N	160	ASP	CB-CG-OD1	5.53	123.27	118.30
1	A	8	VAL	CA-CB-CG1	5.51	119.16	110.90
1	D	170	LEU	CB-CG-CD1	5.46	120.29	111.00
1	A	19	VAL	CB-CA-C	-5.32	101.30	111.40
1	N	29	MET	CG-SD-CE	5.29	108.66	100.20
1	Q	51	LEU	CB-CG-CD2	-5.29	102.01	111.00
1	L	19	VAL	CB-CA-C	-5.26	101.41	111.40
1	P	19	VAL	CB-CA-C	-5.25	101.42	111.40
1	D	130	ARG	NE-CZ-NH1	5.23	122.92	120.30
1	B	147	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	B	161	GLU	CG-CD-OE1	5.21	128.73	118.30
1	Q	87	ARG	CG-CD-NE	5.21	122.73	111.80
1	R	19	VAL	CB-CA-C	-5.18	101.56	111.40
1	E	88	GLY	N-CA-C	-5.17	100.17	113.10
1	N	170	LEU	CA-CB-CG	5.08	126.98	115.30
1	G	147	ARG	NE-CZ-NH2	-5.03	117.79	120.30
1	A	88	GLY	N-CA-C	-5.00	100.59	113.10

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1259	0	1237	29	0
1	B	1280	0	1278	29	0
1	C	1283	0	1273	22	0
1	D	1236	0	1204	34	1
1	E	1293	0	1290	15	0
1	F	1283	0	1268	50	0
1	G	1280	0	1267	12	0
1	H	1293	0	1290	14	0
1	I	1272	0	1265	21	0
1	J	1280	0	1273	23	0
1	K	1256	0	1238	23	0
1	L	1259	0	1237	26	0
1	M	1279	0	1269	21	0
1	N	1255	0	1228	31	0
1	O	1271	0	1265	16	0
1	P	1277	0	1263	19	0
1	Q	1289	0	1284	22	0
1	R	1281	0	1276	16	0
2	A	36	0	21	1	0
2	B	36	0	21	2	0
2	C	36	0	21	2	0
2	D	36	0	21	4	0
2	E	36	0	21	1	0
2	G	36	0	21	1	0
2	H	36	0	21	2	0
2	I	36	0	21	0	0
2	J	36	0	21	1	0
2	K	36	0	21	4	0
2	L	36	0	21	4	0
2	N	36	0	21	1	0
2	O	36	0	21	3	0
2	P	36	0	21	3	0
2	Q	36	0	21	3	0
2	R	36	0	21	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	5	0	0	1	0
3	B	5	0	0	1	0
3	C	5	0	0	2	0
3	D	5	0	0	3	0
3	E	5	0	0	1	0
3	F	5	0	0	0	0
3	G	5	0	0	0	0
3	H	5	0	0	1	0
3	I	5	0	0	0	0
3	J	5	0	0	3	0
3	K	5	0	0	2	0
3	L	5	0	0	1	0
3	M	5	0	0	3	0
3	N	5	0	0	0	0
3	O	5	0	0	3	0
3	P	5	0	0	1	0
3	Q	5	0	0	3	0
3	R	5	0	0	1	0
4	C	4	0	3	0	0
4	J	4	0	3	0	0
4	Q	4	0	3	0	0
5	F	39	0	23	4	0
5	M	39	0	23	6	0
6	A	11	0	0	0	0
6	B	16	0	0	1	0
6	C	10	0	0	0	0
6	D	12	0	0	0	0
6	E	11	0	0	1	0
6	F	10	0	0	0	0
6	G	8	0	0	0	0
6	H	12	0	0	1	0
6	I	12	0	0	0	0
6	J	12	0	0	0	0
6	K	11	0	0	0	0
6	L	11	0	0	2	0
6	M	15	0	0	0	0
6	N	12	0	0	1	0
6	O	11	0	0	0	0
6	P	14	0	0	2	0
6	Q	9	0	0	1	0
6	R	17	0	0	2	0
All	All	23896	0	23096	386	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 8.

