



# Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 05:38 pm BST

PDB ID : 5CMS  
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 : 2015-07-17  
Resolution : 2.98 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 : 2.11  
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

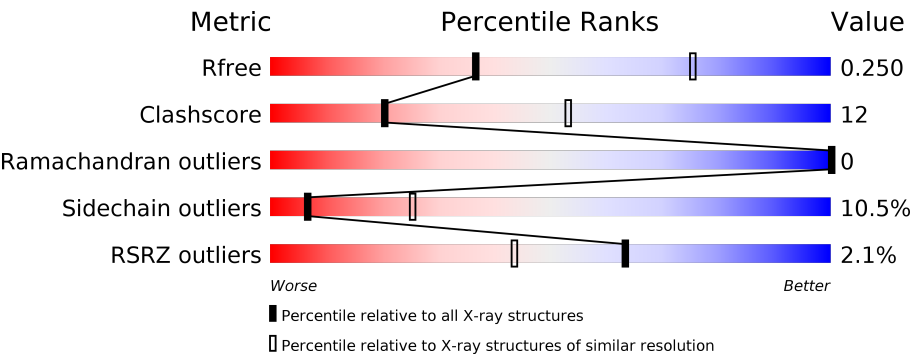
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.98 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.



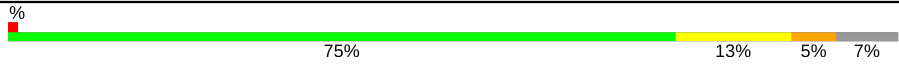



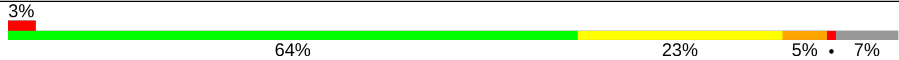
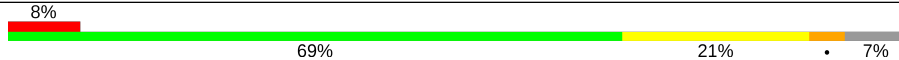
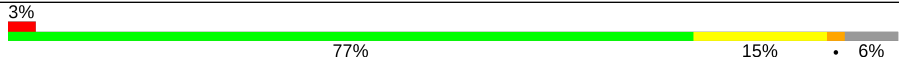
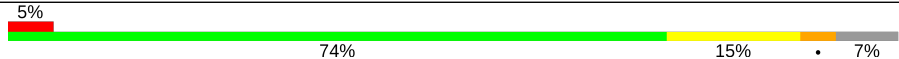
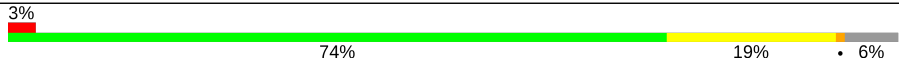
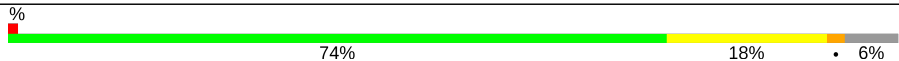
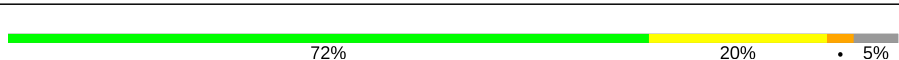
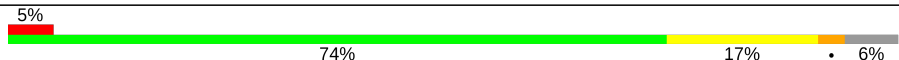
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	2754 (3.00-2.96)
Clashscore	141614	3103 (3.00-2.96)
Ramachandran outliers	138981	2993 (3.00-2.96)
Sidechain outliers	138945	2996 (3.00-2.96)
RSRZ outliers	127900	2644 (3.00-2.96)

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  $\leq 5\%$ . 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	183	<div><div>4%</div><div><div></div><div>74%</div><div>16%</div><div>• 5%</div></div></div>
1	B	183	<div><div>%</div><div><div></div><div>72%</div><div>18%</div><div>5% 5%</div></div></div>
1	C	183	<div><div>%</div><div><div></div><div>75%</div><div>16%</div><div>• 5%</div></div></div>
1	D	183	<div><div></div><div><div></div><div>66%</div><div>23%</div><div>5% 5%</div></div></div>
1	E	183	<div><div></div><div><div></div><div>73%</div><div>16%</div><div>5% 5%</div></div></div>
1	F	183	<div><div></div><div><div></div><div>78%</div><div>13%</div><div>• • 6%</div></div></div>

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Mol	Chain	Length	Quality of chain
1	G	183	
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
2	APR	L	201	-	-	X	-
3	SO4	B	202	-	-	X	-
3	SO4	C	202	-	-	X	-
3	SO4	D	202	-	-	X	-
3	SO4	E	202	-	-	X	-
3	SO4	F	202	-	-	X	-
3	SO4	G	202	-	-	X	-
3	SO4	J	202	-	-	X	-
3	SO4	M	202	-	-	X	-
3	SO4	P	202	-	-	X	-
3	SO4	Q	202	-	-	X	-
3	SO4	R	402	-	-	X	-

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 23519 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	172	Total	C	N	O	S	0	0	0
			1255	790	223	238	4			
1	A	173	Total	C	N	O	S	0	0	0
			1260	795	223	238	4			
1	B	173	Total	C	N	O	S	0	0	0
			1288	810	231	243	4			
1	C	173	Total	C	N	O	S	0	0	0
			1274	803	228	239	4			
1	D	173	Total	C	N	O	S	0	0	0
			1274	802	227	241	4			
1	E	173	Total	C	N	O	S	0	0	0
			1270	800	227	239	4			
1	F	172	Total	C	N	O	S	0	0	0
			1255	790	224	237	4			
1	G	171	Total	C	N	O	S	0	0	0
			1242	784	216	238	4			
1	H	172	Total	C	N	O	S	0	0	0
			1269	798	228	239	4			
1	I	171	Total	C	N	O	S	0	0	0
			1254	789	224	237	4			
1	J	172	Total	C	N	O	S	0	0	0
			1261	794	225	238	4			
1	K	171	Total	C	N	O	S	0	0	0
			1241	785	217	235	4			
1	L	171	Total	C	N	O	S	0	0	0
			1228	774	214	236	4			
1	M	172	Total	C	N	O	S	0	0	0
			1269	799	225	241	4			
1	N	171	Total	C	N	O	S	0	0	0
			1227	776	214	233	4			
1	O	172	Total	C	N	O	S	0	0	0
			1275	802	228	241	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	P	172	Total	C	N	O	S	0	0	0
			1261	794	225	238	4			
1	Q	173	Total	C	N	O	S	0	0	0
			1276	803	224	245	4			

There are 126 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	-5	HIS	-	expression tag	UNP C3TEL7
R	-4	HIS	-	expression tag	UNP C3TEL7
R	-3	HIS	-	expression tag	UNP C3TEL7
R	-2	HIS	-	expression tag	UNP C3TEL7
R	-1	HIS	-	expression tag	UNP C3TEL7
R	0	HIS	-	expression tag	UNP C3TEL7
R	126	ALA	TYR	engineered mutation	UNP C3TEL7
A	-5	HIS	-	expression tag	UNP C3TEL7
A	-4	HIS	-	expression tag	UNP C3TEL7
A	-3	HIS	-	expression tag	UNP C3TEL7
A	-2	HIS	-	expression tag	UNP C3TEL7
A	-1	HIS	-	expression tag	UNP C3TEL7
A	0	HIS	-	expression tag	UNP C3TEL7
A	126	ALA	TYR	engineered mutation	UNP C3TEL7
B	-5	HIS	-	expression tag	UNP C3TEL7
B	-4	HIS	-	expression tag	UNP C3TEL7
B	-3	HIS	-	expression tag	UNP C3TEL7
B	-2	HIS	-	expression tag	UNP C3TEL7
B	-1	HIS	-	expression tag	UNP C3TEL7
B	0	HIS	-	expression tag	UNP C3TEL7
B	126	ALA	TYR	engineered mutation	UNP C3TEL7
C	-5	HIS	-	expression tag	UNP C3TEL7
C	-4	HIS	-	expression tag	UNP C3TEL7
C	-3	HIS	-	expression tag	UNP C3TEL7
C	-2	HIS	-	expression tag	UNP C3TEL7
C	-1	HIS	-	expression tag	UNP C3TEL7
C	0	HIS	-	expression tag	UNP C3TEL7
C	126	ALA	TYR	engineered mutation	UNP C3TEL7
D	-5	HIS	-	expression tag	UNP C3TEL7
D	-4	HIS	-	expression tag	UNP C3TEL7
D	-3	HIS	-	expression tag	UNP C3TEL7
D	-2	HIS	-	expression tag	UNP C3TEL7
D	-1	HIS	-	expression tag	UNP C3TEL7
D	0	HIS	-	expression tag	UNP C3TEL7

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Chain	Residue	Modelled	Actual	Comment	Reference
D	126	ALA	TYR	engineered mutation	UNP C3TEL7
E	-5	HIS	-	expression tag	UNP C3TEL7
E	-4	HIS	-	expression tag	UNP C3TEL7
E	-3	HIS	-	expression tag	UNP C3TEL7
E	-2	HIS	-	expression tag	UNP C3TEL7
E	-1	HIS	-	expression tag	UNP C3TEL7
E	0	HIS	-	expression tag	UNP C3TEL7
E	126	ALA	TYR	engineered mutation	UNP C3TEL7
F	-5	HIS	-	expression tag	UNP C3TEL7
F	-4	HIS	-	expression tag	UNP C3TEL7
F	-3	HIS	-	expression tag	UNP C3TEL7
F	-2	HIS	-	expression tag	UNP C3TEL7
F	-1	HIS	-	expression tag	UNP C3TEL7
F	0	HIS	-	expression tag	UNP C3TEL7
F	126	ALA	TYR	engineered mutation	UNP C3TEL7
G	-5	HIS	-	expression tag	UNP C3TEL7
G	-4	HIS	-	expression tag	UNP C3TEL7
G	-3	HIS	-	expression tag	UNP C3TEL7
G	-2	HIS	-	expression tag	UNP C3TEL7
G	-1	HIS	-	expression tag	UNP C3TEL7
G	0	HIS	-	expression tag	UNP C3TEL7
G	126	ALA	TYR	engineered mutation	UNP C3TEL7
H	-5	HIS	-	expression tag	UNP C3TEL7
H	-4	HIS	-	expression tag	UNP C3TEL7
H	-3	HIS	-	expression tag	UNP C3TEL7
H	-2	HIS	-	expression tag	UNP C3TEL7
H	-1	HIS	-	expression tag	UNP C3TEL7
H	0	HIS	-	expression tag	UNP C3TEL7
H	126	ALA	TYR	engineered mutation	UNP C3TEL7
I	-5	HIS	-	expression tag	UNP C3TEL7
I	-4	HIS	-	expression tag	UNP C3TEL7
I	-3	HIS	-	expression tag	UNP C3TEL7
I	-2	HIS	-	expression tag	UNP C3TEL7
I	-1	HIS	-	expression tag	UNP C3TEL7
I	0	HIS	-	expression tag	UNP C3TEL7
I	126	ALA	TYR	engineered mutation	UNP C3TEL7
J	-5	HIS	-	expression tag	UNP C3TEL7
J	-4	HIS	-	expression tag	UNP C3TEL7
J	-3	HIS	-	expression tag	UNP C3TEL7
J	-2	HIS	-	expression tag	UNP C3TEL7
J	-1	HIS	-	expression tag	UNP C3TEL7
J	0	HIS	-	expression tag	UNP C3TEL7

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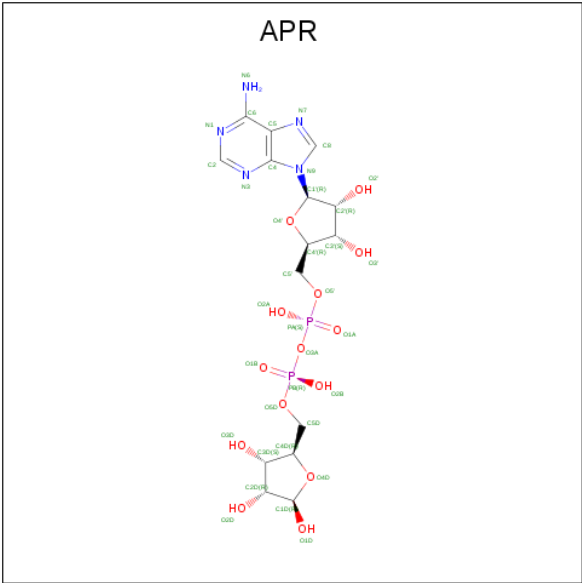
Chain	Residue	Modelled	Actual	Comment	Reference
J	126	ALA	TYR	engineered mutation	UNP C3TEL7
K	-5	HIS	-	expression tag	UNP C3TEL7
K	-4	HIS	-	expression tag	UNP C3TEL7
K	-3	HIS	-	expression tag	UNP C3TEL7
K	-2	HIS	-	expression tag	UNP C3TEL7
K	-1	HIS	-	expression tag	UNP C3TEL7
K	0	HIS	-	expression tag	UNP C3TEL7
K	126	ALA	TYR	engineered mutation	UNP C3TEL7
L	-5	HIS	-	expression tag	UNP C3TEL7
L	-4	HIS	-	expression tag	UNP C3TEL7
L	-3	HIS	-	expression tag	UNP C3TEL7
L	-2	HIS	-	expression tag	UNP C3TEL7
L	-1	HIS	-	expression tag	UNP C3TEL7
L	0	HIS	-	expression tag	UNP C3TEL7
L	126	ALA	TYR	engineered mutation	UNP C3TEL7
M	-5	HIS	-	expression tag	UNP C3TEL7
M	-4	HIS	-	expression tag	UNP C3TEL7
M	-3	HIS	-	expression tag	UNP C3TEL7
M	-2	HIS	-	expression tag	UNP C3TEL7
M	-1	HIS	-	expression tag	UNP C3TEL7
M	0	HIS	-	expression tag	UNP C3TEL7
M	126	ALA	TYR	engineered mutation	UNP C3TEL7
N	-5	HIS	-	expression tag	UNP C3TEL7
N	-4	HIS	-	expression tag	UNP C3TEL7
N	-3	HIS	-	expression tag	UNP C3TEL7
N	-2	HIS	-	expression tag	UNP C3TEL7
N	-1	HIS	-	expression tag	UNP C3TEL7
N	0	HIS	-	expression tag	UNP C3TEL7
N	126	ALA	TYR	engineered mutation	UNP C3TEL7
O	-5	HIS	-	expression tag	UNP C3TEL7
O	-4	HIS	-	expression tag	UNP C3TEL7
O	-3	HIS	-	expression tag	UNP C3TEL7
O	-2	HIS	-	expression tag	UNP C3TEL7
O	-1	HIS	-	expression tag	UNP C3TEL7
O	0	HIS	-	expression tag	UNP C3TEL7
O	126	ALA	TYR	engineered mutation	UNP C3TEL7
P	-5	HIS	-	expression tag	UNP C3TEL7
P	-4	HIS	-	expression tag	UNP C3TEL7
P	-3	HIS	-	expression tag	UNP C3TEL7
P	-2	HIS	-	expression tag	UNP C3TEL7
P	-1	HIS	-	expression tag	UNP C3TEL7
P	0	HIS	-	expression tag	UNP C3TEL7

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Chain	Residue	Modelled	Actual	Comment	Reference
P	126	ALA	TYR	engineered mutation	UNP C3TEL7
Q	-5	HIS	-	expression tag	UNP C3TEL7
Q	-4	HIS	-	expression tag	UNP C3TEL7
Q	-3	HIS	-	expression tag	UNP C3TEL7
Q	-2	HIS	-	expression tag	UNP C3TEL7
Q	-1	HIS	-	expression tag	UNP C3TEL7
Q	0	HIS	-	expression tag	UNP C3TEL7
Q	126	ALA	TYR	engineered mutation	UNP C3TEL7

- Molecule 2 is ADENOSINE-5-DIPHOSPHORIBOSE (three-letter code: APR) (formula: C<sub>15</sub>H<sub>23</sub>N<sub>5</sub>O<sub>14</sub>P<sub>2</sub>).



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
			27	10	5	10	2		
2	E	1	Total	C	N	O	P	0	0
			36	15	5	14	2		
2	F	1	Total	C	N	O	P	0	0
			36	15	5	14	2		

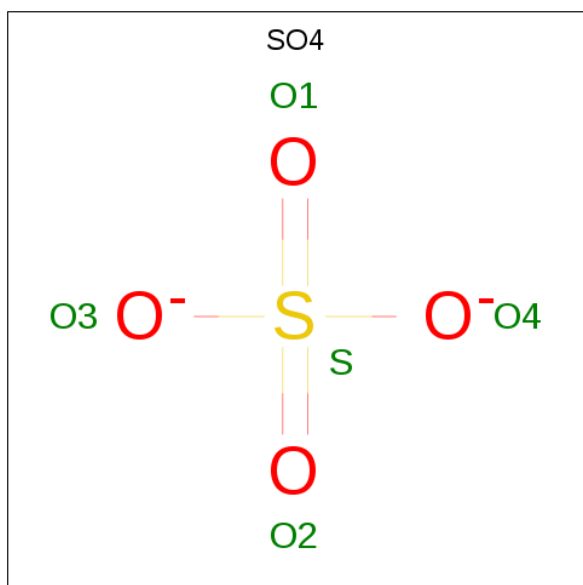
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	G	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	H	1	Total	C	N	O	P	0	0
			36	15	5	14	2		
2	I	1	Total	C	N	O	P	0	0
			36	15	5	14	2		
2	J	1	Total	C	N	O	P	0	0
			36	15	5	14	2		
2	K	1	Total	C	N	O	P	0	0
			36	15	5	14	2		
2	L	1	Total	C	N	O	P	0	0
			36	15	5	14	2		
2	M	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		
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 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0
3	E	1	Total O S 5 4 1	0	0
3	F	1	Total O S 5 4 1	0	0
3	G	1	Total O S 5 4 1	0	0
3	H	1	Total O S 5 4 1	0	0
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 water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	R	4	Total O 4 4	0	0
4	A	5	Total O 5 5	0	0

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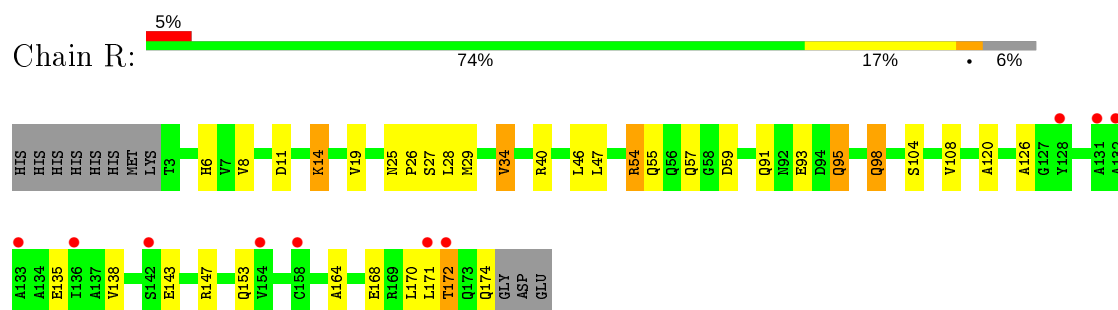
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	9	Total O 9 9	0	0
4	C	12	Total O 12 12	0	0
4	D	6	Total O 6 6	0	0
4	E	12	Total O 12 12	0	0
4	F	8	Total O 8 8	0	0
4	G	7	Total O 7 7	0	0
4	H	6	Total O 6 6	0	0
4	I	3	Total O 3 3	0	0
4	J	7	Total O 7 7	0	0
4	K	7	Total O 7 7	0	0
4	L	7	Total O 7 7	0	0
4	M	7	Total O 7 7	0	0
4	N	6	Total O 6 6	0	0
4	O	3	Total O 3 3	0	0
4	P	6	Total O 6 6	0	0
4	Q	5	Total O 5 5	0	0

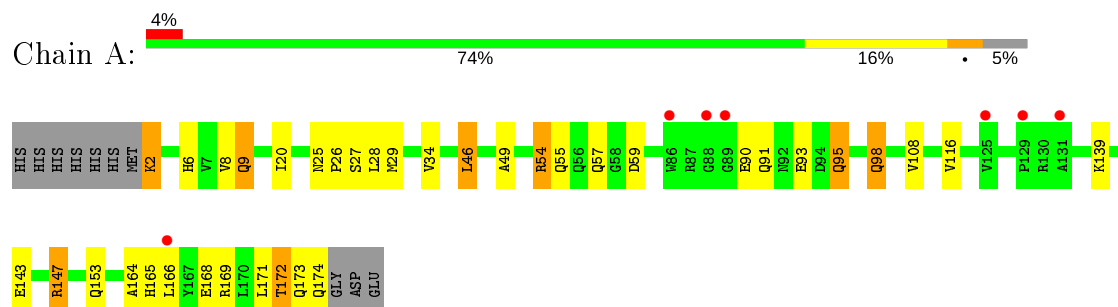
### 3 Residue-property plots [i](#)

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.

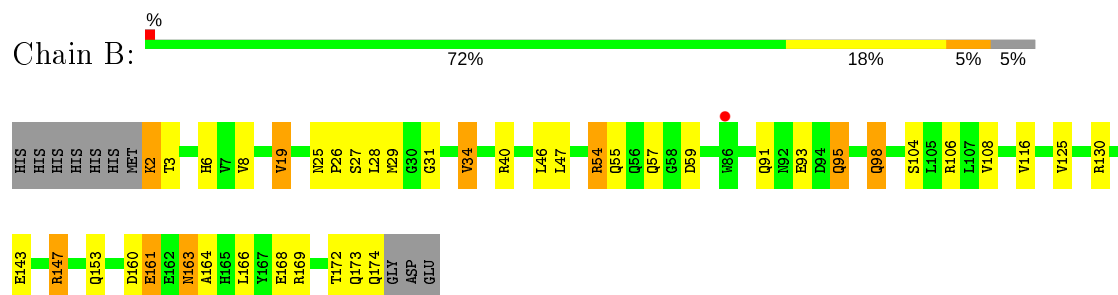
- Molecule 1: O-acetyl-ADP-ribose deacetylase



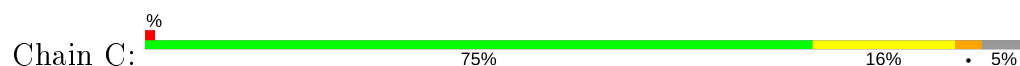
- Molecule 1: O-acetyl-ADP-ribose deacetylase

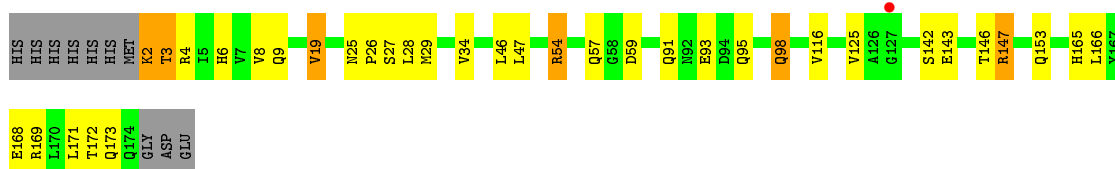


- Molecule 1: O-acetyl-ADP-ribose deacetylase



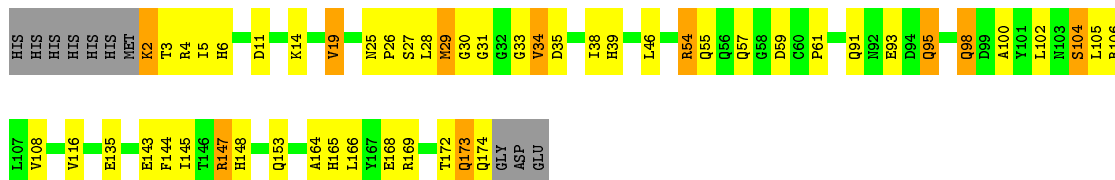
- Molecule 1: O-acetyl-ADP-ribose deacetylase





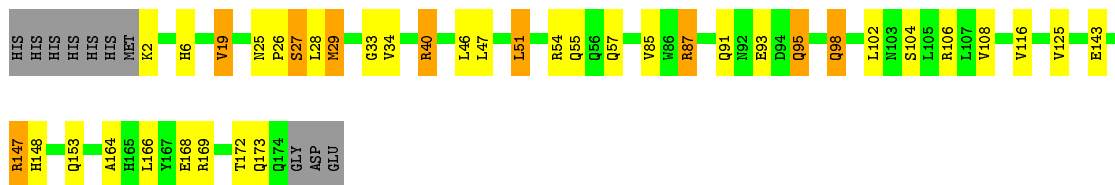
- Molecule 1: O-acetyl-ADP-ribose deacetylase

