



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:40 AM UTC

PDB ID : 2VAR / pdb\_00002var  
Title : Crystal structure of Sulfolobus solfataricus 2-keto-3-deoxygluconate kinase complexed with 2-keto-3-deoxygluconate  
Authors : Potter, J.A.; Theodossis, A.; Kerou, M.; Lamble, H.J.; Bull, S.D.; Hough, D.W.; Danson, M.J.; Taylor, G.L.  
Deposited on : 2007-09-04  
Resolution : 2.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

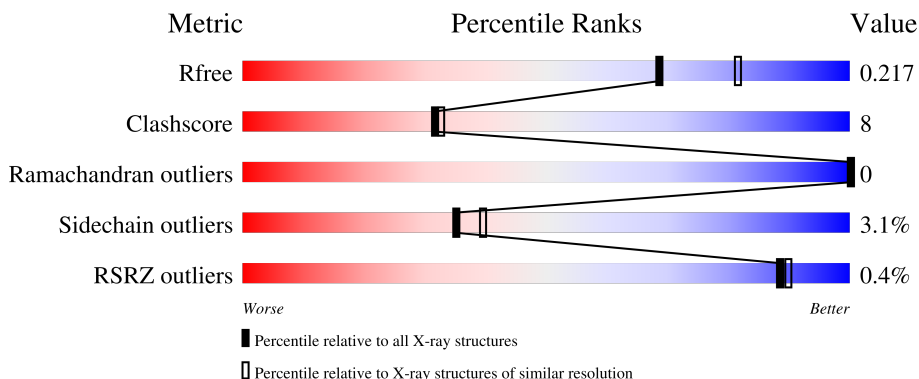
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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))
$R_{free}$	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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

Mol	Chain	Length	Quality of chain
1	A	313	83% 15% ..
1	B	313	84% 15% ..
1	C	313	85% 13% ..

## 2 Entry composition [i](#)

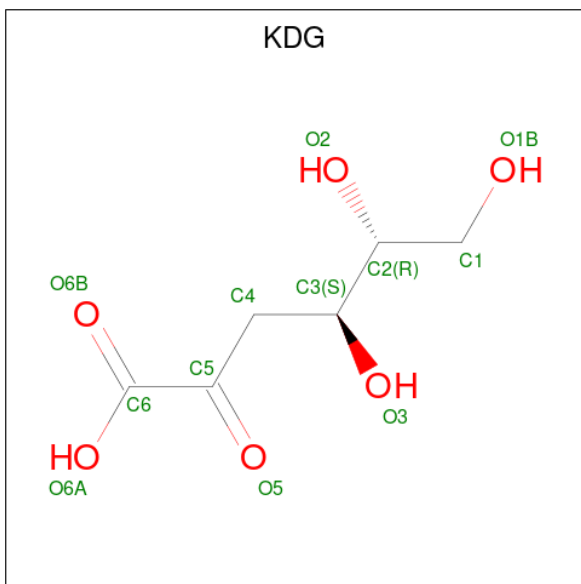
There are 6 unique types of molecules in this entry. The entry contains 8064 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 FRUCTOKINASE.

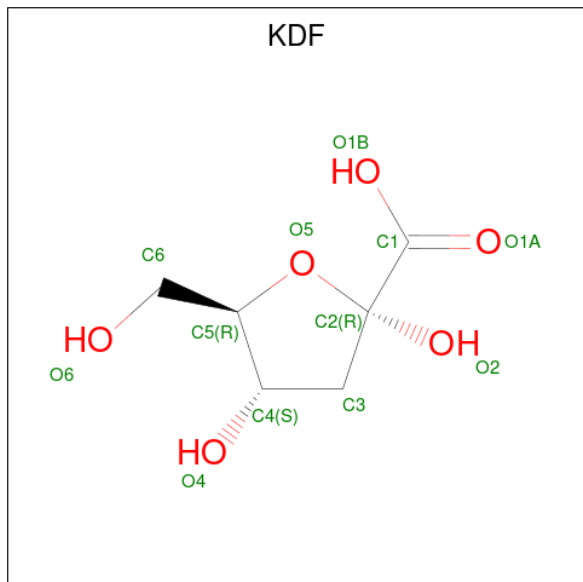
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	311	Total 2472	C 1578	N 411	O 479	S 4	0	28	0
1	B	311	Total 2456	C 1569	N 409	O 474	S 4	0	31	0
1	C	311	Total 2445	C 1562	N 409	O 470	S 4	0	38	0