All (386) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:9:GLN:OE1	1:F:161:GLU:CG	1.68	1.40
1:N:84:PRO:HB3	1:N:96:LEU:CD1	1.60	1.32
1:M:31:GLY:HA3	5:M:201:ZOD:O03	1.16	1.27
1:A:88:GLY:O	1:A:93:GLU:OE1	1.58	1.20
1:F:31:GLY:HA3	5:F:201:ZOD:O03	1.04	1.20
1:N:84:PRO:HB3	1:N:96:LEU:HD12	1.24	1.20
1:F:9:GLN:OE1	1:F:161:GLU:HG3	1.48	1.13
1:F:31:GLY:CA	5:F:201:ZOD:O03	1.99	1.09
1:M:31:GLY:CA	5:M:201:ZOD:O03	1.99	1.08
1:F:9:GLN:OE1	1:F:161:GLU:HG2	1.30	1.08
1:N:84:PRO:CB	1:N:96:LEU:HD12	1.82	1.08
1:C:2:LYS:O	1:C:3:THR:HG22	1.55	1.07
1:N:84:PRO:HB3	1:N:96:LEU:HD13	1.38	1.06
1:F:57:GLN:HB3	1:K:57:GLN:HE22	1.16	1.05
1:A:164:ALA:O	1:A:168:GLU:HG3	1.57	1.03
1:F:57:GLN:HB3	1:K:57:GLN:NE2	1.74	1.02
1:D:62:THR:CG2	1:D:96:LEU:HD23	1.89	1.02
1:B:2:LYS:HG3	1:B:3:THR:H	1.23	1.01
1:F:27:SER:O	1:F:29:MET:HE2	1.61	1.00
1:F:33:GLY:HA3	5:F:201:ZOD:O2A	1.62	0.98
1:Q:147:ARG:NH2	3:Q:403:SO4:O2	1.96	0.97
1:A:139:LYS:O	1:A:143:GLU:HG3	1.65	0.96
1:F:9:GLN:CD	1:F:161:GLU:HG2	1.84	0.96
1:B:29:MET:CE	1:B:51:LEU:HD11	1.94	0.96
1:K:147:ARG:NH2	3:K:202:SO4:O2	1.98	0.96
1:N:135:GLU:HA	1:N:170:LEU:HD21	1.46	0.95
1:O:147:ARG:NH2	3:O:202:SO4:O2	2.01	0.94
1:B:29:MET:HE1	1:B:51:LEU:HD11	1.49	0.92
1:D:62:THR:HG22	1:D:96:LEU:HD23	1.50	0.91
1:D:147:ARG:NH1	3:D:202:SO4:O4	2.03	0.91
1:F:27:SER:O	1:F:29:MET:CE	2.18	0.91
1:N:84:PRO:CB	1:N:96:LEU:CD1	2.43	0.91
1:J:147:ARG:NH2	3:J:202:SO4:O4	2.05	0.90
1:R:147:ARG:NH2	3:R:202:SO4:O2	2.05	0.89
1:R:142:SER:O	1:R:146:THR:CG2	2.20	0.89
1:D:57:GLN:OE1	1:I:57:GLN:CD	2.11	0.88
1:N:2:LYS:N	1:N:3:THR:HA	1.88	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:54:ARG:NH2	1:E:59:ASP:OD1	2.07	0.88
1:L:3:THR:HG23	1:L:4:ARG:H	1.38	0.87
1:A:54:ARG:NH2	1:A:59:ASP:OD1	2.08	0.87
1:D:54:ARG:NH2	1:D:59:ASP:OD1	2.08	0.87
1:B:54:ARG:NH2	1:B:59:ASP:OD1	2.07	0.87
1:G:54:ARG:NH2	1:G:59:ASP:OD1	2.07	0.87
1:R:54:ARG:NH2	1:R:59:ASP:OD1	2.08	0.87
1:R:165:HIS:O	1:R:169:ARG:HG2	1.75	0.86
1:H:54:ARG:NH2	1:H:59:ASP:OD1	2.08	0.86
1:M:106:ARG:NE	3:M:202:SO4:O4	2.07	0.86
1:K:54:ARG:NH2	1:K:59:ASP:OD1	2.08	0.86
1:I:54:ARG:NH2	1:I:59:ASP:OD1	2.08	0.86
1:P:54:ARG:NH2	1:P:59:ASP:OD1	2.08	0.86
1:H:130:ARG:NH2	1:H:160:ASP:OD2	2.08	0.86
1:N:29:MET:CE	1:N:47:LEU:CD1	2.53	0.85
1:Q:54:ARG:NH2	1:Q:59:ASP:OD1	2.08	0.85
1:N:54:ARG:NH2	1:N:59:ASP:OD1	2.09	0.85
1:A:168:GLU:O	1:A:172:THR:HG23	1.75	0.85
1:H:164:ALA:O	1:H:168:GLU:HG3	1.77	0.85
1:L:54:ARG:NH2	1:L:59:ASP:OD1	2.10	0.84
1:D:57:GLN:OE1	1:I:57:GLN:NE2	2.11	0.84
1:N:29:MET:CE	1:N:47:LEU:HD11	2.08	0.84
1:J:29:MET:HE1	1:J:51:LEU:HD23	1.61	0.81
1:M:31:GLY:HA3	5:M:201:ZOD:C02	2.10	0.81
1:R:142:SER:O	1:R:146:THR:HG23	1.80	0.80
1:B:29:MET:SD	1:B:51:LEU:CD1	2.70	0.80
1:D:164:ALA:O	1:D:168:GLU:HG3	1.81	0.80
1:Q:29:MET:HE3	1:Q:51:LEU:HD22	1.66	0.78
1:L:164:ALA:O	1:L:168:GLU:HG3	1.85	0.76
1:I:2:LYS:HB3	1:I:3:THR:HA	1.66	0.76
1:K:164:ALA:O	1:K:168:GLU:HG3	1.85	0.76
1:N:135:GLU:HA	1:N:170:LEU:CD2	2.16	0.75
1:J:147:ARG:NH2	3:J:202:SO4:O1	2.18	0.75
1:M:125:VAL:HG13	5:M:201:ZOD:O1A	1.85	0.75
1:A:108:VAL:HG21	1:A:116:VAL:HG11	1.69	0.75
1:B:2:LYS:HG3	1:B:3:THR:HG22	1.68	0.75
1:A:108:VAL:HG11	1:A:116:VAL:CG1	2.16	0.74
1:C:147:ARG:NH1	3:C:202:SO4:O4	2.21	0.74
1:I:29:MET:HE3	1:I:51:LEU:HD23	1.69	0.74
1:N:29:MET:CE	1:N:47:LEU:HD12	2.18	0.74
1:P:25:ALA:HB2	2:P:201:APR:O3D	1.88	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:88:GLY:O	1:E:93:GLU:OE1	2.06	0.74
1:A:108:VAL:HG11	1:A:116:VAL:HG12	1.70	0.73
1:I:6:HIS:HE1	1:I:153:GLN:OE1	1.72	0.73
1:F:57:GLN:CB	1:K:57:GLN:NE2	2.49	0.73
1:G:57:GLN:OE1	1:Q:57:GLN:OE1	2.07	0.73
1:N:29:MET:HE1	1:N:47:LEU:CD1	2.19	0.73
1:O:87:ARG:N	1:O:93:GLU:OE2	2.20	0.73
1:J:54:ARG:NH2	1:J:59:ASP:OD1	2.22	0.73
1:E:87:ARG:HG2	1:E:87:ARG:HH21	1.54	0.72
1:F:169:ARG:HH11	1:F:169:ARG:HG3	1.54	0.72
1:N:2:LYS:HG3	1:N:4:ARG:H	1.53	0.72
1:P:29:MET:HE3	1:P:51:LEU:HD23	1.70	0.72
1:F:29:MET:CE	1:F:54:ARG:HG3	2.20	0.71
1:P:130:ARG:HD3	1:P:130:ARG:H	1.54	0.71
1:D:62:THR:HG21	1:D:96:LEU:HD23	1.73	0.70
1:O:130:ARG:HD3	1:O:130:ARG:H	1.54	0.70
1:F:54:ARG:NH2	1:F:59:ASP:OD1	2.25	0.70
3:D:202:SO4:O2	1:M:40:ARG:HB3	1.91	0.70
1:B:130:ARG:H	1:B:130:ARG:HE	1.37	0.69
1:R:142:SER:O	1:R:146:THR:HG22	1.93	0.69
1:F:169:ARG:O	1:F:173:GLN:HG3	1.93	0.69
1:J:147:ARG:NH2	3:J:202:SO4:S	2.66	0.68
1:B:2:LYS:HE2	1:B:3:THR:HG22	1.75	0.68
1:F:2:LYS:HG2	1:F:4:ARG:HB2	1.75	0.68
1:R:6:HIS:HE1	1:R:153:GLN:OE1	1.77	0.68
1:M:165:HIS:O	1:M:169:ARG:HG3	1.94	0.67
1:N:2:LYS:HD2	1:N:2:LYS:O	1.94	0.67
1:B:29:MET:SD	1:B:51:LEU:HD11	2.32	0.67
1:K:40:ARG:HB3	3:Q:403:SO4:O4	1.94	0.67
1:F:9:GLN:NE2	1:F:161:GLU:HG2	2.08	0.67
1:N:29:MET:HE2	1:N:47:LEU:HD11	1.75	0.67
1:H:6:HIS:HE1	1:H:153:GLN:OE1	1.77	0.67
1:E:6:HIS:HE1	1:E:153:GLN:OE1	1.77	0.67
1:C:34:VAL:HG23	2:C:201:APR:O2A	1.95	0.66
1:F:29:MET:HG2	1:L:29:MET:HE3	1.76	0.66
1:N:29:MET:HE1	1:N:47:LEU:HD11	1.78	0.66
1:C:29:MET:HE2	1:C:54:ARG:HG3	1.77	0.66
1:O:29:MET:HE2	1:O:54:ARG:HG3	1.78	0.65
1:F:29:MET:HE3	1:F:54:ARG:HG3	1.78	0.65
1:A:6:HIS:HE1	1:A:153:GLN:OE1	1.80	0.65
1:A:168:GLU:OE2	1:D:168:GLU:OE2	2.15	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:40:ARG:HG2	3:H:202:SO4:O1	1.95	0.65
1:A:172:THR:HG21	1:D:9:GLN:HB2	1.79	0.64
1:L:163:ASN:ND2	6:L:301:HOH:O	2.18	0.64
1:B:172:THR:C	1:B:173:GLN:HE21	2.01	0.64
1:M:6:HIS:HE1	1:M:153:GLN:OE1	1.78	0.64
1:L:6:HIS:HE1	1:L:153:GLN:OE1	1.81	0.64
1:D:164:ALA:O	1:D:168:GLU:CG	2.46	0.63
1:A:165:HIS:CE1	1:D:165:HIS:CD2	2.86	0.63
1:N:94:ASP:OD1	1:N:95:GLN:N	2.31	0.63
1:F:2:LYS:HG3	1:F:4:ARG:H	1.64	0.63
1:O:164:ALA:O	1:O:168:GLU:HG3	1.98	0.63
1:B:2:LYS:HE2	1:B:3:THR:CG2	2.29	0.62
1:B:125:VAL:HG13	2:B:201:APR:O1A	1.99	0.62
1:D:161:GLU:HG2	1:D:165:HIS:CE1	2.34	0.62
1:L:158:CYS:HA	6:L:301:HOH:O	2.00	0.62
1:L:3:THR:CG2	1:L:4:ARG:H	2.11	0.62
1:O:147:ARG:NH2	3:O:202:SO4:S	2.71	0.62
1:B:173:GLN:N	1:B:173:GLN:HE21	1.98	0.61
1:L:3:THR:HG23	1:L:4:ARG:N	2.13	0.61
1:C:54:ARG:HH21	1:C:54:ARG:HG3	1.65	0.61
1:O:124:GLY:HA3	2:O:201:APR:O1A	2.01	0.60
1:B:34:VAL:HG23	2:B:201:APR:O2A	2.01	0.60
1:F:163:ASN:ND2	1:F:167:TYR:CD1	2.70	0.60
1:F:29:MET:HG2	1:L:29:MET:CE	2.31	0.60
1:O:106:ARG:NE	3:O:202:SO4:O1	2.31	0.60
1:F:29:MET:HB3	1:L:29:MET:HB2	1.84	0.59
1:A:88:GLY:O	1:A:93:GLU:CD	2.38	0.59
1:F:164:ALA:O	1:F:168:GLU:HG3	2.02	0.59
1:L:147:ARG:HG3	1:L:148:HIS:CD2	2.37	0.59
1:R:130:ARG:NH1	6:R:302:HOH:O	2.34	0.59
1:K:6:HIS:HE1	1:K:153:GLN:OE1	1.86	0.59
1:K:11:ASP:OD1	2:K:201:APR:N6	2.34	0.58
1:N:126:TYR:CE1	2:N:201:APR:HR'4	2.38	0.58
1:D:57:GLN:OE1	1:I:57:GLN:CG	2.52	0.58
1:Q:29:MET:CE	1:Q:51:LEU:HD22	2.32	0.58
1:L:160:ASP:OD1	1:L:163:ASN:HB2	2.04	0.58
1:B:56:GLN:NE2	1:H:53:VAL:HG22	2.18	0.57
1:D:144:PHE:HE2	3:D:202:SO4:O3	1.87	0.57
1:M:29:MET:HE2	1:M:54:ARG:HG3	1.86	0.57
1:A:34:VAL:HG23	2:A:201:APR:O2A	2.04	0.57
1:C:29:MET:HE1	1:C:51:LEU:HA	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:145:ILE:HD11	1:K:154:VAL:HG23	1.86	0.56
1:R:160:ASP:OD1	1:R:163:ASN:HB2	2.05	0.56
1:A:6:HIS:CD2	1:D:6:HIS:CD2	2.93	0.56
1:L:34:VAL:HG23	2:L:201:APR:O2A	2.05	0.56
1:C:29:MET:HE1	1:C:51:LEU:HD23	1.88	0.56
1:F:2:LYS:CG	1:F:4:ARG:H	2.17	0.56
1:C:125:VAL:HG13	2:C:201:APR:O1A	2.06	0.56
1:P:2:LYS:HE3	1:P:145:ILE:HD11	1.87	0.56
1:H:161:GLU:O	1:H:162:GLU:C	2.42	0.56
1:L:165:HIS:O	1:L:169:ARG:HG3	2.06	0.56
1:A:147:ARG:NH1	3:A:202:SO4:O1	2.35	0.56
1:L:147:ARG:NH2	3:L:202:SO4:O4	2.39	0.56
1:C:9:GLN:HB3	1:Q:172:THR:HG21	1.87	0.55
1:N:29:MET:CE	1:N:29:MET:HA	2.37	0.55
1:J:69:LEU:C	1:J:69:LEU:HD23	2.26	0.55
1:I:4:ARG:NH2	1:I:145:ILE:HB	2.21	0.55
1:E:147:ARG:NH1	3:E:202:SO4:O3	2.39	0.55
1:J:29:MET:CE	1:J:51:LEU:HD23	2.34	0.55
1:I:2:LYS:CB	1:I:3:THR:HA	2.34	0.55
1:B:2:LYS:HG3	1:B:3:THR:N	2.07	0.55
1:C:9:GLN:HE22	1:C:161:GLU:HG3	1.72	0.55
1:F:9:GLN:OE1	1:F:161:GLU:CB	2.51	0.55
1:F:29:MET:HE1	1:F:54:ARG:HG3	1.89	0.54
1:B:173:GLN:N	1:B:173:GLN:NE2	2.54	0.54
1:P:126:TYR:CD1	2:P:201:APR:H5R1	2.43	0.54
1:M:29:MET:HE3	1:M:51:LEU:HD23	1.88	0.54
1:P:130:ARG:H	1:P:130:ARG:CD	2.21	0.54
1:G:160:ASP:OD1	1:G:163:ASN:HB2	2.08	0.54
1:R:106:ARG:NH1	1:Q:40:ARG:HH21	2.05	0.54
1:F:132:ALA:O	1:F:135:GLU:HB3	2.07	0.54
1:M:25:ALA:CB	5:M:201:ZOD:H1	2.38	0.54
1:F:29:MET:HB3	1:L:29:MET:CB	2.37	0.53
1:F:9:GLN:OE1	1:F:161:GLU:CA	2.56	0.53
1:F:172:THR:HG22	1:F:172:THR:O	2.08	0.53
1:J:69:LEU:HD23	1:J:69:LEU:O	2.08	0.53
1:C:4:ARG:NH2	1:C:145:ILE:O	2.40	0.53
1:J:29:MET:CE	1:J:51:LEU:CD2	2.87	0.53
1:N:2:LYS:O	1:N:2:LYS:CD	2.57	0.53
1:I:29:MET:HE2	1:I:54:ARG:HG3	1.90	0.53
1:D:141:VAL:HG11	1:D:154:VAL:HG21	1.91	0.52
1:B:2:LYS:CG	1:B:3:THR:H	2.03	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:29:MET:HE3	1:N:29:MET:HA	1.92	0.52
1:F:163:ASN:C	1:F:163:ASN:HD22	2.12	0.52
1:L:135:GLU:HG3	1:L:170:LEU:HD22	1.92	0.52
1:Q:131:ALA:O	1:Q:135:GLU:HG3	2.09	0.52
1:O:29:MET:HE1	1:O:51:LEU:HA	1.92	0.52
1:I:164:ALA:O	1:I:168:GLU:HG3	2.10	0.52
1:P:29:MET:HE3	1:P:51:LEU:CD2	2.40	0.52
1:A:169:ARG:O	1:A:173:GLN:HB2	2.10	0.52
1:O:130:ARG:CD	1:O:130:ARG:H	2.21	0.52
1:P:143:GLU:O	1:P:147:ARG:HG3	2.10	0.52
1:P:173:GLN:O	1:P:173:GLN:HG2	2.10	0.51
1:P:6:HIS:CE1	6:P:307:HOH:O	2.63	0.51
1:C:27:SER:HB2	1:C:54:ARG:HH22	1.74	0.51
1:C:6:HIS:HB3	6:Q:501:HOH:O	2.09	0.51
1:C:27:SER:O	1:C:54:ARG:NH2	2.43	0.51
1:F:29:MET:HG2	1:L:29:MET:HB3	1.91	0.51
1:G:103:ASN:N	1:G:103:ASN:HD22	2.08	0.51
1:C:143:GLU:O	1:C:147:ARG:HG3	2.09	0.51
1:D:143:GLU:O	1:D:147:ARG:HG3	2.10	0.51
1:I:173:GLN:HA	1:I:174:GLN:HB2	1.92	0.51
1:F:2:LYS:HG3	1:F:3:THR:N	2.26	0.51
1:H:143:GLU:O	1:H:147:ARG:HG3	2.10	0.51
1:A:171:LEU:O	1:A:174:GLN:HG2	2.11	0.51
1:G:143:GLU:O	1:G:147:ARG:HG3	2.10	0.51
1:K:160:ASP:OD1	1:K:163:ASN:HB2	2.10	0.51
1:E:143:GLU:O	1:E:147:ARG:HG3	2.11	0.50
1:E:39:HIS:ND1	6:E:301:HOH:O	2.35	0.50
1:J:95:GLN:OE1	1:J:98:GLN:NE2	2.45	0.50
1:G:57:GLN:OE1	1:Q:57:GLN:HB3	2.11	0.50
1:M:106:ARG:NH2	3:M:202:SO4:O4	2.45	0.50
1:M:25:ALA:HB2	5:M:201:ZOD:H1	1.93	0.50
1:R:143:GLU:O	1:R:147:ARG:HG3	2.11	0.50
1:J:143:GLU:O	1:J:147:ARG:HG3	2.12	0.50
1:R:34:VAL:HG23	2:R:201:APR:O2A	2.12	0.50
1:Q:143:GLU:O	1:Q:147:ARG:HG3	2.12	0.50
1:A:139:LYS:HG2	1:A:143:GLU:OE1	2.11	0.49
1:D:95:GLN:NE2	1:D:98:GLN:NE2	2.61	0.49
1:D:95:GLN:HE22	1:D:98:GLN:NE2	2.10	0.49
1:F:29:MET:CG	1:L:29:MET:HE2	2.42	0.49
1:K:143:GLU:O	1:K:147:ARG:HG3	2.12	0.49
1:F:163:ASN:ND2	1:F:167:TYR:HD1	2.09	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:32:GLY:O	2:O:201:APR:O1D	2.30	0.49
1:A:165:HIS:ND1	1:D:165:HIS:CD2	2.81	0.49
1:B:161:GLU:HG3	6:B:314:HOH:O	2.10	0.49
1:R:27:SER:O	1:R:54:ARG:HD2	2.12	0.49
1:D:95:GLN:NE2	1:D:98:GLN:HE21	2.11	0.49
1:F:143:GLU:O	1:F:147:ARG:HG3	2.13	0.49
1:J:122:SER:HA	2:J:201:APR:O1B	2.12	0.49
1:A:29:MET:CE	1:A:51:LEU:HD23	2.43	0.49
1:H:161:GLU:HG3	1:H:162:GLU:N	2.26	0.49
1:K:4:ARG:NH2	1:K:145:ILE:HG23	2.27	0.49
1:M:143:GLU:O	1:M:147:ARG:HG3	2.13	0.49
1:N:143:GLU:O	1:N:147:ARG:HG3	2.12	0.49
1:P:8:VAL:HG23	6:P:314:HOH:O	2.13	0.49
1:F:169:ARG:HH11	1:F:169:ARG:CG	2.23	0.49
1:L:125:VAL:HG13	2:L:201:APR:O1A	2.12	0.49
1:P:29:MET:CE	1:P:51:LEU:HD23	2.40	0.49
1:N:29:MET:HE3	1:N:47:LEU:HD12	1.93	0.49
1:M:106:ARG:CZ	3:M:202:SO4:O4	2.60	0.48
1:F:29:MET:CG	1:L:29:MET:CE	2.91	0.48
1:J:95:GLN:HE22	1:J:98:GLN:HE21	1.59	0.48
1:C:2:LYS:C	1:C:3:THR:HG22	2.32	0.48
1:L:126:TYR:CE1	2:L:201:APR:HR'4	2.48	0.48
1:A:143:GLU:O	1:A:147:ARG:HG3	2.13	0.48
1:B:47:LEU:O	1:B:51:LEU:HD22	2.13	0.48
1:D:120:ALA:O	2:D:201:APR:H'4	2.13	0.48
1:E:51:LEU:HD11	1:Q:51:LEU:HD11	1.96	0.48
1:A:29:MET:HE1	1:A:51:LEU:HD23	1.96	0.48
1:E:125:VAL:HG13	2:E:201:APR:O1A	2.14	0.48
1:H:4:ARG:NH2	1:H:145:ILE:HG23	2.29	0.48
1:I:160:ASP:OD1	1:I:163:ASN:HB2	2.13	0.48
1:C:29:MET:CE	1:C:51:LEU:HD23	2.43	0.48
1:I:72:ASP:OD2	1:P:148:HIS:ND1	2.34	0.48
1:L:32:GLY:O	2:L:201:APR:O1D	2.27	0.47
1:O:29:MET:CE	1:O:51:LEU:HD23	2.44	0.47
1:Q:126:TYR:CE1	2:Q:402:APR:HR'4	2.50	0.47
1:G:34:VAL:HG23	2:G:201:APR:O2A	2.14	0.47
1:J:29:MET:HE1	1:J:51:LEU:CD2	2.37	0.47
1:M:29:MET:CE	1:M:51:LEU:HD23	2.45	0.47
1:O:126:TYR:CE1	2:O:201:APR:HR'4	2.50	0.47
1:K:20:ILE:HG22	1:K:117:ALA:HB3	1.96	0.47
1:D:122:SER:N	2:D:201:APR:O1B	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:27:SER:O	1:F:28:LEU:HB2	2.15	0.46
1:J:29:MET:HE3	1:J:51:LEU:HD21	1.98	0.46
1:M:19:VAL:HG22	1:M:116:VAL:HG23	1.98	0.46
1:F:4:ARG:NH2	1:F:145:ILE:HG23	2.31	0.46
1:Q:147:ARG:NH2	3:Q:403:SO4:S	2.86	0.46
1:Q:34:VAL:HG23	2:Q:402:APR:O2A	2.15	0.46
1:A:108:VAL:HG21	1:A:116:VAL:CG1	2.43	0.46
1:I:143:GLU:O	1:I:147:ARG:HG3	2.15	0.46
1:I:2:LYS:HB3	1:I:3:THR:CA	2.43	0.46
1:R:2:LYS:HG2	1:R:3:THR:H	1.79	0.46
1:J:19:VAL:HG22	1:J:116:VAL:HG23	1.97	0.46
1:N:2:LYS:HE2	1:N:4:ARG:HB2	1.98	0.46
1:I:72:ASP:HB3	1:P:147:ARG:O	2.16	0.46
1:E:87:ARG:HG2	1:E:87:ARG:NH2	2.27	0.46
1:D:123:THR:OG1	2:D:201:APR:O3'	2.27	0.46
1:F:169:ARG:NH1	1:F:169:ARG:HG3	2.28	0.46
1:C:2:LYS:O	1:C:3:THR:CG2	2.44	0.46
1:G:19:VAL:HG22	1:G:116:VAL:HG23	1.97	0.46
1:P:147:ARG:NH1	3:P:202:SO4:O1	2.49	0.46
1:F:163:ASN:HD21	1:F:167:TYR:HE1	1.58	0.45
1:D:122:SER:HA	2:D:201:APR:O1B	2.16	0.45
1:Q:125:VAL:HG13	2:Q:402:APR:O1A	2.17	0.45
1:E:160:ASP:OD1	1:E:163:ASN:HB2	2.16	0.45
1:B:19:VAL:HG22	1:B:116:VAL:HG23	1.99	0.45
1:E:87:ARG:CG	1:E:87:ARG:HH21	2.25	0.45
1:F:164:ALA:O	1:F:168:GLU:CG	2.64	0.45
1:K:120:ALA:O	2:K:201:APR:H5'1	2.16	0.45
1:K:34:VAL:HG23	2:K:201:APR:O2A	2.15	0.45
1:B:160:ASP:OD1	1:B:163:ASN:HB2	2.17	0.45
1:D:62:THR:HG21	1:D:96:LEU:CD2	2.45	0.45
1:N:135:GLU:CA	1:N:170:LEU:HD21	2.32	0.45
1:O:19:VAL:HG22	1:O:116:VAL:HG23	1.99	0.45
1:N:19:VAL:HG22	1:N:116:VAL:HG23	1.98	0.44
1:O:160:ASP:OD1	1:O:163:ASN:HB2	2.17	0.44
1:P:29:MET:HE2	1:P:54:ARG:HG3	1.99	0.44
1:D:19:VAL:HG22	1:D:116:VAL:HG23	1.99	0.44
1:J:34:VAL:HG22	1:J:38:ILE:CD1	2.48	0.44
1:Q:19:VAL:HG22	1:Q:116:VAL:HG23	1.99	0.44
1:C:147:ARG:NH1	3:C:202:SO4:S	2.90	0.44
1:K:9:GLN:HG3	1:K:164:ALA:HB2	1.99	0.44
1:P:2:LYS:HB3	1:P:4:ARG:H	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:160:ASP:OD1	1:Q:163:ASN:HB2	2.17	0.44
1:A:57:GLN:HB3	1:L:57:GLN:HE22	1.81	0.44
1:I:19:VAL:HG22	1:I:116:VAL:HG23	1.98	0.44
1:D:170:LEU:O	1:D:171:LEU:HB2	2.17	0.44
1:M:29:MET:HE1	1:M:51:LEU:HA	1.98	0.44
1:R:169:ARG:HB2	6:R:308:HOH:O	2.17	0.44
1:B:17:VAL:O	1:B:75:ALA:HA	2.18	0.43
1:F:147:ARG:O	1:G:72:ASP:HB3	2.18	0.43
1:B:130:ARG:H	1:B:130:ARG:NE	2.11	0.43
1:C:19:VAL:HG22	1:C:116:VAL:HG23	2.00	0.43
1:Q:161:GLU:HG2	1:Q:165:HIS:CE1	2.53	0.43
1:J:95:GLN:NE2	1:J:98:GLN:HE21	2.16	0.43
1:K:19:VAL:HG22	1:K:116:VAL:HG23	2.01	0.43
1:L:171:LEU:C	1:L:173:GLN:H	2.21	0.43
1:D:88:GLY:N	1:D:93:GLU:OE1	2.52	0.43
1:H:92:ASN:HA	6:H:304:HOH:O	2.18	0.43
1:A:29:MET:HE3	1:A:51:LEU:CD2	2.48	0.43
1:F:33:GLY:HA3	5:F:201:ZOD:PA	2.58	0.43
1:F:95:GLN:CA	1:F:95:GLN:HE21	2.32	0.43
1:I:17:VAL:O	1:I:75:ALA:HA	2.19	0.43
1:G:29:MET:HB3	1:K:29:MET:HG3	2.01	0.43
1:R:57:GLN:HE22	1:E:57:GLN:HB3	1.84	0.42
1:H:34:VAL:HG23	2:H:201:APR:O2A	2.19	0.42
1:N:147:ARG:HD2	6:N:310:HOH:O	2.19	0.42
1:B:147:ARG:NH2	3:B:202:SO4:O2	2.45	0.42
1:D:166:LEU:O	1:D:170:LEU:HD22	2.18	0.42
1:N:84:PRO:CG	1:N:96:LEU:HD12	2.47	0.42
1:J:57:GLN:OE1	1:J:66:VAL:HG11	2.19	0.42
1:F:171:LEU:C	1:F:173:GLN:H	2.21	0.42
1:N:57:GLN:O	1:N:57:GLN:HG3	2.20	0.42
1:A:29:MET:HE3	1:A:51:LEU:HD21	2.02	0.42
1:B:169:ARG:HB2	1:B:169:ARG:HE	1.70	0.42
1:H:19:VAL:HG22	1:H:116:VAL:HG23	2.00	0.42
1:Q:171:LEU:O	1:Q:174:GLN:HB3	2.20	0.42
1:D:148:HIS:CE1	1:M:40:ARG:O	2.73	0.42
1:E:87:ARG:CG	1:E:87:ARG:NH2	2.82	0.42
1:I:6:HIS:CE1	1:I:153:GLN:OE1	2.62	0.41
1:M:9:GLN:HE22	1:M:161:GLU:HB2	1.84	0.41
1:K:40:ARG:O	1:Q:148:HIS:HE1	2.03	0.41
1:A:27:SER:O	1:A:28:LEU:HB2	2.20	0.41
1:J:49:ALA:HB2	1:J:69:LEU:HD21	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:20:ILE:HD11	1:J:73:LEU:HD13	2.02	0.41
1:P:124:GLY:HA3	2:P:201:APR:O1A	2.20	0.41
1:B:51:LEU:HD12	1:B:51:LEU:HA	1.73	0.41
1:C:160:ASP:OD1	1:C:163:ASN:HB2	2.21	0.41
1:I:29:MET:HE3	1:I:51:LEU:CD2	2.44	0.41
1:B:11:ASP:HB3	1:B:14:LYS:CD	2.50	0.41
1:O:87:ARG:HB2	1:O:93:GLU:OE2	2.21	0.41
1:F:9:GLN:HE22	1:F:161:GLU:HG2	1.82	0.41
1:K:124:GLY:HA3	2:K:201:APR:O5'	2.21	0.41
1:D:148:HIS:HE1	1:M:40:ARG:O	2.02	0.41
1:N:92:ASN:O	1:N:96:LEU:HG	2.21	0.41
1:B:57:GLN:HB3	1:H:57:GLN:HE22	1.84	0.41
1:K:147:ARG:NH2	3:K:202:SO4:S	2.92	0.41
1:A:168:GLU:CD	1:D:168:GLU:OE2	2.59	0.40
1:J:160:ASP:OD1	1:J:163:ASN:HB2	2.19	0.40
1:J:171:LEU:HA	1:J:171:LEU:HD23	1.97	0.40
1:G:9:GLN:HE22	1:G:161:GLU:HB2	1.85	0.40
1:H:34:VAL:CG2	2:H:201:APR:H5'2	2.51	0.40
1:K:29:MET:CE	1:K:54:ARG:HG3	2.51	0.40
1:G:57:GLN:OE1	1:Q:57:GLN:CB	2.70	0.40
1:E:51:LEU:CD1	1:Q:51:LEU:HD11	2.49	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:D:29:MET:CE	1:D:29:MET:CE[6_554]	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	171/183 (93%)	166 (97%)	5 (3%)	0	100	100
1	B	170/183 (93%)	166 (98%)	4 (2%)	0	100	100
1	C	171/183 (93%)	168 (98%)	3 (2%)	0	100	100
1	D	168/183 (92%)	162 (96%)	6 (4%)	0	100	100
1	E	171/183 (93%)	167 (98%)	4 (2%)	0	100	100
1	F	171/183 (93%)	165 (96%)	6 (4%)	0	100	100
1	G	171/183 (93%)	166 (97%)	5 (3%)	0	100	100
1	H	171/183 (93%)	167 (98%)	4 (2%)	0	100	100
1	I	171/183 (93%)	165 (96%)	6 (4%)	0	100	100
1	J	170/183 (93%)	165 (97%)	5 (3%)	0	100	100
1	K	170/183 (93%)	168 (99%)	2 (1%)	0	100	100
1	L	170/183 (93%)	168 (99%)	2 (1%)	0	100	100
1	M	171/183 (93%)	167 (98%)	4 (2%)	0	100	100
1	N	171/183 (93%)	168 (98%)	3 (2%)	0	100	100
1	O	169/183 (92%)	166 (98%)	3 (2%)	0	100	100
1	P	171/183 (93%)	167 (98%)	4 (2%)	0	100	100
1	Q	171/183 (93%)	168 (98%)	3 (2%)	0	100	100
1	R	171/183 (93%)	168 (98%)	3 (2%)	0	100	100
All	All	3069/3294 (93%)	2997 (98%)	72 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	124/141 (88%)	116 (94%)	8 (6%)	17	44
1	B	130/141 (92%)	117 (90%)	13 (10%)	7	22
1	C	130/141 (92%)	122 (94%)	8 (6%)	18	47