Chain D: 66% 23% 5% 5%



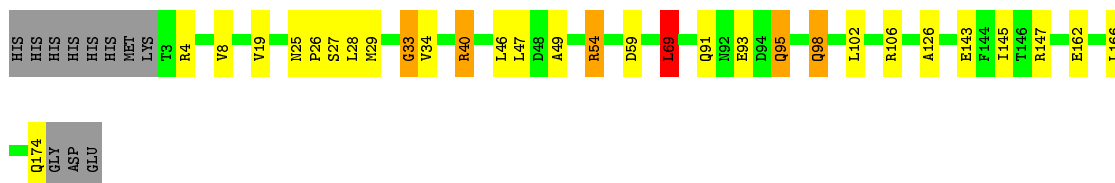
- Molecule 1: O-acetyl-ADP-ribose deacetylase

Chain E: 73% 16% 5% 5%



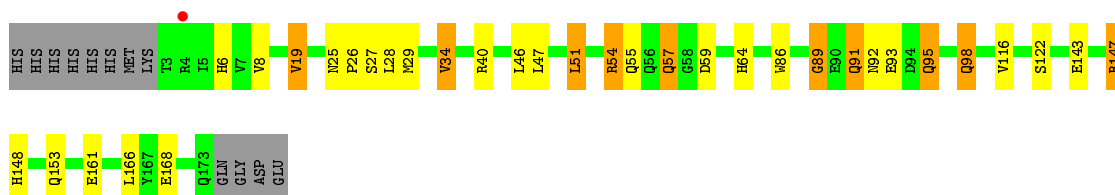
- Molecule 1: O-acetyl-ADP-ribose deacetylase

Chain F: 78% 13% 5% 6%



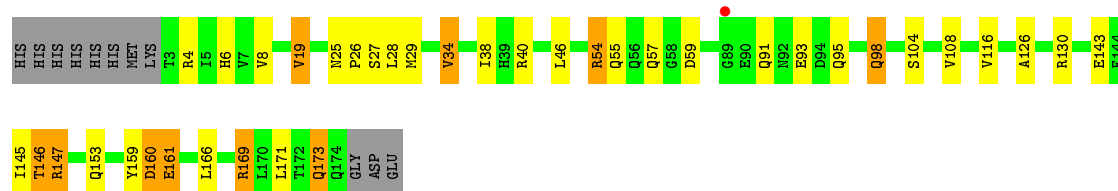
- Molecule 1: O-acetyl-ADP-ribose deacetylase

Chain G: 75% 13% 5% 7%

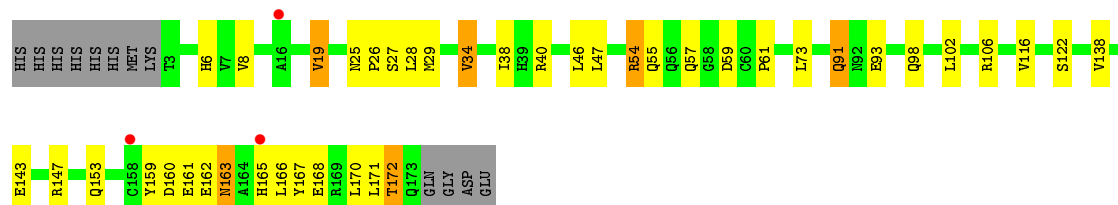


- Molecule 1: O-acetyl-ADP-ribose deacetylase

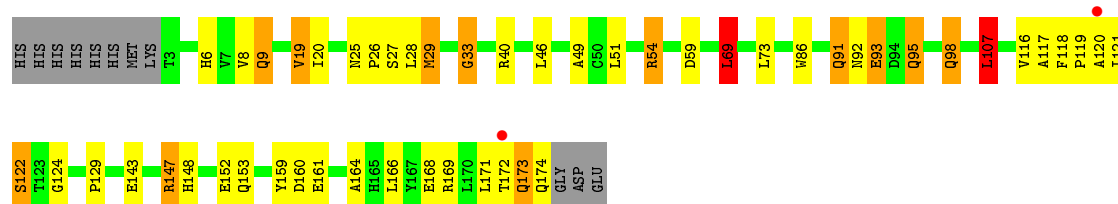
Chain H: 73% 15% 5% 6%



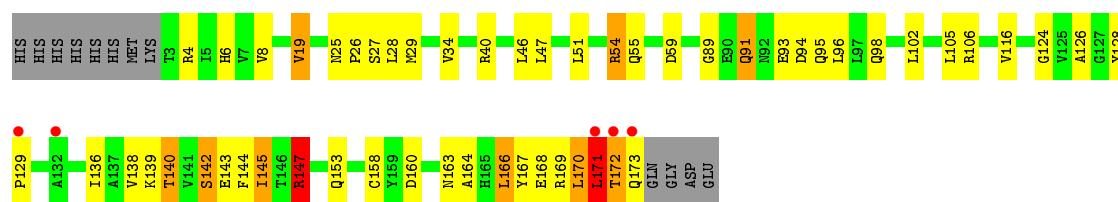
• Molecule 1: O-acetyl-ADP-ribose deacetylase



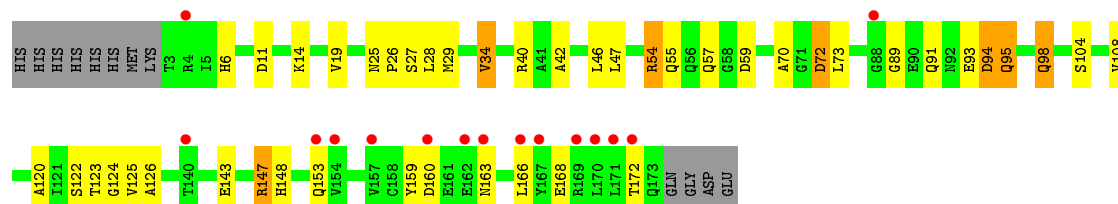
• Molecule 1: O-acetyl-ADP-ribose deacetylase




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

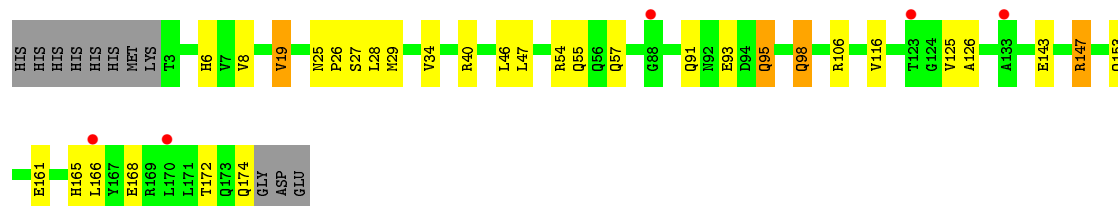


• Molecule 1: O-acetyl-ADP-ribose deacetylase



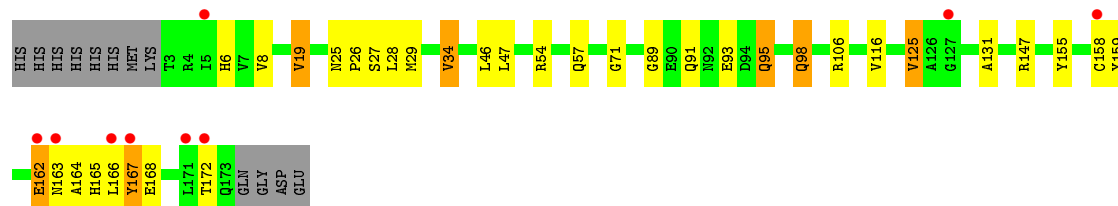
- Molecule 1: O-acetyl-ADP-ribose deacetylase

Chain M: 



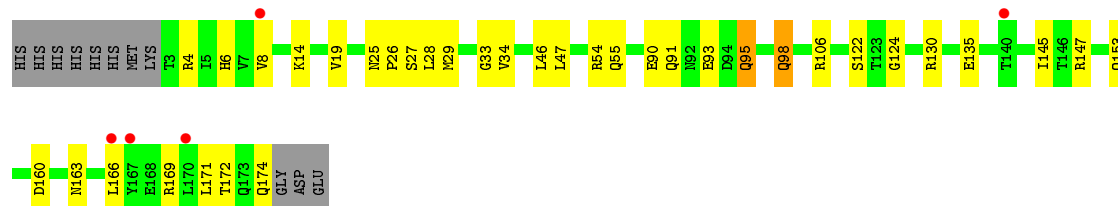
- Molecule 1: O-acetyl-ADP-ribose deacetylase

Chain N: 




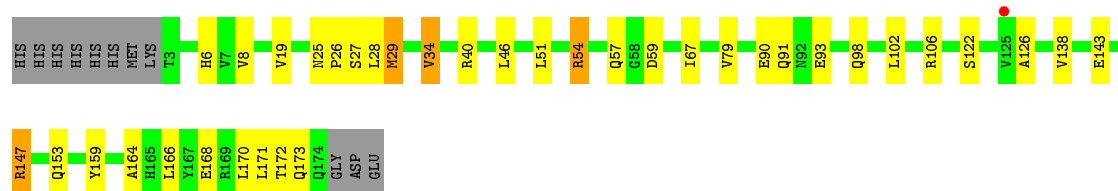
- Molecule 1: O-acetyl-ADP-ribose deacetylase

Chain O: 



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

Chain P: 



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

Chain Q: 



V125	
E143	
R147	
Q153	
E161	
A164	
H165	
L166	
Y167	
E168	
T172	
Q173	
Q174	
GLY	
ASP	
GLU	



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	290.02Å 290.02Å 114.32Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	41.90 – 2.98 41.86 – 2.98	Depositor EDS
% Data completeness (in resolution range)	97.8 (41.90-2.98) 97.9 (41.86-2.98)	Depositor EDS
$R_{merge}$	0.17	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.83 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, $R_{free}$	0.222 , 0.250 0.224 , 0.250	Depositor DCC
$R_{free}$ test set	5499 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	49.4	Xtriage
Anisotropy	0.084	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 33.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.068 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	23519	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	50.0	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 26.27 % 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 2.7183e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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, SO4

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	0.81	0/1284	0.94	2/1758 (0.1%)
1	B	0.82	0/1312	0.92	1/1791 (0.1%)
1	C	0.79	0/1298	0.91	1/1774 (0.1%)
1	D	0.84	0/1298	0.94	4/1775 (0.2%)
1	E	0.83	0/1294	0.97	4/1770 (0.2%)
1	F	0.79	0/1279	0.95	4/1751 (0.2%)
1	G	0.77	0/1266	0.94	3/1736 (0.2%)
1	H	0.78	0/1293	0.95	2/1767 (0.1%)
1	I	0.81	1/1278 (0.1%)	0.92	2/1750 (0.1%)
1	J	0.92	1/1285 (0.1%)	1.03	8/1759 (0.5%)
1	K	0.78	0/1265	0.87	1/1733 (0.1%)
1	L	0.77	0/1250	0.93	5/1714 (0.3%)
1	M	0.73	0/1293	0.86	2/1768 (0.1%)
1	N	0.77	0/1250	0.92	4/1715 (0.2%)
1	O	0.77	0/1299	0.88	0/1775
1	P	0.75	0/1285	0.91	3/1759 (0.2%)
1	Q	0.81	0/1300	0.90	1/1778 (0.1%)
1	R	0.72	0/1279	0.89	1/1751 (0.1%)
All	All	0.79	2/23108 (0.0%)	0.92	48/31624 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	K	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	152	GLU	CD-OE1	-6.21	1.18	1.25
1	I	143	GLU	CD-OE1	-5.23	1.19	1.25

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	33	GLY	N-CA-C	-9.41	89.58	113.10
1	D	33	GLY	N-CA-C	-8.98	90.65	113.10
1	C	147	ARG	NE-CZ-NH1	8.20	124.40	120.30
1	G	89	GLY	N-CA-C	8.16	133.49	113.10
1	H	147	ARG	NE-CZ-NH1	8.10	124.35	120.30
1	J	69	LEU	CA-CB-CG	8.03	133.77	115.30
1	F	69	LEU	CA-CB-CG	7.98	133.65	115.30
1	N	167	TYR	CB-CA-C	-7.79	94.82	110.40
1	L	95	GLN	CB-CA-C	-7.58	95.23	110.40
1	E	147	ARG	NE-CZ-NH1	7.56	124.08	120.30
1	J	107	LEU	CB-CG-CD1	-7.51	98.23	111.00
1	F	33	GLY	N-CA-C	-7.42	94.54	113.10
1	L	147	ARG	NE-CZ-NH2	7.26	123.93	120.30
1	D	147	ARG	NE-CZ-NH1	7.17	123.89	120.30
1	J	107	LEU	CB-CG-CD2	6.92	122.77	111.00
1	M	147	ARG	NE-CZ-NH2	6.91	123.75	120.30
1	L	147	ARG	NE-CZ-NH1	-6.90	116.85	120.30
1	N	162	GLU	CB-CA-C	-6.74	96.92	110.40
1	F	19	VAL	CB-CA-C	-6.71	98.66	111.40
1	B	147	ARG	NE-CZ-NH1	6.58	123.59	120.30
1	K	171	LEU	CB-CA-C	-6.56	97.74	110.20
1	E	33	GLY	N-CA-C	-6.34	97.24	113.10
1	G	147	ARG	NE-CZ-NH2	-6.32	117.14	120.30
1	J	69	LEU	CB-CG-CD1	6.31	121.72	111.00
1	H	147	ARG	NE-CZ-NH2	-6.29	117.16	120.30
1	N	147	ARG	NE-CZ-NH2	6.25	123.42	120.30
1	F	69	LEU	CB-CG-CD1	6.16	121.47	111.00
1	I	147	ARG	NE-CZ-NH2	6.12	123.36	120.30
1	P	147	ARG	NE-CZ-NH1	6.06	123.33	120.30
1	D	147	ARG	NE-CZ-NH2	-6.06	117.27	120.30
1	I	73	LEU	C-N-CD	6.03	141.07	128.40
1	P	19	VAL	CB-CA-C	-6.01	99.97	111.40
1	G	147	ARG	NE-CZ-NH1	5.92	123.26	120.30
1	R	19	VAL	CB-CA-C	-5.91	100.18	111.40
1	J	118	PHE	C-N-CD	5.90	140.79	128.40
1	M	147	ARG	NE-CZ-NH1	-5.87	117.36	120.30
1	N	147	ARG	NE-CZ-NH1	-5.81	117.39	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	147	ARG	NE-CZ-NH1	-5.72	117.44	120.30
1	E	19	VAL	CB-CA-C	-5.71	100.56	111.40
1	L	94	ASP	CB-CA-C	-5.67	99.06	110.40
1	L	19	VAL	CB-CA-C	-5.52	100.90	111.40
1	J	152	GLU	CG-CD-OE2	5.50	129.29	118.30
1	D	31	GLY	N-CA-C	-5.34	99.75	113.10
1	J	147	ARG	NE-CZ-NH2	5.32	122.96	120.30
1	E	147	ARG	NE-CZ-NH2	-5.31	117.64	120.30
1	Q	33	GLY	N-CA-C	-5.06	100.45	113.10
1	P	29	MET	CG-SD-CE	5.04	108.26	100.20
1	A	147	ARG	NE-CZ-NH2	5.01	122.81	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	K	147	ARG	Sidechain

## 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	1260	0	1235	29	0
1	B	1288	0	1282	35	1
1	C	1274	0	1263	28	0
1	D	1274	0	1256	44	0
1	E	1270	0	1252	39	1
1	F	1255	0	1226	24	0
1	G	1242	0	1206	41	0
1	H	1269	0	1252	31	0
1	I	1254	0	1229	24	0
1	J	1261	0	1239	43	0
1	K	1241	0	1216	50	0
1	L	1228	0	1195	39	0
1	M	1269	0	1252	22	0
1	N	1227	0	1190	29	0
1	O	1275	0	1263	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	P	1261	0	1239	29	0
1	Q	1276	0	1253	50	0
1	R	1255	0	1224	36	0
2	A	36	0	21	2	0
2	B	36	0	21	6	0
2	C	36	0	20	0	0
2	D	27	0	12	0	0
2	E	36	0	20	2	0
2	F	36	0	21	4	0
2	G	27	0	12	2	0
2	H	36	0	21	3	0
2	I	36	0	21	1	0
2	J	36	0	21	7	0
2	K	36	0	21	4	0
2	L	36	0	21	9	0
2	M	36	0	21	2	0
2	N	36	0	21	3	0
2	O	36	0	21	5	0
2	P	36	0	21	3	0
2	Q	36	0	21	5	0
2	R	36	0	21	6	0
3	A	5	0	0	1	0
3	B	5	0	0	2	0
3	C	5	0	0	3	0
3	D	5	0	0	2	0
3	E	5	0	0	5	0
3	F	5	0	0	2	0
3	G	5	0	0	2	0
3	H	5	0	0	0	0
3	I	5	0	0	1	0
3	J	5	0	0	3	0
3	K	5	0	0	1	0
3	L	5	0	0	1	0
3	M	5	0	0	3	0
3	N	5	0	0	1	0
3	O	5	0	0	1	0
3	P	5	0	0	3	0
3	Q	5	0	0	4	0
3	R	5	0	0	3	0
4	A	5	0	0	0	0
4	B	9	0	0	1	0
4	C	12	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	6	0	0	0	0
4	E	12	0	0	0	0
4	F	8	0	0	0	0
4	G	7	0	0	2	0
4	H	6	0	0	0	0
4	I	3	0	0	0	0
4	J	7	0	0	0	0
4	K	7	0	0	0	0
4	L	7	0	0	0	0
4	M	7	0	0	0	0
4	N	6	0	0	1	0
4	O	3	0	0	0	0
4	P	6	0	0	0	0
4	Q	5	0	0	0	0
4	R	4	0	0	0	0
All	All	23519	0	22630	571	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 12.