- Molecule 2 is 2-KETO-3-DEOXYGLUCONATE (CCD ID: KDG) (formula: C<sub>6</sub>H<sub>10</sub>O<sub>6</sub>).



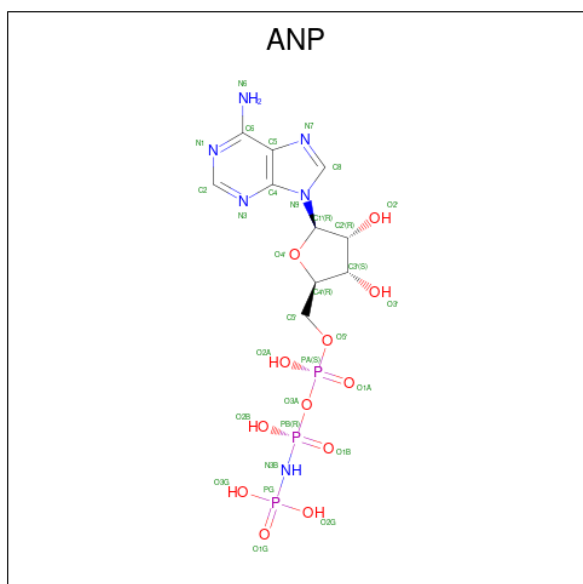
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	Total 12	C 6	O 6	0	0
2	B	1	Total 12	C 6	O 6	0	0
2	C	1	Total 12	C 6	O 6	0	0

- Molecule 3 is 3-deoxy- $\alpha$ -D-erythro-hex-2-ulofuranosonic acid (CCD ID: KDF) (formula:  $C_6H_{10}O_6$ ).



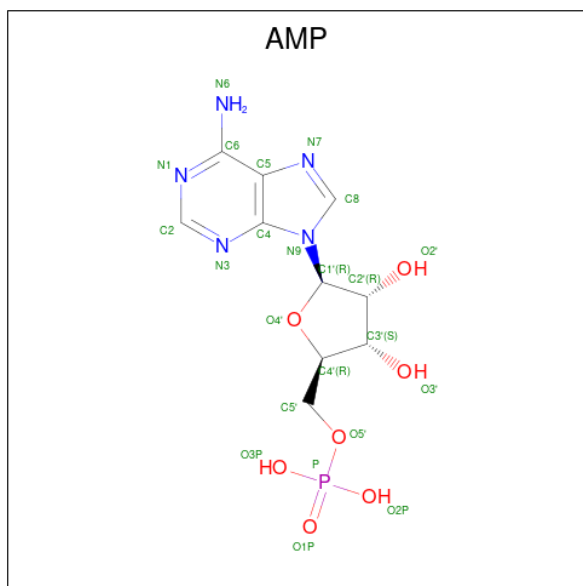
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			12	6	6		
3	B	1	Total	C	O	0	0
			12	6	6		
3	C	1	Total	C	O	0	0
			12	6	6		

- Molecule 4 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula:  $C_{10}H_{17}N_6O_{12}P_3$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
4	A	1	Total 31	C 10	N 6	O 12	P 3	0	0
4	B	1	Total 31	C 10	N 6	O 12	P 3	0	0
4	C	1	Total 31	C 10	N 6	O 12	P 3	0	0