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	121/141 (86%)	110 (91%)	11 (9%)	9	27
1	E	132/141 (94%)	123 (93%)	9 (7%)	16	42
1	F	130/141 (92%)	117 (90%)	13 (10%)	7	22
1	G	128/141 (91%)	117 (91%)	11 (9%)	10	30
1	H	132/141 (94%)	119 (90%)	13 (10%)	8	24
1	I	127/141 (90%)	118 (93%)	9 (7%)	14	39
1	J	130/141 (92%)	119 (92%)	11 (8%)	10	31
1	K	125/141 (89%)	113 (90%)	12 (10%)	8	24
1	L	125/141 (89%)	120 (96%)	5 (4%)	31	65
1	M	129/141 (92%)	118 (92%)	11 (8%)	10	31
1	N	123/141 (87%)	111 (90%)	12 (10%)	8	24
1	O	129/141 (92%)	120 (93%)	9 (7%)	15	40
1	P	128/141 (91%)	120 (94%)	8 (6%)	18	46
1	Q	131/141 (93%)	120 (92%)	11 (8%)	11	31
1	R	129/141 (92%)	119 (92%)	10 (8%)	12	35
All	All	2303/2538 (91%)	2119 (92%)	184 (8%)	12	34

All (184) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	R	14	LYS
1	R	34	VAL
1	R	46	LEU
1	R	54	ARG
1	R	55	GLN
1	R	146	THR
1	R	163	ASN
1	R	166	LEU
1	R	168	GLU
1	R	172	THR
1	A	3	THR
1	A	34	VAL
1	A	46	LEU
1	A	54	ARG
1	A	55	GLN
1	A	57	GLN
1	A	121	ILE

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Mol	Chain	Res	Type
1	A	166	LEU
1	B	19	VAL
1	B	34	VAL
1	B	46	LEU
1	B	51	LEU
1	B	54	ARG
1	B	55	GLN
1	B	57	GLN
1	B	90	GLU
1	B	130	ARG
1	B	161	GLU
1	B	166	LEU
1	B	169	ARG
1	B	173	GLN
1	C	19	VAL
1	C	34	VAL
1	C	40	ARG
1	C	46	LEU
1	C	54	ARG
1	C	130	ARG
1	C	166	LEU
1	C	172	THR
1	D	8	VAL
1	D	19	VAL
1	D	34	VAL
1	D	46	LEU
1	D	52	LYS
1	D	54	ARG
1	D	55	GLN
1	D	95	GLN
1	D	154	VAL
1	D	170	LEU
1	D	171	LEU
1	E	8	VAL
1	E	34	VAL
1	E	46	LEU
1	E	54	ARG
1	E	55	GLN
1	E	130	ARG
1	E	166	LEU
1	E	169	ARG
1	E	173	GLN

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Mol	Chain	Res	Type
1	F	2	LYS
1	F	3	THR
1	F	14	LYS
1	F	34	VAL
1	F	46	LEU
1	F	54	ARG
1	F	69	LEU
1	F	95	GLN
1	F	145	ILE
1	F	163	ASN
1	F	166	LEU
1	F	168	GLU
1	F	174	GLN
1	G	2	LYS
1	G	8	VAL
1	G	15	LEU
1	G	19	VAL
1	G	34	VAL
1	G	46	LEU
1	G	54	ARG
1	G	55	GLN
1	G	147	ARG
1	G	161	GLU
1	G	166	LEU
1	H	8	VAL
1	H	19	VAL
1	H	34	VAL
1	H	46	LEU
1	H	54	ARG
1	H	55	GLN
1	H	90	GLU
1	H	145	ILE
1	H	160	ASP
1	H	161	GLU
1	H	166	LEU
1	H	169	ARG
1	H	174	GLN
1	I	2	LYS
1	I	19	VAL
1	I	34	VAL
1	I	46	LEU
1	I	54	ARG

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Mol	Chain	Res	Type
1	I	55	GLN
1	I	163	ASN
1	I	166	LEU
1	I	169	ARG
1	J	8	VAL
1	J	9	GLN
1	J	19	VAL
1	J	46	LEU
1	J	54	ARG
1	J	57	GLN
1	J	69	LEU
1	J	95	GLN
1	J	98	GLN
1	J	107	LEU
1	J	166	LEU
1	K	3	THR
1	K	19	VAL
1	K	34	VAL
1	K	46	LEU
1	K	54	ARG
1	K	55	GLN
1	K	57	GLN
1	K	96	LEU
1	K	145	ILE
1	K	161	GLU
1	K	166	LEU
1	K	173	GLN
1	L	34	VAL
1	L	46	LEU
1	L	54	ARG
1	L	55	GLN
1	L	147	ARG
1	M	2	LYS
1	M	19	VAL
1	M	34	VAL
1	M	46	LEU
1	M	54	ARG
1	M	55	GLN
1	M	87	ARG
1	M	95	GLN
1	M	98	GLN
1	M	135	GLU

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Mol	Chain	Res	Type
1	M	166	LEU
1	N	2	LYS
1	N	19	VAL
1	N	34	VAL
1	N	46	LEU
1	N	54	ARG
1	N	95	GLN
1	N	96	LEU
1	N	135	GLU
1	N	166	LEU
1	N	169	ARG
1	N	170	LEU
1	N	173	GLN
1	O	19	VAL
1	O	34	VAL
1	O	46	LEU
1	O	54	ARG
1	O	55	GLN
1	O	95	GLN
1	O	130	ARG
1	O	166	LEU
1	O	173	GLN
1	P	34	VAL
1	P	46	LEU
1	P	54	ARG
1	P	87	ARG
1	P	130	ARG
1	P	160	ASP
1	P	166	LEU
1	P	174	GLN
1	Q	3	THR
1	Q	8	VAL
1	Q	19	VAL
1	Q	34	VAL
1	Q	46	LEU
1	Q	51	LEU
1	Q	54	ARG
1	Q	55	GLN
1	Q	87	ARG
1	Q	166	LEU
1	Q	169	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (83) such

sidechains are listed below:

Mol	Chain	Res	Type
1	R	6	HIS
1	R	9	GLN
1	R	56	GLN
1	R	57	GLN
1	R	92	ASN
1	R	103	ASN
1	A	6	HIS
1	A	56	GLN
1	A	103	ASN
1	B	56	GLN
1	B	57	GLN
1	B	103	ASN
1	B	173	GLN
1	C	9	GLN
1	C	92	ASN
1	C	103	ASN
1	C	163	ASN
1	C	174	GLN
1	D	6	HIS
1	D	92	ASN
1	D	95	GLN
1	D	98	GLN
1	D	103	ASN
1	D	148	HIS
1	D	165	HIS
1	E	6	HIS
1	E	92	ASN
1	E	103	ASN
1	F	92	ASN
1	F	95	GLN
1	F	103	ASN
1	F	174	GLN
1	G	9	GLN
1	G	103	ASN
1	H	6	HIS
1	H	9	GLN
1	H	57	GLN
1	H	92	ASN
1	H	103	ASN
1	H	163	ASN
1	H	174	GLN
1	I	6	HIS

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Mol	Chain	Res	Type
1	I	57	GLN
1	I	103	ASN
1	I	163	ASN
1	J	95	GLN
1	J	98	GLN
1	J	103	ASN
1	J	163	ASN
1	J	174	GLN
1	K	6	HIS
1	K	57	GLN
1	K	91	GLN
1	K	95	GLN
1	K	103	ASN
1	K	174	GLN
1	L	6	HIS
1	L	56	GLN
1	L	57	GLN
1	L	92	ASN
1	L	103	ASN
1	L	174	GLN
1	M	6	HIS
1	M	9	GLN
1	M	39	HIS
1	M	57	GLN
1	M	92	ASN
1	M	103	ASN
1	M	174	GLN
1	N	103	ASN
1	N	173	GLN
1	O	98	GLN
1	O	103	ASN
1	P	39	HIS
1	P	92	ASN
1	P	98	GLN
1	P	103	ASN
1	P	163	ASN
1	P	174	GLN
1	Q	56	GLN
1	Q	92	ASN
1	Q	103	ASN
1	Q	173	GLN



### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

39 ligands are modelled in this entry.

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
3	SO4	D	202	-	4,4,4	0.36	0	6,6,6	0.55	0
2	APR	J	201	-	34,39,39	1.02	2 (5%)	40,60,60	1.72	8 (20%)
2	APR	I	201	-	34,39,39	1.24	5 (14%)	40,60,60	1.58	4 (10%)
2	APR	G	201	-	34,39,39	1.21	3 (8%)	40,60,60	1.61	8 (20%)
3	SO4	L	202	-	4,4,4	0.60	0	6,6,6	0.59	0
2	APR	C	201	-	34,39,39	0.89	0	40,60,60	1.52	8 (20%)
4	ACT	J	203	-	1,3,3	3.35	1 (100%)	0,3,3	0.00	-
4	ACT	C	203	-	1,3,3	2.63	1 (100%)	0,3,3	0.00	-
3	SO4	O	202	-	4,4,4	0.55	0	6,6,6	0.98	0
3	SO4	I	202	-	4,4,4	0.43	0	6,6,6	0.58	0
3	SO4	C	202	-	4,4,4	0.55	0	6,6,6	1.08	0
5	ZOD	M	201	-	36,42,42	1.41	6 (16%)	42,64,64	1.51	7 (16%)
2	APR	L	201	-	34,39,39	1.31	4 (11%)	40,60,60	1.91	10 (25%)
3	SO4	K	202	-	4,4,4	0.37	0	6,6,6	0.40	0
2	APR	D	201	-	34,39,39	1.50	3 (8%)	40,60,60	2.05	11 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	SO4	P	202	-	4,4,4	0.42	0	6,6,6	0.33	0
3	SO4	G	202	-	4,4,4	0.65	0	6,6,6	0.69	0
2	APR	R	201	-	34,39,39	1.04	1 (2%)	40,60,60	1.66	7 (17%)
3	SO4	B	202	-	4,4,4	0.46	0	6,6,6	0.41	0
2	APR	Q	402	-	34,39,39	1.15	4 (11%)	40,60,60	1.37	5 (12%)
2	APR	K	201	-	34,39,39	1.25	5 (14%)	40,60,60	1.87	8 (20%)
5	ZOD	F	201	-	36,42,42	1.51	8 (22%)	42,64,64	1.69	7 (16%)
2	APR	E	201	-	34,39,39	0.96	3 (8%)	40,60,60	2.02	12 (30%)
3	SO4	N	202	-	4,4,4	0.35	0	6,6,6	0.99	0
3	SO4	A	202	-	4,4,4	0.50	0	6,6,6	0.49	0
3	SO4	E	202	-	4,4,4	0.35	0	6,6,6	0.71	0
2	APR	O	201	-	34,39,39	0.96	1 (2%)	40,60,60	1.33	4 (10%)
2	APR	N	201	-	34,39,39	1.17	4 (11%)	40,60,60	1.51	8 (20%)
3	SO4	F	202	-	4,4,4	0.50	0	6,6,6	0.36	0
3	SO4	H	202	-	4,4,4	0.28	0	6,6,6	0.99	0
3	SO4	J	202	-	4,4,4	0.46	0	6,6,6	0.72	0
4	ACT	Q	401	-	1,3,3	1.56	0	0,3,3	0.00	-
2	APR	B	201	-	34,39,39	1.14	3 (8%)	40,60,60	1.54	8 (20%)
2	APR	A	201	-	34,39,39	1.15	4 (11%)	40,60,60	1.50	4 (10%)
2	APR	P	201	-	34,39,39	1.19	4 (11%)	40,60,60	1.81	10 (25%)
3	SO4	R	202	-	4,4,4	0.30	0	6,6,6	0.80	0
2	APR	H	201	-	34,39,39	1.20	3 (8%)	40,60,60	1.69	9 (22%)
3	SO4	Q	403	-	4,4,4	0.30	0	6,6,6	0.76	0
3	SO4	M	202	-	4,4,4	0.45	0	6,6,6	0.44	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	APR	N	201	-	-	4/18/54/54	0/4/4/4
2	APR	L	201	-	-	3/18/54/54	0/4/4/4
2	APR	K	201	-	-	7/18/54/54	0/4/4/4
2	APR	J	201	-	-	4/18/54/54	0/4/4/4
2	APR	I	201	-	-	8/18/54/54	0/4/4/4
2	APR	G	201	-	-	7/18/54/54	0/4/4/4
2	APR	E	201	-	-	3/18/54/54	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	APR	D	201	-	-	7/18/54/54	0/4/4/4
2	APR	C	201	-	-	3/18/54/54	0/4/4/4
2	APR	B	201	-	-	1/18/54/54	0/4/4/4
2	APR	Q	402	-	-	5/18/54/54	0/4/4/4
2	APR	P	201	-	-	10/18/54/54	0/4/4/4
2	APR	A	201	-	-	4/18/54/54	0/4/4/4
2	APR	H	201	-	-	6/18/54/54	0/4/4/4
5	ZOD	F	201	-	-	8/22/58/58	0/4/4/4
2	APR	R	201	-	-	8/18/54/54	0/4/4/4
5	ZOD	M	201	-	-	6/22/58/58	0/4/4/4
2	APR	O	201	-	-	4/18/54/54	0/4/4/4

All (65) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	201	APR	O4'-C1'	5.20	1.48	1.41
2	D	201	APR	O4D-C1D	4.10	1.48	1.43
2	K	201	APR	O4'-C1'	4.00	1.46	1.41
5	F	201	ZOD	C2-N3	3.80	1.38	1.32
2	H	201	APR	C2'-C1'	-3.65	1.48	1.53
5	M	201	ZOD	C6-N6	3.64	1.47	1.34
2	Q	402	APR	C1D-C2D	-3.42	1.48	1.52
4	J	203	ACT	CH3-C	3.35	1.53	1.48
5	M	201	ZOD	C2-N3	3.33	1.37	1.32
2	I	201	APR	C2-N3	3.28	1.37	1.32
5	F	201	ZOD	O08-C06	3.20	1.47	1.43
2	P	201	APR	C2-N3	3.15	1.37	1.32
5	F	201	ZOD	C6-N6	3.12	1.45	1.34
2	E	201	APR	C2'-C1'	-3.11	1.49	1.53
2	A	201	APR	C5-C4	3.09	1.49	1.40
2	L	201	APR	O4'-C1'	3.07	1.45	1.41
2	B	201	APR	C5-C4	2.96	1.48	1.40
2	P	201	APR	C5-C4	2.93	1.48	1.40
5	F	201	ZOD	C2'-C1'	-2.92	1.49	1.53
2	R	201	APR	C2'-C1'	-2.88	1.49	1.53
2	L	201	APR	C5-C4	2.88	1.48	1.40
2	K	201	APR	C5-C4	2.87	1.48	1.40
2	L	201	APR	C2'-C1'	-2.86	1.49	1.53
2	A	201	APR	O4'-C1'	2.76	1.44	1.41
5	F	201	ZOD	O4'-C1'	2.75	1.44	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	203	ACT	CH3-C	2.63	1.52	1.48
2	B	201	APR	C2'-C1'	-2.61	1.49	1.53
2	N	201	APR	C5-C4	2.53	1.47	1.40
5	M	201	ZOD	O04-C05	-2.50	1.41	1.44
2	O	201	APR	C5-C4	2.50	1.47	1.40
2	E	201	APR	O4'-C4'	-2.48	1.39	1.45
5	M	201	ZOD	O4'-C1'	2.48	1.44	1.41
2	G	201	APR	O4'-C1'	2.48	1.44	1.41
2	I	201	APR	O4'-C1'	2.47	1.44	1.41
2	N	201	APR	C2-N3	2.47	1.36	1.32
2	I	201	APR	O4D-C1D	2.46	1.46	1.43
5	M	201	ZOD	C4-N3	2.41	1.39	1.35
2	H	201	APR	C2-N3	2.41	1.36	1.32
2	N	201	APR	O4'-C1'	2.33	1.44	1.41
2	A	201	APR	C8-N7	2.32	1.38	1.34
2	P	201	APR	C8-N7	2.28	1.38	1.34
2	A	201	APR	C2-N3	2.28	1.35	1.32
2	K	201	APR	C2-N3	2.27	1.35	1.32
2	J	201	APR	C5-C4	2.26	1.46	1.40
2	B	201	APR	O4D-C1D	2.26	1.46	1.43
2	L	201	APR	C2-N3	2.23	1.35	1.32
2	D	201	APR	C5-N7	-2.22	1.31	1.39
2	K	201	APR	C8-N7	2.18	1.38	1.34
2	G	201	APR	C5-C4	2.18	1.46	1.40
2	P	201	APR	C2'-C1'	-2.17	1.50	1.53
5	F	201	ZOD	C4-N3	2.16	1.38	1.35
2	J	201	APR	C1D-C2D	-2.13	1.50	1.52
2	G	201	APR	O1D-C1D	2.11	1.46	1.39
2	Q	402	APR	C5-C4	2.11	1.46	1.40
2	N	201	APR	O4'-C4'	-2.10	1.40	1.45
2	H	201	APR	C5-C4	2.09	1.46	1.40
5	F	201	ZOD	O04-C05	-2.09	1.41	1.44
2	I	201	APR	C2'-C1'	-2.09	1.50	1.53
2	I	201	APR	C5-C4	2.08	1.46	1.40
2	Q	402	APR	O4D-C1D	2.07	1.45	1.43
5	M	201	ZOD	C2'-C1'	-2.04	1.50	1.53
2	K	201	APR	C6-C5	2.03	1.50	1.43
5	F	201	ZOD	C38-C05	-2.02	1.48	1.52
2	E	201	APR	C5-C4	2.02	1.46	1.40
2	Q	402	APR	C2'-C1'	-2.01	1.50	1.53