All (571) 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:E:25:ASN:HB3	2:E:201:APR:O1D	1.16	1.33
1:D:2:LYS:O	1:D:2:LYS:HD2	1.40	1.20
1:B:106:ARG:NH2	3:B:202:SO4:O3	1.79	1.15
1:L:95:GLN:OE1	1:L:98:GLN:NE2	1.84	1.10
1:K:138:VAL:O	1:K:142:SER:OG	1.68	1.09
1:Q:168:GLU:O	1:Q:172:THR:HG23	1.53	1.08
1:Q:91:GLN:HB2	1:Q:93:GLU:OE2	1.54	1.08
1:A:9:GLN:HG2	1:D:172:THR:HG21	1.34	1.06
1:Q:85:VAL:O	1:Q:87:ARG:NH2	1.88	1.06
1:N:162:GLU:OE2	1:N:162:GLU:N	1.88	1.06
1:L:91:GLN:CA	1:L:93:GLU:OE2	2.05	1.05
1:R:57:GLN:NE2	1:E:57:GLN:OE1	1.90	1.04
1:P:147:ARG:NH1	3:P:202:SO4:O2	1.92	1.02
1:L:91:GLN:HB2	1:L:93:GLU:OE2	1.59	1.01
1:E:25:ASN:CB	2:E:201:APR:O1D	2.10	1.00
1:F:147:ARG:NH1	3:F:202:SO4:O3	1.94	0.99
1:G:57:GLN:OE1	1:Q:57:GLN:OE1	1.81	0.99
1:O:130:ARG:NH2	1:O:160:ASP:OD2	1.96	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:47:LEU:O	1:E:51:LEU:HD12	1.64	0.98
1:A:164:ALA:O	1:A:168:GLU:HG3	1.65	0.97
1:B:57:GLN:OE1	1:H:57:GLN:CD	2.04	0.96
1:L:91:GLN:CB	1:L:93:GLU:OE2	2.13	0.96
1:R:57:GLN:HE22	1:E:57:GLN:HB3	1.29	0.95
1:J:91:GLN:HB2	1:J:93:GLU:OE2	1.68	0.94
1:C:168:GLU:OE1	1:Q:168:GLU:OE2	1.86	0.92
1:G:51:LEU:HD21	1:K:51:LEU:HD11	1.51	0.92
1:L:123:THR:HG1	2:L:201:APR:HO'3	1.08	0.92
1:L:91:GLN:C	1:L:93:GLU:OE2	2.10	0.89
1:K:167:TYR:O	1:K:171:LEU:N	2.04	0.89
1:Q:95:GLN:HE21	1:Q:98:GLN:NE2	1.70	0.89
1:R:57:GLN:HE22	1:E:57:GLN:CB	1.85	0.88
1:B:164:ALA:O	1:B:168:GLU:HG3	1.71	0.88
1:G:86:TRP:CH2	1:G:89:GLY:HA3	2.10	0.88
1:K:171:LEU:O	1:K:171:LEU:HD23	1.74	0.87
1:Q:22:ASN:ND2	1:Q:35:ASP:OD1	2.08	0.87
1:L:25:ASN:HB3	2:L:201:APR:HR'2	1.57	0.86
1:Q:89:GLY:N	1:Q:93:GLU:OE1	2.09	0.86
1:B:57:GLN:OE1	1:H:57:GLN:CG	2.24	0.85
1:K:139:LYS:O	1:K:143:GLU:HG3	1.76	0.85
1:J:124:GLY:HA3	2:J:201:APR:O1A	1.77	0.85
1:L:70:ALA:O	1:L:73:LEU:HD12	1.76	0.85
1:O:130:ARG:HH22	1:O:160:ASP:CG	1.80	0.85
1:C:54:ARG:NH1	1:C:59:ASP:OD1	2.11	0.84
1:E:164:ALA:O	1:E:168:GLU:HG3	1.77	0.84
1:B:57:GLN:OE1	1:H:57:GLN:HG2	1.77	0.84
1:Q:95:GLN:NE2	1:Q:98:GLN:NE2	2.25	0.84
1:E:87:ARG:HG3	1:E:87:ARG:HH21	1.42	0.83
1:J:122:SER:HA	2:J:201:APR:O1B	1.79	0.83
1:J:29:MET:HE2	1:J:51:LEU:HD21	1.61	0.82
1:B:168:GLU:O	1:B:172:THR:HG23	1.80	0.81
1:B:57:GLN:OE1	1:H:57:GLN:NE2	2.13	0.81
1:B:25:ASN:HB3	2:B:201:APR:C1D	2.11	0.80
1:E:29:MET:CE	1:E:51:LEU:HG	2.10	0.80
1:Q:147:ARG:NH2	3:Q:202:SO4:S	2.55	0.79
1:E:29:MET:HE3	1:E:51:LEU:HG	1.61	0.79
1:R:25:ASN:HB3	2:R:401:APR:HR'2	1.63	0.79
1:L:91:GLN:N	1:L:93:GLU:OE2	2.15	0.79
1:P:54:ARG:NH1	1:P:59:ASP:OD1	2.16	0.79
1:I:54:ARG:NH2	1:I:59:ASP:OD1	2.14	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:202:SO4:O1	1:P:40:ARG:HG2	1.84	0.78
1:P:29:MET:HE2	1:P:51:LEU:HD21	1.64	0.78
1:A:168:GLU:OE2	1:D:168:GLU:OE2	2.02	0.78
1:E:168:GLU:O	1:E:172:THR:HG23	1.83	0.78
1:Q:91:GLN:CB	1:Q:93:GLU:OE2	2.31	0.77
1:Q:164:ALA:O	1:Q:168:GLU:HG3	1.84	0.77
1:H:169:ARG:NH2	1:H:173:GLN:OE1	2.15	0.77
1:K:147:ARG:NH1	3:K:202:SO4:O4	2.17	0.77
1:D:168:GLU:O	1:D:172:THR:HG23	1.85	0.76
1:J:29:MET:CE	1:J:51:LEU:CD2	2.64	0.76
1:A:168:GLU:OE1	1:D:168:GLU:OE1	2.04	0.76
1:B:25:ASN:HB3	2:B:201:APR:HR'1	1.65	0.76
1:K:171:LEU:O	1:K:171:LEU:CD2	2.34	0.76
1:K:168:GLU:O	1:K:172:THR:OG1	2.05	0.75
1:M:57:GLN:HE22	1:P:57:GLN:HB3	1.52	0.75
1:R:168:GLU:O	1:R:172:THR:HG23	1.87	0.75
1:R:147:ARG:NH2	3:R:402:SO4:O1	2.20	0.75
1:J:122:SER:CA	2:J:201:APR:O1B	2.35	0.74
1:A:168:GLU:O	1:A:172:THR:OG1	2.06	0.73
1:N:164:ALA:O	1:N:168:GLU:HG2	1.88	0.73
1:C:168:GLU:OE1	1:Q:168:GLU:CD	2.26	0.73
3:D:202:SO4:O2	1:M:40:ARG:HG2	1.89	0.73
1:A:165:HIS:CE1	1:D:165:HIS:CD2	2.77	0.72
1:K:136:ILE:O	1:K:140:THR:OG1	2.04	0.72
1:A:169:ARG:O	1:A:173:GLN:HG3	1.89	0.72
1:D:164:ALA:O	1:D:168:GLU:HG3	1.89	0.72
1:M:168:GLU:O	1:M:172:THR:HG23	1.89	0.72
1:A:165:HIS:ND1	1:D:165:HIS:CD2	2.58	0.72
1:E:106:ARG:NH2	3:E:202:SO4:O1	2.23	0.71
1:H:4:ARG:NH2	1:H:145:ILE:HG23	2.05	0.71
1:R:57:GLN:CD	1:E:57:GLN:OE1	2.28	0.71
1:P:29:MET:CE	1:P:51:LEU:HD21	2.21	0.71
1:N:158:CYS:SG	1:N:167:TYR:CD2	2.83	0.71
1:I:168:GLU:O	1:I:172:THR:OG1	2.09	0.70
1:J:122:SER:N	2:J:201:APR:O1B	2.24	0.70
1:D:27:SER:HB2	1:D:29:MET:HG3	1.72	0.70
1:D:34:VAL:O	1:D:38:ILE:HG13	1.91	0.70
1:J:33:GLY:HA3	2:J:201:APR:O2A	1.92	0.70
1:D:105:LEU:HD13	1:D:144:PHE:CG	2.26	0.69
1:H:4:ARG:NH2	1:H:145:ILE:CG2	2.55	0.69
1:C:6:HIS:HE1	1:C:153:GLN:OE1	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:6:HIS:HE1	1:L:153:GLN:OE1	1.75	0.69
1:O:169:ARG:O	1:O:172:THR:OG1	2.10	0.69
1:L:34:VAL:HG23	2:L:201:APR:O2A	1.91	0.69
1:G:91:GLN:N	1:G:93:GLU:OE2	2.26	0.69
1:Q:147:ARG:NH2	3:Q:202:SO4:O2	2.23	0.68
1:D:100:ALA:O	1:D:104:SER:OG	2.10	0.68
1:C:168:GLU:OE2	1:Q:168:GLU:OE1	2.12	0.68
1:E:169:ARG:O	1:E:173:GLN:HG3	1.94	0.68
1:J:164:ALA:O	1:J:168:GLU:HG3	1.93	0.67
1:R:25:ASN:HB3	2:R:401:APR:C2D	2.24	0.67
1:K:167:TYR:O	1:K:171:LEU:HB2	1.95	0.67
1:O:33:GLY:HA3	2:O:201:APR:O2A	1.95	0.67
1:R:57:GLN:NE2	1:E:57:GLN:HB3	2.08	0.66
1:Q:147:ARG:NH2	3:Q:202:SO4:O1	2.29	0.66
1:P:34:VAL:HG23	2:P:201:APR:O2A	1.95	0.66
1:R:57:GLN:NE2	1:E:57:GLN:CD	2.48	0.65
3:A:202:SO4:O4	1:F:40:ARG:HG2	1.97	0.65
1:E:25:ASN:OD1	1:E:27:SER:OG	2.14	0.65
1:K:40:ARG:HG2	3:Q:202:SO4:O3	1.95	0.65
1:L:89:GLY:HA2	1:L:93:GLU:OE1	1.97	0.65
1:J:29:MET:HE1	1:J:51:LEU:CD2	2.26	0.65
1:Q:95:GLN:HE21	1:Q:98:GLN:HE21	1.43	0.64
1:P:29:MET:CE	1:P:51:LEU:CD2	2.75	0.64
1:R:54:ARG:NH1	1:R:59:ASP:OD1	2.31	0.63
1:G:57:GLN:OE1	1:Q:57:GLN:CG	2.46	0.63
1:J:29:MET:HE2	1:J:51:LEU:CD2	2.25	0.63
1:B:29:MET:HE3	1:B:29:MET:HA	1.80	0.63
1:D:57:GLN:HB3	1:I:57:GLN:OE1	1.98	0.62
1:P:138:VAL:CG1	1:P:171:LEU:HD23	2.29	0.62
1:J:29:MET:HE1	1:J:51:LEU:HG	1.80	0.62
1:N:158:CYS:SG	1:N:167:TYR:CE2	2.92	0.62
1:H:161:GLU:OE1	1:J:169:ARG:NH1	2.33	0.62
1:B:147:ARG:NH2	3:B:202:SO4:O2	2.21	0.62
1:C:142:SER:O	1:C:146:THR:HG23	1.99	0.62
1:K:166:LEU:O	1:K:170:LEU:N	2.25	0.62
1:Q:95:GLN:NE2	1:Q:98:GLN:HE22	1.97	0.62
1:Q:122:SER:HA	2:Q:201:APR:O1B	1.99	0.62
1:D:11:ASP:HB3	1:D:14:LYS:HD2	1.82	0.62
1:K:169:ARG:O	1:K:172:THR:OG1	2.18	0.62
1:L:42:ALA:O	1:L:72:ASP:OD1	2.18	0.61
1:N:25:ASN:HB3	2:N:201:APR:HR'2	1.80	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:34:VAL:O	1:Q:38:ILE:HG13	1.99	0.61
1:C:2:LYS:O	1:C:3:THR:HG22	2.00	0.61
1:J:27:SER:O	1:J:28:LEU:HB2	2.00	0.61
1:N:158:CYS:SG	1:N:167:TYR:HD2	2.24	0.61
1:Q:25:ASN:HB3	2:Q:201:APR:HR'2	1.81	0.61
1:L:168:GLU:O	1:L:172:THR:HG23	1.99	0.61
1:R:126:ALA:HB2	2:R:401:APR:HR'4	1.83	0.61
1:N:168:GLU:OE2	1:N:168:GLU:HA	2.00	0.61
1:C:29:MET:HA	1:C:29:MET:HE3	1.82	0.60
1:B:25:ASN:CB	2:B:201:APR:HR'1	2.31	0.60
1:G:86:TRP:CH2	1:G:89:GLY:CA	2.84	0.60
1:D:29:MET:CE	1:D:54:ARG:HE	2.14	0.60
1:C:2:LYS:HD3	1:C:2:LYS:O	2.01	0.60
1:E:27:SER:O	1:E:28:LEU:HB2	2.02	0.60
1:P:106:ARG:NH2	3:P:202:SO4:O4	2.33	0.60
1:Q:161:GLU:HG2	1:Q:165:HIS:CE1	2.37	0.60
1:N:29:MET:HE3	1:N:29:MET:HA	1.82	0.59
1:O:29:MET:HA	1:O:29:MET:HE3	1.83	0.59
1:L:29:MET:HE3	1:L:29:MET:HA	1.84	0.59
1:J:124:GLY:CA	2:J:201:APR:O1A	2.50	0.59
1:D:104:SER:O	1:D:108:VAL:HG23	2.02	0.59
1:R:29:MET:HA	1:R:29:MET:HE3	1.82	0.59
1:I:27:SER:O	1:I:28:LEU:HB2	2.03	0.59
1:H:6:HIS:HE1	1:H:153:GLN:OE1	1.86	0.59
1:C:165:HIS:CD2	1:Q:165:HIS:CD2	2.90	0.59
1:G:89:GLY:HA2	1:G:93:GLU:OE1	2.02	0.59
1:N:168:GLU:O	1:N:172:THR:HG23	2.03	0.59
1:G:57:GLN:OE1	1:Q:57:GLN:CD	2.41	0.59
1:G:91:GLN:HB2	1:G:93:GLU:OE2	2.03	0.59
1:N:57:GLN:O	1:N:57:GLN:HG2	2.03	0.59
1:P:138:VAL:HG13	1:P:171:LEU:HD23	1.85	0.59
1:I:29:MET:CE	1:I:47:LEU:HD11	2.31	0.58
1:L:89:GLY:CA	1:L:93:GLU:OE1	2.51	0.58
1:E:29:MET:HE1	1:E:51:LEU:HG	1.86	0.58
1:D:6:HIS:HE1	1:D:153:GLN:OE1	1.87	0.58
1:G:89:GLY:N	1:G:93:GLU:OE1	2.37	0.58
1:I:34:VAL:O	1:I:38:ILE:HG13	2.04	0.58
1:K:27:SER:O	1:K:28:LEU:HB2	2.04	0.58
1:K:29:MET:CE	1:K:47:LEU:HD11	2.33	0.58
1:M:29:MET:HE3	1:M:29:MET:HA	1.84	0.58
1:N:131:ALA:HA	1:N:166:LEU:HD11	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:173:GLN:O	1:D:174:GLN:HB2	2.04	0.58
1:F:126:ALA:HB2	2:F:201:APR:HR'4	1.86	0.58
1:P:126:ALA:HB2	2:P:201:APR:HR'4	1.86	0.58
1:Q:89:GLY:CA	1:Q:93:GLU:OE1	2.51	0.58
1:R:57:GLN:HE22	1:E:57:GLN:CG	2.17	0.57
1:F:29:MET:CE	1:F:47:LEU:HD11	2.34	0.57
1:Q:168:GLU:O	1:Q:172:THR:CG2	2.43	0.57
1:G:29:MET:HE3	1:G:29:MET:HA	1.86	0.57
1:P:29:MET:HE2	1:P:51:LEU:CD2	2.34	0.57
1:A:108:VAL:HG11	1:A:116:VAL:CG1	2.35	0.57
1:O:6:HIS:HE1	1:O:153:GLN:OE1	1.87	0.57
1:E:87:ARG:HG3	1:E:87:ARG:NH2	2.16	0.57
1:L:6:HIS:CE1	1:L:153:GLN:OE1	2.57	0.56
1:R:29:MET:CE	1:R:47:LEU:HD11	2.35	0.56
1:B:169:ARG:O	1:B:173:GLN:HG3	2.04	0.56
1:K:164:ALA:O	1:K:168:GLU:HG3	2.04	0.56
1:H:27:SER:O	1:H:28:LEU:HB2	2.04	0.56
1:I:6:HIS:HE1	1:I:153:GLN:OE1	1.89	0.56
1:A:29:MET:HA	1:A:29:MET:HE3	1.88	0.56
1:F:25:ASN:HB3	2:F:201:APR:HR'2	1.87	0.56
1:L:29:MET:CE	1:L:47:LEU:HD11	2.36	0.56
1:R:57:GLN:NE2	1:E:57:GLN:CB	2.65	0.55
1:D:61:PRO:HG3	1:I:61:PRO:HG2	1.89	0.55
1:D:2:LYS:O	1:D:2:LYS:CD	2.35	0.55
1:D:61:PRO:HG2	1:I:61:PRO:HG3	1.89	0.55
1:A:6:HIS:HE1	1:A:153:GLN:OE1	1.90	0.55
1:M:106:ARG:NE	3:M:202:SO4:O3	2.39	0.55
1:D:27:SER:HB2	1:D:29:MET:CG	2.37	0.55
1:Q:27:SER:O	1:Q:28:LEU:HB2	2.06	0.55
1:G:6:HIS:HE1	1:G:153:GLN:OE1	1.90	0.54
1:J:9:GLN:HE22	1:J:161:GLU:HG3	1.72	0.54
1:N:106:ARG:NH2	3:N:202:SO4:O3	2.40	0.54
1:C:57:GLN:OE1	1:N:57:GLN:HG3	2.07	0.54
1:H:130:ARG:NH2	1:H:160:ASP:OD1	2.32	0.54
1:O:29:MET:CE	1:O:47:LEU:HD11	2.38	0.54
1:A:173:GLN:O	1:A:174:GLN:HG3	2.08	0.53
1:J:29:MET:HE1	1:J:51:LEU:HD23	1.90	0.53
1:J:92:ASN:OD1	1:J:95:GLN:HB2	2.07	0.53
1:K:168:GLU:O	1:K:172:THR:HG23	2.08	0.53
1:Q:91:GLN:CA	1:Q:93:GLU:OE2	2.55	0.53
1:G:64:HIS:CE1	1:Q:61:PRO:HB3	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:27:SER:O	1:F:28:LEU:HB2	2.08	0.53
1:J:120:ALA:O	2:J:201:APR:H5'2	2.09	0.53
1:D:102:LEU:O	1:D:106:ARG:HG3	2.08	0.53
1:G:148:HIS:NE2	3:G:202:SO4:O3	2.35	0.53
1:I:29:MET:HE3	1:I:29:MET:HA	1.91	0.53
1:J:29:MET:CE	1:J:51:LEU:HD23	2.39	0.53
1:G:92:ASN:ND2	1:G:95:GLN:HB2	2.24	0.53
1:L:42:ALA:HB2	1:L:73:LEU:HD11	1.89	0.53
1:K:126:ALA:HB2	2:K:201:APR:HR'4	1.91	0.53
1:A:57:GLN:HB3	1:L:57:GLN:HE22	1.73	0.53
1:B:57:GLN:HB3	1:H:57:GLN:HE22	1.74	0.53
1:N:29:MET:CE	1:N:47:LEU:HD11	2.39	0.53
1:D:5:ILE:HD11	1:D:145:ILE:HD11	1.91	0.53
1:P:170:LEU:O	1:P:173:GLN:HB3	2.08	0.53
1:F:25:ASN:CB	2:F:201:APR:HR'2	2.38	0.52
1:G:29:MET:CE	1:G:47:LEU:HD11	2.39	0.52
1:N:71:GLY:HA2	4:N:302:HOH:O	2.09	0.52
1:F:29:MET:HA	1:F:29:MET:HE3	1.90	0.52
1:G:64:HIS:HB3	4:G:305:HOH:O	2.09	0.52
1:O:4:ARG:CZ	1:O:145:ILE:HG23	2.39	0.52
4:C:312:HOH:O	1:P:40:ARG:HD2	2.10	0.52
1:H:126:ALA:HB2	2:H:201:APR:HR'4	1.91	0.52
1:Q:91:GLN:N	1:Q:93:GLU:OE2	2.43	0.52
1:A:25:ASN:OD1	1:A:27:SER:OG	2.27	0.52
1:G:91:GLN:O	1:G:92:ASN:HB3	2.10	0.52
1:C:147:ARG:NH1	3:C:202:SO4:O3	2.42	0.52
1:E:106:ARG:NE	3:E:202:SO4:O1	2.41	0.52
1:M:125:VAL:HG13	2:M:201:APR:O1A	2.09	0.52
1:M:29:MET:CE	1:M:47:LEU:HD11	2.40	0.52
1:C:6:HIS:CE1	1:C:153:GLN:OE1	2.61	0.52
1:F:4:ARG:CZ	1:F:145:ILE:HG23	2.40	0.52
1:H:4:ARG:CZ	1:H:145:ILE:HG23	2.40	0.52
1:H:4:ARG:NH2	1:H:145:ILE:HG22	2.25	0.51
1:I:167:TYR:HA	1:I:170:LEU:HD12	1.92	0.51
1:Q:95:GLN:NE2	1:Q:98:GLN:HE21	1.99	0.51
1:E:40:ARG:HG2	3:G:202:SO4:O2	2.10	0.51
1:O:4:ARG:NH2	1:O:145:ILE:CG2	2.74	0.51
1:R:34:VAL:HG23	2:R:401:APR:O2A	2.10	0.51
1:F:54:ARG:NH2	1:F:59:ASP:OD1	2.43	0.51
1:R:6:HIS:HE1	1:R:153:GLN:OE1	1.93	0.51
1:D:169:ARG:O	1:D:173:GLN:HG2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:121:ILE:O	1:J:122:SER:HB2	2.10	0.51
1:Q:95:GLN:HE21	1:Q:98:GLN:HE22	1.52	0.51
1:C:168:GLU:CD	1:Q:168:GLU:OE1	2.48	0.51
1:H:54:ARG:NH2	1:H:59:ASP:OD1	2.44	0.51
1:P:164:ALA:O	1:P:168:GLU:HG3	2.10	0.51
1:P:29:MET:HE1	1:P:51:LEU:CD2	2.41	0.51
1:D:29:MET:HE2	1:D:54:ARG:HE	1.76	0.51
1:H:34:VAL:O	1:H:38:ILE:HG13	2.10	0.51
1:P:106:ARG:NE	3:P:202:SO4:O4	2.43	0.51
1:I:29:MET:CE	1:I:47:LEU:CD1	2.89	0.50
1:L:25:ASN:OD1	1:L:27:SER:OG	2.29	0.50
1:R:25:ASN:HB3	2:R:401:APR:O2D	2.11	0.50
1:B:31:GLY:HA3	4:B:303:HOH:O	2.12	0.50
1:G:89:GLY:CA	1:G:93:GLU:OE1	2.59	0.50
2:L:201:APR:H5'1	2:L:201:APR:PB	2.52	0.50
1:A:54:ARG:NH2	1:A:59:ASP:OD1	2.44	0.50
1:J:49:ALA:HB2	1:J:69:LEU:HD21	1.93	0.50
1:N:25:ASN:OD1	1:N:27:SER:OG	2.29	0.50
1:K:170:LEU:O	1:K:170:LEU:HD23	2.11	0.50
1:G:92:ASN:HD21	1:G:95:GLN:HB2	1.77	0.50
1:A:2:LYS:HE2	1:A:2:LYS:HA	1.92	0.50
1:D:91:GLN:N	1:D:93:GLU:OE2	2.42	0.50
1:E:6:HIS:HE1	1:E:153:GLN:OE1	1.93	0.50
1:J:19:VAL:HG22	1:J:116:VAL:HG23	1.93	0.50
1:J:148:HIS:NE2	3:J:202:SO4:O3	2.40	0.50
1:J:29:MET:HE1	1:J:51:LEU:CG	2.41	0.50
1:K:158:CYS:SG	1:K:167:TYR:CD2	3.05	0.50
1:O:106:ARG:NH2	3:O:202:SO4:O3	2.42	0.50
1:C:25:ASN:OD1	1:C:27:SER:OG	2.29	0.49
1:J:91:GLN:O	1:J:92:ASN:HB3	2.12	0.49
1:P:91:GLN:N	1:P:93:GLU:OE2	2.42	0.49
1:Q:29:MET:CE	1:Q:47:LEU:HD11	2.42	0.49
1:Q:54:ARG:NH2	1:Q:59:ASP:OD1	2.45	0.49
1:M:25:ASN:OD1	1:M:27:SER:OG	2.30	0.49
1:E:91:GLN:N	1:E:93:GLU:OE2	2.41	0.49
1:F:95:GLN:OE1	1:F:98:GLN:NE2	2.46	0.49
1:L:54:ARG:NH2	1:L:59:ASP:OD1	2.45	0.49
1:J:25:ASN:OD1	1:J:27:SER:OG	2.30	0.49
1:A:91:GLN:N	1:A:93:GLU:OE2	2.42	0.49
1:J:95:GLN:OE1	1:J:98:GLN:NE2	2.45	0.49
1:P:138:VAL:HG13	1:P:171:LEU:CD2	2.41	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:6:HIS:HE1	1:Q:153:GLN:OE1	1.95	0.49
1:F:33:GLY:HA3	2:F:201:APR:O2A	2.13	0.49
1:F:49:ALA:HB2	1:F:69:LEU:HD21	1.94	0.49
1:B:130:ARG:NH2	1:B:160:ASP:OD2	2.45	0.49
1:L:126:ALA:HB2	2:L:201:APR:HR'4	1.94	0.49
1:C:91:GLN:N	1:C:93:GLU:OE2	2.43	0.49
1:G:54:ARG:NH1	1:G:59:ASP:OD1	2.46	0.49
1:K:94:ASP:OD1	1:K:94:ASP:N	2.45	0.49
1:M:6:HIS:HE1	1:M:153:GLN:OE1	1.94	0.49
1:O:25:ASN:OD1	1:O:27:SER:OG	2.30	0.49
1:O:91:GLN:N	1:O:93:GLU:OE2	2.43	0.49
1:J:143:GLU:O	1:J:147:ARG:HG3	2.13	0.49
1:J:54:ARG:NH2	1:J:59:ASP:OD1	2.44	0.49
1:K:29:MET:HE3	1:K:47:LEU:CD1	2.43	0.49
1:N:34:VAL:HG23	2:N:201:APR:O2A	2.13	0.49
1:O:124:GLY:HA3	2:O:201:APR:O1A	2.13	0.49
1:B:29:MET:CE	1:B:47:LEU:HD11	2.43	0.48
1:H:95:GLN:OE1	1:H:98:GLN:NE2	2.47	0.48
1:B:54:ARG:NH2	1:B:59:ASP:OD1	2.46	0.48
1:G:25:ASN:OD1	1:G:27:SER:OG	2.31	0.48
1:K:54:ARG:NH2	1:K:59:ASP:OD1	2.46	0.48
1:B:125:VAL:HG13	2:B:201:APR:O1A	2.14	0.48
1:G:92:ASN:HD21	1:G:95:GLN:CB	2.26	0.48
1:D:25:ASN:OD1	1:D:27:SER:OG	2.29	0.48
1:D:54:ARG:NH2	1:D:59:ASP:OD1	2.45	0.48
1:A:25:ASN:HB3	2:A:201:APR:C2D	2.44	0.48
1:K:171:LEU:CD2	1:K:171:LEU:C	2.80	0.48
1:E:25:ASN:HB2	1:E:26:PRO:HD2	1.96	0.48
1:F:25:ASN:OD1	1:F:27:SER:OG	2.31	0.48
1:O:25:ASN:HB3	2:O:201:APR:HR'2	1.96	0.48
1:B:25:ASN:OD1	1:B:27:SER:OG	2.29	0.48
1:R:91:GLN:N	1:R:93:GLU:OE2	2.42	0.48
1:G:91:GLN:CA	1:G:93:GLU:OE2	2.61	0.48
1:K:166:LEU:O	1:K:170:LEU:HB2	2.14	0.48
1:R:164:ALA:O	1:R:168:GLU:HG3	2.14	0.47
1:F:29:MET:CE	1:F:47:LEU:CD1	2.91	0.47
1:G:51:LEU:HD11	1:K:51:LEU:HD21	1.96	0.47
1:B:91:GLN:N	1:B:93:GLU:OE2	2.42	0.47
1:P:122:SER:N	2:P:201:APR:O1B	2.40	0.47
1:C:147:ARG:NH1	3:C:202:SO4:S	2.88	0.47
1:D:57:GLN:CB	1:I:57:GLN:OE1	2.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:6:HIS:HE1	1:J:153:GLN:OE1	1.97	0.47
1:L:25:ASN:HB2	1:L:26:PRO:HD2	1.97	0.47
1:M:106:ARG:NH2	3:M:202:SO4:O3	2.43	0.47
1:A:95:GLN:OE1	1:A:98:GLN:NE2	2.48	0.47
1:R:95:GLN:OE1	1:R:98:GLN:NE2	2.48	0.47
1:I:122:SER:N	2:I:201:APR:O1B	2.48	0.47
1:R:120:ALA:O	2:R:401:APR:H'4	2.15	0.47
1:A:108:VAL:HG11	1:A:116:VAL:HG12	1.95	0.47
1:R:25:ASN:OD1	1:R:27:SER:OG	2.30	0.47
1:L:124:GLY:N	2:L:201:APR:O2B	2.45	0.47
1:O:95:GLN:OE1	1:O:98:GLN:NE2	2.48	0.47
1:Q:122:SER:CA	2:Q:201:APR:O1B	2.62	0.47
1:A:108:VAL:HG21	1:A:116:VAL:HG11	1.95	0.47
3:D:202:SO4:O2	1:M:40:ARG:CG	2.61	0.47
1:R:29:MET:CE	1:R:47:LEU:CD1	2.93	0.47
1:M:147:ARG:NH1	3:M:202:SO4:O1	2.48	0.46
1:A:29:MET:HA	1:A:29:MET:CE	2.45	0.46
1:J:29:MET:CE	1:J:51:LEU:HG	2.45	0.46
1:N:25:ASN:HB2	1:N:26:PRO:HD2	1.97	0.46
1:F:147:ARG:CZ	3:F:202:SO4:O3	2.62	0.46
1:F:4:ARG:NH2	1:F:145:ILE:CG2	2.79	0.46
1:B:95:GLN:OE1	1:B:98:GLN:NE2	2.48	0.46
1:C:9:GLN:HB3	1:Q:172:THR:HG21	1.98	0.46
1:I:25:ASN:OD1	1:I:27:SER:OG	2.31	0.46
1:R:147:ARG:NH2	3:R:402:SO4:S	2.89	0.46
1:H:25:ASN:HB2	1:H:26:PRO:HD2	1.97	0.46
1:M:95:GLN:OE1	1:M:98:GLN:NE2	2.49	0.46
1:D:25:ASN:HB2	1:D:26:PRO:HD2	1.97	0.46
1:J:147:ARG:NH2	3:J:202:SO4:O2	2.49	0.46
1:L:42:ALA:HB2	1:L:73:LEU:CD1	2.46	0.46
1:B:25:ASN:HB2	1:B:26:PRO:HD2	1.96	0.46
1:H:25:ASN:OD1	1:H:27:SER:OG	2.30	0.46
1:O:171:LEU:HA	1:O:171:LEU:HD23	1.83	0.46
1:D:27:SER:O	1:D:28:LEU:HB2	2.17	0.46
1:D:29:MET:HE1	1:D:54:ARG:HE	1.80	0.46
1:I:106:ARG:NH2	3:I:202:SO4:O4	2.43	0.46
1:J:147:ARG:NH2	3:J:202:SO4:S	2.89	0.46
1:Q:24:ALA:O	2:Q:201:APR:HR'3	2.16	0.46
1:C:25:ASN:HB2	1:C:26:PRO:HD2	1.99	0.45
1:F:4:ARG:NH2	1:F:145:ILE:HG23	2.31	0.45
1:H:29:MET:HB3	1:O:29:MET:HG3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:95:GLN:OE1	1:D:98:GLN:NE2	2.49	0.45
1:J:19:VAL:O	1:J:116:VAL:HA	2.16	0.45
1:P:25:ASN:HB2	1:P:26:PRO:HD2	1.98	0.45
1:A:25:ASN:HB3	2:A:201:APR:HR'2	1.97	0.45
1:G:51:LEU:HD21	1:K:51:LEU:CD1	2.36	0.45
1:O:145:ILE:HG23	1:O:145:ILE:HD12	1.78	0.45
1:O:122:SER:N	2:O:201:APR:O1B	2.46	0.45
1:O:25:ASN:HB2	1:O:26:PRO:HD2	1.97	0.45
1:O:4:ARG:NH2	1:O:145:ILE:HG23	2.31	0.45
1:P:25:ASN:OD1	1:P:27:SER:OG	2.29	0.45
1:Q:25:ASN:OD1	1:Q:27:SER:OG	2.30	0.45
1:K:25:ASN:HB3	2:K:201:APR:C2D	2.46	0.45
1:N:131:ALA:HA	1:N:166:LEU:CD1	2.46	0.45
1:Q:25:ASN:HB2	1:Q:26:PRO:HD2	1.97	0.45
1:Q:29:MET:HE2	1:Q:29:MET:HB3	1.88	0.45
1:G:91:GLN:CB	1:G:93:GLU:OE2	2.64	0.45
1:C:29:MET:HA	1:C:29:MET:CE	2.46	0.45
1:K:29:MET:HE3	1:K:47:LEU:HD11	1.98	0.45
1:H:146:THR:HG22	1:H:147:ARG:N	2.31	0.45
1:H:91:GLN:N	1:H:93:GLU:OE2	2.43	0.45
1:K:124:GLY:HA3	2:K:201:APR:O1A	2.17	0.45
1:L:29:MET:CE	1:L:47:LEU:CD1	2.95	0.45
1:Q:122:SER:N	2:Q:201:APR:O1B	2.49	0.45
1:C:169:ARG:O	1:C:173:GLN:HG3	2.17	0.45
1:E:95:GLN:OE1	1:E:98:GLN:NE2	2.49	0.45
1:M:25:ASN:HB2	1:M:26:PRO:HD2	1.98	0.45
1:D:35:ASP:OD1	1:D:39:HIS:CE1	2.71	0.44
1:G:27:SER:O	1:G:28:LEU:HB2	2.17	0.44
1:R:25:ASN:HB2	1:R:26:PRO:HD2	2.00	0.44
1:B:161:GLU:HG3	1:B:161:GLU:O	2.18	0.44
1:I:25:ASN:HB2	1:I:26:PRO:HD2	1.98	0.44
1:N:91:GLN:N	1:N:93:GLU:OE2	2.44	0.44
1:D:19:VAL:HG22	1:D:116:VAL:HG23	1.99	0.44
1:K:4:ARG:NH2	1:K:145:ILE:O	2.50	0.44
1:R:27:SER:O	1:R:28:LEU:HB2	2.17	0.44
1:R:57:GLN:HE22	1:E:57:GLN:CD	2.21	0.44
1:B:34:VAL:CG2	2:B:201:APR:H5'2	2.48	0.44
1:G:95:GLN:OE1	1:G:98:GLN:NE2	2.50	0.44
1:F:25:ASN:HB2	1:F:26:PRO:HD2	1.99	0.44
1:I:91:GLN:N	1:I:93:GLU:OE2	2.44	0.44
1:K:143:GLU:O	1:K:147:ARG:CG	2.66	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:147:ARG:NH2	3:R:402:SO4:O2	2.50	0.44
1:G:34:VAL:HG23	2:G:201:APR:O1A	2.16	0.44
1:L:27:SER:O	1:L:28:LEU:HB2	2.18	0.44
1:O:4:ARG:NH2	1:O:145:ILE:HG22	2.33	0.44
1:K:25:ASN:HB3	2:K:201:APR:O2D	2.17	0.44
1:E:85:VAL:O	1:E:87:ARG:HD2	2.18	0.43
1:M:27:SER:O	1:M:28:LEU:HB2	2.18	0.43
1:K:25:ASN:HB2	1:K:26:PRO:HD2	2.00	0.43
1:D:29:MET:HE2	1:D:54:ARG:HH11	1.84	0.43
1:H:34:VAL:HG23	2:H:201:APR:O2A	2.18	0.43
1:I:171:LEU:HD23	1:I:171:LEU:HA	1.84	0.43
1:J:173:GLN:O	1:J:173:GLN:HG3	2.19	0.43
1:K:144:PHE:O	1:K:147:ARG:HG3	2.19	0.43
1:L:160:ASP:OD1	1:L:163:ASN:HB2	2.19	0.43
1:G:122:SER:HA	2:G:201:APR:O5D	2.19	0.43
1:K:6:HIS:CE1	1:K:153:GLN:OE1	2.71	0.43
1:L:122:SER:N	2:L:201:APR:O1B	2.44	0.43
1:B:6:HIS:HE1	1:B:153:GLN:OE1	2.02	0.43
1:D:105:LEU:HD13	1:D:144:PHE:CB	2.49	0.43
1:F:91:GLN:N	1:F:93:GLU:OE2	2.51	0.43
1:G:29:MET:CE	1:G:29:MET:HA	2.48	0.43
1:M:126:ALA:HB2	2:M:201:APR:HR'4	2.00	0.43
1:N:19:VAL:HG22	1:N:116:VAL:HG23	2.00	0.43
1:A:27:SER:O	1:A:28:LEU:HB2	2.19	0.43
1:M:161:GLU:HG2	1:M:165:HIS:NE2	2.34	0.43
1:N:163:ASN:C	1:N:165:HIS:N	2.72	0.43
1:N:27:SER:O	1:N:28:LEU:HB2	2.19	0.43
1:N:95:GLN:OE1	1:N:98:GLN:NE2	2.51	0.43
1:O:27:SER:O	1:O:28:LEU:HB2	2.19	0.43
1:B:2:LYS:HB2	1:B:2:LYS:HE3	1.77	0.43
1:F:143:GLU:O	1:F:147:ARG:HG3	2.18	0.43
1:K:93:GLU:O	1:K:96:LEU:N	2.52	0.43
1:P:6:HIS:HE1	1:P:153:GLN:OE1	2.02	0.43
1:Q:91:GLN:O	1:Q:92:ASN:HB3	2.17	0.43
1:R:11:ASP:OD2	1:R:14:LYS:HD2	2.19	0.43
1:F:145:ILE:HA	1:F:145:ILE:HD13	1.82	0.43
1:H:25:ASN:HB3	2:H:201:APR:O1D	2.18	0.43
1:L:11:ASP:HB3	1:L:14:LYS:HG3	2.01	0.43
1:D:11:ASP:OD2	1:D:14:LYS:HD2	2.19	0.43
1:G:25:ASN:HB2	1:G:26:PRO:HD2	1.99	0.43
1:L:148:HIS:NE2	3:L:202:SO4:O4	2.40	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:29:MET:CE	1:O:47:LEU:CD1	2.97	0.43
1:P:67:ILE:HD12	1:P:79:VAL:HG23	2.01	0.43
1:B:143:GLU:O	1:B:147:ARG:HG3	2.18	0.42
1:D:143:GLU:O	1:D:147:ARG:HG3	2.18	0.42
1:L:120:ALA:O	2:L:201:APR:H'4	2.19	0.42
1:R:138:VAL:HG13	1:R:171:LEU:HD23	2.00	0.42
1:H:104:SER:O	1:H:108:VAL:HG23	2.19	0.42
1:K:143:GLU:O	1:K:147:ARG:HG2	2.19	0.42
1:K:168:GLU:O	1:K:172:THR:N	2.51	0.42
1:E:148:HIS:NE2	3:E:202:SO4:O3	2.51	0.42
1:E:27:SER:C	1:E:29:MET:N	2.73	0.42
1:H:6:HIS:CE1	1:H:153:GLN:OE1	2.71	0.42
1:P:6:HIS:CE1	1:P:153:GLN:OE1	2.71	0.42
1:B:29:MET:CE	1:B:29:MET:HA	2.48	0.42
1:G:57:GLN:OE1	1:Q:57:GLN:CB	2.67	0.42
1:A:25:ASN:HB2	1:A:26:PRO:HD2	2.01	0.42
1:D:25:ASN:ND2	1:D:30:GLY:O	2.53	0.42
1:I:138:VAL:HG13	1:I:171:LEU:CD2	2.49	0.42
1:K:89:GLY:HA2	1:K:93:GLU:OE2	2.19	0.42
1:N:166:LEU:HA	1:N:166:LEU:HD23	1.78	0.42
1:C:19:VAL:HG22	1:C:116:VAL:HG23	2.02	0.42
1:K:6:HIS:HE1	1:K:153:GLN:OE1	2.03	0.42
1:N:29:MET:CE	1:N:47:LEU:CD1	2.98	0.42
1:O:25:ASN:HB3	2:O:201:APR:C2D	2.50	0.42
1:E:143:GLU:O	1:E:147:ARG:HG3	2.19	0.42
1:K:91:GLN:HB3	1:K:91:GLN:HE21	1.62	0.42
1:M:143:GLU:O	1:M:147:ARG:HG3	2.20	0.42
1:M:19:VAL:HG22	1:M:116:VAL:HG23	2.01	0.42
1:P:27:SER:O	1:P:28:LEU:HB2	2.19	0.42
1:A:143:GLU:O	1:A:147:ARG:HG3	2.20	0.42
1:A:57:GLN:HB3	1:L:57:GLN:NE2	2.34	0.42
1:B:57:GLN:HB3	1:H:57:GLN:NE2	2.34	0.42
1:H:171:LEU:HA	1:H:171:LEU:HD23	1.89	0.42
1:I:160:ASP:OD1	1:I:163:ASN:HB2	2.20	0.42
1:J:49:ALA:HB2	1:J:69:LEU:CD2	2.50	0.42
1:K:105:LEU:HB3	1:K:144:PHE:CE2	2.55	0.42
1:R:135:GLU:HA	1:R:170:LEU:HD13	2.02	0.42
1:A:2:LYS:HA	1:A:2:LYS:CE	2.49	0.42
1:F:102:LEU:O	1:F:106:ARG:HG3	2.20	0.42
1:H:19:VAL:HG22	1:H:116:VAL:HG23	2.00	0.42
1:C:29:MET:CE	1:C:47:LEU:HD11	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:6:HIS:CD2	1:Q:6:HIS:CD2	3.08	0.42
1:G:19:VAL:HG22	1:G:116:VAL:HG23	2.00	0.42
1:I:19:VAL:HG22	1:I:116:VAL:HG23	2.02	0.42
1:L:91:GLN:HB2	1:L:93:GLU:CD	2.36	0.42
1:J:171:LEU:HA	1:J:171:LEU:HD23	1.80	0.41
1:B:19:VAL:HG22	1:B:116:VAL:HG23	2.02	0.41
1:C:27:SER:O	1:C:28:LEU:HB2	2.19	0.41
1:E:47:LEU:C	1:E:51:LEU:HD12	2.36	0.41
1:G:29:MET:CE	1:G:47:LEU:CD1	2.98	0.41
1:K:160:ASP:OD1	1:K:163:ASN:HB2	2.20	0.41
1:N:125:VAL:CG2	2:N:201:APR:O1A	2.68	0.41
1:N:6:HIS:HD2	1:N:155:TYR:CE2	2.38	0.41
1:C:143:GLU:O	1:C:147:ARG:HG3	2.20	0.41
1:J:86:TRP:CD1	1:J:129:PRO:HD3	2.54	0.41
1:Q:19:VAL:HG22	1:Q:116:VAL:HG23	2.02	0.41
1:R:143:GLU:O	1:R:147:ARG:HG3	2.21	0.41
1:D:102:LEU:HA	1:D:102:LEU:HD23	1.85	0.41
1:B:163:ASN:HD22	1:B:163:ASN:HA	1.61	0.41
1:E:106:ARG:CZ	3:E:202:SO4:O1	2.68	0.41
1:E:147:ARG:NH2	3:E:202:SO4:O4	2.52	0.41
1:J:25:ASN:HB2	1:J:26:PRO:HD2	2.02	0.41
1:D:6:HIS:CE1	1:D:153:GLN:OE1	2.70	0.41
1:K:19:VAL:HG22	1:K:116:VAL:HG23	2.01	0.41
1:P:143:GLU:O	1:P:147:ARG:HG3	2.20	0.41
1:Q:143:GLU:O	1:Q:147:ARG:HG3	2.21	0.41
1:E:19:VAL:O	1:E:116:VAL:HA	2.21	0.41
1:G:57:GLN:HB2	4:G:306:HOH:O	2.20	0.41
1:I:102:LEU:O	1:I:106:ARG:HG3	2.21	0.41
1:J:107:LEU:HD12	1:J:107:LEU:HA	1.52	0.41
1:K:29:MET:CE	1:K:47:LEU:CD1	2.98	0.41
1:L:104:SER:O	1:L:108:VAL:HG23	2.21	0.41
1:H:143:GLU:O	1:H:147:ARG:HG3	2.20	0.41
1:I:162:GLU:O	1:I:165:HIS:HB3	2.19	0.41
1:B:27:SER:O	1:B:28:LEU:HB2	2.20	0.41
1:L:143:GLU:O	1:L:147:ARG:HG3	2.21	0.41
1:K:128:TYR:O	1:K:129:PRO:C	2.58	0.41
1:M:29:MET:CE	1:M:47:LEU:CD1	2.99	0.41
1:A:46:LEU:O	1:A:49:ALA:HB3	2.21	0.41
1:G:19:VAL:O	1:G:116:VAL:HA	2.21	0.41
1:G:57:GLN:OE1	1:Q:57:GLN:HG2	2.21	0.41
1:N:89:GLY:N	1:N:93:GLU:OE1	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:104:SER:O	1:R:108:VAL:HG23	2.21	0.41
1:C:95:GLN:HE21	1:C:98:GLN:NE2	2.19	0.40
1:P:102:LEU:O	1:P:106:ARG:HG3	2.21	0.40
1:E:102:LEU:O	1:E:106:ARG:HG3	2.21	0.40
1:G:143:GLU:O	1:G:147:ARG:HG3	2.20	0.40
1:J:116:VAL:HG22	1:J:117:ALA:N	2.36	0.40
1:K:171:LEU:HD22	1:K:171:LEU:O	2.19	0.40
1:F:29:MET:HB3	1:L:29:MET:HG3	2.02	0.40
1:B:104:SER:O	1:B:108:VAL:HG23	2.21	0.40
1:D:148:HIS:HE1	1:M:40:ARG:O	2.04	0.40
1:C:171:LEU:HA	1:C:171:LEU:HD23	1.90	0.40
1:E:104:SER:O	1:E:108:VAL:HG23	2.21	0.40
1:G:51:LEU:HD11	1:K:51:LEU:CD2	2.52	0.40
1:K:102:LEU:O	1:K:106:ARG:HG3	2.21	0.40
1:L:125:VAL:HG13	2:L:201:APR:O1A	2.21	0.40
1:M:91:GLN:N	1:M:93:GLU:OE2	2.48	0.40
1:O:130:ARG:NH2	1:O:163:ASN:HB2	2.36	0.40
1:R:138:VAL:CG1	1:R:171:LEU:HD23	2.51	0.40
1:B:25:ASN:CB	2:B:201:APR:C1D	2.89	0.40
1:J:20:ILE:HD11	1:J:73:LEU:HD13	2.02	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:B:168:GLU:OE2	1:E:168:GLU:OE2[2_564]	2.11	0.09

