



# Full wwPDB X-ray Structure Validation Report i

Aug 7, 2020 – 07:19 AM BST

PDB ID : 2JG1  
Title : STRUCTURE OF Staphylococcus aureus D-TAGATOSE-6-PHOSPHATE KINASE with cofactor and substrate  
Authors : Miallau, L.; Hunter, W.N.; McSweeney, S.M.; Leonard, G.A.  
Deposited on : 2007-02-07  
Resolution : 2.00 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 i symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13.1

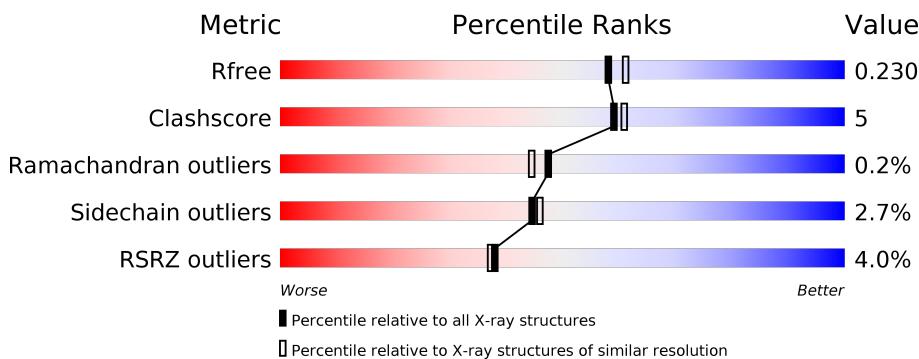
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## X-RAY DIFFRACTION

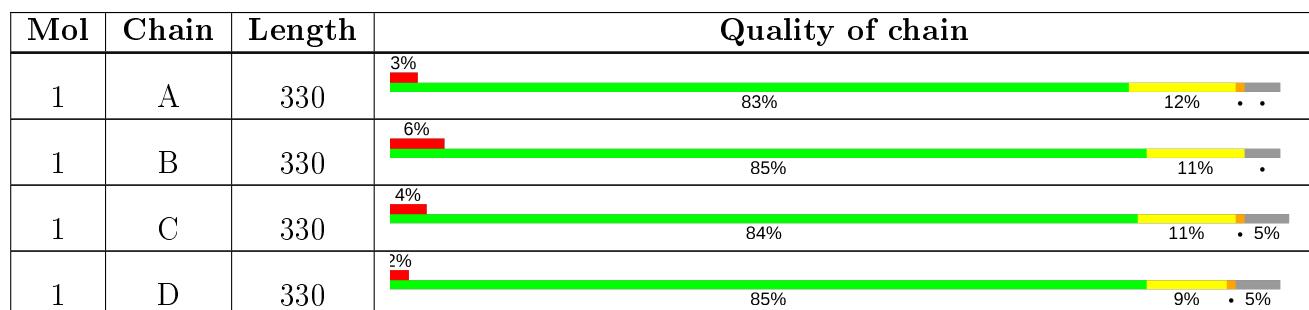
The reported resolution of this entry is 2.00 Å.

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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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



## 2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 10894 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 TAGATOSE-6-PHOSPHATE KINASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	318	Total	C 2498	N 1583	O 424	S 482	Se 4	0	13	0
1	B	318	Total	C 2475	N 1567	O 418	S 481	Se 4	0	7	0
1	C	315	Total	C 2451	N 1552	O 416	S 476	Se 3	0	7	0
1	D	313	Total	C 2450	N 1553	O 411	S 478	Se 3	0	12	0

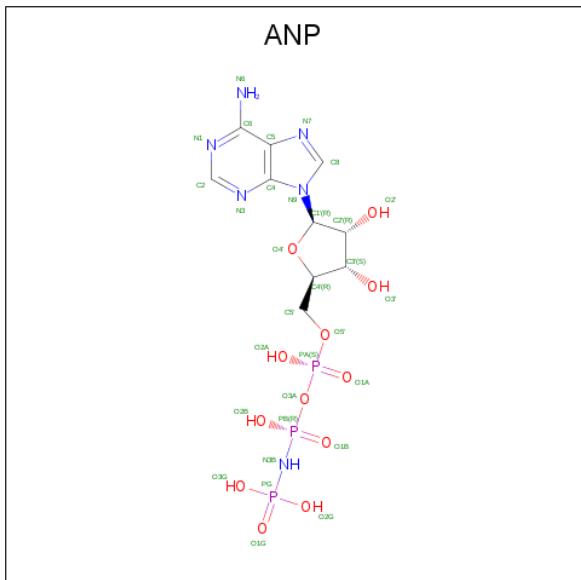
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	124	MSE	LEU	engineered mutation	UNP P0A0B9
A	125	MSE	LEU	engineered mutation	UNP P0A0B9
B	124	MSE	LEU	engineered mutation	UNP P0A0B9
B	125	MSE	LEU	engineered mutation	UNP P0A0B9
C	124	MSE	LEU	engineered mutation	UNP P0A0B9
C	125	MSE	LEU	engineered mutation	UNP P0A0B9
D	124	MSE	LEU	engineered mutation	UNP P0A0B9
D	125	MSE	LEU	engineered mutation	UNP P0A0B9

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

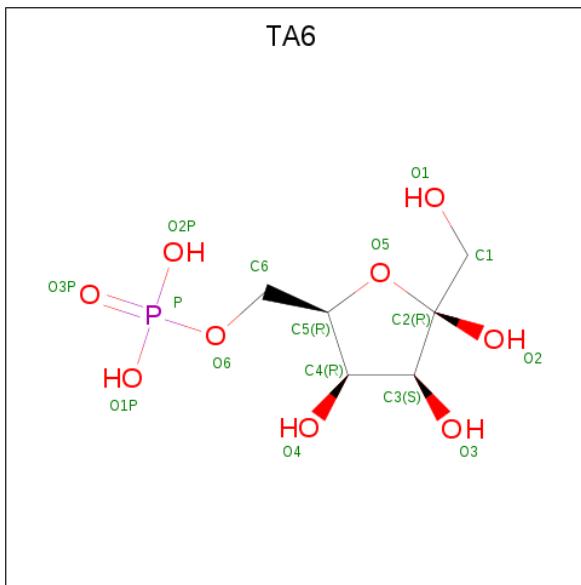
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mg 1 1	0	0
2	A	1	Total	Mg 1 1	0	0
2	D	1	Total	Mg 1 1	0	0
2	C	2	Total	Mg 2 2	0	0

- Molecule 3 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: C<sub>10</sub>H<sub>17</sub>N<sub>6</sub>O<sub>12</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total		C	N	O	P	
			31	10	6	12	3		
3	B	1	Total		C	N	O	P	
			31	10	6	12	3		
3	C	1	Total		C	N	O	P	
			31	10	6	12	3		
3	D	1	Total		C	N	O	P	
			31	10	6	12	3		

- Molecule 4 is 6-O-phosphono-beta-D-tagatofuranose (three-letter code: TA6) (formula: C<sub>6</sub>H<sub>13</sub>O<sub>9</sub>P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total    C    O    P 16    6    9    1	0	0

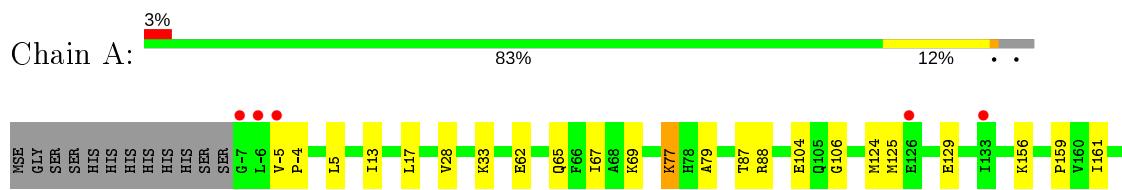
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	221	Total    O 221    221	0	0
5	B	214	Total    O 214    214	0	0
5	C	201	Total    O 201    201	0	0
5	D	239	Total    O 239    239	0	0