All (138) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	201	APR	C1'-N9-C4	-6.63	115.00	126.64
2	K	201	APR	C1'-N9-C4	-5.53	116.92	126.64
2	I	201	APR	C4-C5-N7	-5.09	104.10	109.40
5	F	201	ZOD	O04-C02-O03	-4.97	113.08	122.96
2	D	201	APR	O2'-C2'-C3'	-4.85	96.12	111.82
2	A	201	APR	O3'-C3'-C4'	-4.68	97.51	111.05
2	R	201	APR	N3-C2-N1	-4.67	121.37	128.68
2	K	201	APR	PB-O3A-PA	-4.57	117.15	132.83
2	L	201	APR	C1'-N9-C4	-4.53	118.67	126.64
2	D	201	APR	O1D-C1D-O4D	4.43	116.80	111.13
2	J	201	APR	O1D-C1D-O4D	-4.40	105.50	111.13
2	K	201	APR	C1D-C2D-C3D	4.37	107.78	102.30
2	J	201	APR	C1'-N9-C4	-4.29	119.10	126.64
2	I	201	APR	PB-O3A-PA	-4.29	118.10	132.83
2	G	201	APR	C1'-N9-C4	-4.26	119.16	126.64
2	L	201	APR	C1D-C2D-C3D	4.25	107.61	102.30
2	J	201	APR	N3-C2-N1	-4.21	122.09	128.68
5	M	201	ZOD	C1'-N9-C4	-4.13	119.39	126.64
2	P	201	APR	C4-C5-N7	-4.10	105.13	109.40
5	F	201	ZOD	N3-C2-N1	-4.08	122.30	128.68
2	H	201	APR	C1'-N9-C4	-4.07	119.49	126.64
2	B	201	APR	C1'-N9-C4	-4.07	119.49	126.64
2	E	201	APR	O3'-C3'-C2'	-4.03	98.79	111.82
2	R	201	APR	C1'-N9-C4	-4.00	119.61	126.64
2	H	201	APR	O3'-C3'-C2'	-3.99	98.93	111.82
2	I	201	APR	C1'-N9-C4	-3.94	119.72	126.64
2	D	201	APR	O3'-C3'-C2'	-3.88	99.27	111.82
2	L	201	APR	N3-C2-N1	-3.88	122.62	128.68
5	F	201	ZOD	O04-C02-C01	3.86	118.19	111.09
2	P	201	APR	PB-O3A-PA	-3.76	119.94	132.83
2	N	201	APR	O1D-C1D-O4D	-3.75	106.33	111.13
2	C	201	APR	N3-C2-N1	-3.75	122.82	128.68
2	H	201	APR	N3-C2-N1	-3.74	122.83	128.68
2	P	201	APR	C1D-C2D-C3D	3.72	106.96	102.30
2	R	201	APR	O1D-C1D-O4D	-3.63	106.48	111.13
2	G	201	APR	N3-C2-N1	-3.59	123.06	128.68
2	L	201	APR	C4-C5-N7	-3.55	105.69	109.40
2	D	201	APR	C3'-C2'-C1'	3.54	106.31	100.98
2	D	201	APR	C4-C5-N7	-3.54	105.71	109.40
2	C	201	APR	C2'-C3'-C4'	3.52	109.48	102.64
2	O	201	APR	C1'-N9-C4	-3.49	120.51	126.64
2	H	201	APR	C2'-C3'-C4'	3.44	109.33	102.64
2	E	201	APR	C2'-C3'-C4'	3.41	109.27	102.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Q	402	APR	C1'-N9-C4	-3.40	120.66	126.64
5	M	201	ZOD	O04-C02-O03	-3.40	116.21	122.96
2	D	201	APR	N3-C2-N1	-3.39	123.38	128.68
2	E	201	APR	C4-C5-N7	-3.37	105.89	109.40
5	M	201	ZOD	N3-C2-N1	-3.34	123.45	128.68
2	N	201	APR	PB-O3A-PA	-3.33	121.40	132.83
2	A	201	APR	N3-C2-N1	-3.33	123.48	128.68
5	M	201	ZOD	O04-C05-C06	3.31	117.83	108.37
2	D	201	APR	C2'-C3'-C4'	3.31	109.07	102.64
2	E	201	APR	N3-C2-N1	-3.29	123.54	128.68
2	L	201	APR	O2D-C2D-C3D	-3.19	101.50	111.82
2	C	201	APR	O3'-C3'-C4'	-3.15	101.95	111.05
2	I	201	APR	N3-C2-N1	-3.15	123.76	128.68
2	L	201	APR	O3D-C3D-C4D	-3.14	101.98	111.05
2	P	201	APR	O4'-C1'-C2'	-3.13	102.36	106.93
2	P	201	APR	O3'-C3'-C4'	-3.12	102.01	111.05
2	R	201	APR	C2-N1-C6	3.11	124.08	118.75
2	B	201	APR	O4D-C1D-C2D	3.10	108.28	104.46
2	D	201	APR	C1'-N9-C4	-3.07	121.25	126.64
2	O	201	APR	N3-C2-N1	-3.07	123.88	128.68
2	E	201	APR	PB-O3A-PA	-3.06	122.33	132.83
2	J	201	APR	C2-N1-C6	3.01	123.90	118.75
2	L	201	APR	C2-N1-C6	2.99	123.88	118.75
2	H	201	APR	PB-O3A-PA	-2.98	122.60	132.83
2	C	201	APR	C1'-N9-C4	-2.98	121.41	126.64
2	H	201	APR	O2'-C2'-C3'	-2.97	102.21	111.82
2	P	201	APR	N3-C2-N1	-2.95	124.07	128.68
2	J	201	APR	C2D-C3D-C4D	2.93	108.34	102.64
2	H	201	APR	C4-C5-N7	-2.92	106.35	109.40
2	K	201	APR	C4-C5-N7	-2.87	106.41	109.40
2	Q	402	APR	N3-C2-N1	-2.87	124.19	128.68
2	D	201	APR	C5-C6-N6	2.86	124.69	120.35
2	N	201	APR	N3-C2-N1	-2.84	124.24	128.68
2	B	201	APR	O2'-C2'-C3'	-2.83	102.67	111.82
2	K	201	APR	N3-C2-N1	-2.82	124.27	128.68
2	G	201	APR	O3D-C3D-C4D	-2.79	102.99	111.05
2	O	201	APR	PB-O3A-PA	-2.70	123.57	132.83
2	D	201	APR	O3'-C3'-C4'	-2.66	103.35	111.05
2	Q	402	APR	O1D-C1D-O4D	2.65	114.52	111.13
2	P	201	APR	C5-C6-N6	2.63	124.35	120.35
2	A	201	APR	C1'-N9-C4	-2.63	122.02	126.64
2	R	201	APR	C5D-C4D-C3D	-2.62	105.36	115.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	201	APR	C5-C6-N6	2.62	124.33	120.35
2	N	201	APR	C1'-N9-C4	-2.61	122.05	126.64
2	G	201	APR	C2D-C3D-C4D	2.59	107.68	102.64
5	M	201	ZOD	C5'-C4'-C3'	-2.59	105.46	115.18
2	E	201	APR	C2-N1-C6	2.59	123.19	118.75
2	L	201	APR	C5-C6-N6	2.58	124.28	120.35
2	N	201	APR	C5'-C4'-C3'	-2.56	105.59	115.18
2	E	201	APR	O5'-PA-O1A	-2.55	99.11	109.07
2	E	201	APR	O1D-C1D-O4D	-2.51	107.92	111.13
2	G	201	APR	O4'-C1'-C2'	2.50	110.58	106.93
2	N	201	APR	O3'-C3'-C4'	-2.46	103.94	111.05
5	F	201	ZOD	O1B-C10-C09	-2.46	100.53	108.99
2	B	201	APR	O3'-C3'-C4'	-2.43	104.03	111.05
2	N	201	APR	C2'-C3'-C4'	2.39	107.29	102.64
2	J	201	APR	PB-O3A-PA	-2.39	124.61	132.83
2	A	201	APR	O4'-C1'-C2'	-2.39	103.43	106.93
2	N	201	APR	C4-C5-N7	-2.39	106.91	109.40
2	B	201	APR	C4-C5-N7	-2.38	106.91	109.40
2	J	201	APR	O3D-C3D-C4D	-2.37	104.21	111.05
2	E	201	APR	C3'-C2'-C1'	-2.36	97.42	100.98
2	Q	402	APR	O2B-PB-O1B	2.35	123.85	112.24
5	F	201	ZOD	C10-C09-C38	-2.32	106.50	115.18
2	B	201	APR	PB-O3A-PA	-2.31	124.89	132.83
2	K	201	APR	O3D-C3D-C4D	-2.30	104.41	111.05
2	P	201	APR	C1'-N9-C4	-2.25	122.68	126.64
5	F	201	ZOD	C05-O04-C02	-2.25	114.24	117.72
2	E	201	APR	O2'-C2'-C3'	-2.25	104.56	111.82
2	L	201	APR	PB-O3A-PA	-2.22	125.20	132.83
2	Q	402	APR	O5D-C5D-C4D	-2.21	101.39	108.99
2	L	201	APR	PB-O5D-C5D	-2.20	108.78	121.68
2	B	201	APR	C2-N1-C6	2.19	122.50	118.75
5	F	201	ZOD	O07-C06-O08	2.18	113.93	111.13
2	R	201	APR	PB-O3A-PA	-2.18	125.34	132.83
2	C	201	APR	O3D-C3D-C2D	-2.15	104.86	111.82
2	C	201	APR	C1D-C2D-C3D	-2.15	99.61	102.30
2	J	201	APR	C5-C6-N6	2.13	123.59	120.35
2	C	201	APR	C4-C5-N7	-2.13	107.18	109.40
2	R	201	APR	C4-C5-N7	-2.13	107.18	109.40
2	K	201	APR	C2'-C3'-C4'	2.12	106.76	102.64
2	G	201	APR	C2-N1-C6	2.09	122.33	118.75
2	G	201	APR	O4D-C1D-C2D	2.09	107.03	104.46
2	H	201	APR	O3D-C3D-C4D	-2.08	105.03	111.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	201	APR	O2A-PA-O5'	2.08	117.39	107.75
5	M	201	ZOD	O07-C06-O08	-2.07	108.48	111.13
2	B	201	APR	N3-C2-N1	-2.07	125.45	128.68
5	M	201	ZOD	C2'-C3'-C4'	2.05	106.63	102.64
2	P	201	APR	O2D-C2D-C3D	-2.04	105.22	111.82
2	G	201	APR	N6-C6-N1	2.03	122.80	118.57
2	E	201	APR	C5-C6-N6	2.03	123.44	120.35
2	O	201	APR	O5D-C5D-C4D	-2.02	102.03	108.99
2	P	201	APR	O3'-C3'-C2'	2.02	118.35	111.82
2	C	201	APR	PB-O3A-PA	-2.01	125.92	132.83
2	H	201	APR	C2-N1-C6	2.00	122.18	118.75

There are no chirality outliers.

All (98) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	J	201	APR	C5'-O5'-PA-O1A
2	J	201	APR	C5'-O5'-PA-O2A
2	J	201	APR	C5'-O5'-PA-O3A
2	I	201	APR	C5D-O5D-PB-O3A
2	G	201	APR	C5'-O5'-PA-O3A
2	G	201	APR	C5D-O5D-PB-O1B
2	C	201	APR	C5'-O5'-PA-O3A
5	M	201	ZOD	C06-C05-O04-C02
5	M	201	ZOD	C5'-O5'-PA-O3A
5	M	201	ZOD	C5'-O5'-PA-O2A
5	M	201	ZOD	C5'-O5'-PA-O1A
2	L	201	APR	C5'-O5'-PA-O3A
2	D	201	APR	C5'-O5'-PA-O1A
2	D	201	APR	C5'-O5'-PA-O2A
2	D	201	APR	C5'-O5'-PA-O3A
2	D	201	APR	C5D-O5D-PB-O3A
2	D	201	APR	C5D-O5D-PB-O1B
2	R	201	APR	C5D-O5D-PB-O1B
2	Q	402	APR	C5'-O5'-PA-O3A
2	Q	402	APR	C5D-O5D-PB-O1B
2	K	201	APR	PA-O3A-PB-O5D
2	K	201	APR	C5D-O5D-PB-O1B
5	F	201	ZOD	PA-O3A-PB-O1B
5	F	201	ZOD	C5'-O5'-PA-O3A
5	F	201	ZOD	C5'-O5'-PA-O2A
5	F	201	ZOD	C5'-O5'-PA-O1A

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Mol	Chain	Res	Type	Atoms
2	O	201	APR	C5'-O5'-PA-O1A
2	O	201	APR	C5'-O5'-PA-O2A
2	O	201	APR	C5'-O5'-PA-O3A
2	N	201	APR	C5'-O5'-PA-O1A
2	N	201	APR	C5'-O5'-PA-O2A
2	N	201	APR	C5'-O5'-PA-O3A
2	P	201	APR	C5'-O5'-PA-O1A
2	P	201	APR	C5'-O5'-PA-O2A
2	P	201	APR	C5'-O5'-PA-O3A
2	P	201	APR	C5D-O5D-PB-O1B
5	M	201	ZOD	C01-C02-O04-C05
5	M	201	ZOD	O03-C02-O04-C05
5	F	201	ZOD	C01-C02-O04-C05
5	F	201	ZOD	O03-C02-O04-C05
2	I	201	APR	O4'-C4'-C5'-O5'
2	R	201	APR	C3'-C4'-C5'-O5'
2	R	201	APR	C3D-C4D-C5D-O5D
2	P	201	APR	O4D-C4D-C5D-O5D
2	H	201	APR	O4'-C4'-C5'-O5'
2	R	201	APR	O4'-C4'-C5'-O5'
2	E	201	APR	C3'-C4'-C5'-O5'
2	P	201	APR	C3D-C4D-C5D-O5D
2	H	201	APR	C3'-C4'-C5'-O5'
2	R	201	APR	O4D-C4D-C5D-O5D
2	E	201	APR	O4'-C4'-C5'-O5'
2	I	201	APR	C3D-C4D-C5D-O5D
2	I	201	APR	C3'-C4'-C5'-O5'
2	A	201	APR	O4'-C4'-C5'-O5'
2	I	201	APR	O4D-C4D-C5D-O5D
2	J	201	APR	PA-O3A-PB-O5D
2	G	201	APR	C5D-O5D-PB-O3A
2	R	201	APR	C5D-O5D-PB-O3A
2	K	201	APR	C5D-O5D-PB-O3A
2	B	201	APR	C5'-O5'-PA-O3A
2	A	201	APR	C3'-C4'-C5'-O5'
2	A	201	APR	C3D-C4D-C5D-O5D
2	R	201	APR	PA-O3A-PB-O2B
5	F	201	ZOD	PB-O3A-PA-O1A
2	N	201	APR	PB-O3A-PA-O1A
2	H	201	APR	PA-O3A-PB-O1B
2	I	201	APR	C5D-O5D-PB-O1B
2	I	201	APR	C5D-O5D-PB-O2B

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Mol	Chain	Res	Type	Atoms
2	G	201	APR	C5'-O5'-PA-O1A
2	G	201	APR	C5'-O5'-PA-O2A
2	D	201	APR	C5D-O5D-PB-O2B
2	Q	402	APR	C5'-O5'-PA-O1A
2	Q	402	APR	C5'-O5'-PA-O2A
2	K	201	APR	C5D-O5D-PB-O2B
5	F	201	ZOD	C10-O1B-PB-O2B
2	K	201	APR	C3D-C4D-C5D-O5D
2	P	201	APR	O4'-C4'-C5'-O5'
2	G	201	APR	C3D-C4D-C5D-O5D
2	K	201	APR	O4D-C4D-C5D-O5D
2	H	201	APR	PA-O3A-PB-O2B
2	H	201	APR	C3D-C4D-C5D-O5D
2	G	201	APR	PA-O3A-PB-O1B
2	D	201	APR	PA-O3A-PB-O1B
2	E	201	APR	PA-O3A-PB-O1B
2	O	201	APR	PB-O3A-PA-O1A
2	P	201	APR	PA-O3A-PB-O1B
2	P	201	APR	PA-O3A-PB-O5D
2	A	201	APR	O4D-C4D-C5D-O5D
2	P	201	APR	C5D-O5D-PB-O3A
2	Q	402	APR	C3D-C4D-C5D-O5D
2	I	201	APR	PA-O3A-PB-O2B
2	R	201	APR	PA-O3A-PB-O1B
2	C	201	APR	C5'-O5'-PA-O1A
2	C	201	APR	C5'-O5'-PA-O2A
2	L	201	APR	C5'-O5'-PA-O1A
2	L	201	APR	C5'-O5'-PA-O2A
2	H	201	APR	C5D-O5D-PB-O1B
2	K	201	APR	C4'-C5'-O5'-PA

There are no ring outliers.