## 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%)	162 (95%)	9 (5%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	171/183 (93%)	164 (96%)	7 (4%)	0	100	100
1	C	171/183 (93%)	164 (96%)	7 (4%)	0	100	100
1	D	171/183 (93%)	161 (94%)	10 (6%)	0	100	100
1	E	171/183 (93%)	164 (96%)	7 (4%)	0	100	100
1	F	170/183 (93%)	161 (95%)	9 (5%)	0	100	100
1	G	169/183 (92%)	163 (96%)	6 (4%)	0	100	100
1	H	170/183 (93%)	162 (95%)	8 (5%)	0	100	100
1	I	169/183 (92%)	162 (96%)	7 (4%)	0	100	100
1	J	170/183 (93%)	162 (95%)	8 (5%)	0	100	100
1	K	169/183 (92%)	160 (95%)	9 (5%)	0	100	100
1	L	169/183 (92%)	162 (96%)	7 (4%)	0	100	100
1	M	170/183 (93%)	163 (96%)	7 (4%)	0	100	100
1	N	169/183 (92%)	160 (95%)	9 (5%)	0	100	100
1	O	170/183 (93%)	164 (96%)	6 (4%)	0	100	100
1	P	170/183 (93%)	165 (97%)	5 (3%)	0	100	100
1	Q	171/183 (93%)	165 (96%)	6 (4%)	0	100	100
1	R	170/183 (93%)	164 (96%)	6 (4%)	0	100	100
All	All	3061/3294 (93%)	2928 (96%)	133 (4%)	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	126/142 (89%)	111 (88%)	15 (12%)	5	21
1	B	132/142 (93%)	117 (89%)	15 (11%)	5	22
1	C	129/142 (91%)	117 (91%)	12 (9%)	9	31
1	D	129/142 (91%)	114 (88%)	15 (12%)	5	21

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	128/142 (90%)	114 (89%)	14 (11%)	6	24
1	F	125/142 (88%)	114 (91%)	11 (9%)	10	34
1	G	124/142 (87%)	109 (88%)	15 (12%)	5	20
1	H	128/142 (90%)	113 (88%)	15 (12%)	5	21
1	I	126/142 (89%)	112 (89%)	14 (11%)	6	23
1	J	127/142 (89%)	106 (84%)	21 (16%)	2	10
1	K	124/142 (87%)	106 (86%)	18 (14%)	3	14
1	L	122/142 (86%)	112 (92%)	10 (8%)	11	37
1	M	129/142 (91%)	119 (92%)	10 (8%)	12	40
1	N	120/142 (84%)	111 (92%)	9 (8%)	13	41
1	O	130/142 (92%)	116 (89%)	14 (11%)	6	24
1	P	127/142 (89%)	118 (93%)	9 (7%)	14	44
1	Q	130/142 (92%)	118 (91%)	12 (9%)	9	32
1	R	125/142 (88%)	114 (91%)	11 (9%)	10	34
All	All	2281/2556 (89%)	2041 (90%)	240 (10%)	7	25

All (240) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	R	8	VAL
1	R	14	LYS
1	R	34	VAL
1	R	40	ARG
1	R	46	LEU
1	R	54	ARG
1	R	55	GLN
1	R	95	GLN
1	R	98	GLN
1	R	172	THR
1	R	174	GLN
1	A	2	LYS
1	A	8	VAL
1	A	9	GLN
1	A	20	ILE
1	A	34	VAL
1	A	46	LEU
1	A	54	ARG

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Mol	Chain	Res	Type
1	A	55	GLN
1	A	90	GLU
1	A	95	GLN
1	A	98	GLN
1	A	139	LYS
1	A	166	LEU
1	A	171	LEU
1	A	172	THR
1	B	2	LYS
1	B	3	THR
1	B	8	VAL
1	B	19	VAL
1	B	34	VAL
1	B	40	ARG
1	B	46	LEU
1	B	54	ARG
1	B	55	GLN
1	B	95	GLN
1	B	98	GLN
1	B	161	GLU
1	B	163	ASN
1	B	166	LEU
1	B	174	GLN
1	C	2	LYS
1	C	3	THR
1	C	4	ARG
1	C	8	VAL
1	C	19	VAL
1	C	34	VAL
1	C	46	LEU
1	C	54	ARG
1	C	98	GLN
1	C	125	VAL
1	C	166	LEU
1	C	172	THR
1	D	2	LYS
1	D	3	THR
1	D	4	ARG
1	D	19	VAL
1	D	29	MET
1	D	34	VAL
1	D	46	LEU

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Mol	Chain	Res	Type
1	D	54	ARG
1	D	55	GLN
1	D	95	GLN
1	D	98	GLN
1	D	104	SER
1	D	135	GLU
1	D	166	LEU
1	D	173	GLN
1	E	2	LYS
1	E	27	SER
1	E	29	MET
1	E	34	VAL
1	E	40	ARG
1	E	46	LEU
1	E	51	LEU
1	E	54	ARG
1	E	55	GLN
1	E	87	ARG
1	E	95	GLN
1	E	98	GLN
1	E	125	VAL
1	E	166	LEU
1	F	8	VAL
1	F	34	VAL
1	F	40	ARG
1	F	46	LEU
1	F	54	ARG
1	F	69	LEU
1	F	95	GLN
1	F	98	GLN
1	F	162	GLU
1	F	166	LEU
1	F	174	GLN
1	G	8	VAL
1	G	19	VAL
1	G	34	VAL
1	G	40	ARG
1	G	46	LEU
1	G	51	LEU
1	G	54	ARG
1	G	55	GLN
1	G	57	GLN

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Mol	Chain	Res	Type
1	G	91	GLN
1	G	95	GLN
1	G	98	GLN
1	G	161	GLU
1	G	166	LEU
1	G	168	GLU
1	H	8	VAL
1	H	19	VAL
1	H	34	VAL
1	H	40	ARG
1	H	46	LEU
1	H	54	ARG
1	H	55	GLN
1	H	98	GLN
1	H	146	THR
1	H	159	TYR
1	H	160	ASP
1	H	161	GLU
1	H	166	LEU
1	H	169	ARG
1	H	173	GLN
1	I	8	VAL
1	I	19	VAL
1	I	34	VAL
1	I	40	ARG
1	I	46	LEU
1	I	54	ARG
1	I	55	GLN
1	I	91	GLN
1	I	98	GLN
1	I	159	TYR
1	I	161	GLU
1	I	163	ASN
1	I	166	LEU
1	I	172	THR
1	J	8	VAL
1	J	9	GLN
1	J	19	VAL
1	J	29	MET
1	J	40	ARG
1	J	46	LEU
1	J	54	ARG

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Mol	Chain	Res	Type
1	J	69	LEU
1	J	91	GLN
1	J	93	GLU
1	J	95	GLN
1	J	98	GLN
1	J	107	LEU
1	J	119	PRO
1	J	122	SER
1	J	159	TYR
1	J	160	ASP
1	J	166	LEU
1	J	172	THR
1	J	173	GLN
1	J	174	GLN
1	K	8	VAL
1	K	19	VAL
1	K	34	VAL
1	K	46	LEU
1	K	54	ARG
1	K	55	GLN
1	K	91	GLN
1	K	95	GLN
1	K	98	GLN
1	K	140	THR
1	K	142	SER
1	K	145	ILE
1	K	147	ARG
1	K	166	LEU
1	K	170	LEU
1	K	171	LEU
1	K	172	THR
1	K	173	GLN
1	L	34	VAL
1	L	40	ARG
1	L	46	LEU
1	L	54	ARG
1	L	55	GLN
1	L	72	ASP
1	L	94	ASP
1	L	98	GLN
1	L	159	TYR
1	L	166	LEU

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Mol	Chain	Res	Type
1	M	8	VAL
1	M	19	VAL
1	M	34	VAL
1	M	46	LEU
1	M	54	ARG
1	M	55	GLN
1	M	95	GLN
1	M	98	GLN
1	M	166	LEU
1	M	174	GLN
1	N	8	VAL
1	N	19	VAL
1	N	34	VAL
1	N	46	LEU
1	N	54	ARG
1	N	95	GLN
1	N	98	GLN
1	N	125	VAL
1	N	159	TYR
1	O	8	VAL
1	O	14	LYS
1	O	19	VAL
1	O	34	VAL
1	O	46	LEU
1	O	54	ARG
1	O	55	GLN
1	O	90	GLU
1	O	95	GLN
1	O	98	GLN
1	O	135	GLU
1	O	147	ARG
1	O	166	LEU
1	O	174	GLN
1	P	8	VAL
1	P	34	VAL
1	P	46	LEU
1	P	54	ARG
1	P	90	GLU
1	P	98	GLN
1	P	159	TYR
1	P	166	LEU
1	P	172	THR

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Mol	Chain	Res	Type
1	Q	19	VAL
1	Q	34	VAL
1	Q	40	ARG
1	Q	46	LEU
1	Q	54	ARG
1	Q	55	GLN
1	Q	87	ARG
1	Q	95	GLN
1	Q	98	GLN
1	Q	125	VAL
1	Q	166	LEU
1	Q	174	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (92) such sidechains are listed below:

Mol	Chain	Res	Type
1	R	6	HIS
1	R	57	GLN
1	R	95	GLN
1	R	98	GLN
1	R	103	ASN
1	A	6	HIS
1	A	56	GLN
1	A	57	GLN
1	A	92	ASN
1	A	98	GLN
1	A	103	ASN
1	A	174	GLN
1	B	6	HIS
1	B	92	ASN
1	B	98	GLN
1	B	103	ASN
1	B	163	ASN
1	B	165	HIS
1	C	6	HIS
1	C	98	GLN
1	C	103	ASN
1	C	165	HIS
1	D	6	HIS
1	D	92	ASN
1	D	98	GLN
1	D	103	ASN

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Mol	Chain	Res	Type
1	D	165	HIS
1	E	6	HIS
1	E	95	GLN
1	E	98	GLN
1	E	103	ASN
1	F	98	GLN
1	F	103	ASN
1	F	173	GLN
1	F	174	GLN
1	G	6	HIS
1	G	9	GLN
1	G	92	ASN
1	G	95	GLN
1	G	98	GLN
1	G	103	ASN
1	H	6	HIS
1	H	9	GLN
1	H	57	GLN
1	H	95	GLN
1	H	98	GLN
1	H	103	ASN
1	H	174	GLN
1	I	6	HIS
1	I	92	ASN
1	I	103	ASN
1	I	163	ASN
1	J	6	HIS
1	J	9	GLN
1	J	98	GLN
1	J	103	ASN
1	J	165	HIS
1	J	174	GLN
1	K	6	HIS
1	K	91	GLN
1	K	95	GLN
1	K	98	GLN
1	K	103	ASN
1	L	6	HIS
1	L	56	GLN
1	L	57	GLN
1	L	103	ASN
1	M	6	HIS