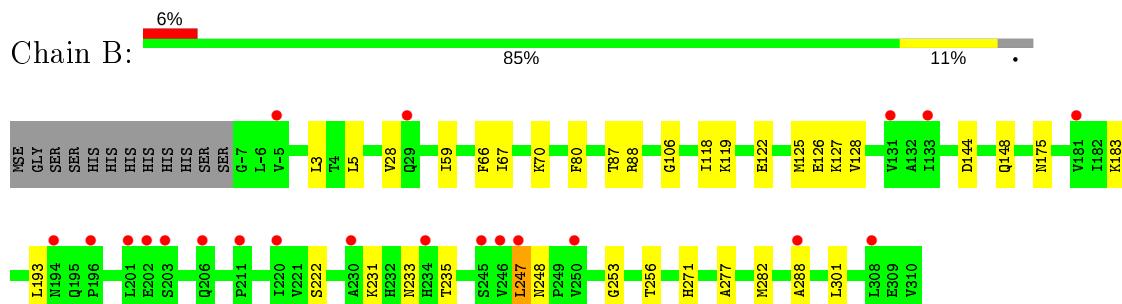
### 3 Residue-property plots

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

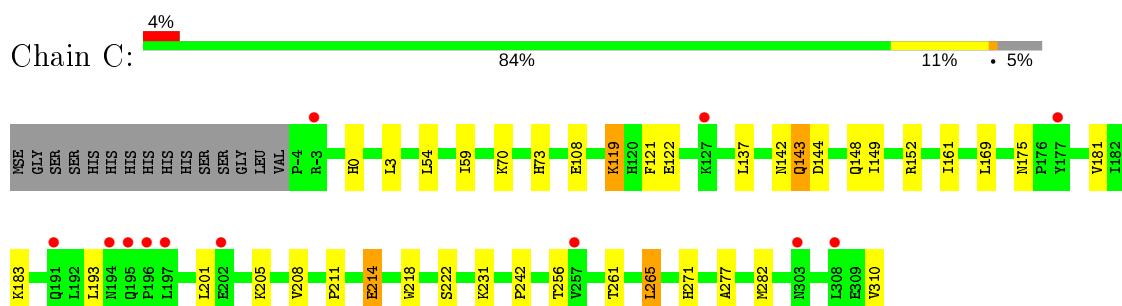
- Molecule 1: TAGATOSE-6-PHOSPHATE KINASE



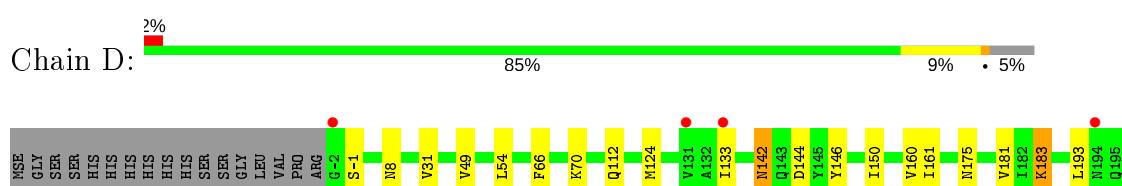
- Molecule 1: TAGATOSE-6-PHOSPHATE KINASE

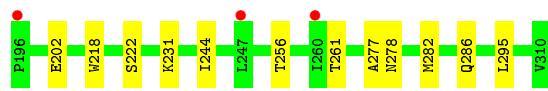


- Molecule 1: TAGATOSE-6-PHOSPHATE KINASE



- Molecule 1: TAGATOSE-6-PHOSPHATE KINASE





## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	95.20 Å   97.09 Å   154.47 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	24.85 – 2.00 24.85 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.8 (24.85-2.00) 99.8 (24.85-2.00)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle^1$	1.55 (at 1.99 Å)	Xtriage
Refinement program	REFMAC 5.3.0011	Depositor
$R$ , $R_{free}$	0.190 , 0.234 0.189 , 0.230	Depositor DCC
$R_{free}$ test set	4857 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	28.7	Xtriage
Anisotropy	0.010	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 50.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.029 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	10894	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.56% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality [\(i\)](#)

### 5.1 Standard geometry [\(i\)](#)

Bond lengths and bond angles in the following residue types are not validated in this section: TA6, ANP, MG

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	0.66	2/2585 (0.1%)	0.56	2/3495 (0.1%)
1	B	0.44	0/2538	0.56	0/3437
1	C	0.45	0/2517	0.61	0/3409
1	D	0.52	2/2540 (0.1%)	0.55	0/3440
All	All	0.53	4/10180 (0.0%)	0.57	2/13781 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	77[A]	LYS	CD-CE	17.30	1.94	1.51
1	A	77[B]	LYS	CD-CE	17.30	1.94	1.51
1	D	202[A]	GLU	CB-CG	8.83	1.69	1.52
1	D	202[B]	GLU	CB-CG	8.83	1.69	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	77[A]	LYS	CD-CE-NZ	-5.16	99.84	111.70
1	A	77[B]	LYS	CD-CE-NZ	-5.16	99.84	111.70