31 monomers are involved in 69 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	202	SO4	3	0
2	J	201	APR	1	0
2	G	201	APR	1	0
3	L	202	SO4	1	0
2	C	201	APR	2	0
3	O	202	SO4	3	0
3	C	202	SO4	2	0

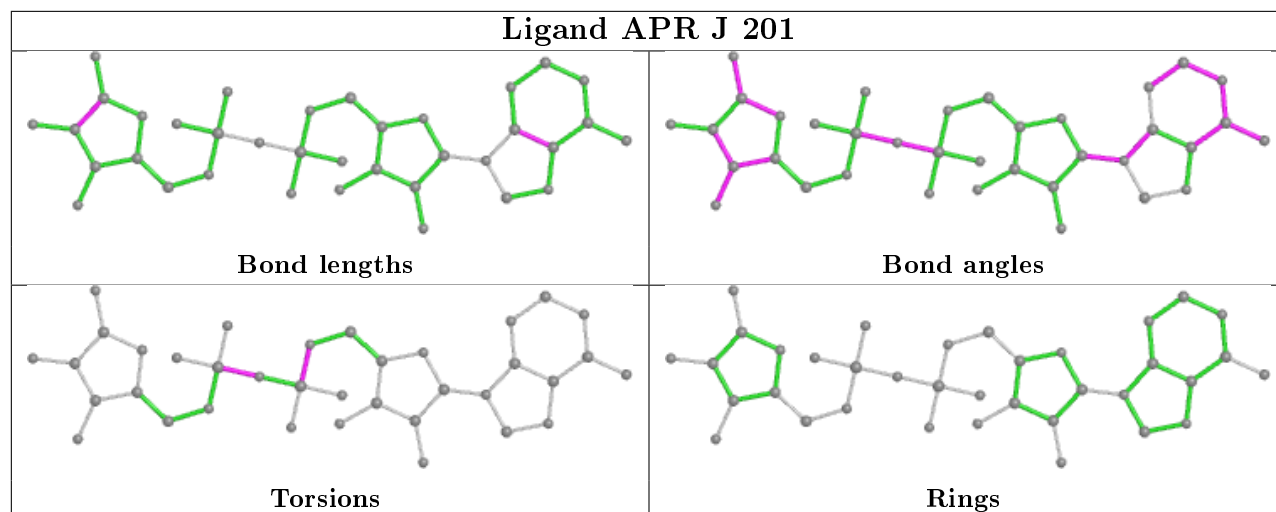
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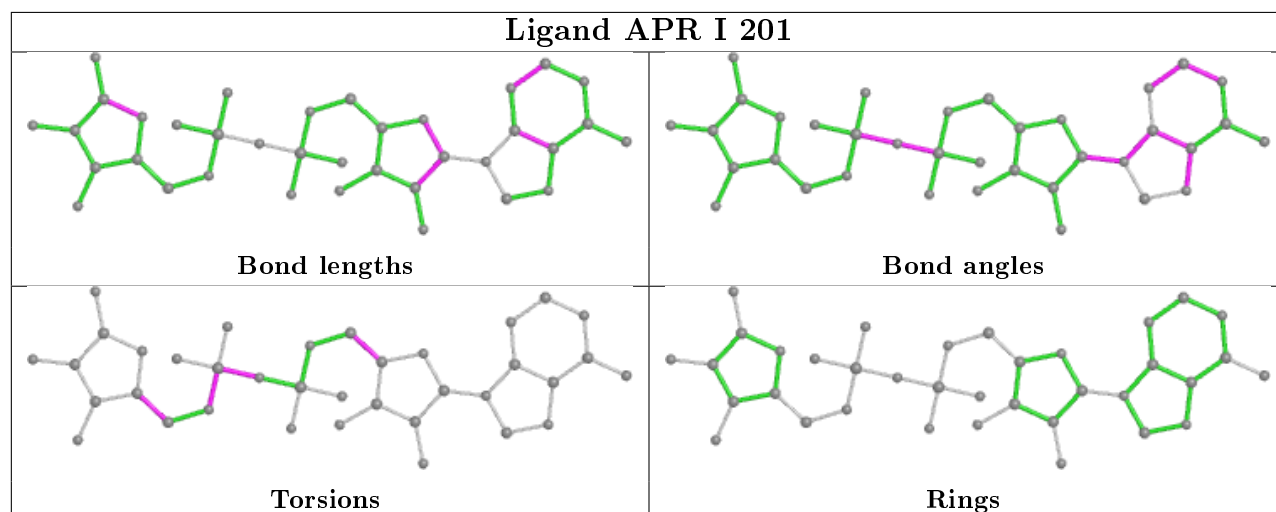
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	M	201	ZOD	6	0
2	L	201	APR	4	0
3	K	202	SO4	2	0
2	D	201	APR	4	0
3	P	202	SO4	1	0
2	R	201	APR	1	0
3	B	202	SO4	1	0
2	Q	402	APR	3	0
2	K	201	APR	4	0
5	F	201	ZOD	4	0
2	E	201	APR	1	0
3	A	202	SO4	1	0
3	E	202	SO4	1	0
2	O	201	APR	3	0
2	N	201	APR	1	0
3	H	202	SO4	1	0
3	J	202	SO4	3	0
2	B	201	APR	2	0
2	A	201	APR	1	0
2	P	201	APR	3	0
3	R	202	SO4	1	0
2	H	201	APR	2	0
3	Q	403	SO4	3	0
3	M	202	SO4	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

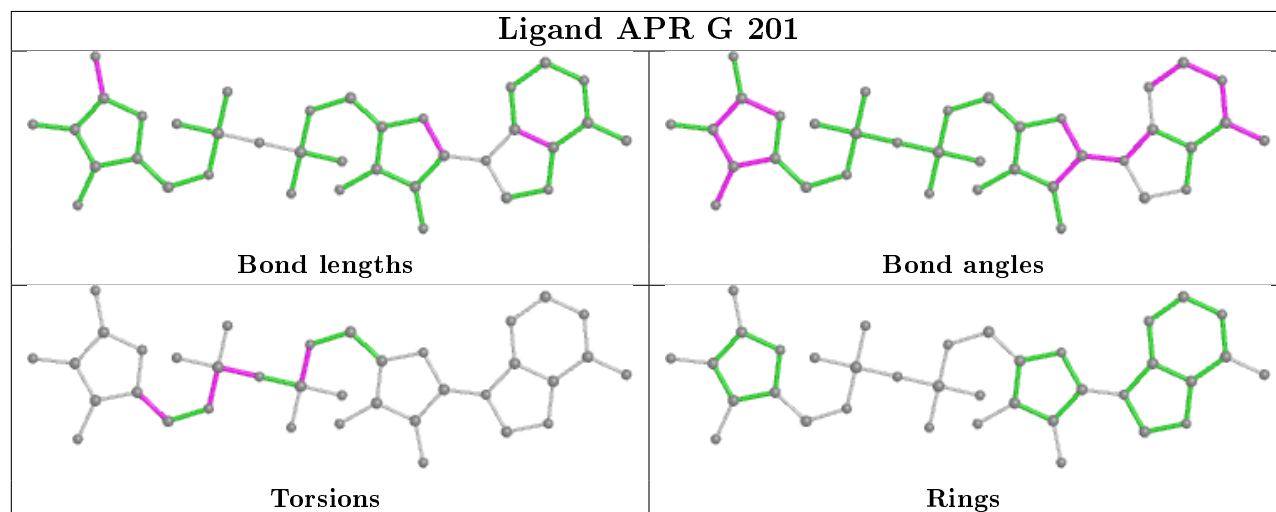
## Ligand APR J 201

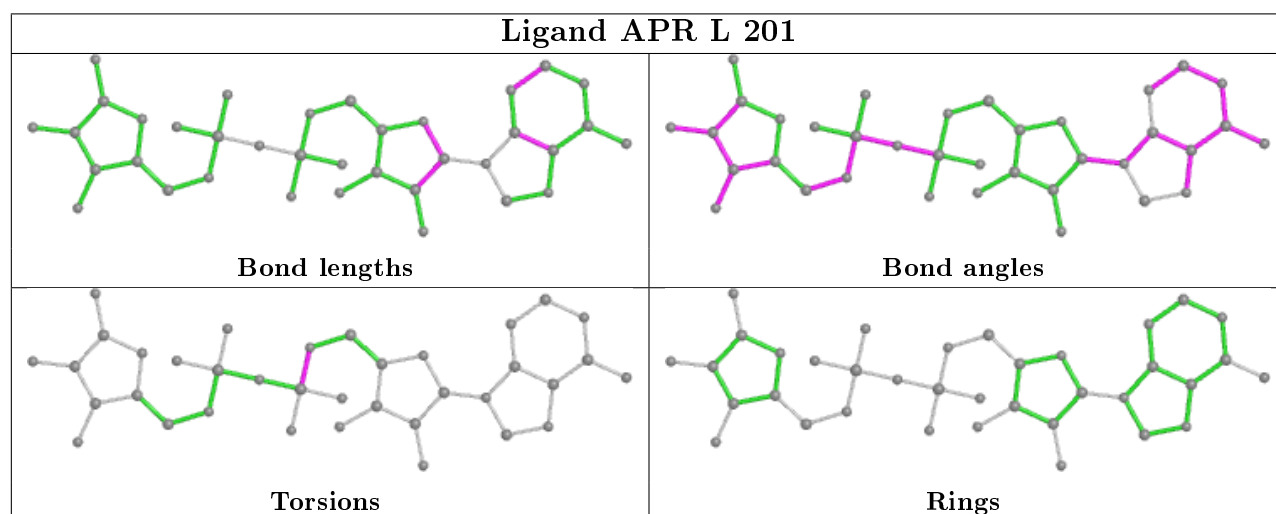
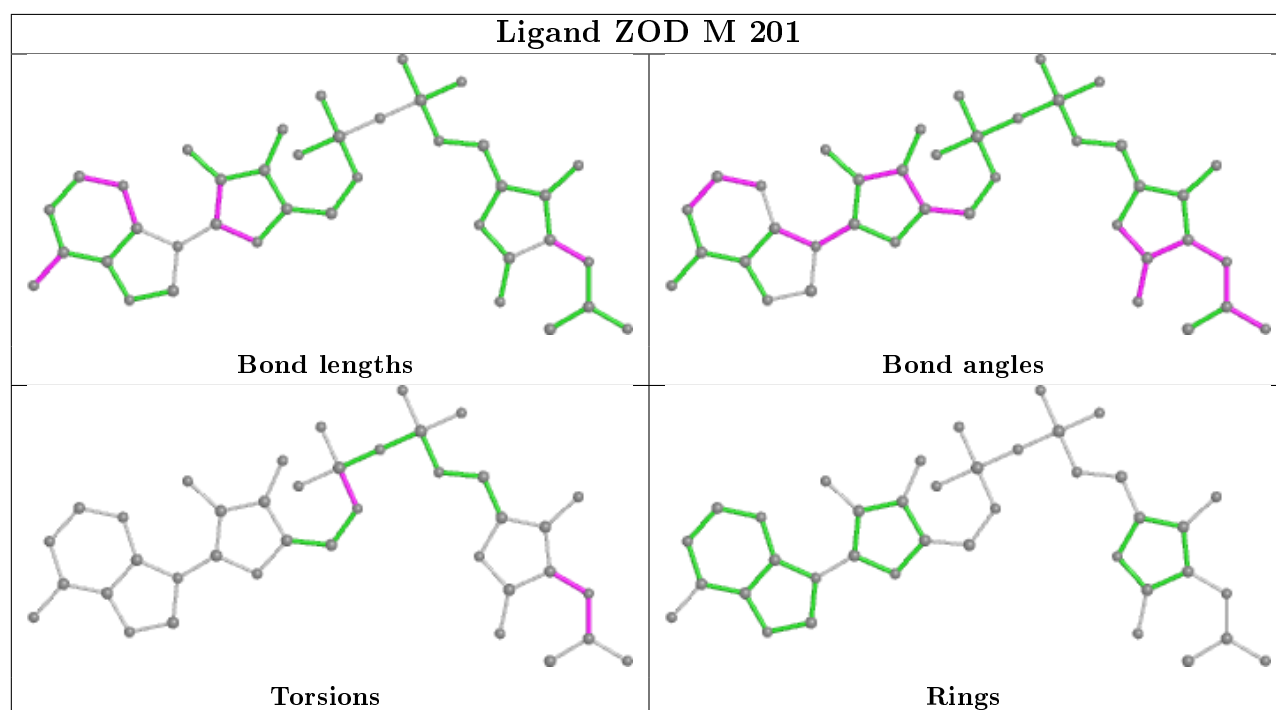
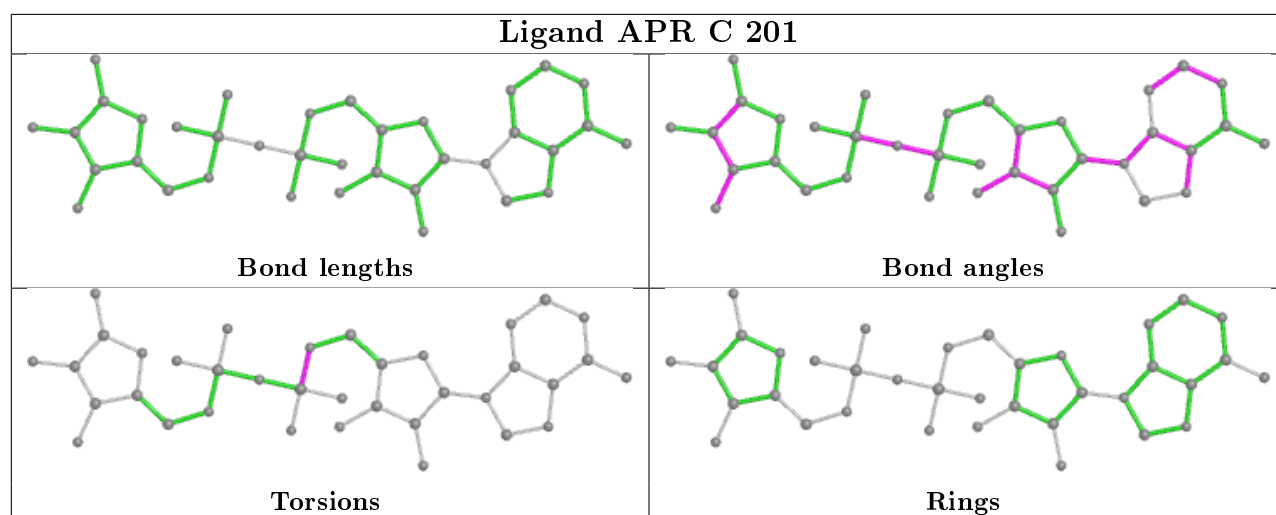


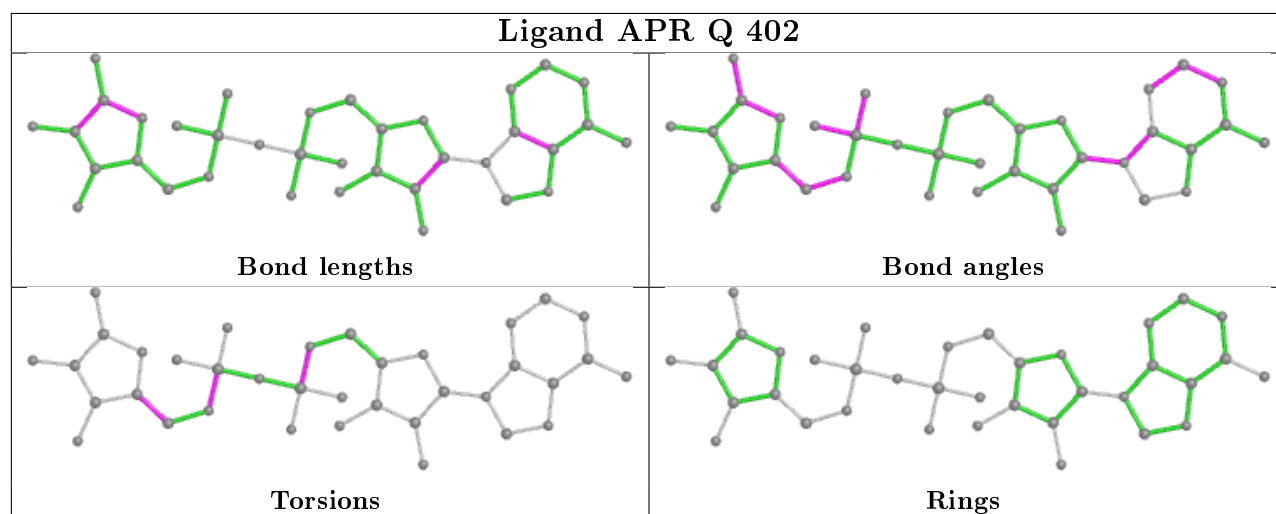
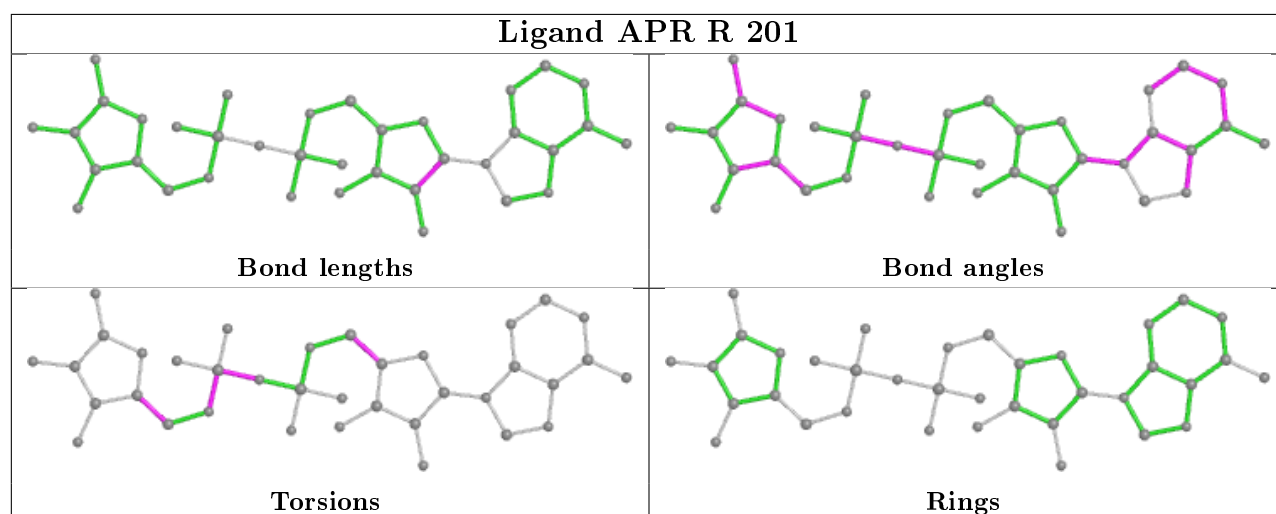
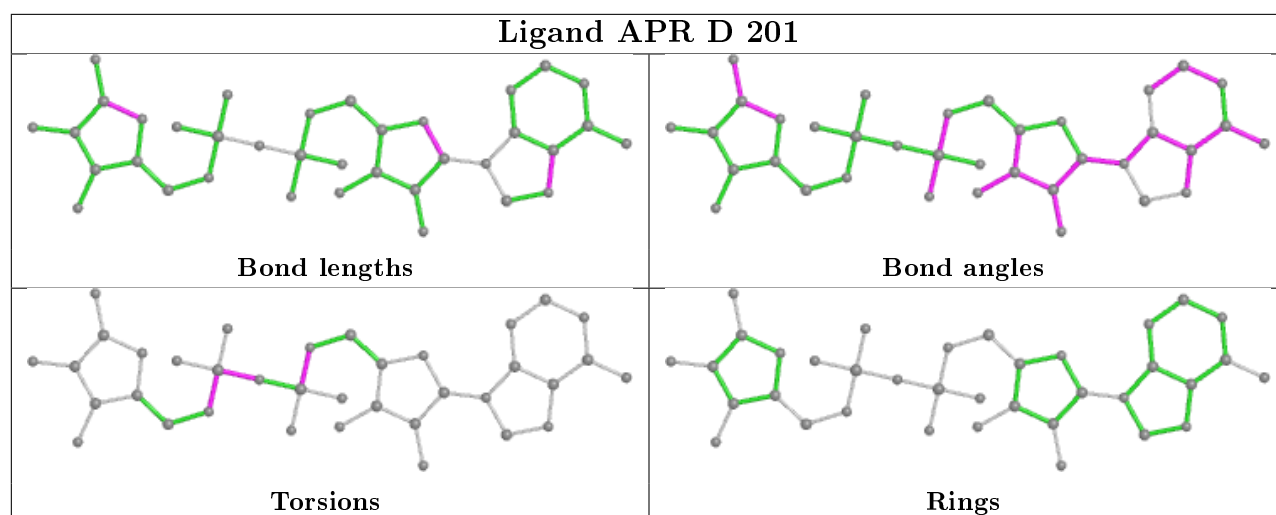
## Ligand APR I 201