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Mol	Chain	Res	Type
1	M	57	GLN
1	M	95	GLN
1	M	98	GLN
1	M	103	ASN
1	M	174	GLN
1	N	98	GLN
1	N	103	ASN
1	O	6	HIS
1	O	92	ASN
1	O	98	GLN
1	O	103	ASN
1	P	6	HIS
1	P	57	GLN
1	P	92	ASN
1	P	98	GLN
1	P	103	ASN
1	P	174	GLN
1	Q	6	HIS
1	Q	56	GLN
1	Q	92	ASN
1	Q	98	GLN
1	Q	103	ASN
1	Q	165	HIS
1	Q	174	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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](#)

36 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	Q	202	-	4,4,4	0.55	0	6,6,6	1.30	0
3	SO4	L	202	-	4,4,4	0.44	0	6,6,6	1.46	1 (16%)
3	SO4	J	202	-	4,4,4	0.55	0	6,6,6	0.65	0
3	SO4	R	402	-	4,4,4	0.51	0	6,6,6	1.38	1 (16%)
2	APR	N	201	-	34,39,39	1.07	2 (5%)	40,60,60	1.52	6 (15%)
3	SO4	H	202	-	4,4,4	0.48	0	6,6,6	0.84	0
3	SO4	E	202	-	4,4,4	0.28	0	6,6,6	1.29	0
2	APR	J	201	-	34,39,39	1.07	2 (5%)	40,60,60	1.66	10 (25%)
3	SO4	K	202	-	4,4,4	0.72	0	6,6,6	1.15	1 (16%)
2	APR	D	201	-	24,29,39	1.36	3 (12%)	29,45,60	1.77	7 (24%)
3	SO4	I	202	-	4,4,4	0.28	0	6,6,6	0.54	0
2	APR	R	401	-	34,39,39	1.09	3 (8%)	40,60,60	1.74	8 (20%)
2	APR	Q	201	-	34,39,39	1.05	4 (11%)	40,60,60	1.41	4 (10%)
3	SO4	N	202	-	4,4,4	0.44	0	6,6,6	0.56	0
2	APR	C	201	-	34,39,39	1.15	4 (11%)	40,60,60	1.60	7 (17%)
2	APR	L	201	-	34,39,39	1.03	2 (5%)	40,60,60	1.72	8 (20%)
3	SO4	A	202	-	4,4,4	0.18	0	6,6,6	1.76	1 (16%)
2	APR	O	201	-	34,39,39	1.09	2 (5%)	40,60,60	1.33	6 (15%)
2	APR	G	201	-	24,29,39	1.57	4 (16%)	29,45,60	1.46	4 (13%)
3	SO4	M	202	-	4,4,4	0.72	0	6,6,6	0.77	0
2	APR	B	201	-	34,39,39	1.63	6 (17%)	40,60,60	2.23	13 (32%)
3	SO4	B	202	-	4,4,4	0.59	0	6,6,6	0.45	0
3	SO4	F	202	-	4,4,4	0.24	0	6,6,6	0.88	0
2	APR	K	201	-	34,39,39	1.03	3 (8%)	40,60,60	1.21	4 (10%)
2	APR	P	201	-	34,39,39	1.18	4 (11%)	40,60,60	1.84	13 (32%)
2	APR	H	201	-	34,39,39	1.22	2 (5%)	40,60,60	1.65	9 (22%)
2	APR	I	201	-	34,39,39	1.11	2 (5%)	40,60,60	1.52	9 (22%)
2	APR	E	201	-	34,39,39	2.14	9 (26%)	40,60,60	3.84	9 (22%)
2	APR	F	201	-	34,39,39	1.07	3 (8%)	40,60,60	1.50	8 (20%)
3	SO4	P	202	-	4,4,4	0.70	0	6,6,6	0.64	0
3	SO4	D	202	-	4,4,4	0.32	0	6,6,6	0.04	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	SO4	C	202	-	4,4,4	0.45	0	6,6,6	0.63	0
2	APR	M	201	-	34,39,39	1.03	2 (5%)	40,60,60	1.58	7 (17%)
3	SO4	G	202	-	4,4,4	0.18	0	6,6,6	0.79	0
3	SO4	O	202	-	4,4,4	0.38	0	6,6,6	0.90	0
2	APR	A	201	-	34,39,39	1.07	3 (8%)	40,60,60	1.30	4 (10%)

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	K	201	-	-	8/18/54/54	0/4/4/4
2	APR	R	401	-	-	10/18/54/54	0/4/4/4
2	APR	P	201	-	-	6/18/54/54	0/4/4/4
2	APR	Q	201	-	-	11/18/54/54	0/4/4/4
2	APR	C	201	-	-	9/18/54/54	0/4/4/4
2	APR	L	201	-	-	6/18/54/54	0/4/4/4
2	APR	M	201	-	-	8/18/54/54	0/4/4/4
2	APR	N	201	-	-	9/18/54/54	0/4/4/4
2	APR	O	201	-	-	9/18/54/54	0/4/4/4
2	APR	H	201	-	-	11/18/54/54	0/4/4/4
2	APR	I	201	-	-	9/18/54/54	0/4/4/4
2	APR	J	201	-	-	7/18/54/54	0/4/4/4
2	APR	D	201	-	-	3/12/32/54	0/3/3/4
2	APR	E	201	-	-	9/18/54/54	0/4/4/4
2	APR	F	201	-	-	5/18/54/54	0/4/4/4
2	APR	G	201	-	-	2/12/32/54	0/3/3/4
2	APR	A	201	-	-	13/18/54/54	0/4/4/4
2	APR	B	201	-	-	3/18/54/54	0/4/4/4

All (60) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	201	APR	C1D-C2D	5.46	1.59	1.52
2	B	201	APR	O4D-C1D	5.31	1.49	1.43
2	E	201	APR	O1D-C1D	-5.07	1.23	1.39
2	G	201	APR	PB-O1B	4.45	1.64	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	201	APR	C4-N3	4.34	1.41	1.35
2	E	201	APR	O3D-C3D	3.95	1.52	1.43
2	E	201	APR	O4D-C1D	3.78	1.47	1.43
2	H	201	APR	C2-N3	3.69	1.38	1.32
2	D	201	APR	PB-O1B	3.67	1.62	1.50
2	E	201	APR	O4'-C1'	3.53	1.46	1.41
2	B	201	APR	C5-C4	3.41	1.50	1.40
2	I	201	APR	C2-N3	3.23	1.37	1.32
2	G	201	APR	C2-N3	3.19	1.37	1.32
2	N	201	APR	C2-N3	3.17	1.37	1.32
2	I	201	APR	C5-C4	3.16	1.49	1.40
2	Q	201	APR	C5-C4	3.12	1.49	1.40
2	H	201	APR	C5-C4	3.07	1.49	1.40
2	P	201	APR	C2-N3	3.00	1.36	1.32
2	O	201	APR	C5-C4	2.90	1.48	1.40
2	R	401	APR	C2-N3	2.85	1.36	1.32
2	G	201	APR	C5-C4	2.84	1.48	1.40
2	A	201	APR	C2-N3	2.79	1.36	1.32
2	N	201	APR	C5-C4	2.78	1.48	1.40
2	R	401	APR	C5-C4	2.75	1.48	1.40
2	J	201	APR	C2-N3	2.74	1.36	1.32
2	O	201	APR	C2-N3	2.70	1.36	1.32
2	M	201	APR	C5-C4	2.70	1.48	1.40
2	K	201	APR	C5-C4	2.68	1.48	1.40
2	L	201	APR	C5-C4	2.66	1.48	1.40
2	D	201	APR	O4'-C1'	2.65	1.44	1.41
2	J	201	APR	C5-C4	2.65	1.47	1.40
2	E	201	APR	C8-N7	2.64	1.39	1.34
2	F	201	APR	C5-C4	2.63	1.47	1.40
2	L	201	APR	C2-N3	2.62	1.36	1.32
2	Q	201	APR	O4'-C1'	2.59	1.44	1.41
2	P	201	APR	O4'-C1'	2.58	1.44	1.41
2	E	201	APR	C5-C4	2.57	1.47	1.40
2	F	201	APR	C2-N3	2.57	1.36	1.32
2	P	201	APR	C5-C4	2.54	1.47	1.40
2	A	201	APR	C5-C4	2.50	1.47	1.40
2	D	201	APR	C5-C4	2.49	1.47	1.40
2	F	201	APR	C1D-C2D	2.47	1.55	1.52
2	B	201	APR	C2-N3	2.47	1.36	1.32
2	B	201	APR	O4'-C1'	2.46	1.44	1.41
2	M	201	APR	C2-N3	2.43	1.36	1.32
2	K	201	APR	O4'-C1'	2.42	1.44	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	201	APR	C2-N3	2.36	1.35	1.32
2	K	201	APR	C2-N3	2.34	1.35	1.32
2	B	201	APR	O1D-C1D	2.29	1.46	1.39
2	C	201	APR	C5-N7	-2.23	1.31	1.39
2	A	201	APR	C1D-C2D	2.22	1.55	1.52
2	G	201	APR	O4'-C1'	2.21	1.44	1.41
2	Q	201	APR	C4-N3	2.16	1.38	1.35
2	C	201	APR	PB-O2B	-2.16	1.45	1.55
2	P	201	APR	C1D-C2D	2.12	1.55	1.52
2	Q	201	APR	C2-N3	2.08	1.35	1.32
2	C	201	APR	O4'-C4'	-2.08	1.40	1.45
2	R	401	APR	C6-C5	2.07	1.51	1.43
2	B	201	APR	C8-N7	2.04	1.38	1.34
2	C	201	APR	C3'-C2'	-2.03	1.47	1.53

All (140) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	201	APR	O1D-C1D-O4D	-20.13	85.35	111.13
2	E	201	APR	C1D-C2D-C3D	-8.12	92.14	102.30
2	B	201	APR	O1D-C1D-O4D	7.16	120.30	111.13
2	E	201	APR	N3-C2-N1	-5.76	119.68	128.68
2	B	201	APR	O4D-C1D-C2D	5.74	111.53	104.46
2	L	201	APR	C1D-C2D-C3D	5.55	109.24	102.30
2	R	401	APR	C1D-C2D-C3D	5.13	108.72	102.30
2	M	201	APR	C1D-C2D-C3D	4.62	108.08	102.30
2	M	201	APR	C1'-N9-C4	-4.58	118.59	126.64
2	C	201	APR	O2'-C2'-C3'	-4.51	97.22	111.82
2	Q	201	APR	N3-C2-N1	-4.47	121.68	128.68
2	D	201	APR	N3-C2-N1	-4.42	121.76	128.68
2	H	201	APR	C1D-C2D-C3D	4.29	107.67	102.30
2	C	201	APR	N3-C2-N1	-4.27	122.01	128.68
2	R	401	APR	C1'-N9-C4	-4.19	119.29	126.64
2	G	201	APR	N3-C2-N1	-4.12	122.23	128.68
2	P	201	APR	N6-C6-N1	4.10	127.09	118.57
2	P	201	APR	O4D-C1D-C2D	4.10	109.50	104.46
2	N	201	APR	C1D-C2D-C3D	4.08	107.41	102.30
2	E	201	APR	O2D-C2D-C1D	3.93	122.68	111.82
2	M	201	APR	N3-C2-N1	-3.89	122.60	128.68
2	O	201	APR	N3-C2-N1	-3.80	122.75	128.68
2	K	201	APR	N3-C2-N1	-3.75	122.81	128.68
2	C	201	APR	O3'-C3'-C2'	-3.73	99.75	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	201	APR	PB-O3A-PA	-3.68	120.19	132.83
2	N	201	APR	N3-C2-N1	-3.66	122.96	128.68
2	E	201	APR	C1'-N9-C4	-3.63	120.26	126.64
2	L	201	APR	N3-C2-N1	-3.57	123.10	128.68
2	A	201	APR	C1D-C2D-C3D	3.57	106.76	102.30
2	P	201	APR	C5-C6-N6	-3.55	114.96	120.35
2	R	401	APR	C4-C5-N7	-3.54	105.71	109.40
2	C	201	APR	C1D-C2D-C3D	-3.49	97.93	102.30
2	L	201	APR	C4-C5-N7	-3.49	105.76	109.40
2	L	201	APR	C3'-C2'-C1'	3.47	106.20	100.98
2	H	201	APR	O1D-C1D-O4D	-3.46	106.70	111.13
2	N	201	APR	C1'-N9-C4	-3.41	120.65	126.64
2	B	201	APR	O1D-C1D-C2D	-3.41	94.12	110.39
2	D	201	APR	C2-N1-C6	3.40	124.58	118.75
2	H	201	APR	O4D-C1D-C2D	3.39	108.63	104.46
2	B	201	APR	PB-O3A-PA	-3.38	121.22	132.83
2	B	201	APR	C4-C5-N7	-3.36	105.89	109.40
2	J	201	APR	C1'-N9-C4	-3.33	120.79	126.64
2	F	201	APR	N3-C2-N1	-3.33	123.48	128.68
3	A	202	SO4	O4-S-O3	3.33	123.27	109.06
2	A	201	APR	N3-C2-N1	-3.29	123.54	128.68
2	F	201	APR	C5-C6-N6	-3.26	115.41	120.35
2	B	201	APR	C2'-C3'-C4'	3.25	108.95	102.64
2	E	201	APR	C4-C5-N7	-3.25	106.02	109.40
2	J	201	APR	O1D-C1D-O4D	-3.24	106.98	111.13
2	I	201	APR	O5D-PB-O1B	-3.22	96.47	109.07
2	J	201	APR	N3-C2-N1	-3.20	123.67	128.68
2	Q	201	APR	O4D-C1D-C2D	-3.11	100.64	104.46
2	A	201	APR	C4-C5-N7	-3.07	106.20	109.40
2	F	201	APR	N6-C6-N1	3.04	124.89	118.57
2	H	201	APR	O4D-C4D-C3D	3.01	111.08	105.11
2	P	201	APR	N3-C2-N1	-3.00	123.99	128.68
2	G	201	APR	C1'-N9-C4	-3.00	121.37	126.64
2	O	201	APR	C1D-C2D-C3D	2.99	106.04	102.30
2	P	201	APR	O1D-C1D-O4D	-2.99	107.31	111.13
2	D	201	APR	N6-C6-N1	2.98	124.77	118.57
2	L	201	APR	O4D-C4D-C3D	2.95	110.95	105.11
2	E	201	APR	C2D-C3D-C4D	-2.94	96.93	102.64
2	L	201	APR	O5D-C5D-C4D	-2.92	98.94	108.99
2	N	201	APR	O5D-C5D-C4D	-2.91	98.99	108.99
2	F	201	APR	C1D-C2D-C3D	2.88	105.91	102.30
2	J	201	APR	PB-O3A-PA	-2.85	123.04	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	201	APR	N3-C2-N1	-2.84	124.24	128.68
2	B	201	APR	C2D-C3D-C4D	2.84	108.16	102.64
2	R	401	APR	N3-C2-N1	-2.82	124.27	128.68
2	I	201	APR	N3-C2-N1	-2.82	124.27	128.68
2	Q	201	APR	C2-N1-C6	2.79	123.52	118.75
2	I	201	APR	O4D-C1D-C2D	2.72	107.82	104.46
2	D	201	APR	O5D-PB-O2B	2.72	118.04	107.64
2	R	401	APR	O4D-C4D-C3D	2.64	110.33	105.11
2	E	201	APR	C2'-C3'-C4'	2.64	107.76	102.64
2	H	201	APR	N6-C6-N1	2.63	124.04	118.57
2	P	201	APR	O3'-C3'-C2'	-2.62	103.35	111.82
2	B	201	APR	N3-C2-N1	-2.60	124.61	128.68
2	R	401	APR	O3D-C3D-C2D	2.59	120.20	111.82
2	B	201	APR	C2-N1-C6	2.58	123.17	118.75
2	M	201	APR	C2-N1-C6	2.54	123.10	118.75
2	P	201	APR	O5D-C5D-C4D	-2.53	100.27	108.99
2	F	201	APR	O5'-C5'-C4'	2.53	117.71	108.99
2	P	201	APR	O5'-C5'-C4'	2.53	117.71	108.99
2	O	201	APR	O5D-C5D-C4D	2.52	117.66	108.99
2	E	201	APR	C2-N1-C6	2.52	123.06	118.75
2	J	201	APR	O2B-PB-O1B	2.51	124.66	112.24
2	J	201	APR	N6-C6-N1	2.51	123.79	118.57
2	N	201	APR	O4'-C1'-C2'	2.51	110.60	106.93
2	K	201	APR	C1'-N9-C4	-2.51	122.23	126.64
2	B	201	APR	C3'-C2'-C1'	2.49	104.72	100.98
2	G	201	APR	C5-C6-N6	-2.47	116.59	120.35
2	F	201	APR	C1'-N9-C4	-2.45	122.33	126.64
2	H	201	APR	O3D-C3D-C4D	2.44	118.10	111.05
2	H	201	APR	O5'-C5'-C4'	2.43	117.36	108.99
2	I	201	APR	N6-C6-N1	2.42	123.59	118.57
2	M	201	APR	PB-O3A-PA	-2.40	124.59	132.83
2	P	201	APR	C1'-N9-C4	-2.39	122.44	126.64
2	P	201	APR	C1D-C2D-C3D	2.39	105.29	102.30
2	P	201	APR	O4D-C4D-C3D	2.39	109.84	105.11
2	B	201	APR	O2A-PA-O5'	2.39	118.83	107.75
2	I	201	APR	O5D-C5D-C4D	-2.38	100.78	108.99
2	J	201	APR	C3'-C2'-C1'	-2.36	97.42	100.98
2	J	201	APR	O3'-C3'-C2'	-2.36	104.20	111.82
2	I	201	APR	O2B-PB-O1B	2.34	123.83	112.24
2	C	201	APR	C2'-C3'-C4'	2.34	107.18	102.64
2	D	201	APR	O2A-PA-O1A	2.34	123.79	112.24
2	O	201	APR	C2-N1-C6	2.31	122.70	118.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	201	APR	O5D-C5D-C4D	-2.29	101.12	108.99
2	R	401	APR	C5-C6-N6	2.27	123.81	120.35
2	F	201	APR	O4D-C4D-C3D	2.27	109.61	105.11
2	O	201	APR	N6-C6-N1	2.27	123.28	118.57
2	R	401	APR	O4'-C1'-C2'	2.26	110.23	106.93
2	K	201	APR	C2-N1-C6	2.26	122.62	118.75
2	J	201	APR	O2D-C2D-C3D	2.25	119.10	111.82
2	B	201	APR	O4D-C4D-C5D	2.25	116.77	109.37
3	R	402	SO4	O4-S-O2	-2.25	97.58	109.31
2	O	201	APR	C1'-N9-C4	-2.24	122.70	126.64
2	I	201	APR	C1D-C2D-C3D	2.22	105.08	102.30
2	N	201	APR	PB-O3A-PA	-2.22	125.21	132.83
2	C	201	APR	C2-N1-C6	2.22	122.54	118.75
2	P	201	APR	C3'-C2'-C1'	-2.18	97.70	100.98
3	K	202	SO4	O3-S-O2	2.17	120.62	109.31
2	A	201	APR	C1'-N9-C4	-2.16	122.84	126.64
2	P	201	APR	C2'-C3'-C4'	2.13	106.78	102.64
2	Q	201	APR	O4'-C1'-C2'	-2.12	103.83	106.93
2	L	201	APR	O2B-PB-O1B	2.11	122.69	112.24
2	K	201	APR	C4-C5-N7	-2.10	107.21	109.40
2	M	201	APR	C4-C5-N7	-2.10	107.21	109.40
2	L	201	APR	O4'-C4'-C3'	2.09	109.25	105.11
2	B	201	APR	C5-C6-N1	-2.09	115.62	120.35
2	I	201	APR	C4-C5-N7	-2.09	107.23	109.40
2	D	201	APR	C3'-C2'-C1'	2.08	104.12	100.98
2	G	201	APR	O2'-C2'-C3'	2.06	118.48	111.82
3	L	202	SO4	O4-S-O1	2.05	120.03	109.31
2	M	201	APR	N6-C6-N1	2.04	122.80	118.57
2	C	201	APR	C4-C5-N7	-2.02	107.29	109.40
2	F	201	APR	O4D-C1D-C2D	2.01	106.94	104.46
2	D	201	APR	C5-C6-N1	-2.00	115.81	120.35
2	J	201	APR	O4D-C4D-C3D	-2.00	101.16	105.11

There are no chirality outliers.

All (138) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	N	201	APR	C5D-O5D-PB-O1B
2	N	201	APR	C3D-C4D-C5D-O5D
2	J	201	APR	C5D-O5D-PB-O3A
2	J	201	APR	C5D-O5D-PB-O2B
2	R	401	APR	C5'-O5'-PA-O3A

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Mol	Chain	Res	Type	Atoms
2	R	401	APR	C5D-O5D-PB-O1B
2	R	401	APR	C5D-O5D-PB-O2B
2	R	401	APR	O4D-C4D-C5D-O5D
2	R	401	APR	C3D-C4D-C5D-O5D
2	Q	201	APR	C5'-O5'-PA-O3A
2	Q	201	APR	PA-O3A-PB-O5D
2	Q	201	APR	C5D-O5D-PB-O3A
2	Q	201	APR	C5D-O5D-PB-O2B
2	Q	201	APR	C4D-C5D-O5D-PB
2	C	201	APR	C5'-O5'-PA-O3A
2	C	201	APR	C5D-O5D-PB-O1B
2	C	201	APR	C5D-O5D-PB-O2B
2	C	201	APR	O4D-C4D-C5D-O5D
2	C	201	APR	C3D-C4D-C5D-O5D
2	L	201	APR	C5'-O5'-PA-O1A
2	L	201	APR	C5'-O5'-PA-O2A
2	L	201	APR	C5'-O5'-PA-O3A
2	O	201	APR	C5'-O5'-PA-O1A
2	O	201	APR	C5D-O5D-PB-O1B
2	O	201	APR	C5D-O5D-PB-O2B
2	O	201	APR	O4D-C4D-C5D-O5D
2	O	201	APR	C3D-C4D-C5D-O5D
2	B	201	APR	O4'-C4'-C5'-O5'
2	K	201	APR	C5'-O5'-PA-O3A
2	K	201	APR	PA-O3A-PB-O5D
2	K	201	APR	C5D-O5D-PB-O1B
2	P	201	APR	C5D-O5D-PB-O3A
2	H	201	APR	C5'-O5'-PA-O1A
2	H	201	APR	C5'-O5'-PA-O2A
2	H	201	APR	C5D-O5D-PB-O3A
2	I	201	APR	O4'-C4'-C5'-O5'
2	I	201	APR	PB-O3A-PA-O5'
2	I	201	APR	C5D-O5D-PB-O3A
2	I	201	APR	C5D-O5D-PB-O1B
2	I	201	APR	C5D-O5D-PB-O2B
2	I	201	APR	O4D-C4D-C5D-O5D
2	I	201	APR	C3D-C4D-C5D-O5D
2	E	201	APR	C5'-O5'-PA-O1A
2	E	201	APR	C5'-O5'-PA-O2A
2	E	201	APR	C5'-O5'-PA-O3A
2	E	201	APR	C5D-O5D-PB-O3A
2	E	201	APR	C5D-O5D-PB-O2B

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Mol	Chain	Res	Type	Atoms
2	E	201	APR	O4D-C4D-C5D-O5D
2	E	201	APR	C3D-C4D-C5D-O5D
2	F	201	APR	C3D-C4D-C5D-O5D
2	M	201	APR	C5'-O5'-PA-O1A
2	M	201	APR	C5'-O5'-PA-O2A
2	M	201	APR	C5'-O5'-PA-O3A
2	M	201	APR	C5D-O5D-PB-O1B
2	M	201	APR	C5D-O5D-PB-O2B
2	A	201	APR	C5'-O5'-PA-O1A
2	A	201	APR	C5'-O5'-PA-O3A
2	A	201	APR	PA-O3A-PB-O5D
2	A	201	APR	C5D-O5D-PB-O1B
2	A	201	APR	C3D-C4D-C5D-O5D
2	J	201	APR	O4D-C4D-C5D-O5D
2	Q	201	APR	O4'-C4'-C5'-O5'
2	G	201	APR	C3'-C4'-C5'-O5'
2	P	201	APR	C3'-C4'-C5'-O5'
2	H	201	APR	O4'-C4'-C5'-O5'
2	I	201	APR	C3'-C4'-C5'-O5'
2	F	201	APR	O4'-C4'-C5'-O5'
2	A	201	APR	O4'-C4'-C5'-O5'
2	J	201	APR	O4'-C4'-C5'-O5'
2	J	201	APR	C3D-C4D-C5D-O5D
2	Q	201	APR	C3'-C4'-C5'-O5'
2	G	201	APR	O4'-C4'-C5'-O5'
2	P	201	APR	O4'-C4'-C5'-O5'
2	F	201	APR	O4D-C4D-C5D-O5D
2	A	201	APR	C3'-C4'-C5'-O5'
2	A	201	APR	O4D-C4D-C5D-O5D
2	J	201	APR	C3'-C4'-C5'-O5'
2	D	201	APR	C3'-C4'-C5'-O5'
2	N	201	APR	O4'-C4'-C5'-O5'
2	D	201	APR	O4'-C4'-C5'-O5'
2	F	201	APR	C3'-C4'-C5'-O5'
2	L	201	APR	PA-O3A-PB-O1B
2	H	201	APR	C3'-C4'-C5'-O5'
2	N	201	APR	O4D-C4D-C5D-O5D
2	J	201	APR	C4D-C5D-O5D-PB
2	K	201	APR	C4D-C5D-O5D-PB
2	A	201	APR	C4D-C5D-O5D-PB
2	N	201	APR	PB-O3A-PA-O5'
2	R	401	APR	PB-O3A-PA-O5'

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Mol	Chain	Res	Type	Atoms
2	P	201	APR	PB-O3A-PA-O5'
2	H	201	APR	PB-O3A-PA-O5'
2	E	201	APR	PA-O3A-PB-O5D
2	M	201	APR	PA-O3A-PB-O5D
2	M	201	APR	C4D-C5D-O5D-PB
2	D	201	APR	C5'-O5'-PA-O3A
2	O	201	APR	C5'-O5'-PA-O3A
2	O	201	APR	C5D-O5D-PB-O3A
2	K	201	APR	C5D-O5D-PB-O3A
2	A	201	APR	C5D-O5D-PB-O3A
2	N	201	APR	PA-O3A-PB-O2B
2	R	401	APR	PA-O3A-PB-O2B
2	L	201	APR	PA-O3A-PB-O2B
2	O	201	APR	PA-O3A-PB-O2B
2	I	201	APR	C4D-C5D-O5D-PB
2	F	201	APR	C4D-C5D-O5D-PB
2	Q	201	APR	C5'-O5'-PA-O1A
2	Q	201	APR	C5'-O5'-PA-O2A
2	C	201	APR	C5'-O5'-PA-O1A
2	C	201	APR	C5'-O5'-PA-O2A
2	K	201	APR	C5'-O5'-PA-O1A
2	K	201	APR	C5'-O5'-PA-O2A
2	K	201	APR	C5D-O5D-PB-O2B
2	A	201	APR	C5D-O5D-PB-O2B
2	N	201	APR	C3'-C4'-C5'-O5'
2	R	401	APR	PA-O3A-PB-O1B
2	Q	201	APR	PB-O3A-PA-O2A
2	H	201	APR	C4D-C5D-O5D-PB
2	H	201	APR	PB-O3A-PA-O1A
2	H	201	APR	O4D-C4D-C5D-O5D
2	R	401	APR	C5D-O5D-PB-O3A
2	C	201	APR	C5D-O5D-PB-O3A
2	H	201	APR	C5'-O5'-PA-O3A
2	M	201	APR	C5D-O5D-PB-O3A
2	N	201	APR	PA-O3A-PB-O1B
2	Q	201	APR	PA-O3A-PB-O1B
2	C	201	APR	PB-O3A-PA-O1A
2	O	201	APR	PA-O3A-PB-O1B
2	B	201	APR	PA-O3A-PB-O2B
2	E	201	APR	PA-O3A-PB-O1B
2	A	201	APR	PB-O3A-PA-O2A
2	N	201	APR	C5D-O5D-PB-O2B

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Mol	Chain	Res	Type	Atoms
2	R	401	APR	C5'-O5'-PA-O1A
2	P	201	APR	C5D-O5D-PB-O1B
2	H	201	APR	C5D-O5D-PB-O1B
2	A	201	APR	C5'-O5'-PA-O2A
2	B	201	APR	O4D-C4D-C5D-O5D
2	P	201	APR	O4D-C4D-C5D-O5D
2	L	201	APR	C3D-C4D-C5D-O5D

There are no ring outliers.