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [\(i\)](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2498	0	2519	33	0
1	B	2475	0	2487	17	0
1	C	2451	0	2450	22	0
1	D	2450	0	2453	21	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	2	0	0	0	0
2	D	1	0	0	0	0
3	A	31	0	13	1	0
3	B	31	0	13	2	0
3	C	31	0	13	2	0
3	D	31	0	13	0	0
4	C	16	0	11	0	0
5	A	221	0	0	1	0
5	B	214	0	0	2	0
5	C	201	0	0	2	0
5	D	239	0	0	3	0
All	All	10894	0	9972	95	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (95) 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:A:77[A]:LYS:CE	1:A:77[A]:LYS:CD	1.94	1.45
1:C:211:PRO:O	1:C:214:GLU:HG3	1.88	0.73
1:D:150[B]:ILE:HD12	1:D:160:VAL:HG11	1.72	0.72
1:C:70:LYS:O	1:C:73[B]:HIS:HD2	1.73	0.71
1:D:142:ASN:HD22	1:D:144:ASP:H	1.41	0.68
1:D:146:TYR:O	1:D:150[B]:ILE:HG12	1.95	0.67
1:C:70:LYS:O	1:C:73[B]:HIS:CD2	2.48	0.67
1:A:183:LYS:HE2	1:A:183:LYS:O	1.96	0.65
1:A:77[A]:LYS:CE	1:A:77[A]:LYS:CB	2.76	0.64
1:D:54:LEU:HD21	1:D:124[A]:MSE:HE1	1.80	0.63
1:A:79:ALA:CB	1:A:124[A]:MSE:HE1	2.29	0.62
1:B:231:LYS:HE2	1:B:233:ASN:O	2.00	0.61
1:D:54:LEU:HD21	1:D:124[A]:MSE:CE	2.29	0.61
1:A:77[A]:LYS:CB	1:A:77[A]:LYS:HE3	2.31	0.60
1:C:119:LYS:NZ	1:C:122:GLU:OE1	2.34	0.59
1:A:17:LEU:CD2	1:A:28[A]:VAL:CG1	2.80	0.59
1:A:17:LEU:HD21	1:A:28[A]:VAL:CG1	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77[A]:LYS:CE	1:A:77[A]:LYS:CG	2.76	0.58
1:D:150[B]:ILE:CD1	1:D:160:VAL:HG11	2.33	0.58
1:B:118:ILE:O	1:B:122:GLU:HG3	2.04	0.57
1:A:125:MSE:HE2	1:A:125:MSE:HA	1.87	0.57
1:D:278:ASN:O	1:D:282:MSE:HG3	2.04	0.56
1:A:62:GLU:HA	1:A:65[B]:GLN:HE21	1.71	0.56
1:A:77[A]:LYS:NZ	1:A:77[A]:LYS:CD	2.65	0.56
1:A:17:LEU:CD2	1:A:28[A]:VAL:HG12	2.35	0.55
1:C:201:LEU:HD12	1:C:310:VAL:HG11	1.87	0.55
1:B:144:ASP:OD1	1:B:148:GLN:NE2	2.36	0.55
1:A:79:ALA:HB3	1:A:124[A]:MSE:HE1	1.89	0.54
1:C:122:GLU:OE2	1:C:152:ARG:NH1	2.35	0.54
1:A:77[A]:LYS:HB2	1:A:77[A]:LYS:HE3	1.89	0.53
1:B:126:GLU:HG3	1:B:127:LYS:HG3	1.90	0.53
1:C:181:VAL:HG22	1:C:218:TRP:HB2	1.92	0.52
1:C:142[B]:ASN:HD21	1:C:148:GLN:HE22	1.57	0.51
1:C:271:HIS:HD2	5:C:2172:HOH:O	1.94	0.51
1:B:183:LYS:HE3	1:B:253:GLY:HA2	1.93	0.51
1:A:181:VAL:HG11	1:A:260:ILE:HG21	1.93	0.51
1:A:129:GLU:O	1:A:159:PRO:HD2	2.12	0.50
1:D:256:THR:HG23	1:D:277:ALA:HB1	1.93	0.50
1:D:133:ILE:HD12	1:D:150[B]:ILE:HD11	1.93	0.50
1:C:256:THR:HG23	1:C:277:ALA:HB1	1.92	0.50
1:C:208:VAL:HG12	1:C:231:LYS:HD3	1.94	0.49
3:A:1312:ANP:H8	3:A:1312:ANP:O5'	2.13	0.49
1:D:181:VAL:HG22	1:D:218:TRP:HB2	1.94	0.48
1:D:49:VAL:HA	1:D:295:LEU:HD11	1.95	0.48
1:C:205:LYS:HE3	1:C:310:VAL:HG12	1.95	0.48
1:A:104:GLU:HG2	1:D:31[A]:VAL:HG21	1.94	0.48
1:B:271:HIS:HE1	5:B:2211:HOH:O	1.97	0.48
1:C:142[B]:ASN:HD21	1:C:148:GLN:NE2	2.11	0.47
1:D:8:ASN:OD1	5:D:2006:HOH:O	2.20	0.47
1:B:247:LEU:HD12	1:B:288:ALA:HB2	1.97	0.47
1:B:59:ILE:HG12	1:B:80:PHE:HB3	1.97	0.47
1:A:161:ILE:N	1:A:161:ILE:HD12	2.31	0.46
1:A:77[A]:LYS:CE	1:A:77[A]:LYS:HB2	2.45	0.46
1:A:244:ILE:HD13	1:A:286:GLN:HG3	1.98	0.46
1:B:66:PHE:CZ	1:B:70:LYS:HE2	2.51	0.45
1:A:13:ILE:HG12	1:A:33:LYS:HG2	1.97	0.45
1:A:242:PRO:HG2	1:A:282:MSE:HE1	1.98	0.45
1:B:67:ILE:HD12	1:B:87:THR:HG21	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:LEU:HD21	1:A:238:ARG:HD3	1.98	0.44
1:C:121:PHE:CZ	1:C:149:ILE:HG23	2.52	0.44
1:B:282:MSE:HE2	1:B:301:LEU:HD13	2.00	0.44
1:D:231:LYS:HE2	5:D:2181:HOH:O	2.17	0.44
1:C:242:PRO:HG2	1:C:282:MSE:HE1	2.00	0.44
3:B:1312:ANP:H8	3:B:1312:ANP:O5'	2.18	0.44
1:A:17:LEU:HD23	1:A:28[A]:VAL:HG12	1.99	0.43
1:B:3:LEU:HB2	1:B:128:VAL:HG11	2.00	0.43
1:D:244:ILE:HD12	1:D:286:GLN:HG3	1.99	0.43
1:A:213:PHE:HB3	1:A:219:ILE:HD11	1.99	0.43
1:B:256:THR:HG23	1:B:277:ALA:HB1	2.01	0.43
1:D:183:LYS:HE3	1:D:222:SER:OG	2.17	0.43
1:D:66:PHE:CZ	1:D:70:LYS:HE2	2.53	0.43
1:A:256:THR:HG23	1:A:277:ALA:HB1	2.01	0.43
1:B:125:MSE:HA	1:B:125:MSE:HE2	2.01	0.42
1:D:161:ILE:HD13	1:D:261:THR:HG23	2.02	0.42
1:C:143[B]:GLN:HG3	1:C:144:ASP:N	2.34	0.42
1:D:112:GLN:HG2	5:D:2108:HOH:O	2.20	0.42
1:C:161:ILE:HD13	1:C:261:THR:HG23	2.02	0.42
1:C:231:LYS:HE2	5:C:2154:HOH:O	2.19	0.42
1:A:156:LYS:HE3	5:A:2124:HOH:O	2.20	0.41
1:A:88:ARG:HB3	1:A:106:GLY:HA2	2.02	0.41
1:A:-5:VAL:HA	1:A:-4:PRO:HD3	1.92	0.41
1:C:222:SER:HB2	3:C:1313:ANP:H5'2	2.03	0.41
1:B:119:LYS:NZ	5:B:2120:HOH:O	2.52	0.41
1:A:173:LEU:HD11	1:A:192:LEU:HD21	2.03	0.41
1:C:122:GLU:OE2	1:C:152:ARG:HD3	2.21	0.41
1:B:222:SER:HB2	3:B:1312:ANP:H5'2	2.02	0.41
1:D:183:LYS:HE3	1:D:222:SER:HB3	2.02	0.41
1:A:67:ILE:HD12	1:A:87:THR:HG21	2.02	0.41
3:C:1313:ANP:H8	3:C:1313:ANP:O5'	2.22	0.40
1:C:0[B]:HIS:CE1	1:C:265:LEU:HD22	2.56	0.40
1:B:88:ARG:HB3	1:B:106:GLY:HA2	2.04	0.40
1:D:183:LYS:HE3	1:D:222:SER:CB	2.51	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [\(i\)](#)

### 5.3.1 Protein backbone [\(i\)](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	329/330 (100%)	326 (99%)	2 (1%)	1 (0%)	41 37
1	B	323/330 (98%)	317 (98%)	5 (2%)	1 (0%)	41 37
1	C	320/330 (97%)	311 (97%)	9 (3%)	0	100 100
1	D	323/330 (98%)	318 (98%)	4 (1%)	1 (0%)	41 37
All	All	1295/1320 (98%)	1272 (98%)	20 (2%)	3 (0%)	47 44

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	233	ASN
1	D	-1	SER
1	B	248	ASN

### 5.3.2 Protein sidechains [\(i\)](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	281/275 (102%)	275 (98%)	6 (2%)	53 57
1	B	276/275 (100%)	270 (98%)	6 (2%)	52 55
1	C	272/275 (99%)	258 (95%)	14 (5%)	24 19
1	D	276/275 (100%)	272 (99%)	4 (1%)	67 72
All	All	1105/1100 (100%)	1075 (97%)	30 (3%)	44 46

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LEU
1	A	175	ASN
1	A	183	LYS
1	A	193	LEU
1	A	195	GLN
1	A	212	LEU
1	B	5	LEU
1	B	28	VAL
1	B	175	ASN
1	B	193	LEU
1	B	235	THR
1	B	247	LEU
1	C	3	LEU
1	C	54	LEU
1	C	59	ILE
1	C	108	GLU
1	C	119	LYS
1	C	137	LEU
1	C	143[A]	GLN
1	C	143[B]	GLN
1	C	169	LEU
1	C	175	ASN
1	C	183	LYS
1	C	193	LEU
1	C	214	GLU
1	C	265	LEU
1	D	142	ASN
1	D	175	ASN
1	D	183	LYS
1	D	193	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	155	ASN
1	A	191	GLN
1	A	195	GLN
1	A	278	ASN
1	B	271	HIS
1	B	296	ASN
1	C	111	ASN
1	C	148	GLN
1	C	191	GLN

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Mol	Chain	Res	Type
1	C	278	ASN
1	D	65	GLN
1	D	105	GLN
1	D	142	ASN
1	D	155	ASN
1	D	233	ASN
1	D	278	ASN

### 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 monosaccharides in this entry.

### 5.6 Ligand geometry [\(i\)](#)

Of 10 ligands modelled in this entry, 5 are monoatomic - leaving 5 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	ANP	D	1312	2	29,33,33	1.88	8 (27%)	31,52,52	1.85	5 (16%)
3	ANP	A	1312	2	29,33,33	1.95	9 (31%)	31,52,52	1.69	5 (16%)
3	ANP	C	1313	2	29,33,33	1.91	6 (20%)	31,52,52	1.69	5 (16%)
3	ANP	B	1312	2	29,33,33	1.94	9 (31%)	31,52,52	1.50	4 (12%)
4	TA6	C	1312	-	15,16,16	1.28	1 (6%)	17,25,25	0.96	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ANP	D	1312	2	-	2/14/38/38	0/3/3/3
3	ANP	A	1312	2	-	1/14/38/38	0/3/3/3
3	ANP	C	1313	2	-	2/14/38/38	0/3/3/3
3	ANP	B	1312	2	-	1/14/38/38	0/3/3/3
4	TA6	C	1312	-	-	1/9/28/28	0/1/1/1