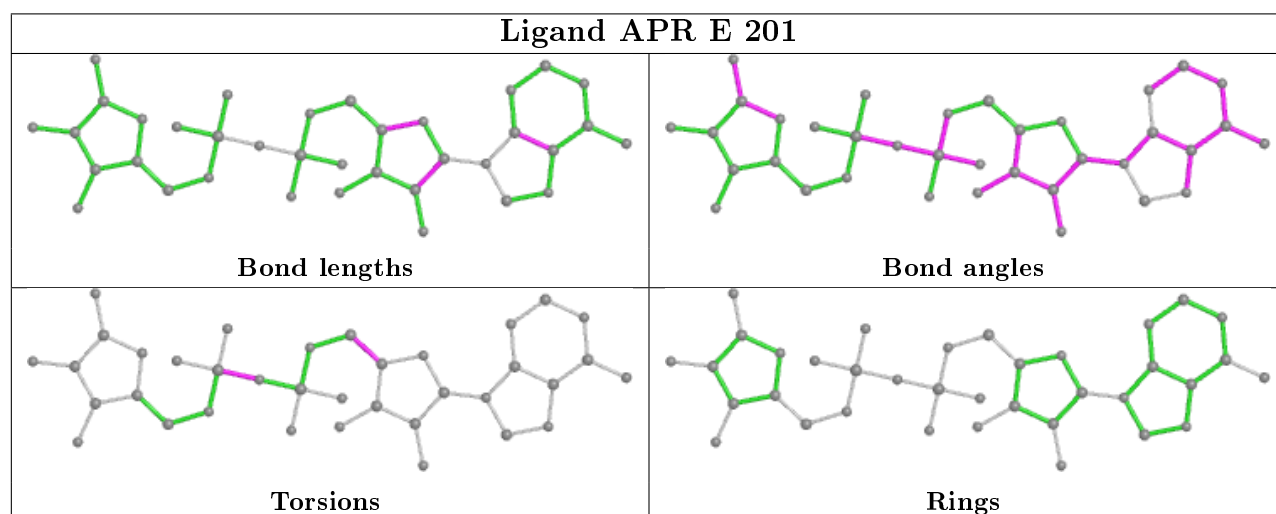
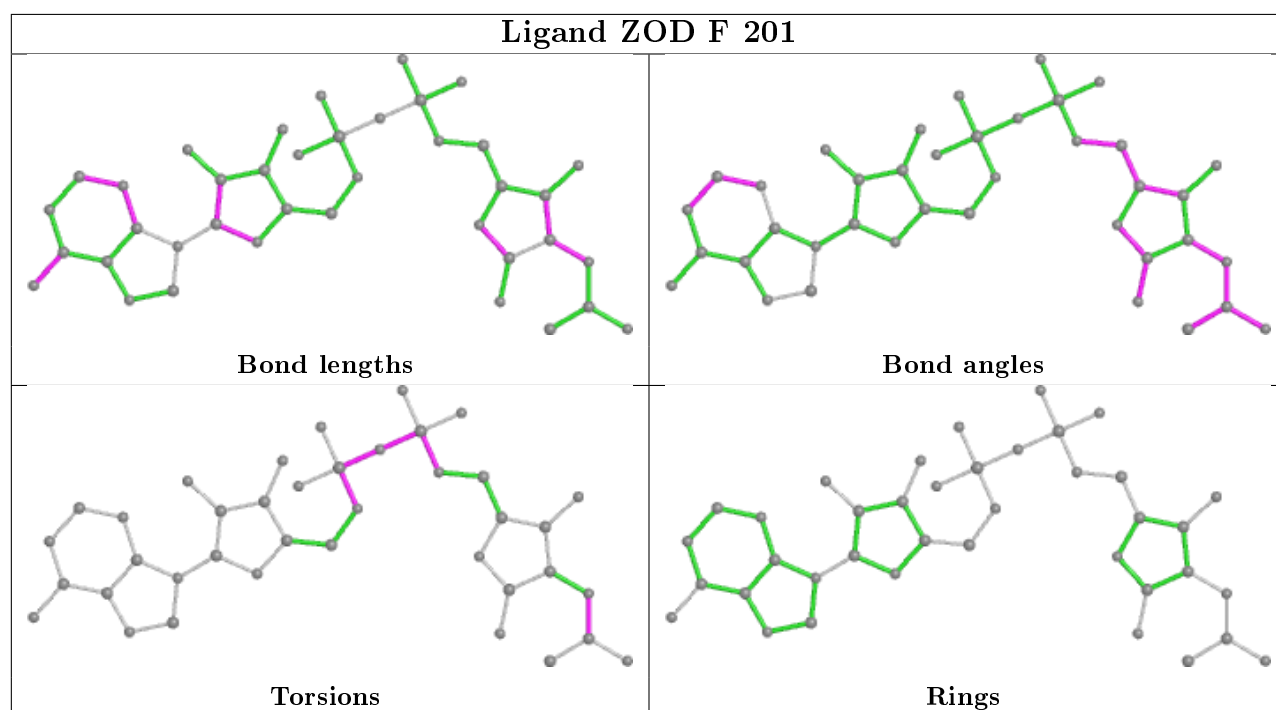
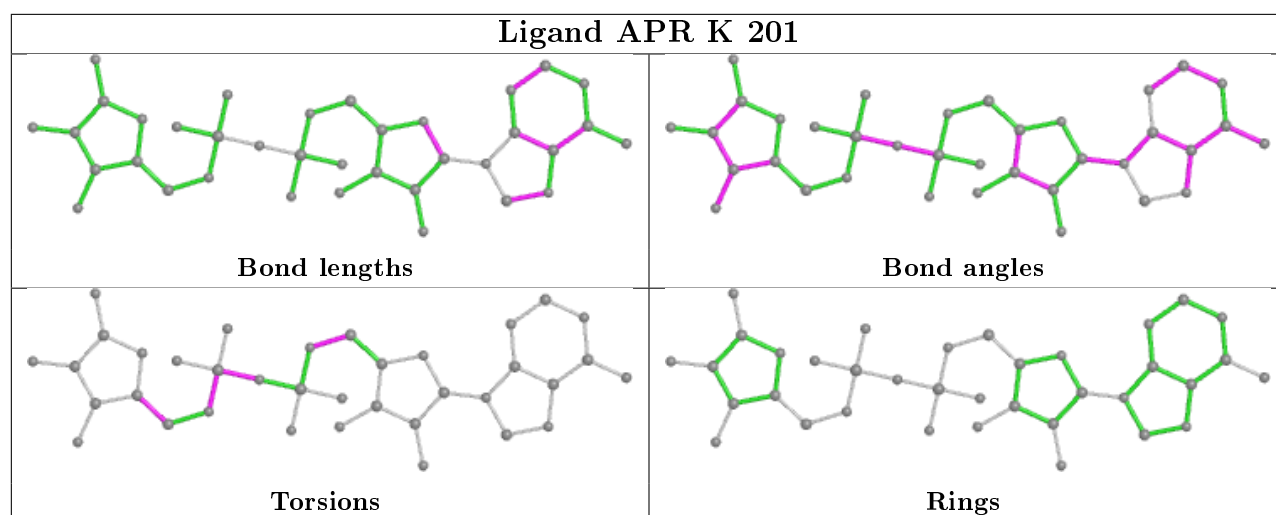


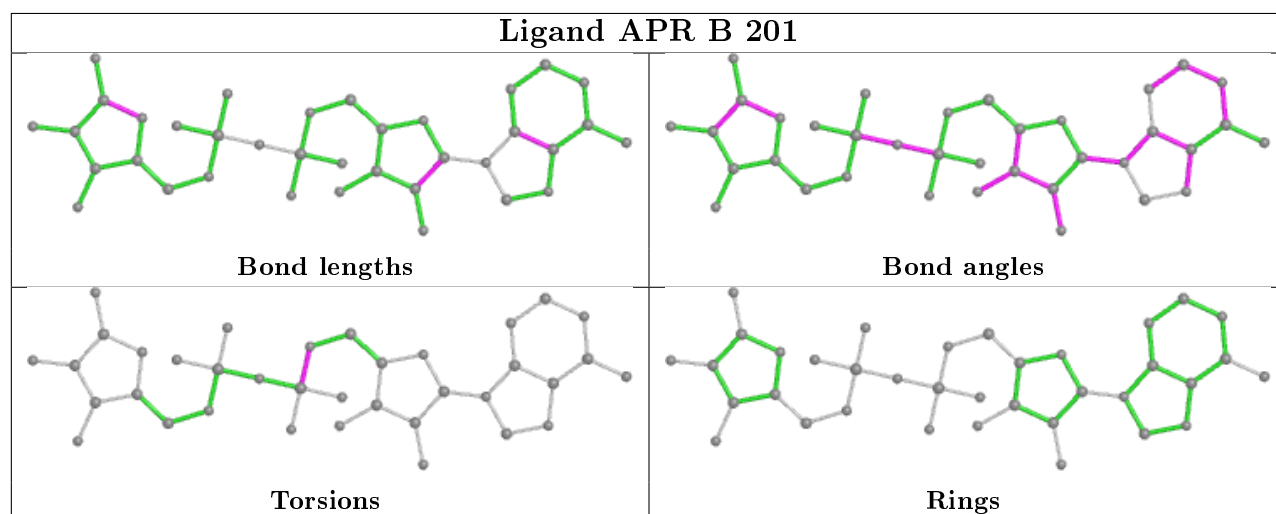
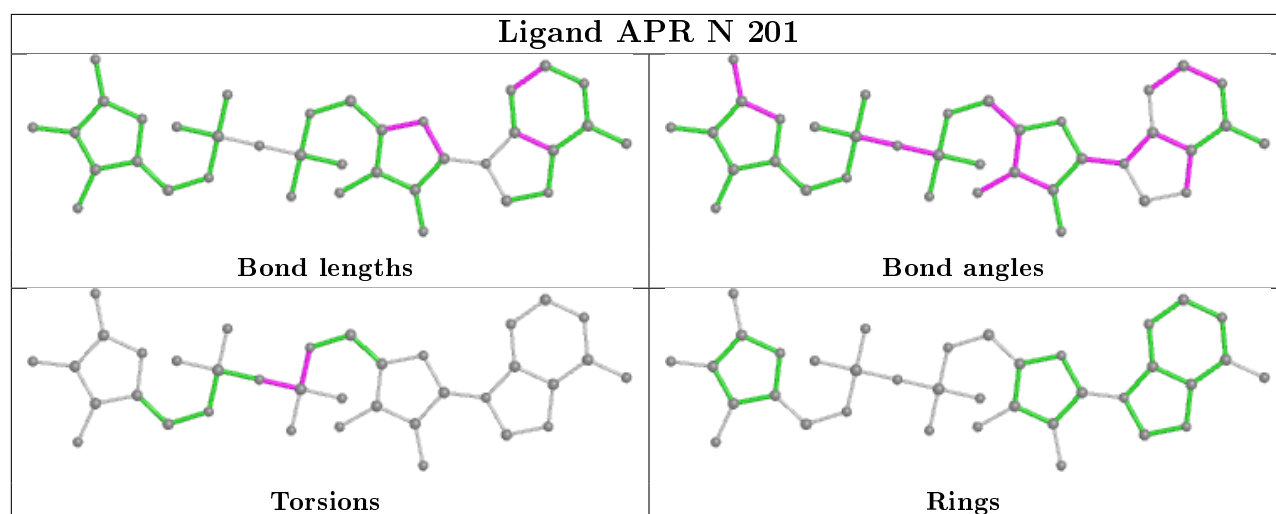
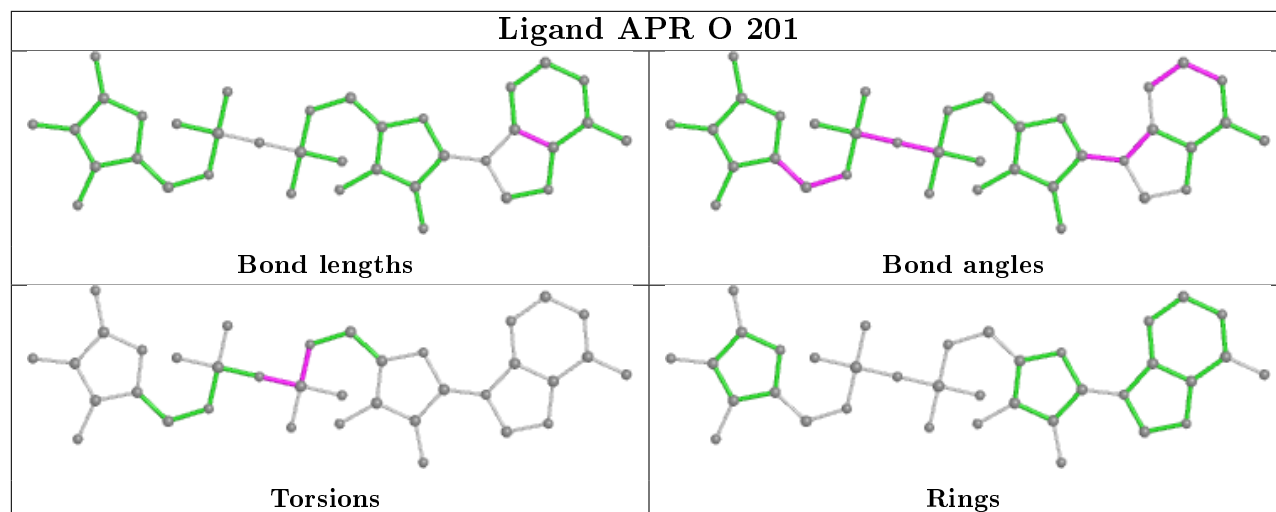
## Ligand APR G 201



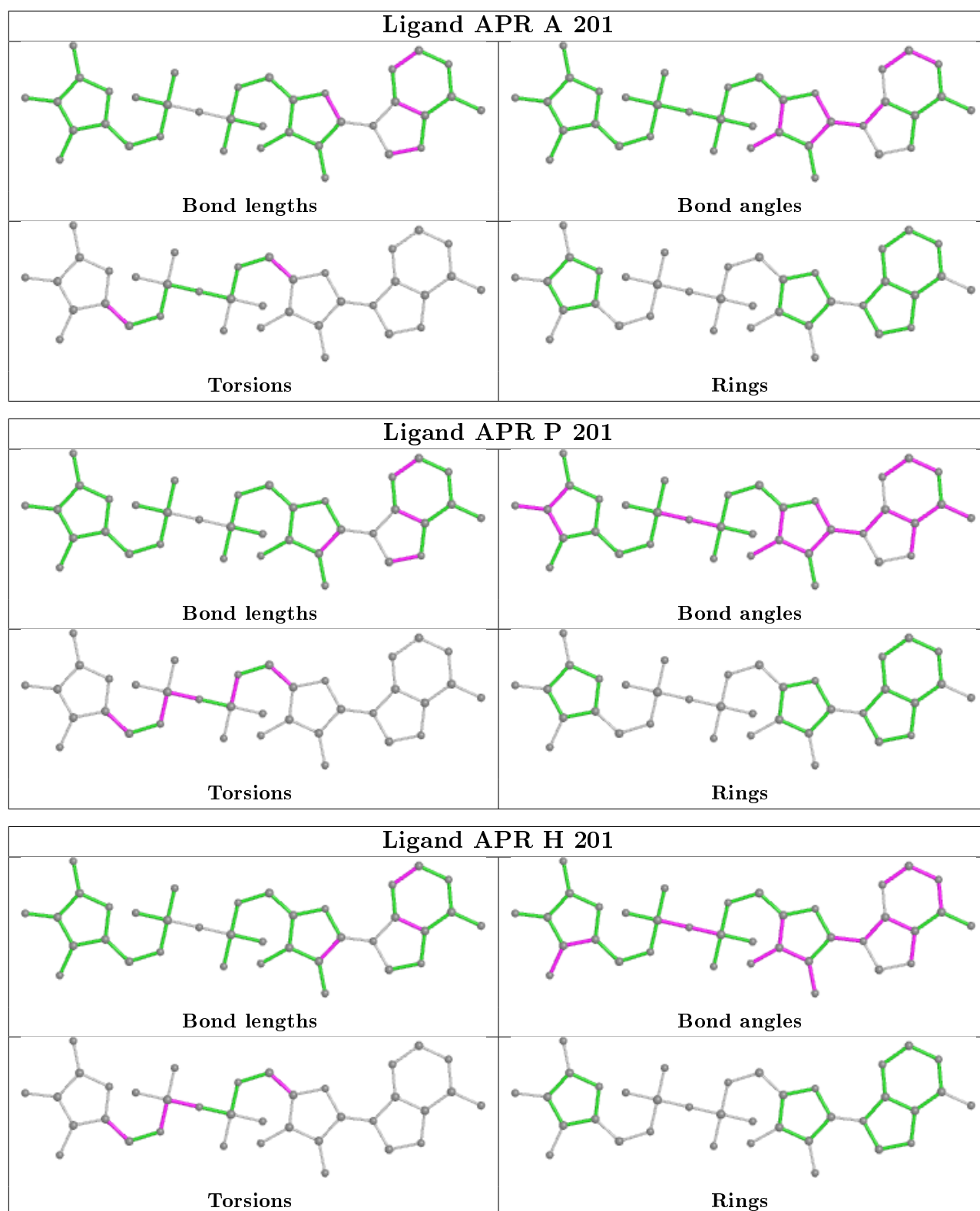












## 5.7 Other polymers ⓘ

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 ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