33 monomers are involved in 102 short contacts:

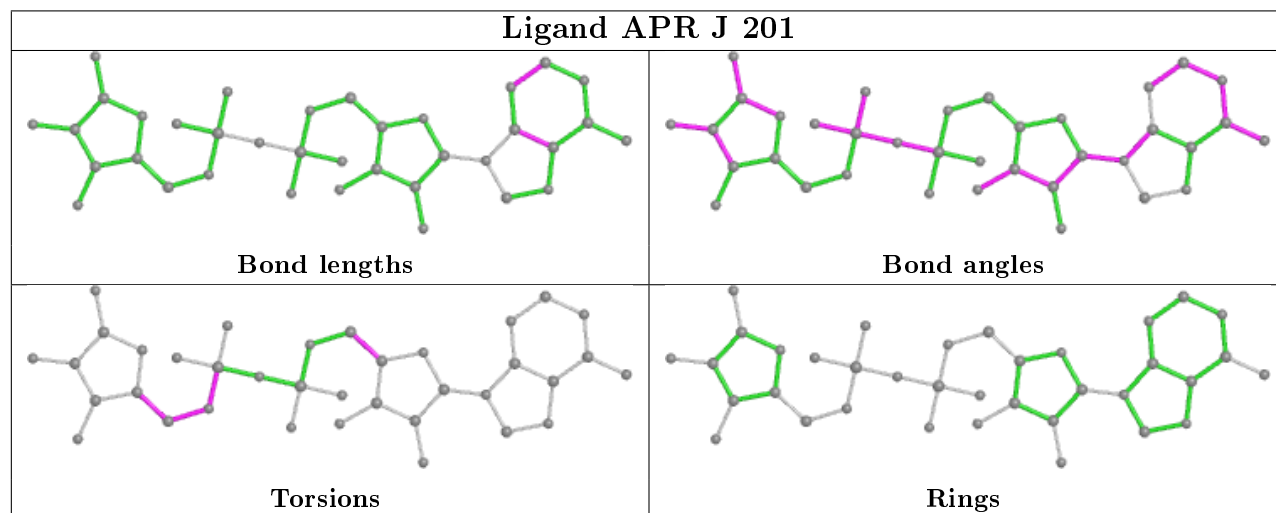
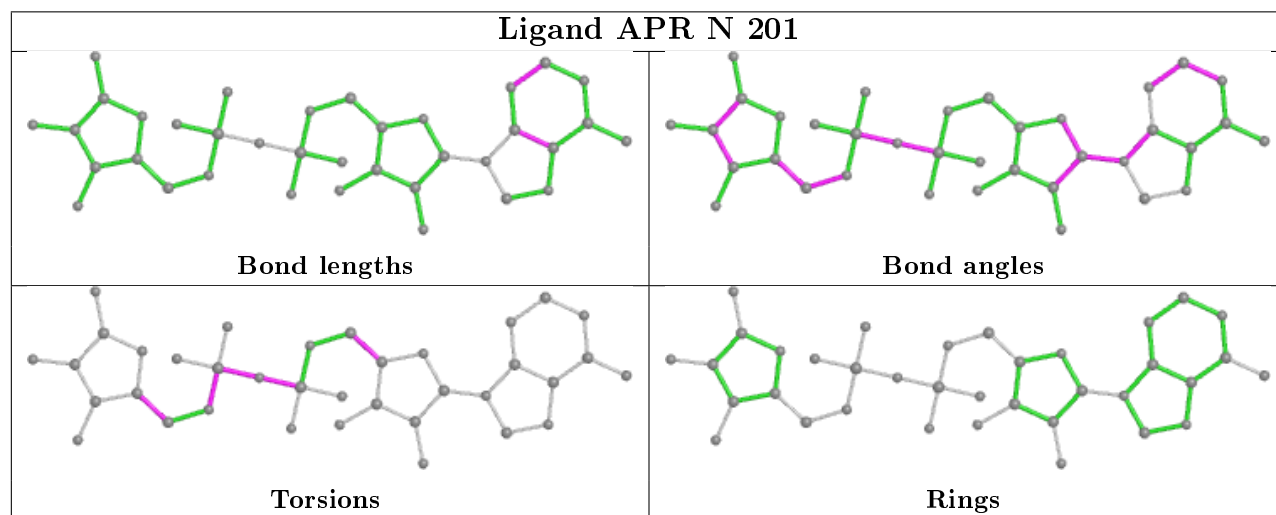
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	Q	202	SO4	4	0
3	L	202	SO4	1	0
3	J	202	SO4	3	0
3	R	402	SO4	3	0
2	N	201	APR	3	0
3	E	202	SO4	5	0
2	J	201	APR	7	0
3	K	202	SO4	1	0
3	I	202	SO4	1	0
2	R	401	APR	6	0
2	Q	201	APR	5	0
3	N	202	SO4	1	0
2	L	201	APR	9	0
3	A	202	SO4	1	0
2	O	201	APR	5	0
2	G	201	APR	2	0
3	M	202	SO4	3	0
2	B	201	APR	6	0
3	B	202	SO4	2	0
3	F	202	SO4	2	0
2	K	201	APR	4	0
2	P	201	APR	3	0
2	H	201	APR	3	0
2	I	201	APR	1	0
2	E	201	APR	2	0
2	F	201	APR	4	0
3	P	202	SO4	3	0
3	D	202	SO4	2	0
3	C	202	SO4	3	0
2	M	201	APR	2	0

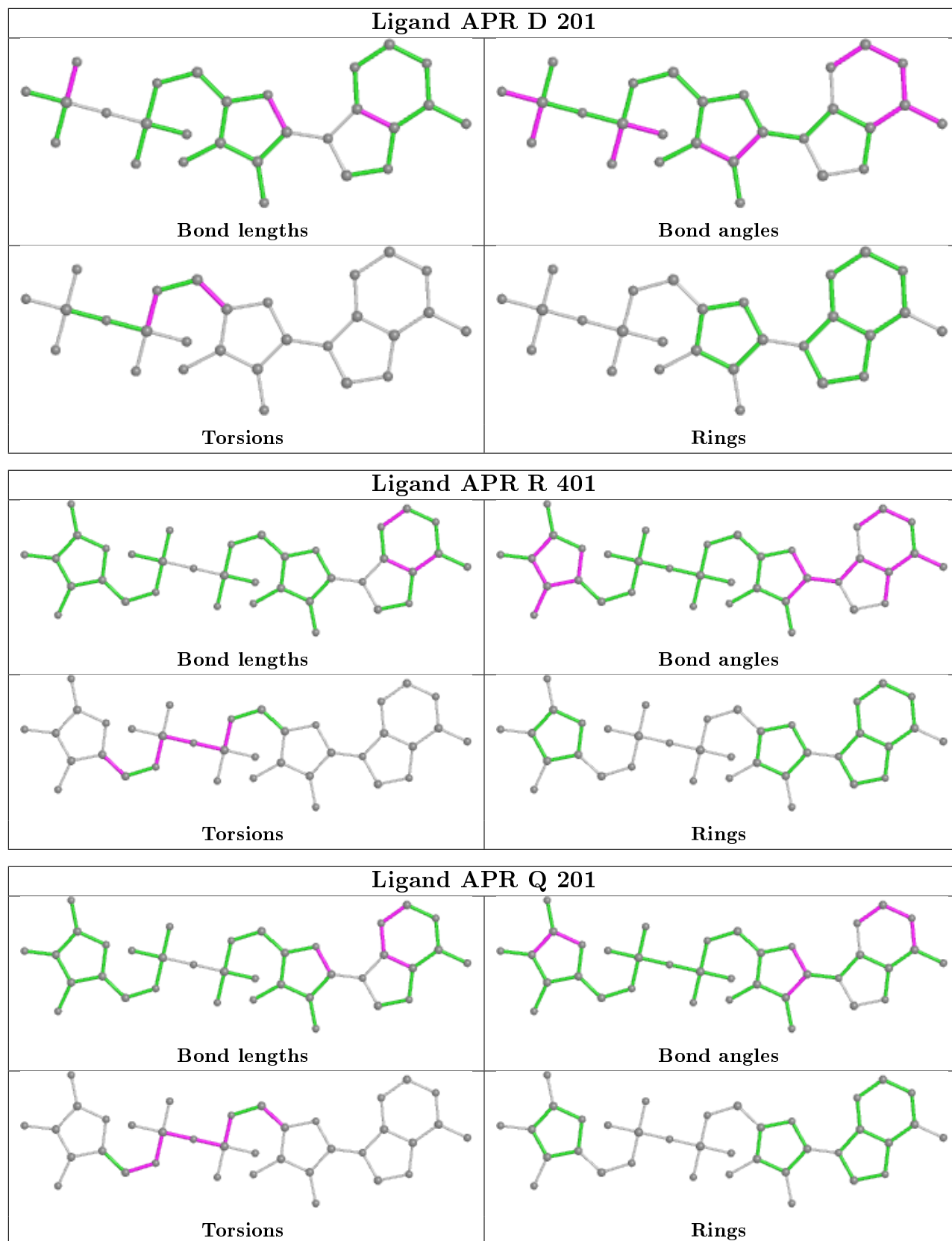
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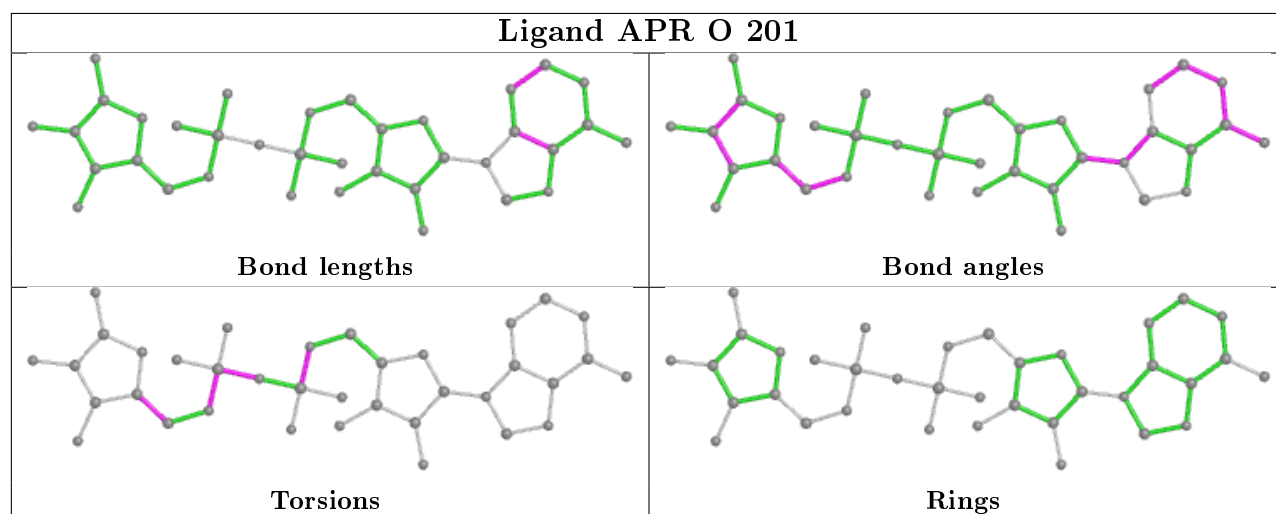
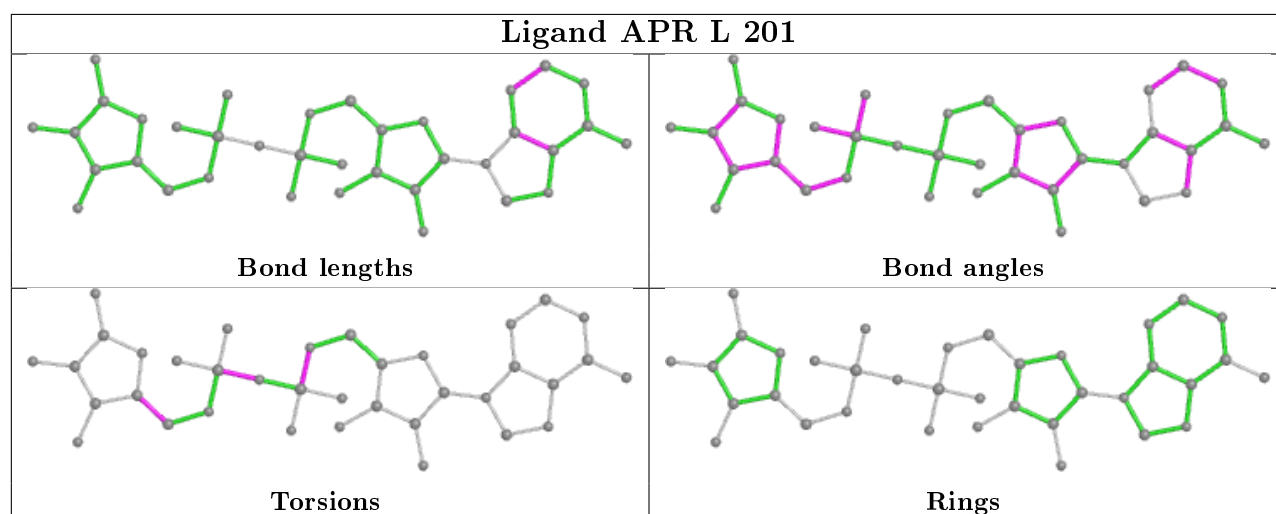
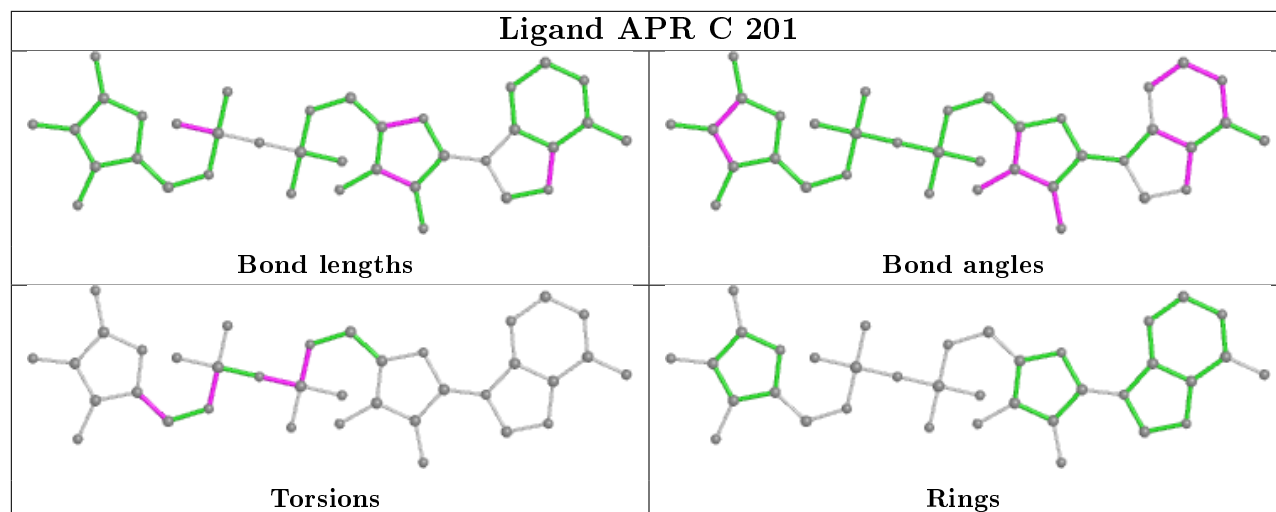
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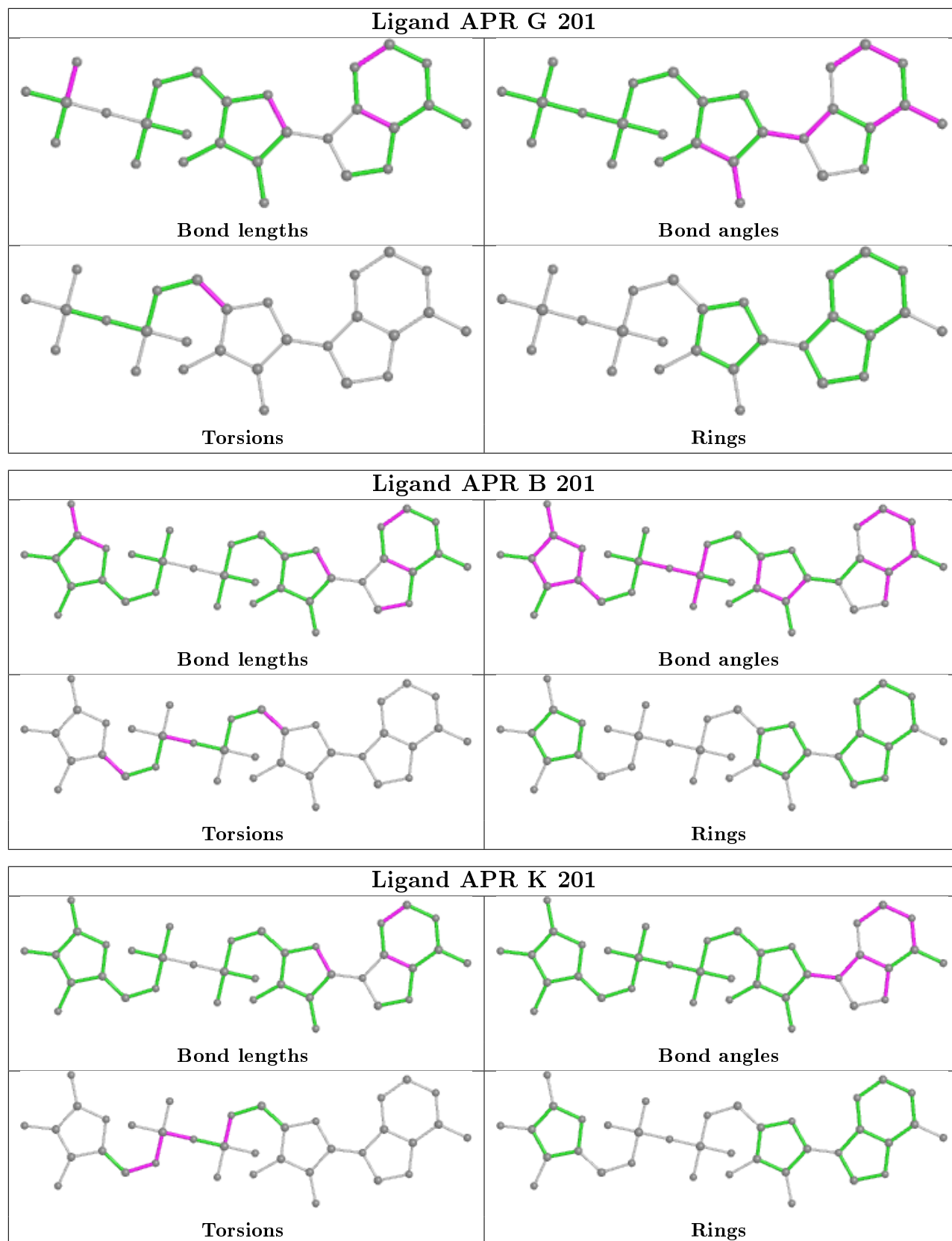
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	202	SO4	2	0
3	O	202	SO4	1	0
2	A	201	APR	2	0