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1313	ANP	PG-N3B	5.14	1.76	1.63
3	B	1312	ANP	PG-N3B	4.94	1.76	1.63
3	B	1312	ANP	PB-N3B	4.74	1.75	1.63
3	A	1312	ANP	PB-N3B	4.74	1.75	1.63
3	D	1312	ANP	PG-N3B	4.71	1.75	1.63
3	A	1312	ANP	PG-N3B	4.68	1.75	1.63
3	C	1313	ANP	PB-N3B	4.62	1.75	1.63
3	D	1312	ANP	PB-N3B	4.25	1.74	1.63
3	C	1313	ANP	PG-O1G	3.63	1.51	1.46
3	D	1312	ANP	PB-O3A	3.62	1.63	1.59
3	B	1312	ANP	PG-O1G	3.39	1.51	1.46
3	D	1312	ANP	PG-O1G	3.19	1.51	1.46
3	A	1312	ANP	PB-O1B	3.18	1.51	1.46
3	B	1312	ANP	PB-O1B	3.01	1.50	1.46
3	A	1312	ANP	PB-O3A	3.00	1.62	1.59
3	A	1312	ANP	PG-O1G	2.93	1.50	1.46
3	B	1312	ANP	C5-C4	2.83	1.48	1.40
3	C	1313	ANP	PB-O1B	2.68	1.50	1.46
3	A	1312	ANP	C5-C4	2.66	1.48	1.40
4	C	1312	TA6	O2-C2	2.61	1.45	1.40
3	C	1313	ANP	C5-C4	2.61	1.47	1.40
3	D	1312	ANP	PB-O1B	2.57	1.50	1.46
3	D	1312	ANP	C5-C4	2.46	1.47	1.40
3	B	1312	ANP	PB-O3A	2.32	1.62	1.59
3	A	1312	ANP	C2-N3	2.19	1.35	1.32
3	C	1313	ANP	PB-O3A	2.15	1.61	1.59
3	A	1312	ANP	O4'-C1'	2.15	1.44	1.41
3	A	1312	ANP	PG-O3G	-2.14	1.51	1.56
3	D	1312	ANP	PG-O2G	-2.11	1.51	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1312	ANP	C2-N3	2.08	1.35	1.32
3	B	1312	ANP	PG-O3G	-2.02	1.51	1.56
3	D	1312	ANP	C2-N3	2.01	1.35	1.32
3	B	1312	ANP	PG-O2G	-2.01	1.51	1.56

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1312	ANP	O1G-PG-N3B	-6.99	101.48	111.77
3	C	1313	ANP	O1G-PG-N3B	-5.94	103.03	111.77
3	A	1312	ANP	O1G-PG-N3B	-5.09	104.28	111.77
3	B	1312	ANP	O1G-PG-N3B	-4.74	104.80	111.77
3	D	1312	ANP	N3-C2-N1	-3.83	122.70	128.68
3	A	1312	ANP	N3-C2-N1	-3.60	123.05	128.68
3	A	1312	ANP	O2B-PB-O1B	3.51	117.28	109.92
3	A	1312	ANP	O1B-PB-N3B	-3.20	107.06	111.77
3	C	1313	ANP	O2B-PB-O1B	3.17	116.57	109.92
3	C	1313	ANP	C4-C5-N7	-3.16	106.11	109.40
3	B	1312	ANP	N3-C2-N1	-3.10	123.83	128.68
3	C	1313	ANP	N3-C2-N1	-2.95	124.06	128.68
3	B	1312	ANP	O2B-PB-O1B	2.90	115.99	109.92
3	C	1313	ANP	O1B-PB-N3B	-2.49	108.10	111.77
3	D	1312	ANP	C4-C5-N7	-2.48	106.81	109.40
3	D	1312	ANP	O2B-PB-O1B	2.48	115.12	109.92
3	D	1312	ANP	C2-N1-C6	2.34	122.75	118.75
3	B	1312	ANP	C4-C5-N7	-2.26	107.04	109.40
3	A	1312	ANP	C4-C5-N7	-2.07	107.25	109.40

There are no chirality outliers.

All (7) torsion outliers are listed below:

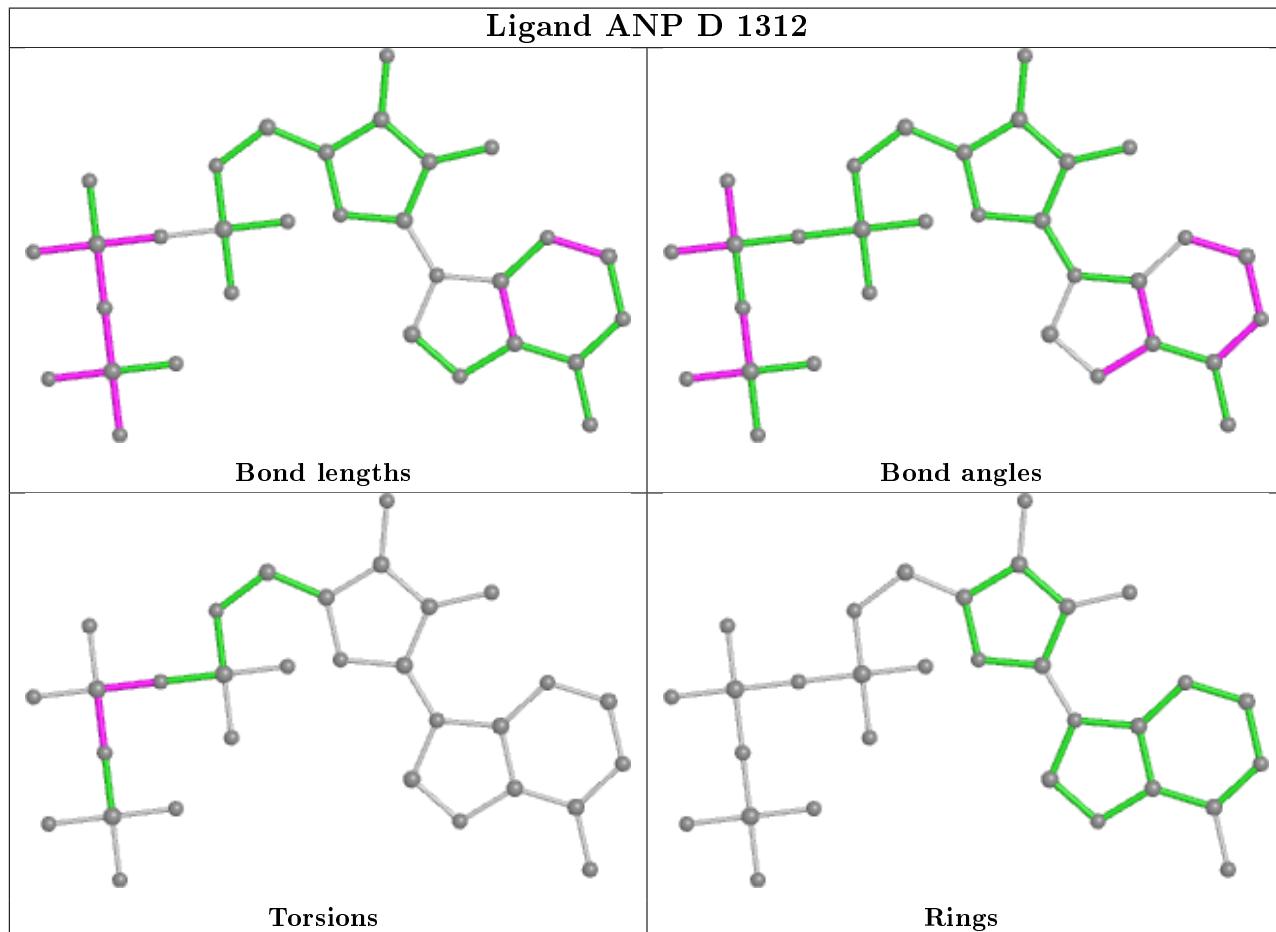
Mol	Chain	Res	Type	Atoms
3	C	1313	ANP	PB-N3B-PG-O1G
3	C	1313	ANP	PG-N3B-PB-O1B
3	B	1312	ANP	PG-N3B-PB-O1B
3	D	1312	ANP	PG-N3B-PB-O1B
3	A	1312	ANP	PG-N3B-PB-O1B
3	D	1312	ANP	PA-O3A-PB-O2B
4	C	1312	TA6	O1-C1-C2-C3