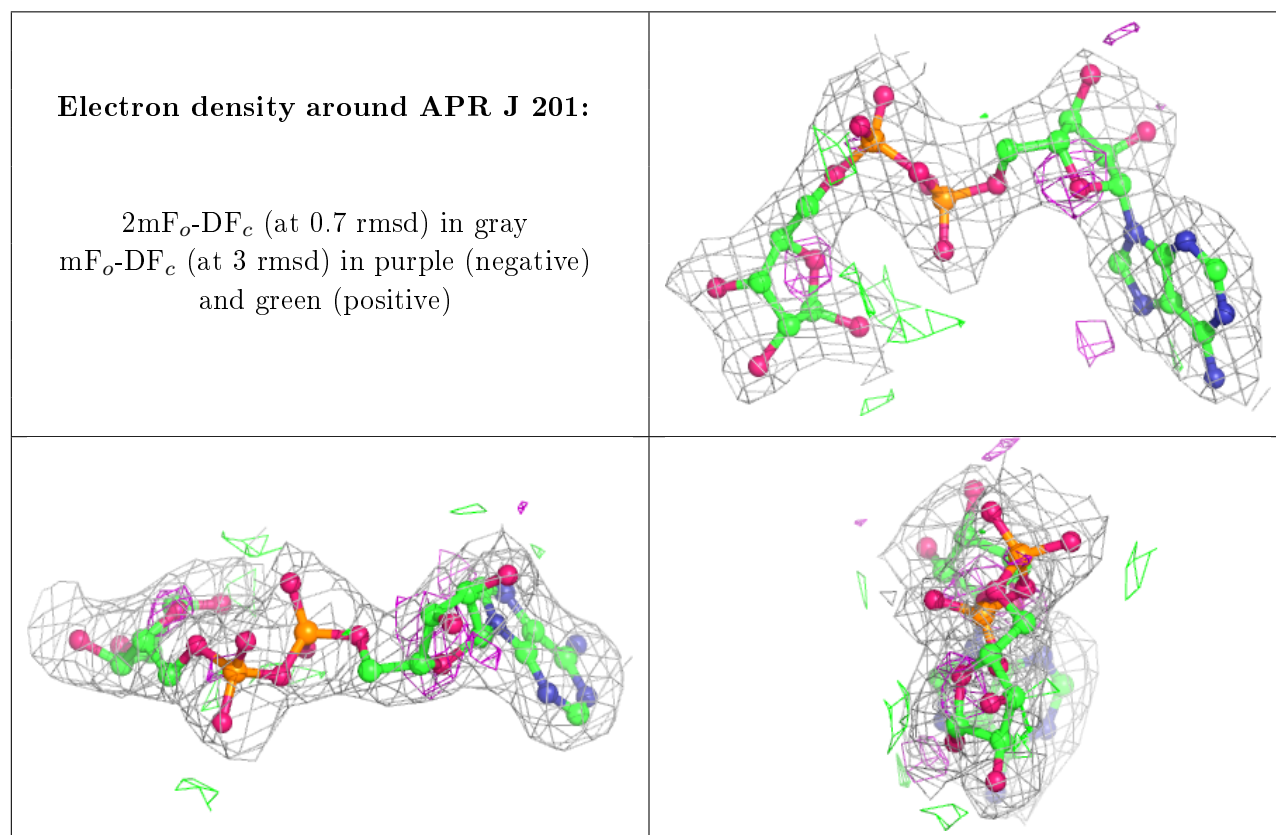
### 6.3 Carbohydrates ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.4 Ligands ⓘ

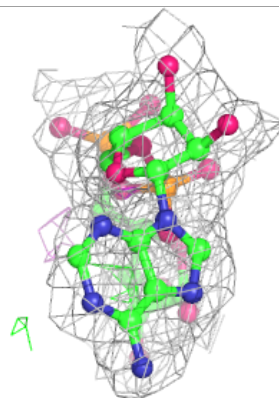
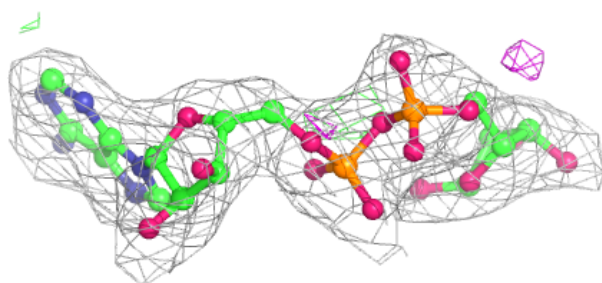
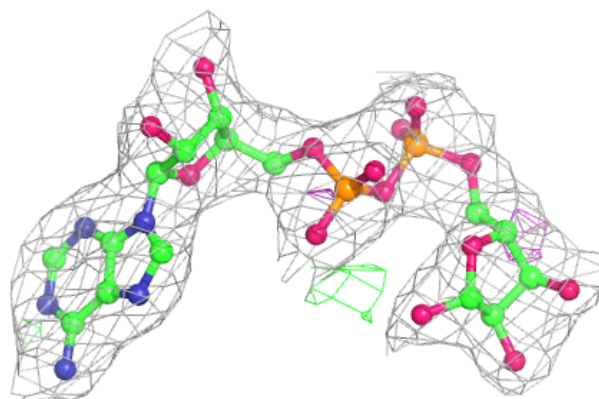
Unable to reproduce the depositors R factor - this section is therefore empty.

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.

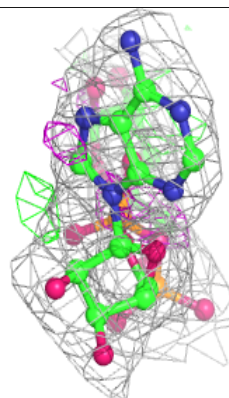
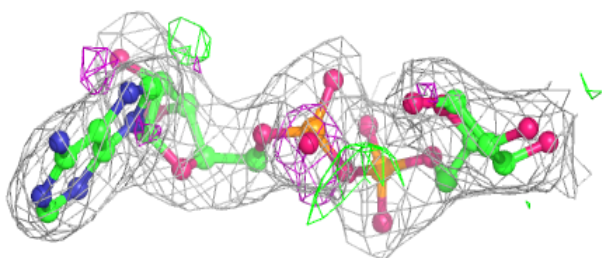
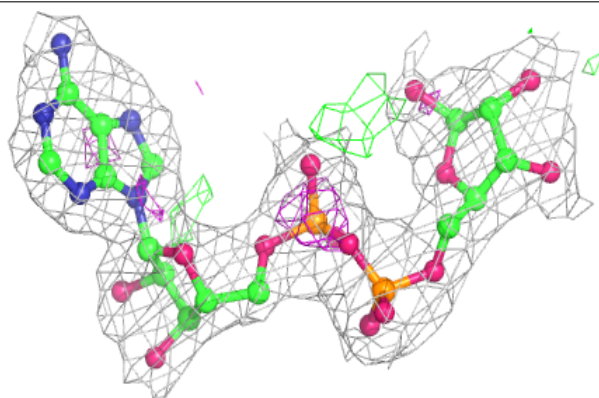


**Electron density around APR I 201:**

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

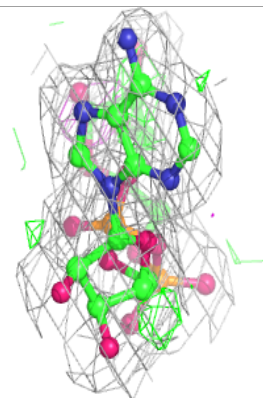
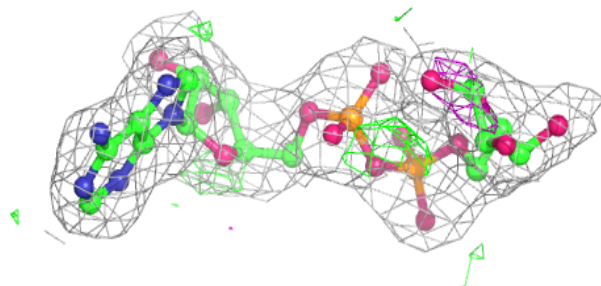
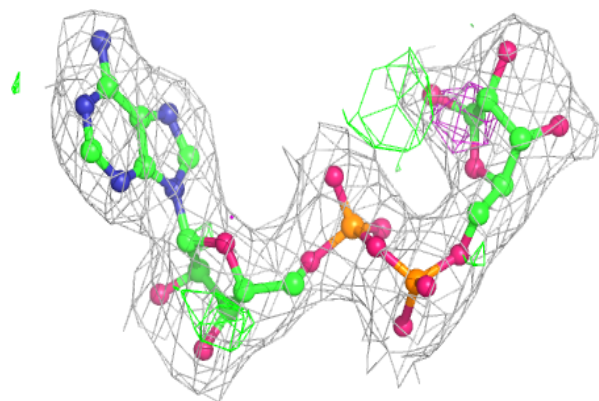
**Electron density around APR G 201:**

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

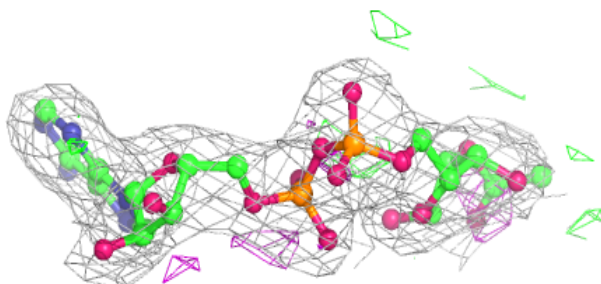
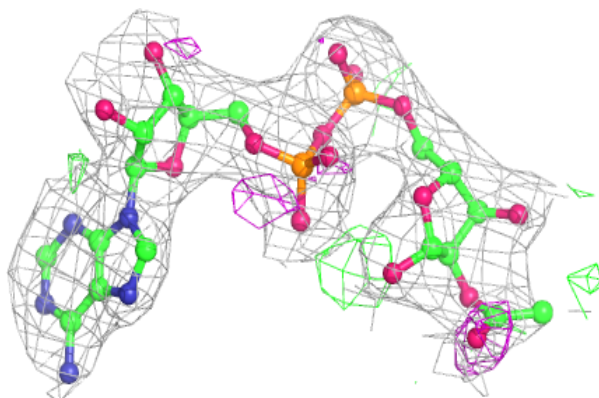


**Electron density around APR C 201:**

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

**Electron density around ZOD M 201:**

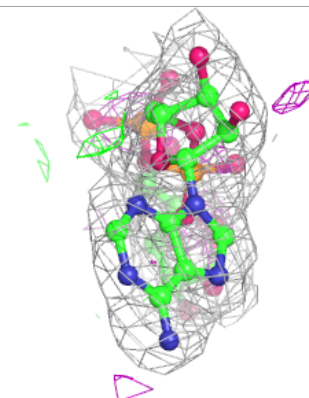
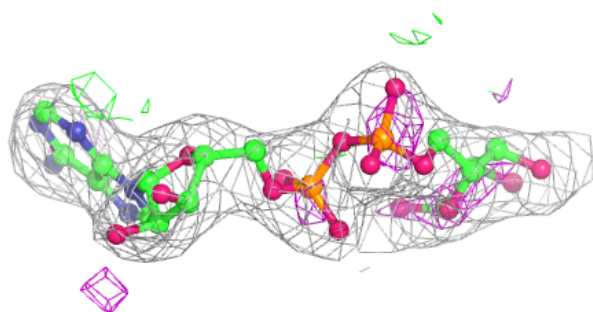
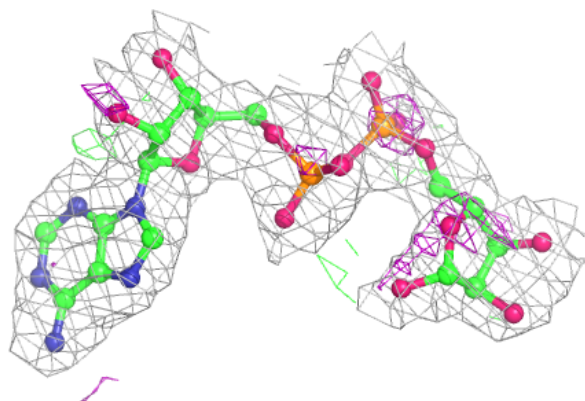
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



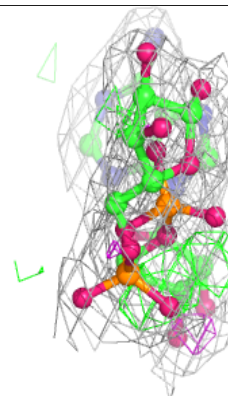
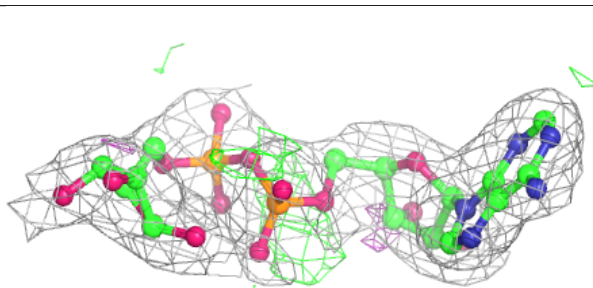
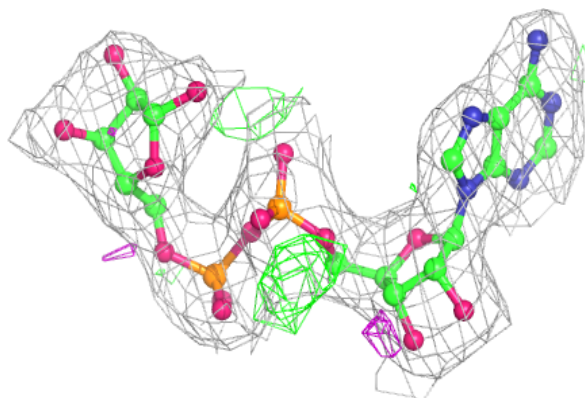


**Electron density around APR L 201:**

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

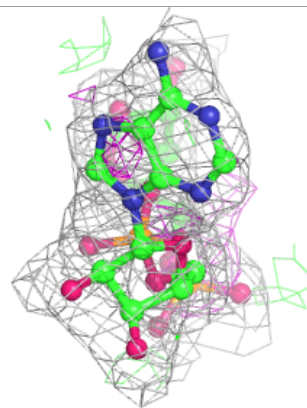
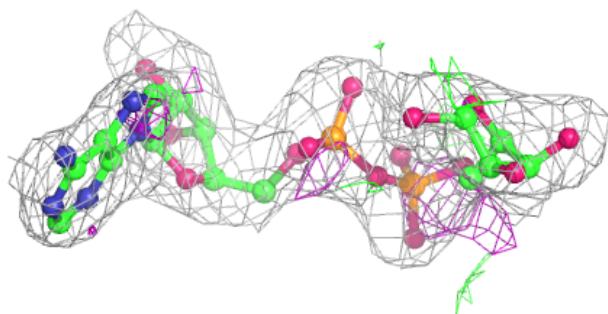
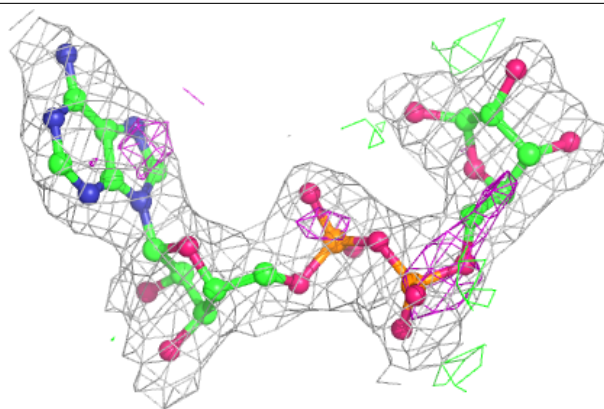
**Electron density around APR D 201:**

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

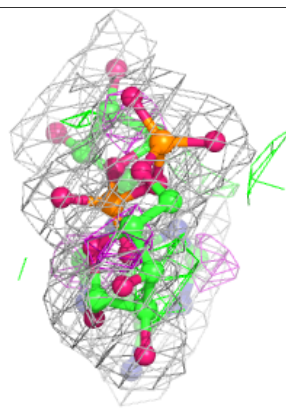
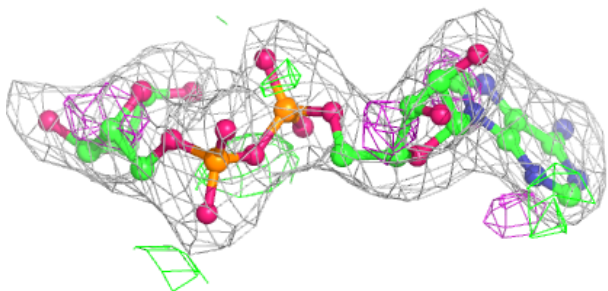
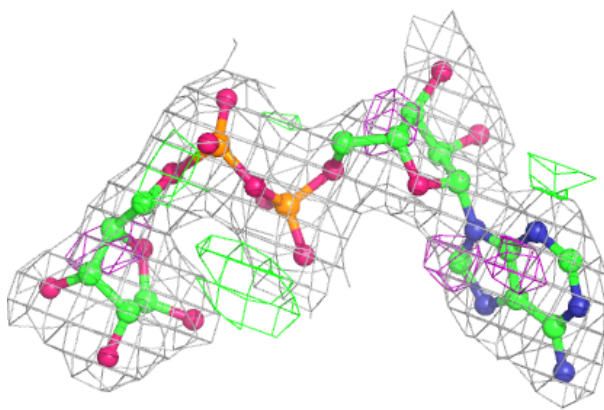