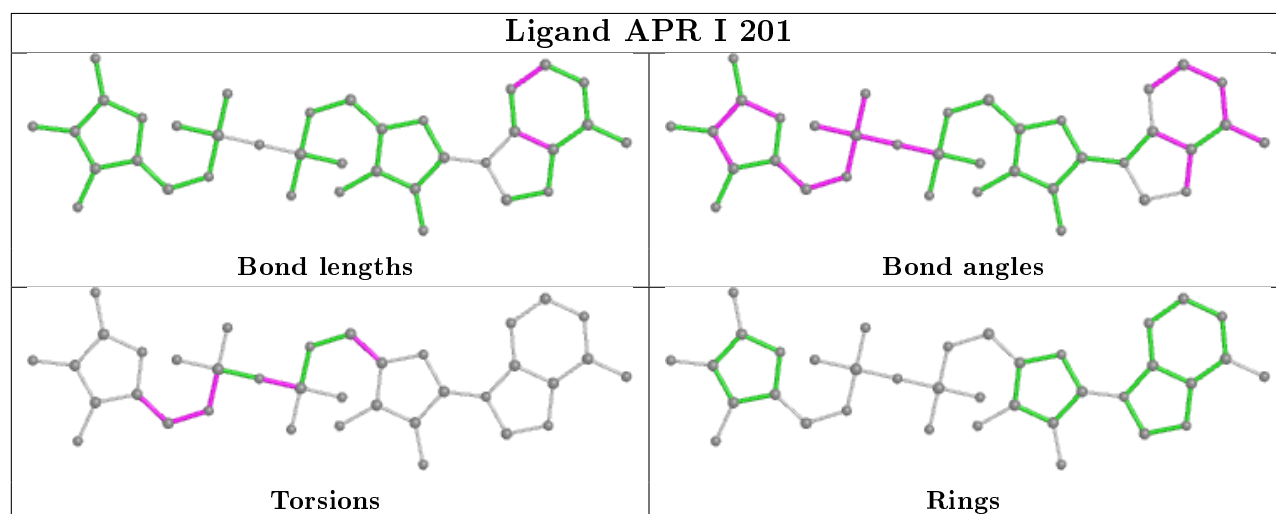
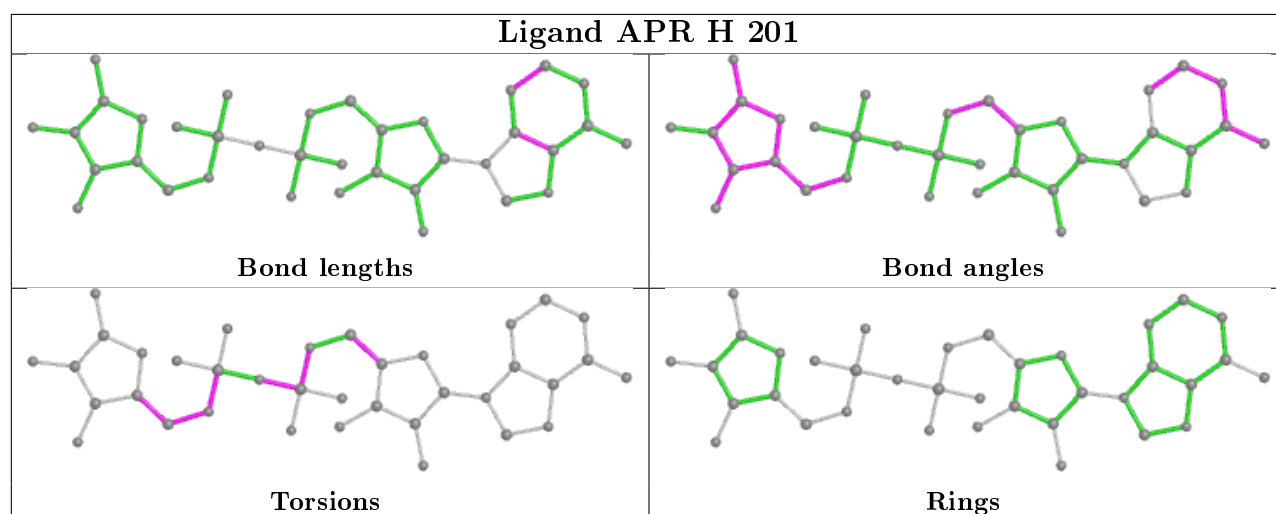
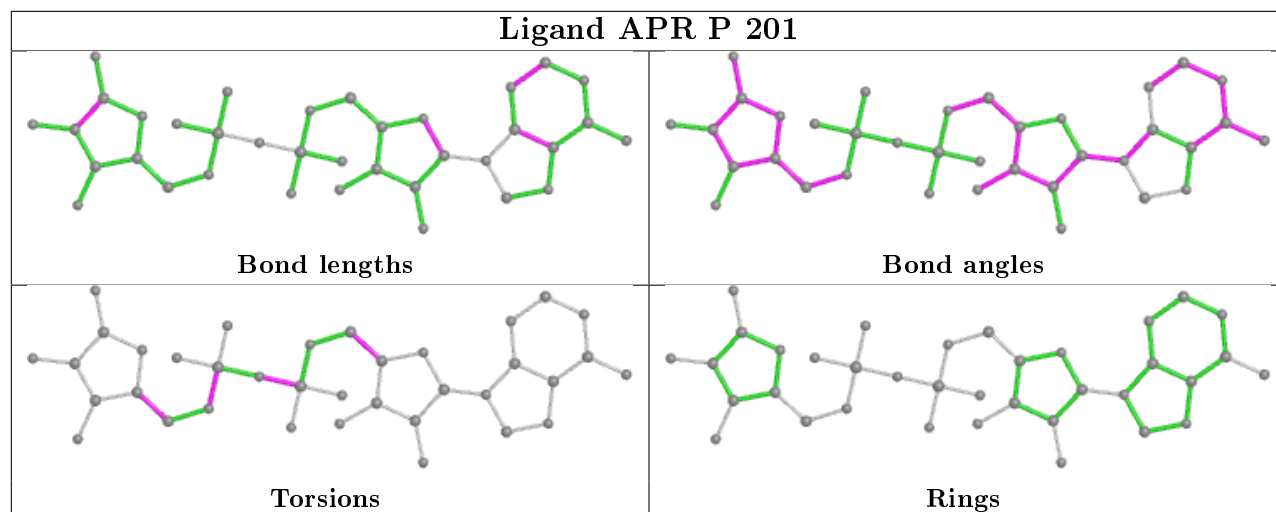
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

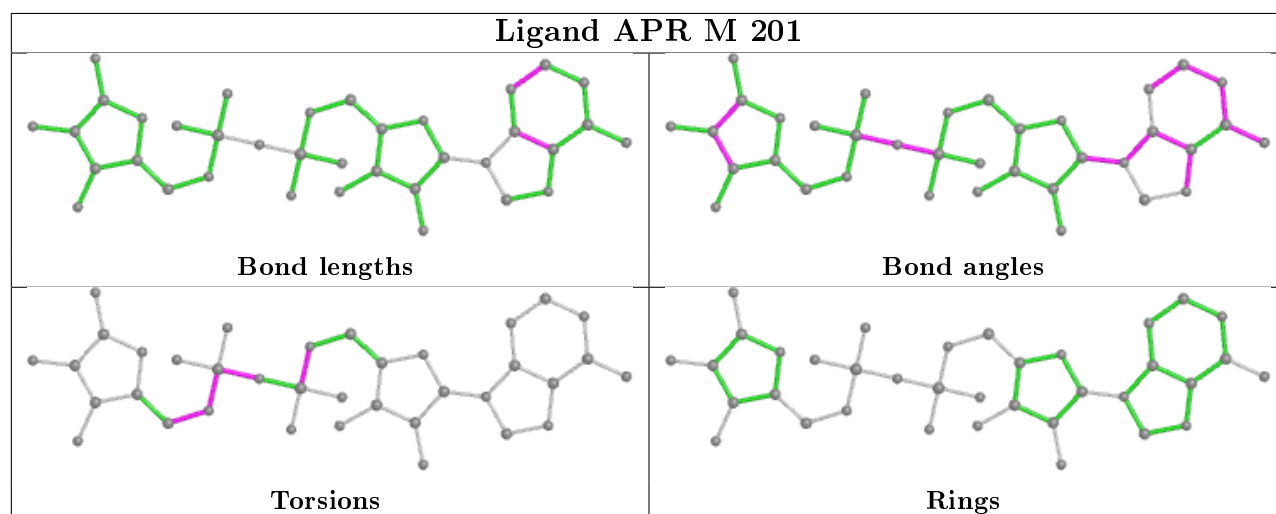
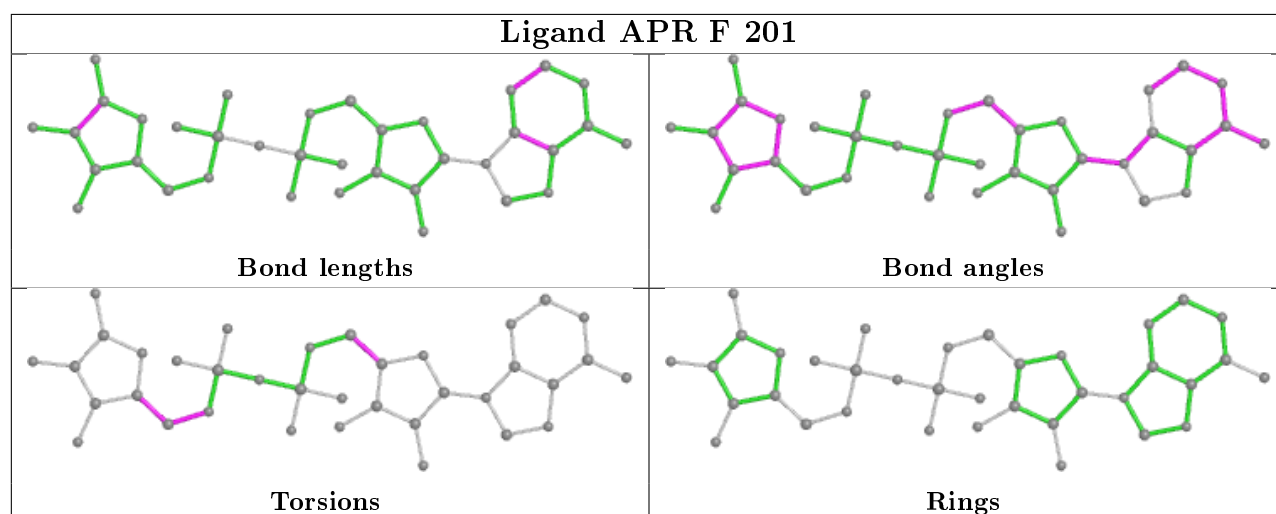
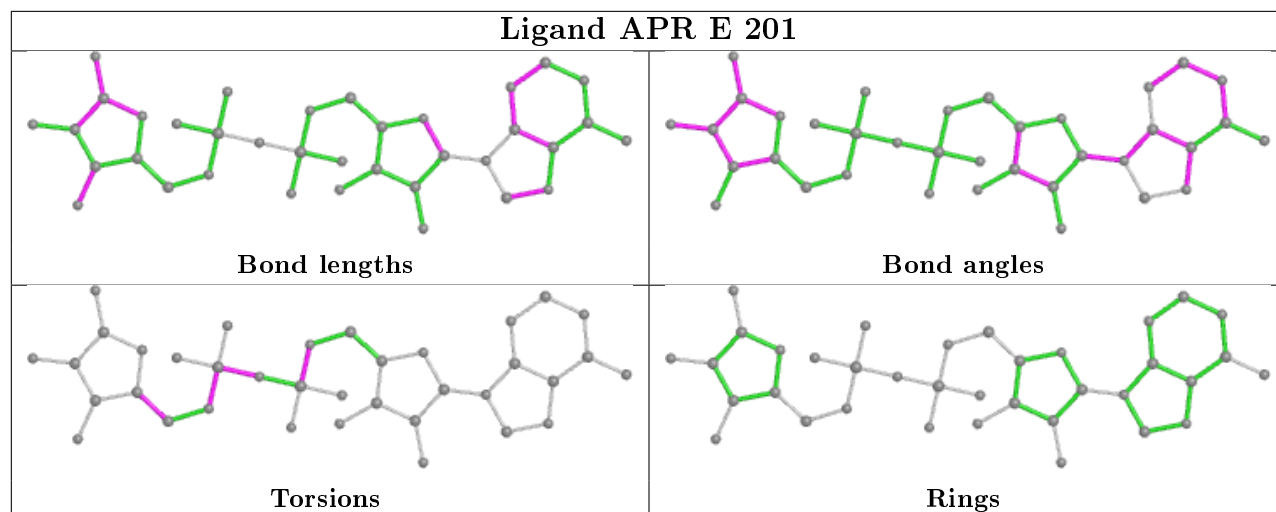


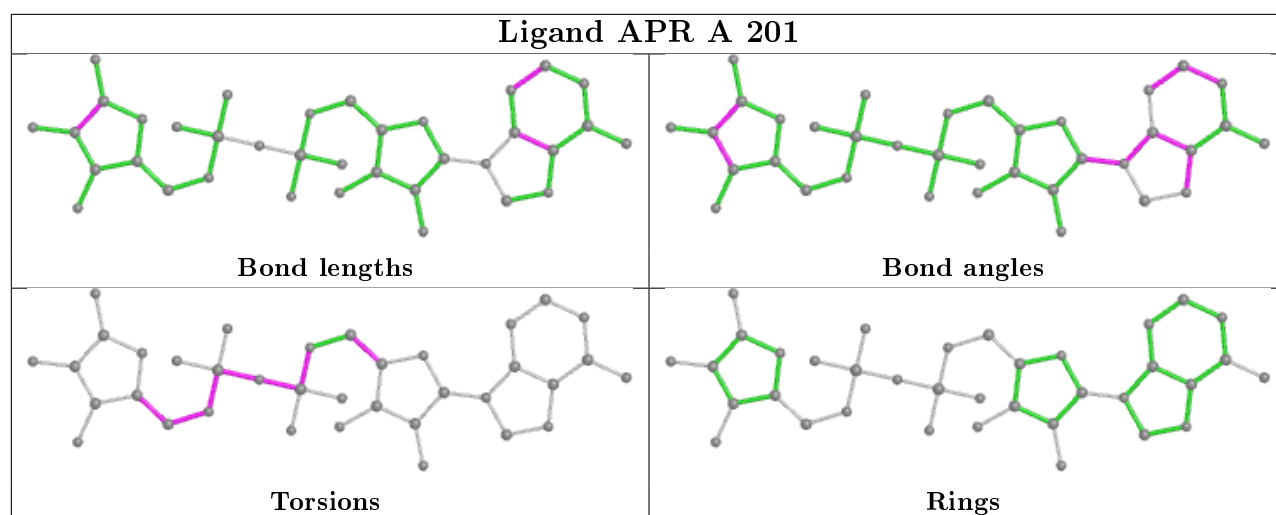












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.



## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	173/183 (94%)	0.05	7 (4%) 38 23	32, 51, 77, 83	0
1	B	173/183 (94%)	-0.11	1 (0%) 89 77	26, 41, 66, 78	0
1	C	173/183 (94%)	-0.06	1 (0%) 89 77	25, 42, 66, 83	0
1	D	173/183 (94%)	-0.01	0 100 100	29, 46, 70, 85	0
1	E	173/183 (94%)	-0.15	0 100 100	24, 42, 62, 82	0
1	F	172/183 (93%)	0.06	0 100 100	30, 48, 80, 87	0
1	G	171/183 (93%)	-0.03	1 (0%) 89 77	30, 47, 72, 86	0
1	H	172/183 (93%)	0.01	1 (0%) 89 77	27, 43, 69, 85	0
1	I	171/183 (93%)	0.10	3 (1%) 68 48	28, 49, 75, 89	0
1	J	172/183 (93%)	0.07	2 (1%) 79 61	26, 44, 72, 90	0
1	K	171/183 (93%)	0.12	5 (2%) 51 32	30, 54, 80, 97	0
1	L	171/183 (93%)	0.38	15 (8%) 10 5	34, 60, 82, 95	0
1	M	172/183 (93%)	0.08	5 (2%) 51 32	30, 48, 77, 87	0
1	N	171/183 (93%)	0.25	9 (5%) 26 15	27, 53, 79, 90	0
1	O	172/183 (93%)	0.12	5 (2%) 51 32	31, 47, 74, 93	0
1	P	172/183 (93%)	0.07	1 (0%) 89 77	29, 49, 74, 95	0
1	Q	173/183 (94%)	-0.11	0 100 100	28, 44, 65, 75	0
1	R	172/183 (93%)	0.23	10 (5%) 23 12	28, 56, 82, 100	0
All	All	3097/3294 (94%)	0.06	66 (2%) 63 43	24, 48, 76, 100	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	N	163	ASN	4.9
1	L	163	ASN	4.2
1	L	167	TYR	3.9

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Mol	Chain	Res	Type	RSRZ
1	O	170	LEU	3.8
1	R	132	ALA	3.4
1	R	172	THR	3.2
1	A	86	TRP	3.2
1	M	170	LEU	3.2
1	J	172	THR	3.1
1	R	171	LEU	3.0
1	L	88	GLY	2.9
1	I	165	HIS	2.8
1	A	88	GLY	2.8
1	N	172	THR	2.8
1	N	167	TYR	2.8
1	H	89	GLY	2.7
1	A	131	ALA	2.7
1	K	132	ALA	2.7
1	P	125	VAL	2.7
1	L	4	ARG	2.7
1	L	154	VAL	2.6
1	N	158	CYS	2.6
1	R	158	CYS	2.6
1	N	162	GLU	2.6
1	R	133	ALA	2.6
1	J	120	ALA	2.5
1	L	169	ARG	2.5
1	K	173	GLN	2.4
1	A	166	LEU	2.4
1	A	129	PRO	2.4
1	L	171	LEU	2.4
1	L	166	LEU	2.4
1	L	162	GLU	2.4
1	K	171	LEU	2.4
1	A	89	GLY	2.3
1	R	142	SER	2.3
1	N	127	GLY	2.3
1	R	128	TYR	2.3
1	K	172	THR	2.3
1	L	172	THR	2.2
1	O	8	VAL	2.2
1	L	170	LEU	2.2
1	M	133	ALA	2.2
1	L	140	THR	2.2
1	R	154	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	M	166	LEU	2.2
1	O	166	LEU	2.2
1	R	131	ALA	2.2
1	M	123	THR	2.1
1	A	125	VAL	2.1
1	K	129	PRO	2.1
1	N	166	LEU	2.1
1	N	171	LEU	2.1
1	C	127	GLY	2.1
1	L	157	VAL	2.1
1	B	86	TRP	2.0
1	L	160	ASP	2.0
1	I	16	ALA	2.0
1	N	5	ILE	2.0
1	M	88	GLY	2.0
1	O	140	THR	2.0
1	L	153	GLN	2.0
1	G	4	ARG	2.0
1	I	158	CYS	2.0
1	R	136	ILE	2.0
1	O	167	TYR	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<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	SO4	D	202	5/5	0.89	0.21	51,59,62,65	0
2	APR	H	201	36/36	0.92	0.19	39,58,90,92	0

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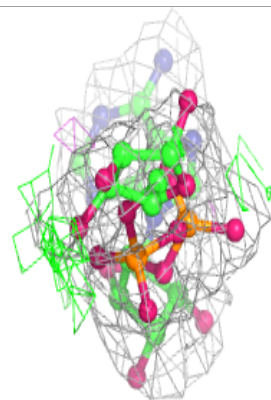
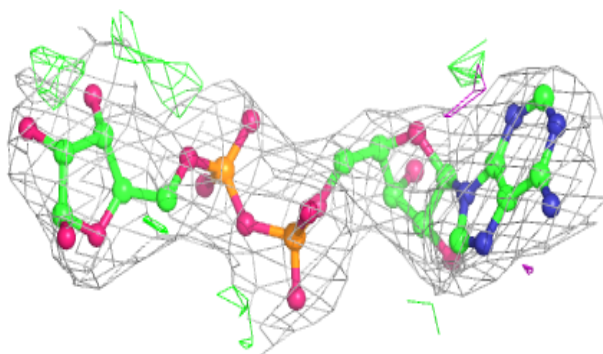
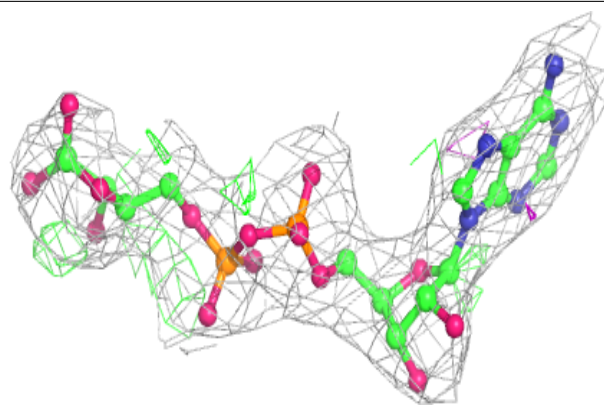
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	APR	R	401	36/36	0.92	0.23	44,68,98,102	0
2	APR	G	201	27/36	0.93	0.23	46,63,77,79	0
2	APR	B	201	36/36	0.93	0.28	33,42,68,74	0
2	APR	K	201	36/36	0.93	0.23	53,66,108,113	0
2	APR	N	201	36/36	0.93	0.20	49,67,97,98	0
2	APR	L	201	36/36	0.93	0.17	55,77,101,103	0
2	APR	J	201	36/36	0.94	0.27	54,61,84,95	0
2	APR	Q	201	36/36	0.94	0.20	54,66,92,96	0
2	APR	C	201	36/36	0.94	0.31	16,21,26,32	0
2	APR	P	201	36/36	0.94	0.23	51,62,72,76	0
2	APR	D	201	27/36	0.94	0.20	39,57,64,69	0
2	APR	I	201	36/36	0.94	0.19	39,58,79,85	0
2	APR	E	201	36/36	0.94	0.21	32,41,58,66	0
2	APR	F	201	36/36	0.94	0.21	51,62,73,76	0
2	APR	O	201	36/36	0.94	0.22	45,62,98,107	0
2	APR	A	201	36/36	0.94	0.24	59,69,100,111	0
3	SO4	I	202	5/5	0.95	0.13	49,49,52,59	0
2	APR	M	201	36/36	0.95	0.18	55,61,79,90	0
3	SO4	L	202	5/5	0.95	0.16	41,49,50,50	0
3	SO4	Q	202	5/5	0.96	0.16	45,52,52,59	0
3	SO4	O	202	5/5	0.96	0.14	54,55,58,67	0
3	SO4	K	202	5/5	0.96	0.11	55,62,65,65	0
3	SO4	B	202	5/5	0.97	0.17	44,51,57,62	0
3	SO4	F	202	5/5	0.97	0.11	44,48,53,62	0
3	SO4	P	202	5/5	0.97	0.10	43,51,51,53	0
3	SO4	A	202	5/5	0.97	0.14	41,43,50,52	0
3	SO4	C	202	5/5	0.97	0.17	36,40,42,44	0
3	SO4	N	202	5/5	0.97	0.19	43,44,49,50	0
3	SO4	J	202	5/5	0.97	0.13	39,41,44,44	0
3	SO4	H	202	5/5	0.97	0.16	36,38,41,47	0
3	SO4	G	202	5/5	0.98	0.13	37,38,40,45	0
3	SO4	E	202	5/5	0.98	0.14	41,41,46,53	0
3	SO4	R	402	5/5	0.98	0.14	37,38,39,41	0
3	SO4	M	202	5/5	0.99	0.09	44,49,55,57	0

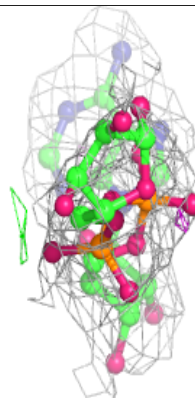
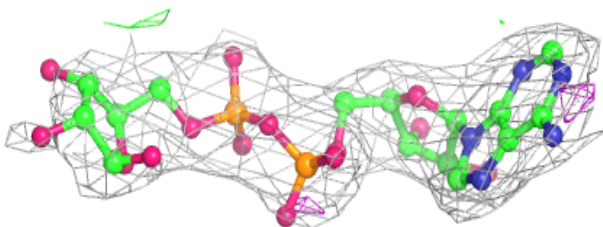
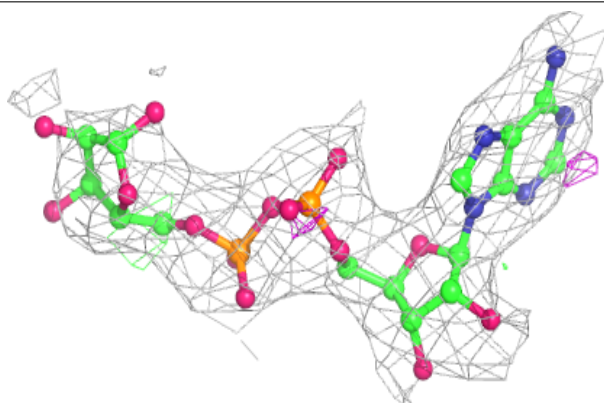
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around APR H 201:**

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

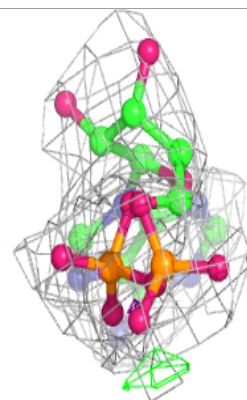
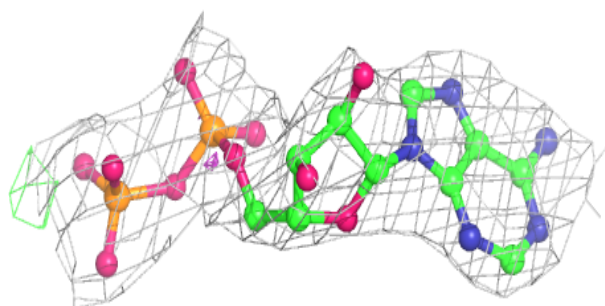
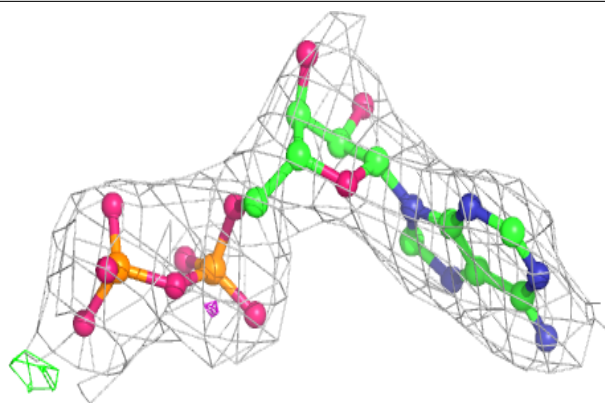
**Electron density around APR R 401:**