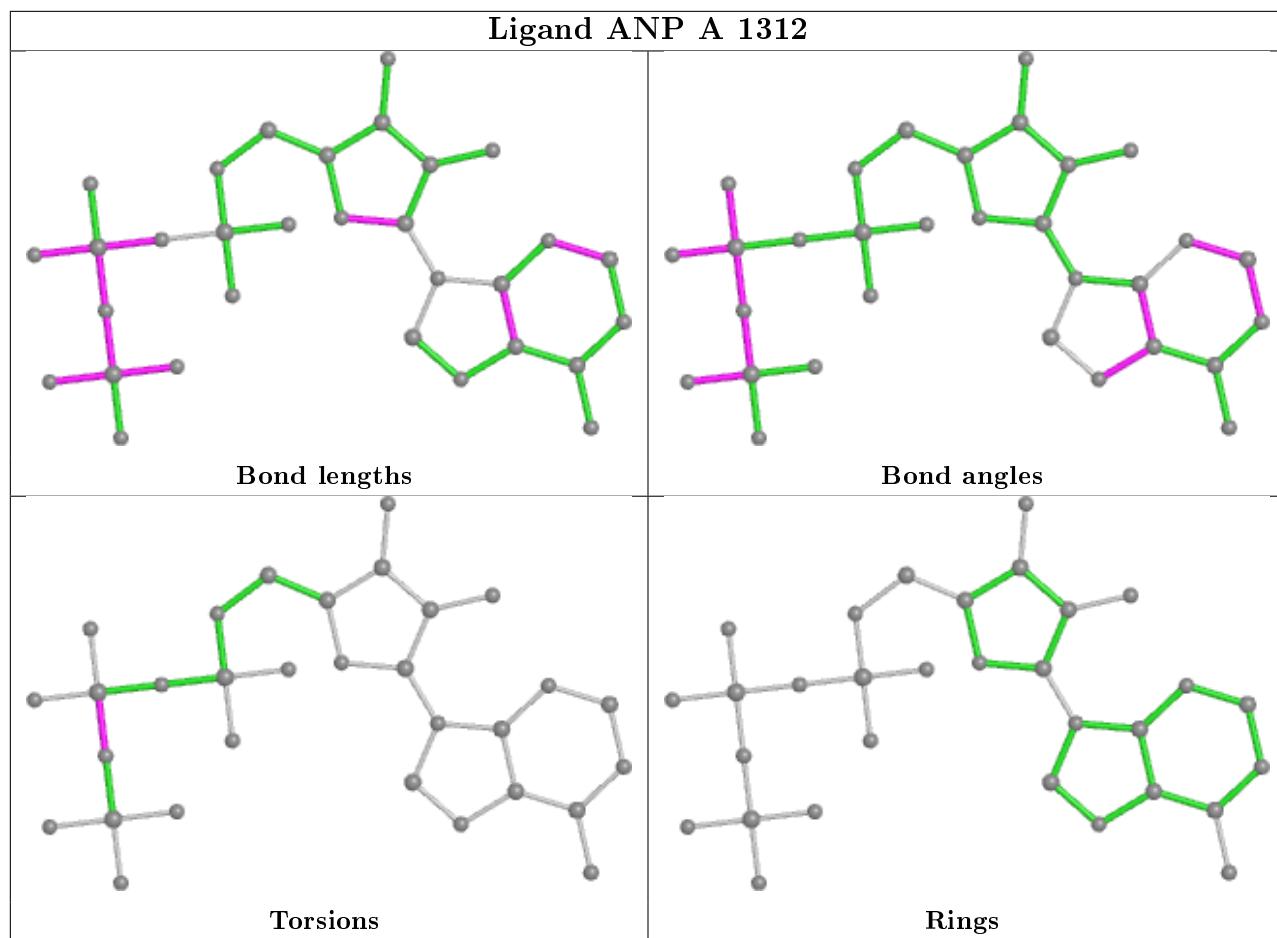
There are no ring outliers.

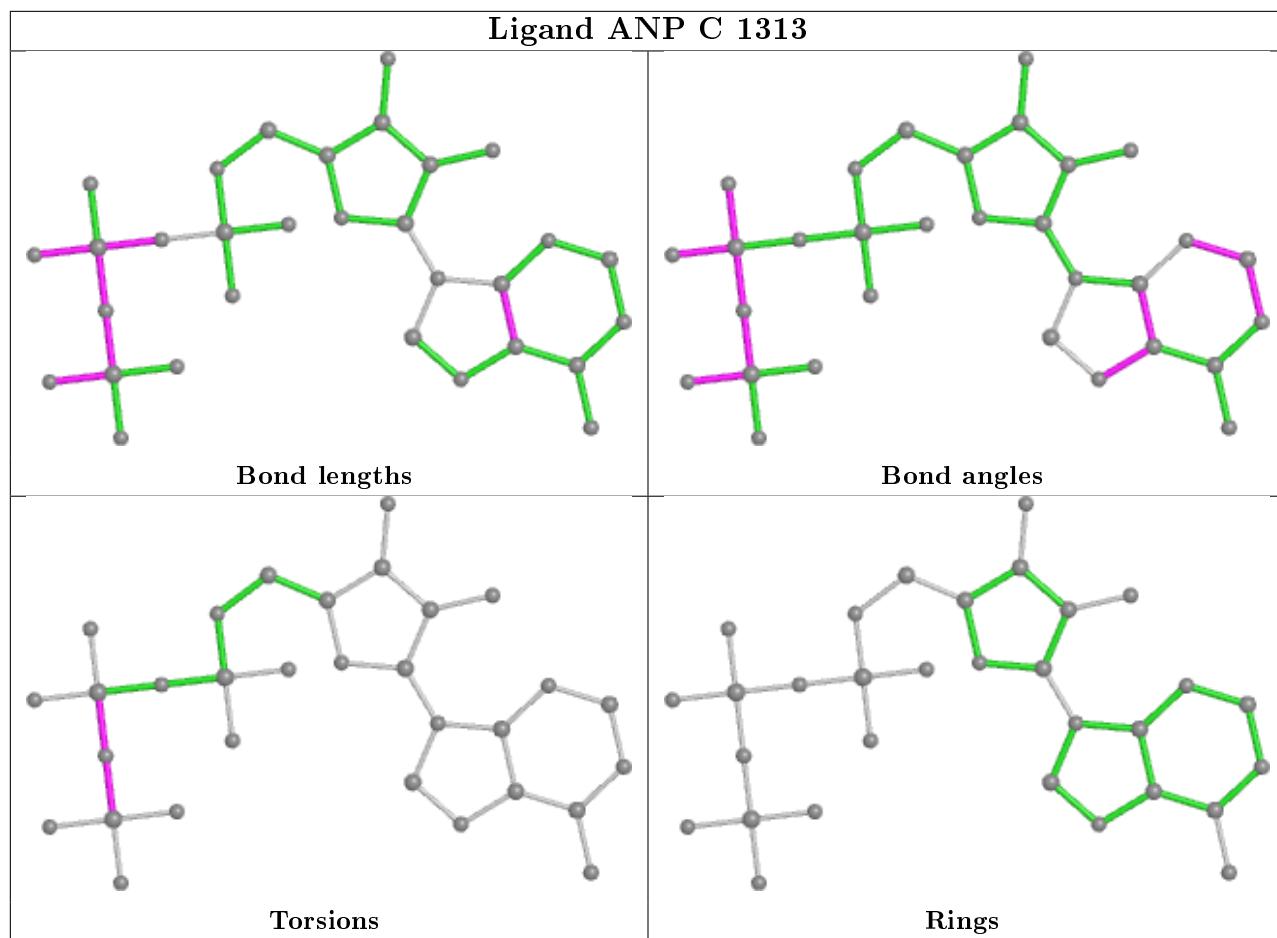
3 monomers are involved in 5 short contacts:

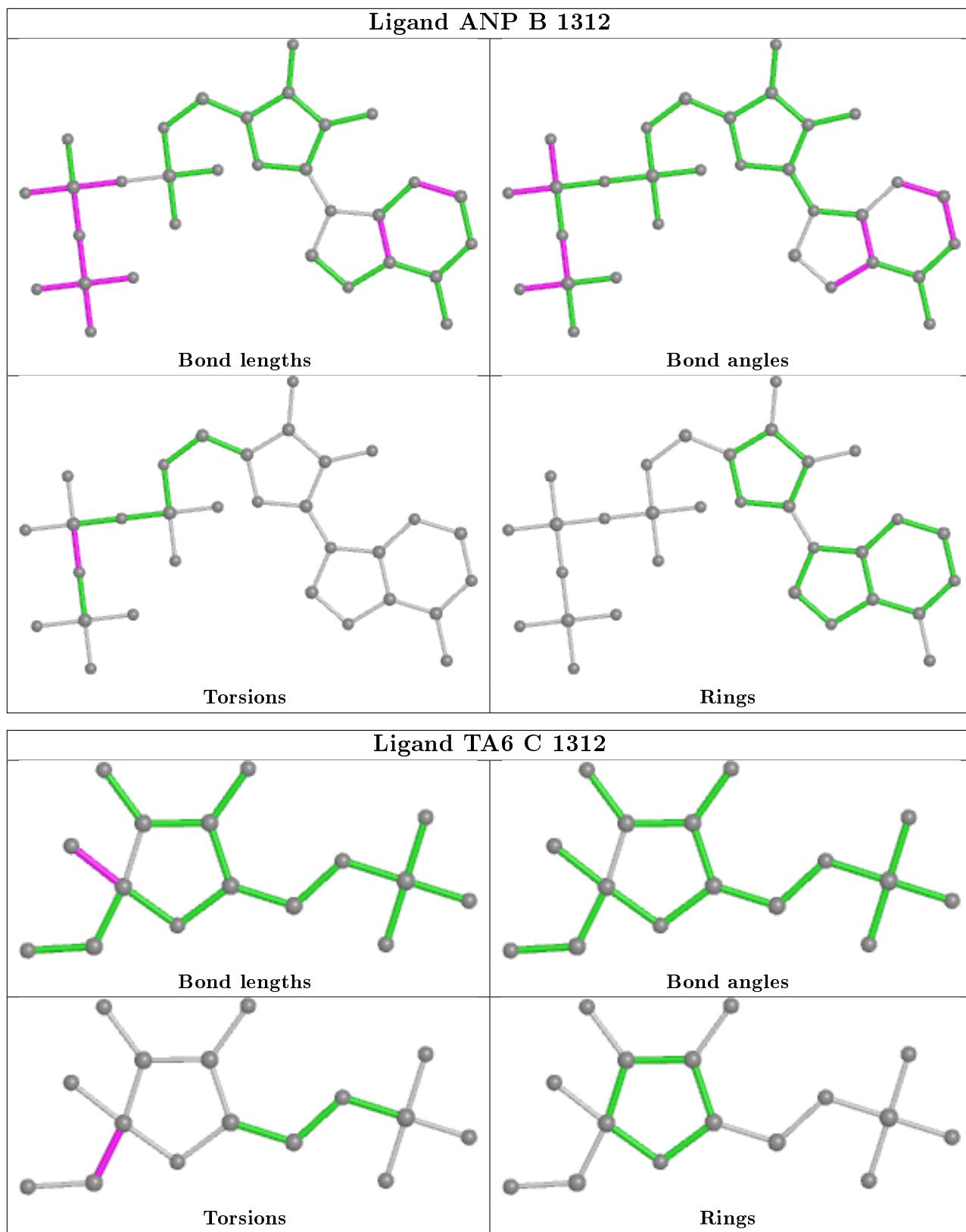
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1312	ANP	1	0
3	C	1313	ANP	2	0
3	B	1312	ANP	2	0

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 (i)

### 6.1 Protein, DNA and RNA chains (i)

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	314/330 (95%)	0.14	10 (3%) 47 46	14, 27, 51, 66	10 (3%)
1	B	314/330 (95%)	0.31	21 (6%) 17 17	16, 28, 55, 70	7 (2%)
1	C	311/330 (94%)	0.19	12 (3%) 39 38	15, 30, 49, 63	6 (1%)
1	D	309/330 (93%)	0.01	7 (2%) 60 59	16, 26, 41, 47	16 (5%)
All	All	1248/1320 (94%)	0.16	50 (4%) 38 37	14, 28, 50, 70	39 (3%)

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	-7	GLY	6.1
1	B	246	VAL	5.9
1	B	247	LEU	5.0
1	B	194	ASN	4.5
1	B	206	GLN	4.0
1	C	196	PRO	4.0
1	C	194	ASN	3.7
1	B	308	LEU	3.6
1	D	-2	GLY	3.5
1	C	127	LYS	3.3
1	B	202	GLU	3.2
1	B	245	SER	3.0
1	C	-3	ARG	2.9
1	C	197	LEU	2.9
1	B	230	ALA	2.7
1	B	201	LEU	2.7
1	B	-5	VAL	2.7
1	C	191	GLN	2.7
1	A	243	THR	2.7
1	B	211	PRO	2.7
1	B	234	HIS	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	202	GLU	2.6
1	D	194[A]	ASN	2.6
1	C	308	LEU	2.6
1	D	131	VAL	2.5
1	C	177	TYR	2.5
1	A	133	ILE	2.5
1	A	220	ILE	2.5
1	B	220	ILE	2.4
1	B	288	ALA	2.4
1	B	250	VAL	2.4
1	B	133	ILE	2.4
1	B	29	GLN	2.4
1	B	196	PRO	2.3
1	B	131	VAL	2.3
1	C	257	VAL	2.3
1	D	247	LEU	2.2
1	C	195	GLN	2.2
1	A	-6	LEU	2.2
1	A	257	VAL	2.2
1	A	196	PRO	2.2
1	A	-5	VAL	2.1
1	C	202	GLU	2.1
1	D	133	ILE	2.1
1	A	126	GLU	2.0
1	C	303	ASN	2.0
1	D	260	ILE	2.0
1	D	196	PRO	2.0
1	B	181	VAL	2.0
1	B	203	SER	2.0

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

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

## 6.3 Carbohydrates [\(i\)](#)

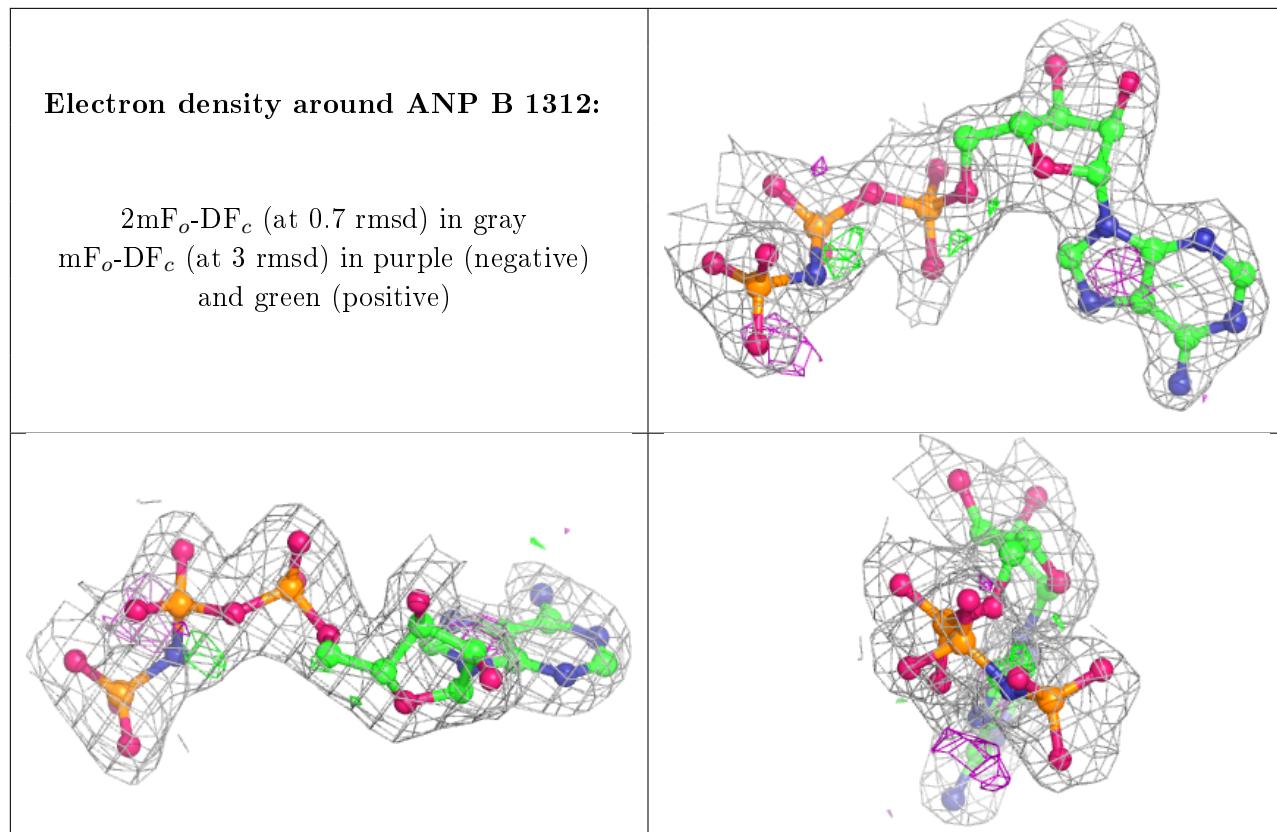
There are no monosaccharides in this entry.