**Electron density around APR R 201:**

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

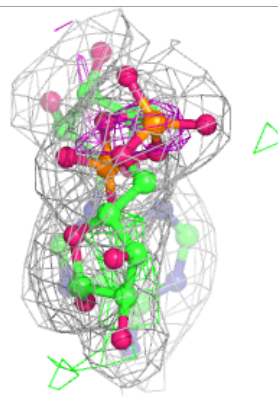
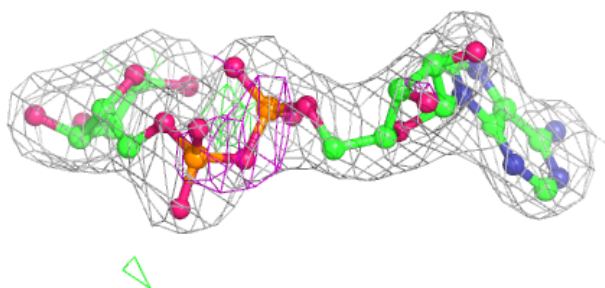
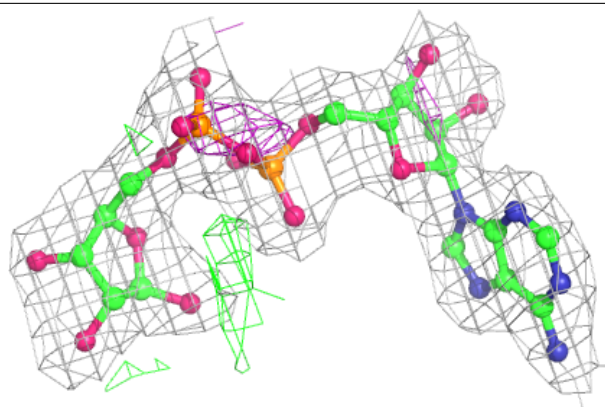
**Electron density around APR Q 402:**

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

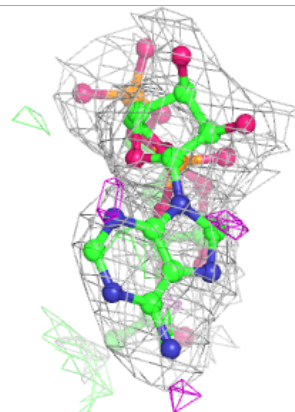
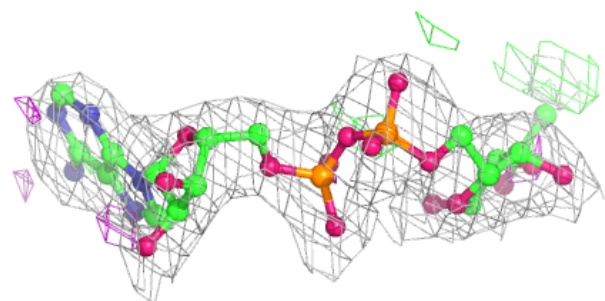
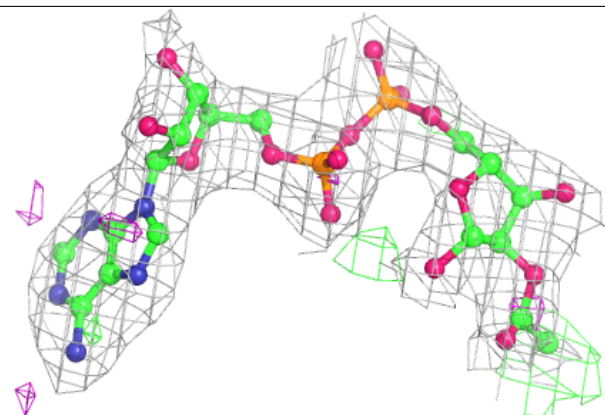


**Electron density around APR K 201:**

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

**Electron density around ZOD F 201:**

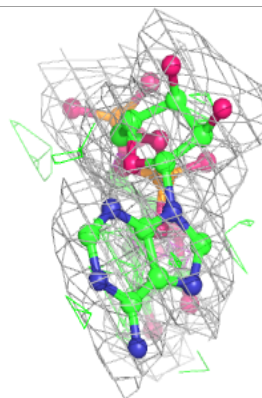
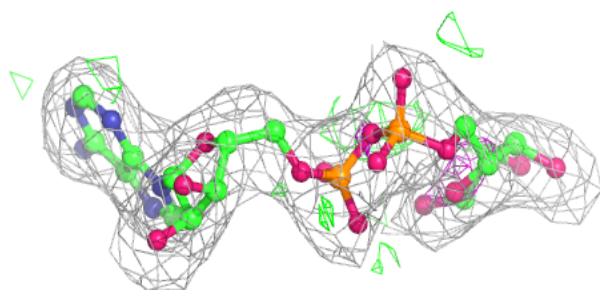
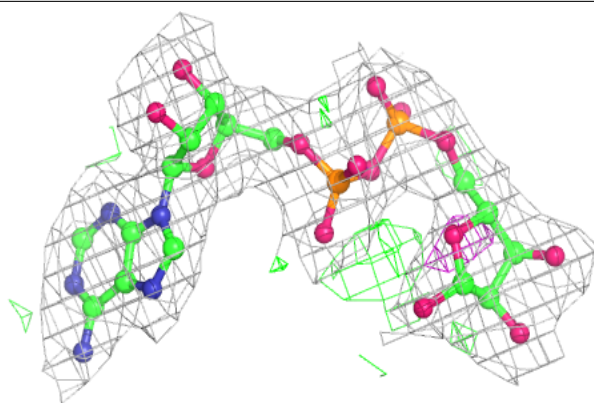
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



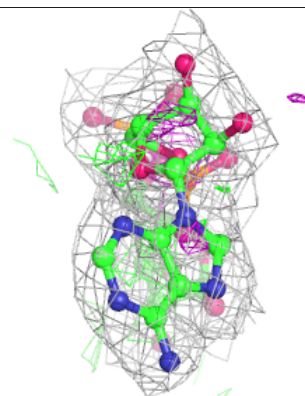
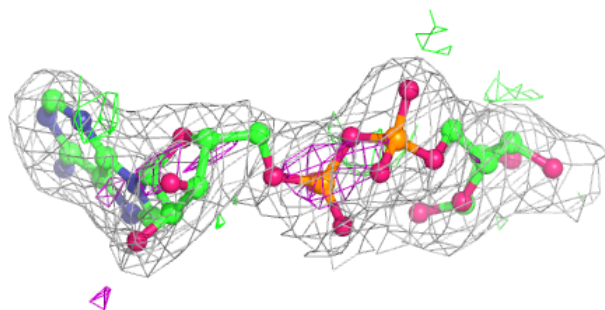
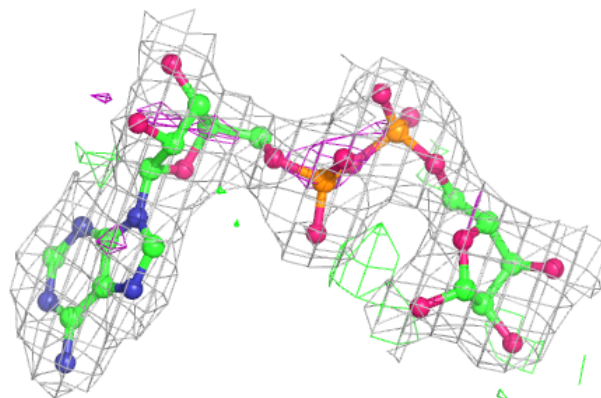


**Electron density around APR E 201:**

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

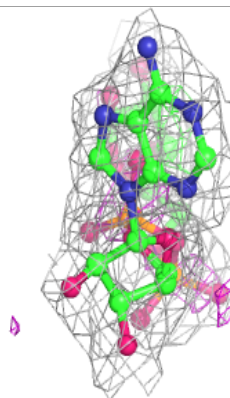
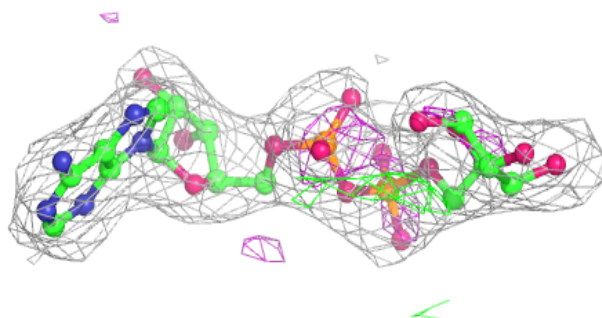
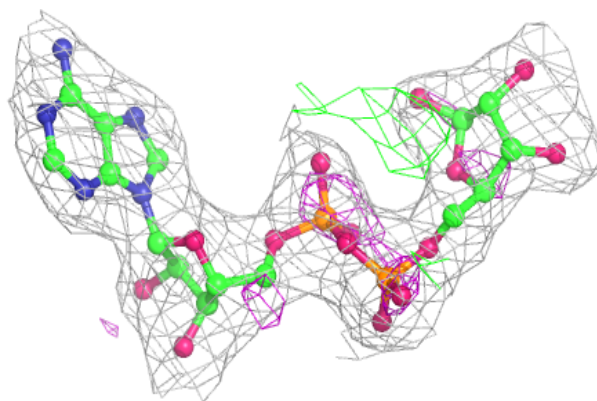
**Electron density around APR O 201:**

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

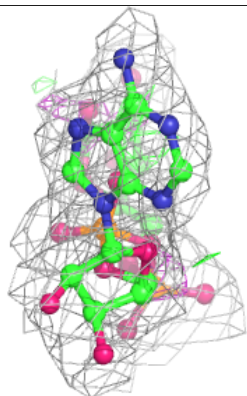
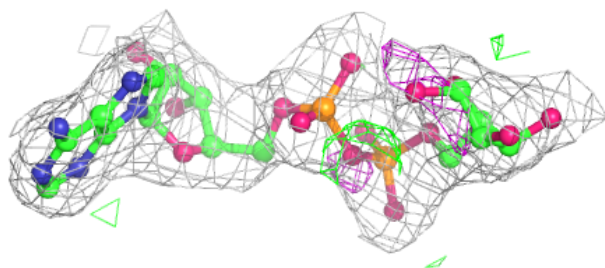
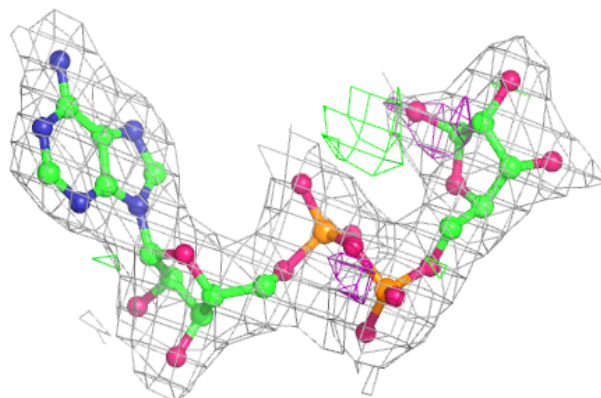


**Electron density around APR N 201:**

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

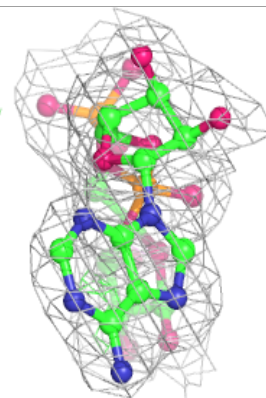
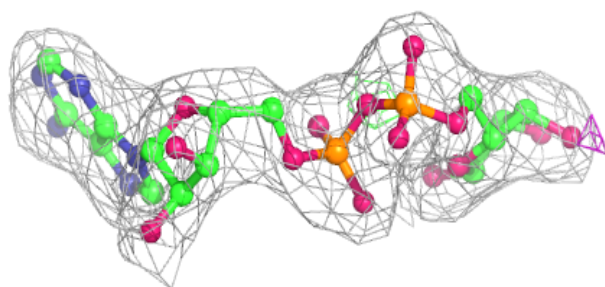
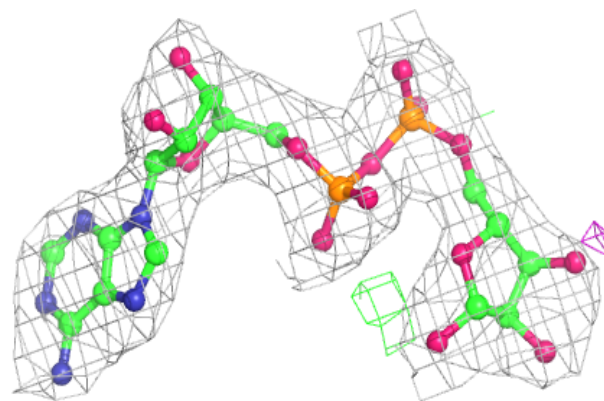
**Electron density around APR B 201:**

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

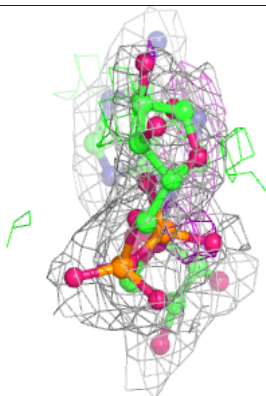
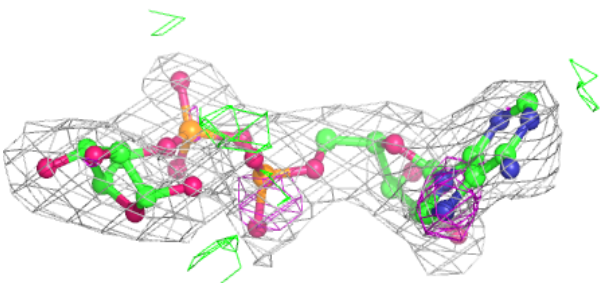
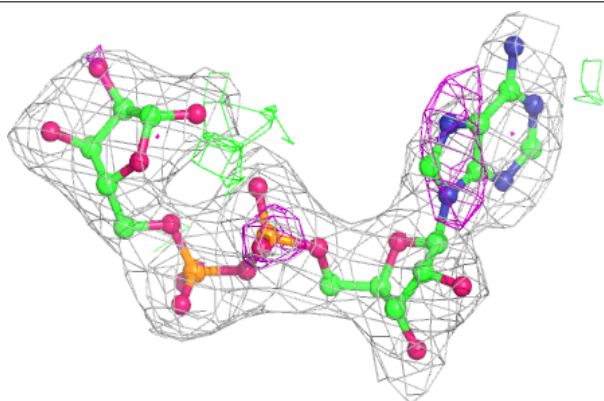


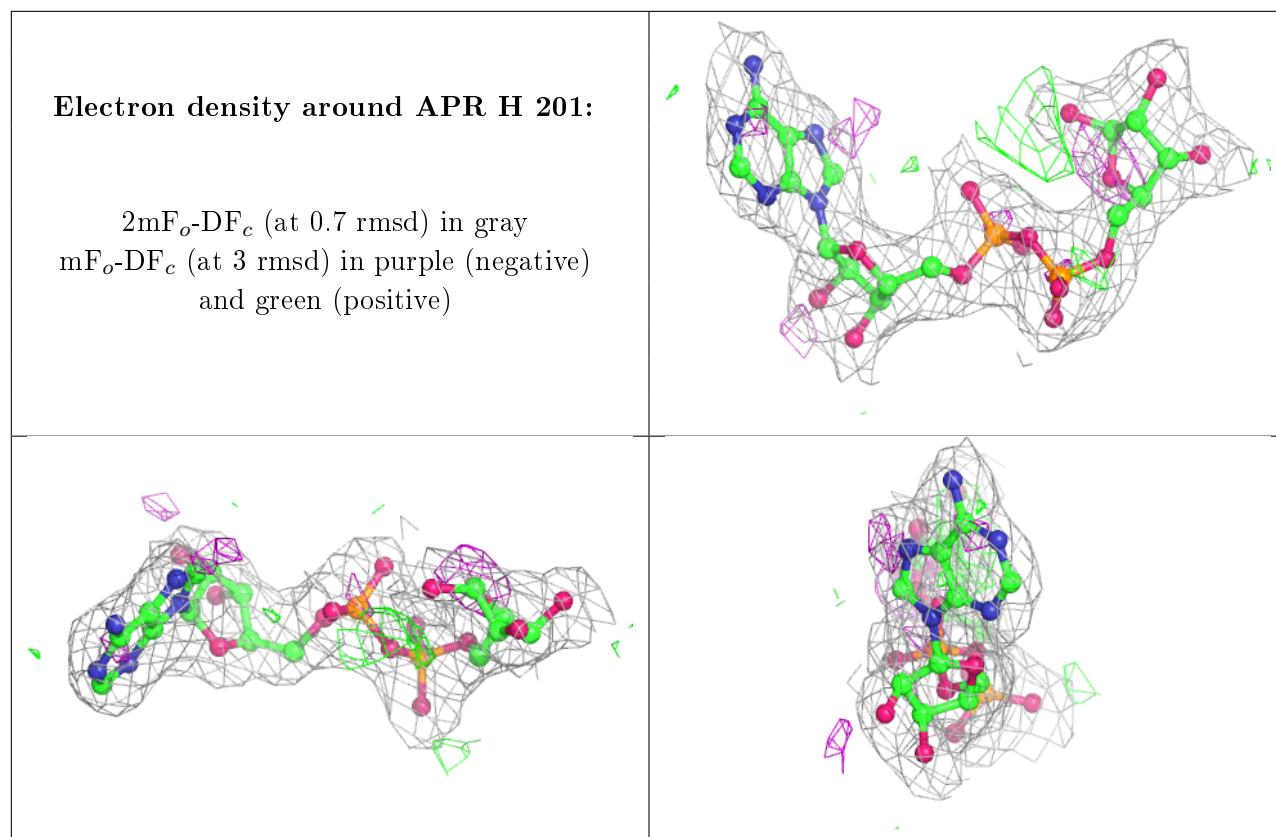
**Electron density around APR A 201:**

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

**Electron density around APR P 201:**

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





## 6.5 Other polymers [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.