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

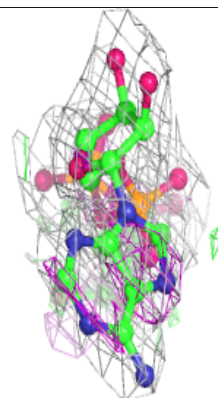
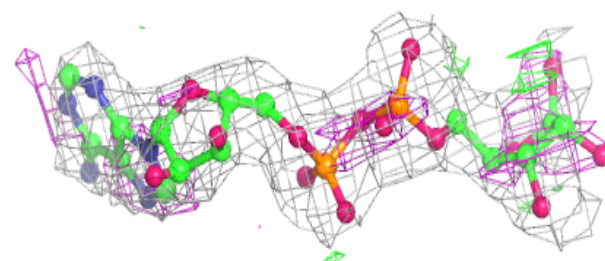
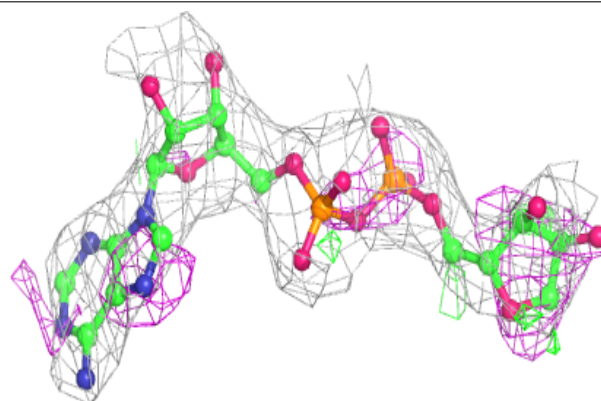


**Electron density around APR G 201:**

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

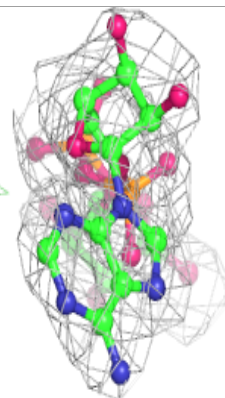
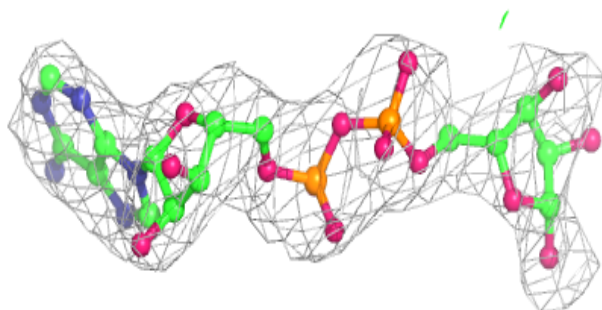
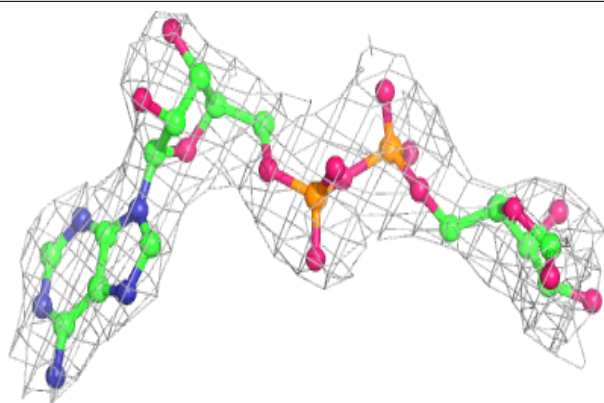
**Electron density around APR B 201:**

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

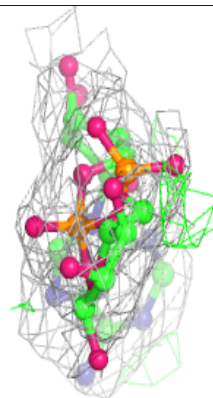
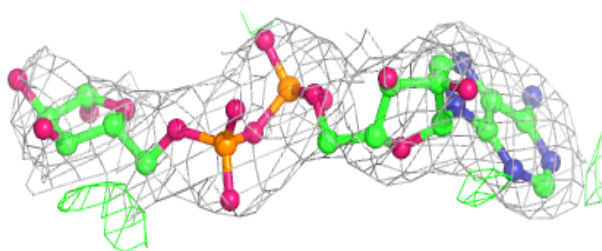
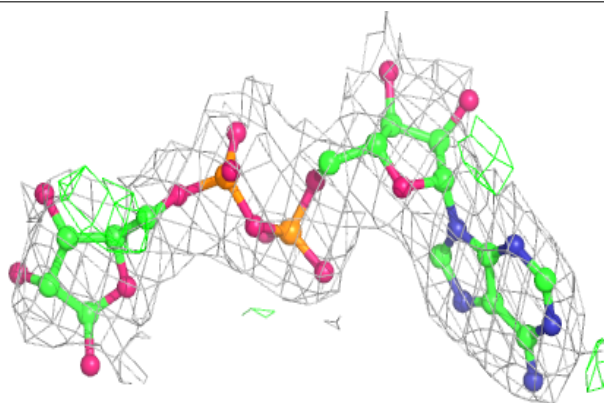


**Electron density around APR K 201:**

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

**Electron density around APR N 201:**

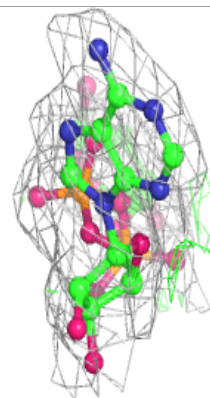
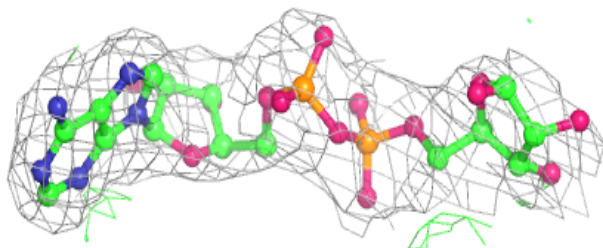
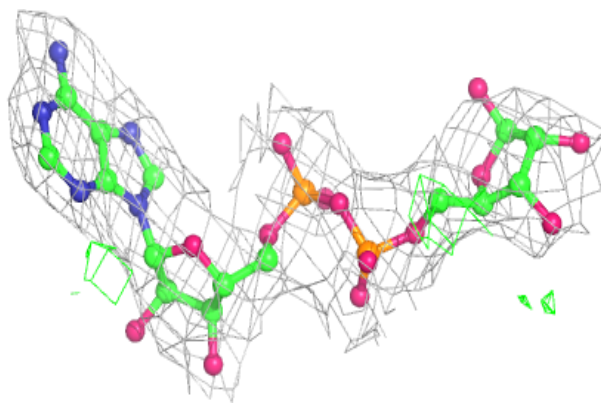
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



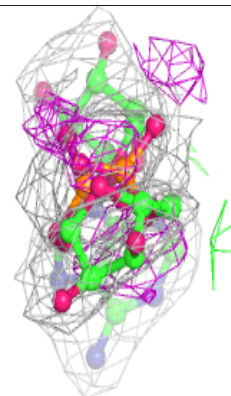
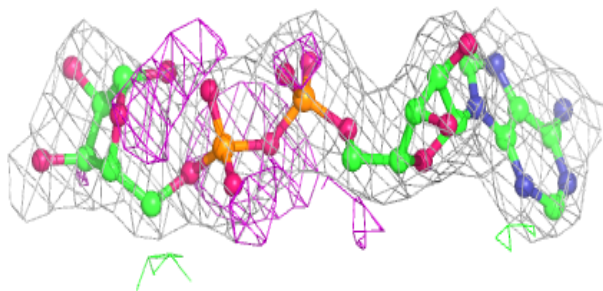
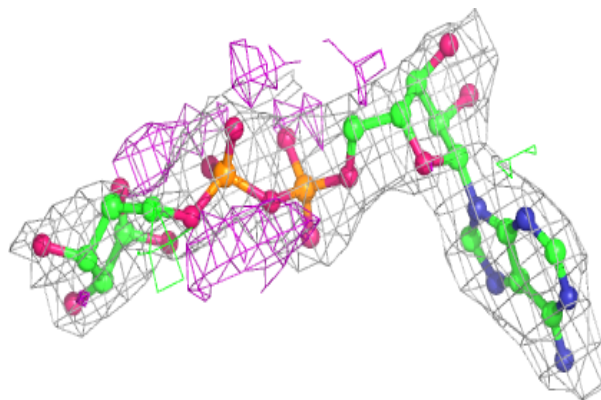


**Electron density around APR L 201:**

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

**Electron density around APR J 201:**

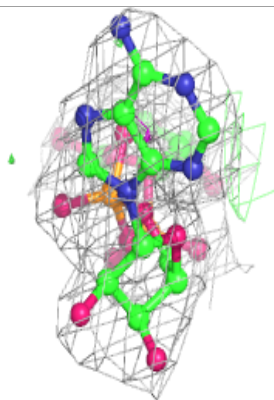
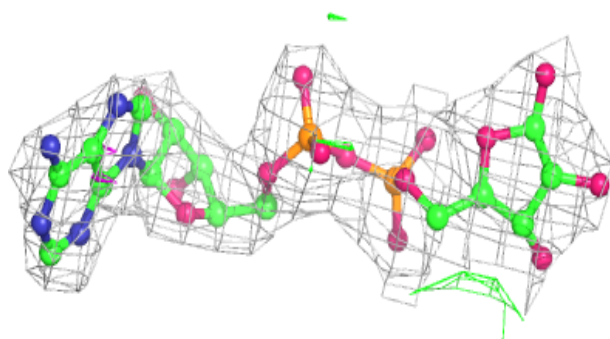
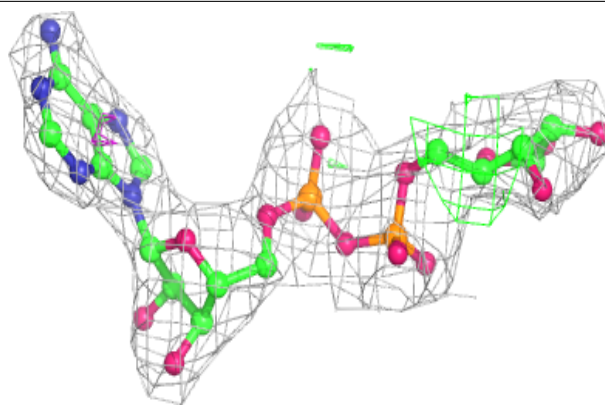
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



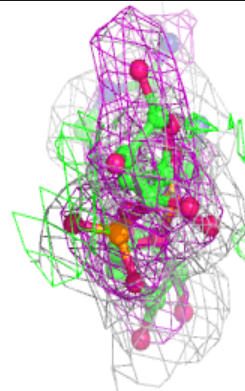
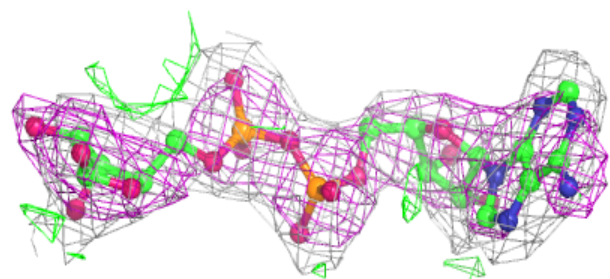
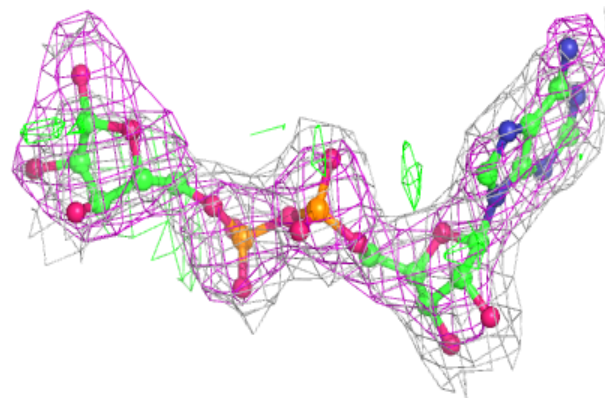


**Electron density around APR Q 201:**

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

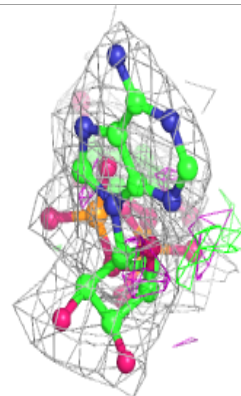
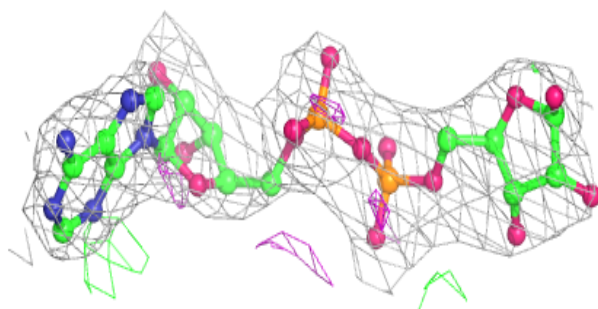
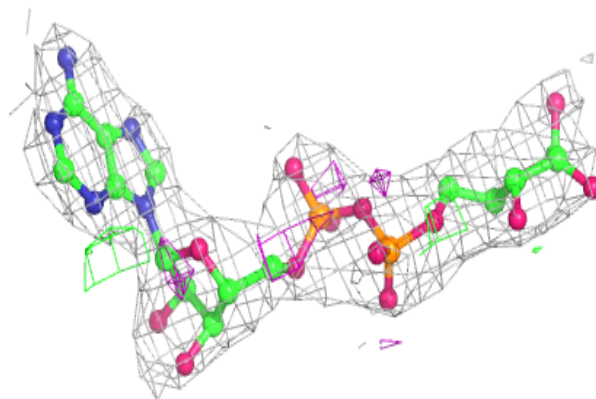
**Electron density around APR C 201:**

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

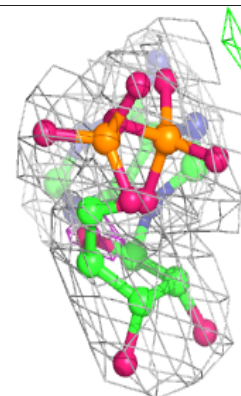
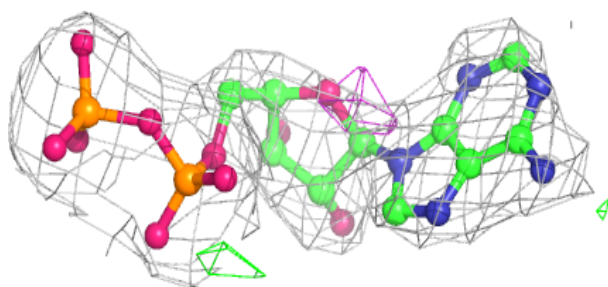
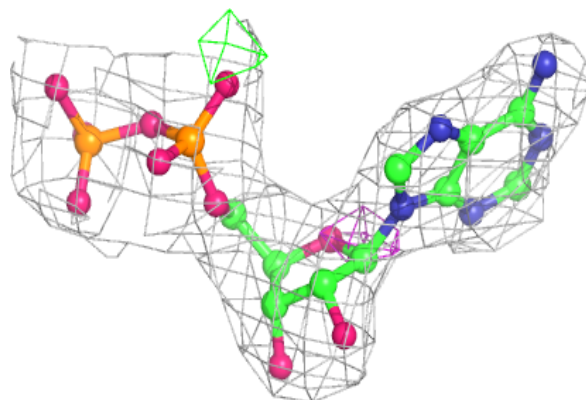


**Electron density around APR P 201:**

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

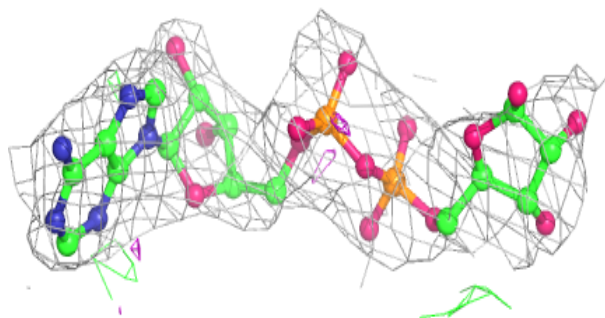
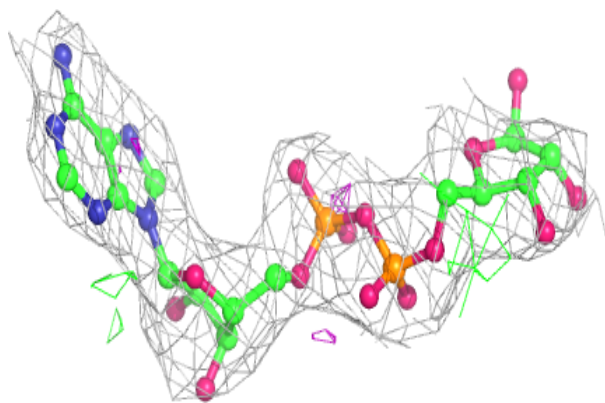
**Electron density around APR D 201:**

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

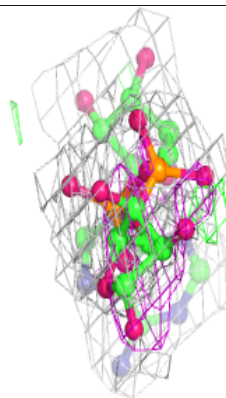
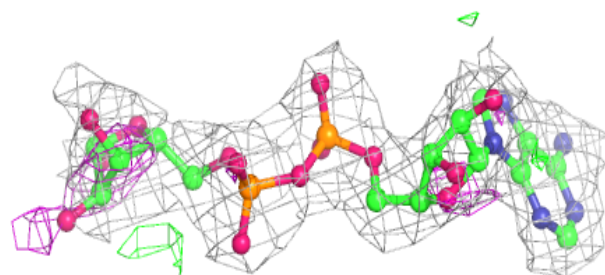
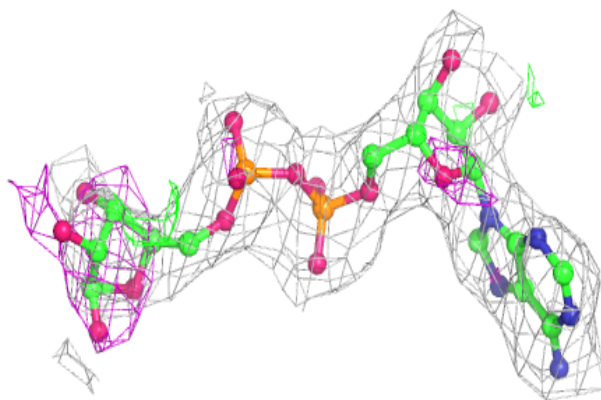


**Electron density around APR I 201:**

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

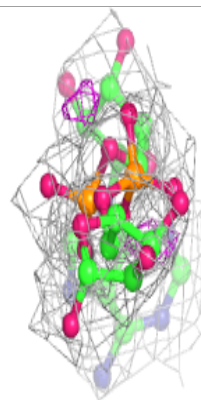
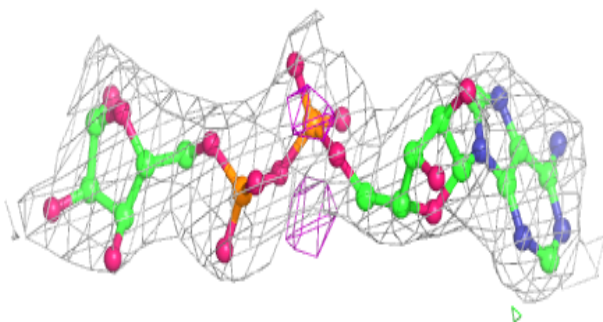
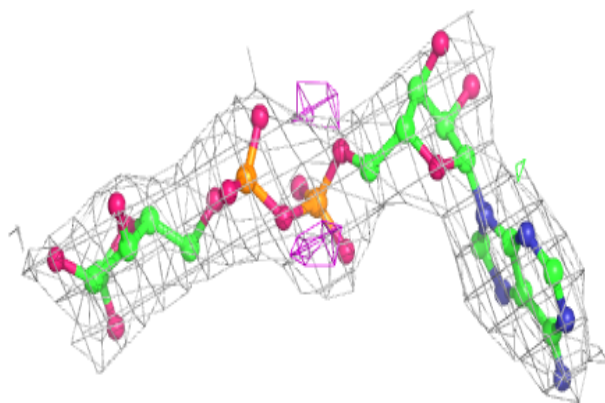
**Electron density around APR E 201:**

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

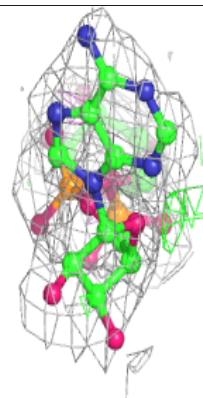
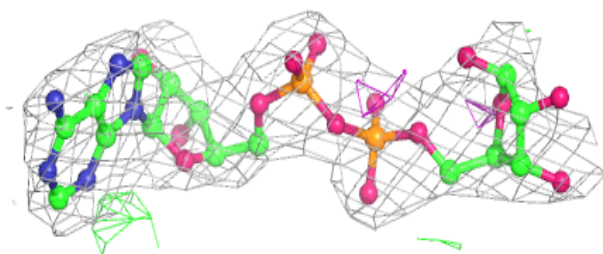
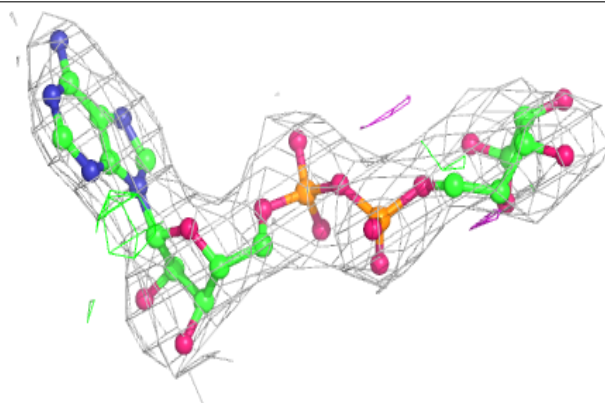


**Electron density around APR F 201:**

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

**Electron density around APR O 201:**

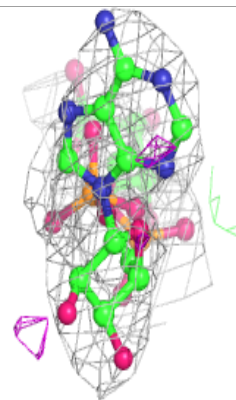
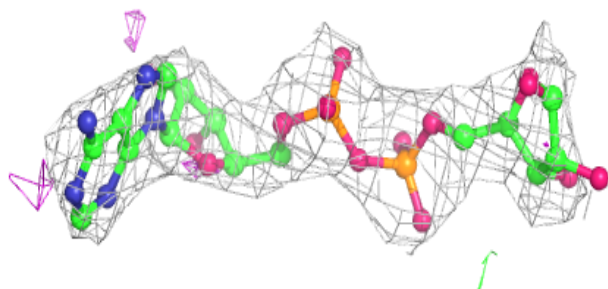
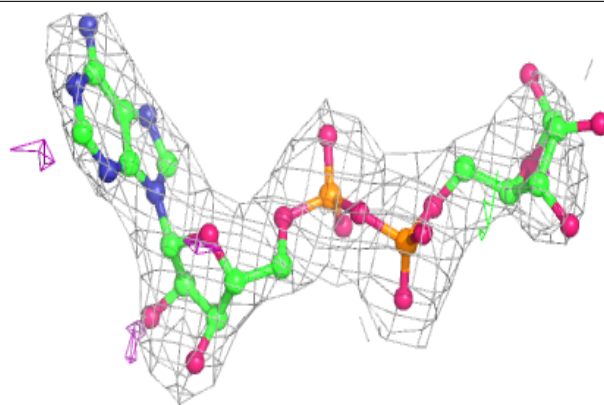
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



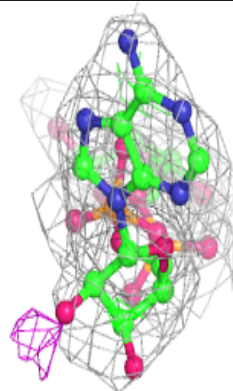
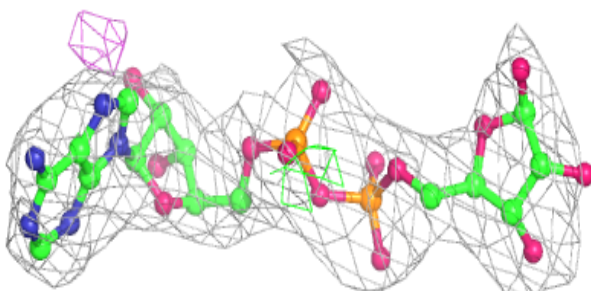
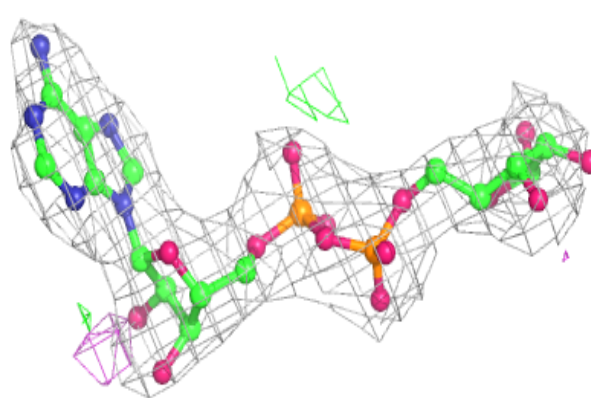


**Electron density around APR A 201:**

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

**Electron density around APR 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)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.