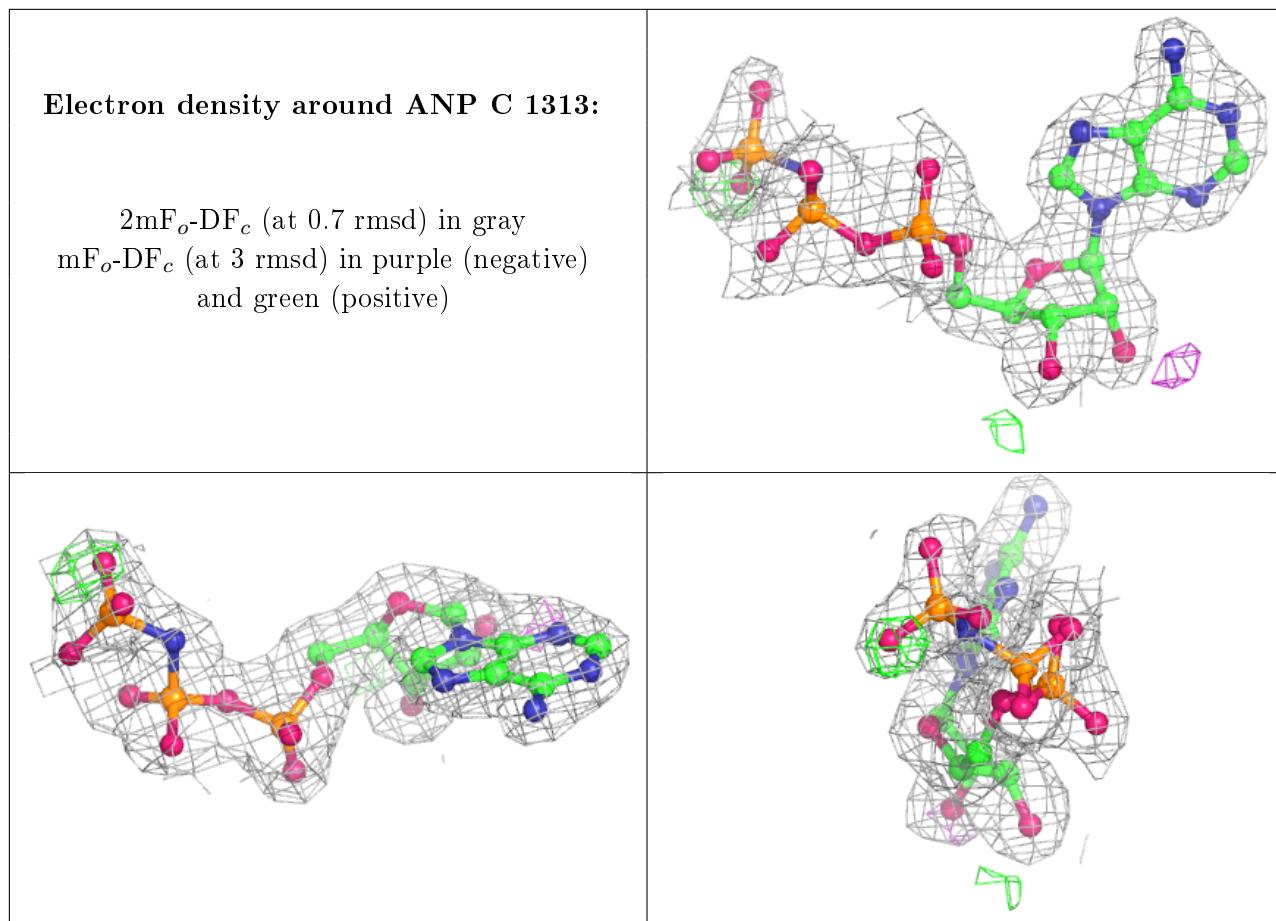
## 6.4 Ligands [\(i\)](#)

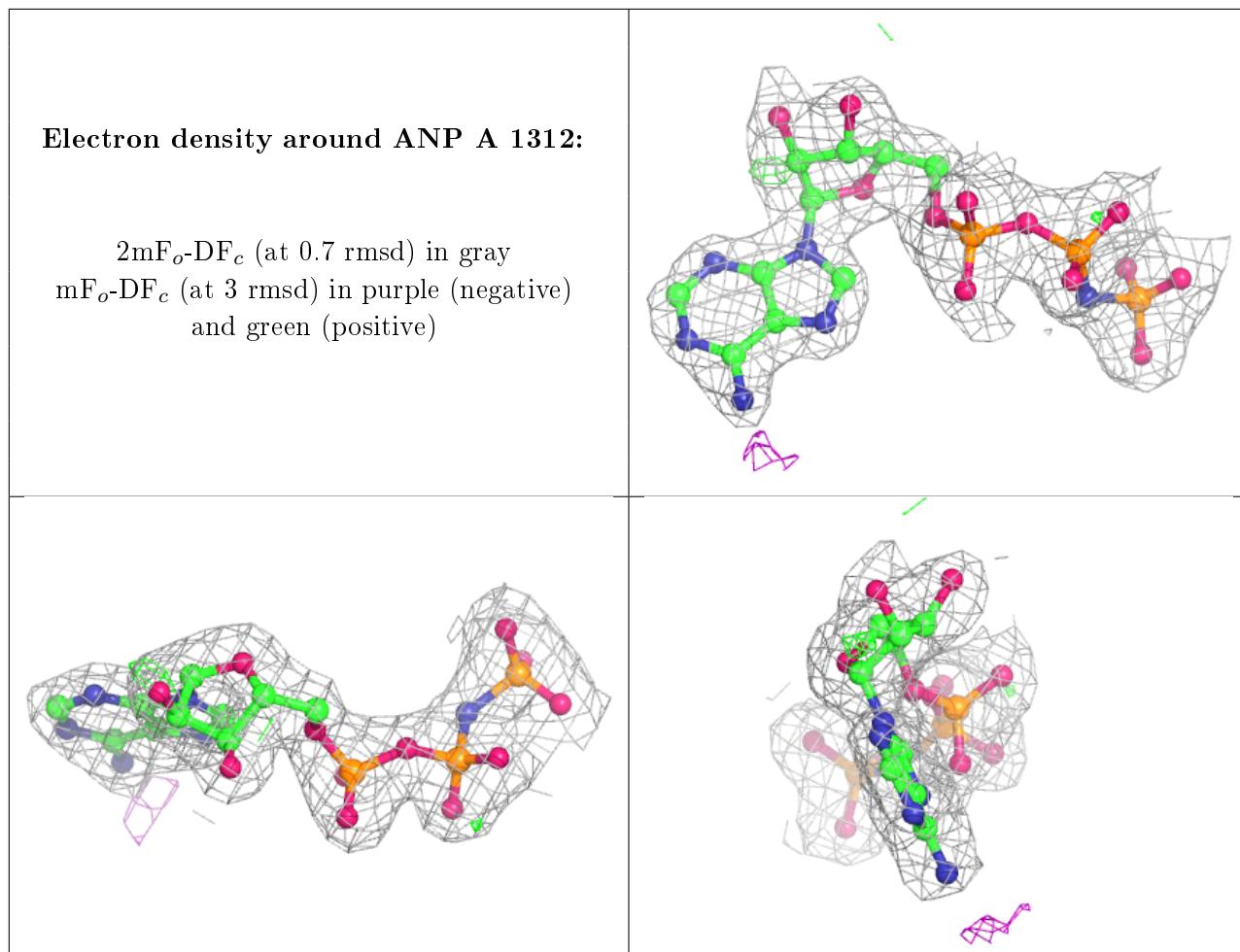
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q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