- Molecule 5 is ADENOSINE MONOPHOSPHATE (CCD ID: AMP) (formula: C<sub>10</sub>H<sub>14</sub>N<sub>5</sub>O<sub>7</sub>P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
5	A	1	Total 23	C 10	N 5	O 7	P 1	0	0
5	B	1	Total 23	C 10	N 5	O 7	P 1	0	0
5	C	1	Total 23	C 10	N 5	O 7	P 1	0	0

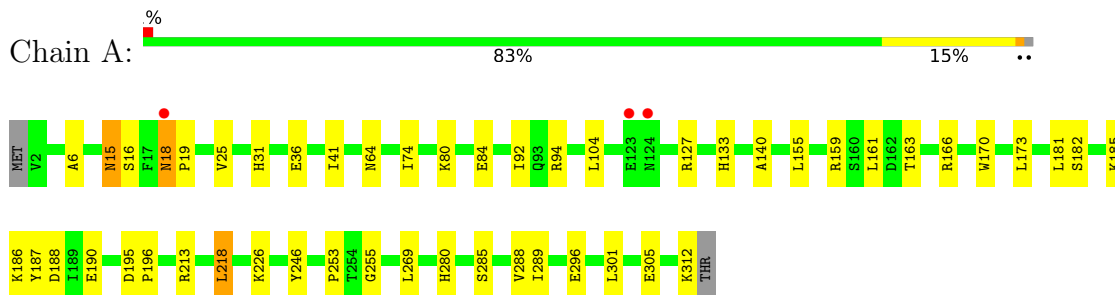
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	139	Total 139	O 139	0	0
6	B	164	Total 164	O 164	0	0
6	C	154	Total 154	O 154	0	0

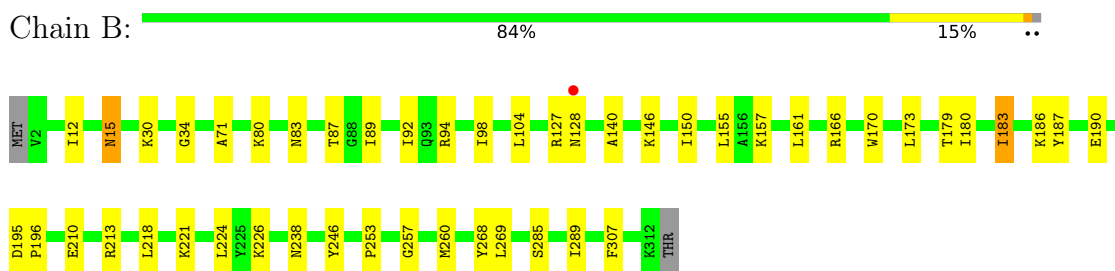
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

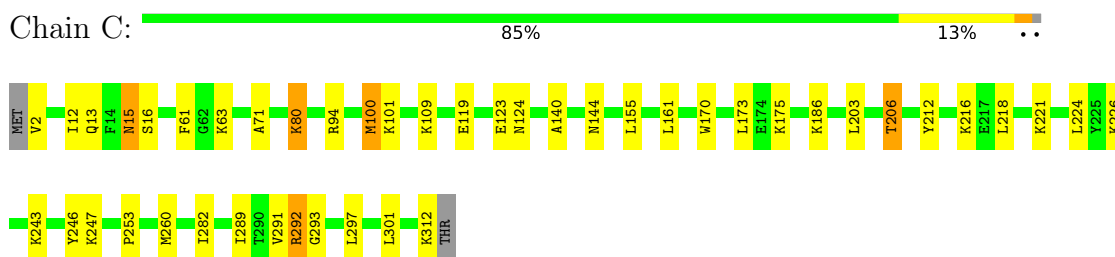
- Molecule 1: FRUCTOKINASE



- Molecule 1: FRUCTOKINASE



- Molecule 1: FRUCTOKINASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	104.55Å 104.55Å 420.78Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	61.66 – 2.10 61.66 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.6 (61.66-2.10) 99.6 (61.66-2.10)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.04 (at 2.10Å)	Xtrriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.181 , 0.218 (Not available) , 0.217	Depositor DCC
$R_{free}$ test set	4008 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	25.0	Xtrriage
Anisotropy	0.072	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 43.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	8064	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.68% 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: AMP, KDG, ANP, KDF