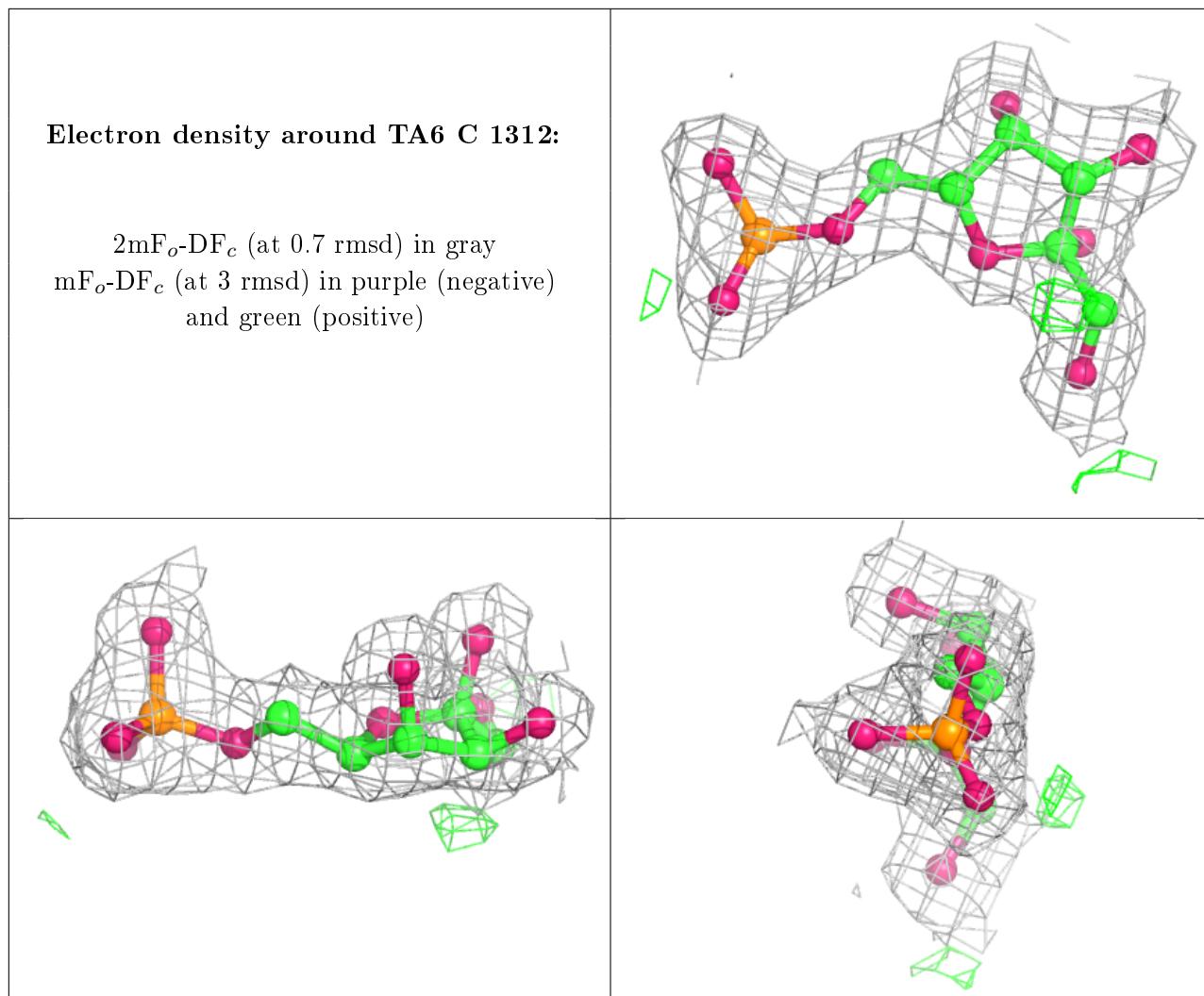
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	MG	B	1311	1/1	0.92	0.07	34,34,34,34	0
3	ANP	B	1312	31/31	0.92	0.14	34,41,47,48	0
3	ANP	C	1313	31/31	0.95	0.12	27,28,30,32	4
3	ANP	A	1312	31/31	0.96	0.11	28,33,38,38	0
2	MG	D	1311	1/1	0.97	0.04	26,26,26,26	0
2	MG	A	1311	1/1	0.97	0.04	27,27,27,27	0
4	TA6	C	1312	16/16	0.97	0.08	24,26,28,29	0
3	ANP	D	1312	31/31	0.97	0.08	19,22,24,26	0
2	MG	C	1310	1/1	0.97	0.07	37,37,37,37	0
2	MG	C	1311	1/1	0.98	0.05	42,42,42,42	0

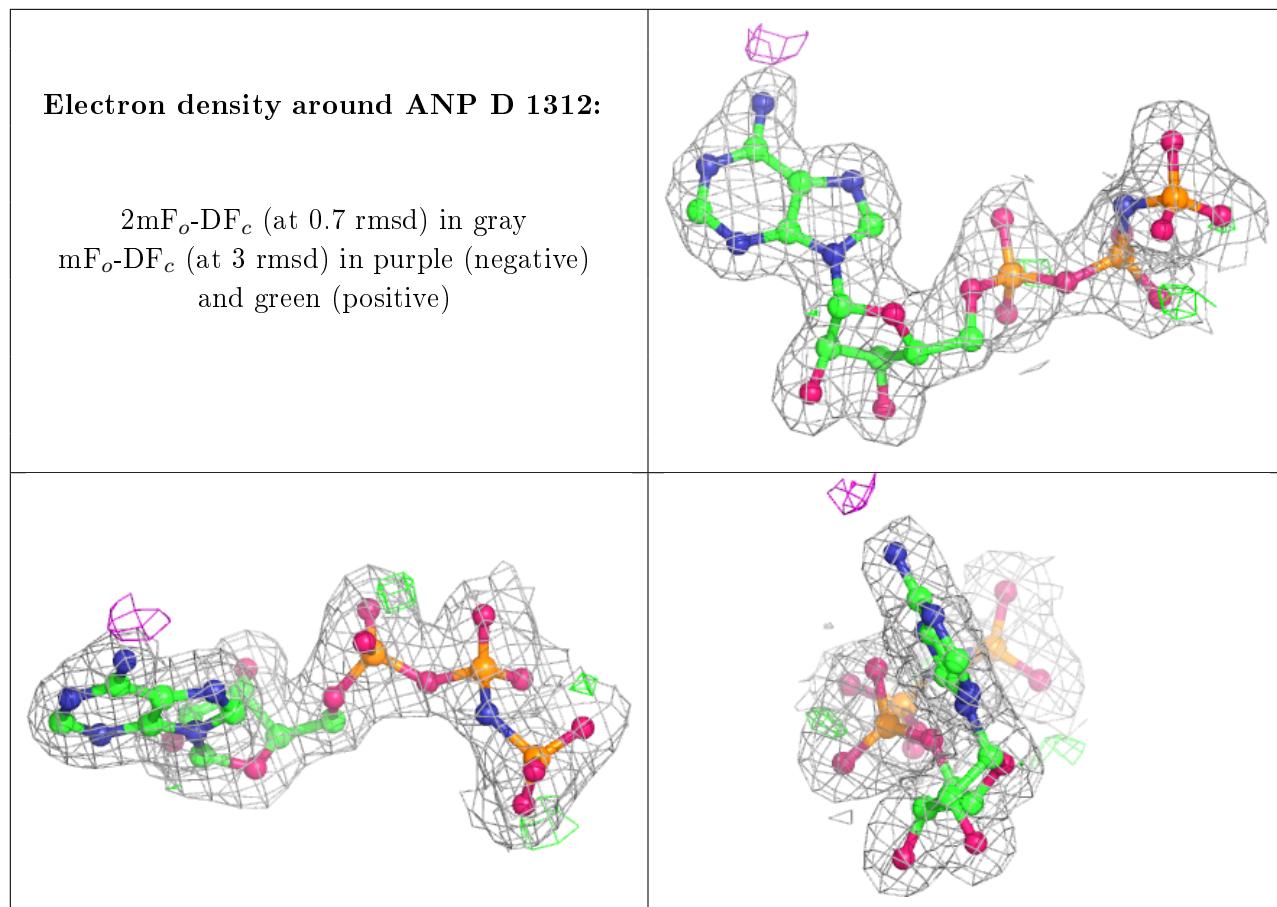
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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











## 6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.