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	1.02	1/2524 (0.0%)	1.02	1/3414 (0.0%)
1	B	0.99	1/2511 (0.0%)	0.97	2/3397 (0.1%)
1	C	0.97	1/2491 (0.0%)	1.01	3/3370 (0.1%)
All	All	1.00	3/7526 (0.0%)	1.00	6/10181 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	15	ASN	CB-CG	-5.30	1.38	1.52
1	B	98	ILE	CA-CB	5.18	1.58	1.54
1	A	64	ASN	CA-C	5.11	1.59	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	292	ARG	N-CA-C	7.96	120.66	111.11
1	C	15	ASN	CB-CA-C	-7.69	96.84	109.53
1	A	288	VAL	N-CA-C	7.62	118.39	110.62
1	C	186[A]	LYS	N-CA-C	5.57	117.43	111.36
1	B	87	THR	CA-C-N	5.28	125.11	120.10
1	B	87	THR	C-N-CA	5.28	125.11	120.10

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	2472	0	2393	43	0
1	B	2456	0	2371	38	0
1	C	2445	0	2320	39	0
2	A	12	0	5	3	0
2	B	12	0	4	1	0
2	C	12	0	5	0	0
3	A	12	0	0	0	0
3	B	12	0	0	0	0
3	C	12	0	1	0	0
4	A	31	0	8	3	0
4	B	31	0	10	4	0
4	C	31	0	9	2	0
5	A	23	0	5	1	0
5	B	23	0	9	1	0
5	C	23	0	5	1	0
6	A	139	0	0	19	0
6	B	164	0	0	10	0
6	C	154	0	0	26	0
All	All	8064	0	7145	122	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 8.

All (122) 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:94:ARG:NH1	6:A:2042:HOH:O	1.60	1.31
1:C:63[A]:LYS:HE2	6:C:2029:HOH:O	1.32	1.29
1:B:80[A]:LYS:HD2	6:B:2070:HOH:O	1.28	1.27
1:C:15:ASN:HB3	6:C:2004:HOH:O	1.37	1.23
1:B:238[A]:ASN:HB3	6:B:2126:HOH:O	1.62	0.99
1:B:257:GLY:H	4:B:1315:ANP:HNB1	1.08	0.95
1:A:16:SER:HB3	6:A:2004:HOH:O	0.78	0.94
1:B:166[A]:ARG:CZ	6:B:2096:HOH:O	2.16	0.92
1:A:15:ASN:HD21	1:A:94:ARG:HD3	1.36	0.91
1:C:15:ASN:CB	6:C:2004:HOH:O	2.06	0.89
1:C:15:ASN:ND2	6:C:2004:HOH:O	1.93	0.89
1:C:144[A]:ASN:HB3	6:C:2081:HOH:O	1.73	0.88
1:C:94:ARG:HG3	6:C:2043:HOH:O	1.73	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:206[A]:THR:HG23	6:C:2103:HOH:O	1.74	0.86
1:A:166[A]:ARG:CZ	6:A:2080:HOH:O	2.22	0.86
1:A:213:ARG:HD3	6:A:2106:HOH:O	1.80	0.80
1:B:257:GLY:N	4:B:1315:ANP:HNB1	1.80	0.79
1:A:133:HIS:HD2	6:A:2067:HOH:O	1.66	0.78
1:C:312:LYS:HE2	6:C:2149:HOH:O	1.84	0.77
1:B:221:LYS:HD3	6:B:2035:HOH:O	1.85	0.76
1:A:133:HIS:CD2	6:A:2067:HOH:O	2.39	0.74
1:B:166[A]:ARG:NE	6:B:2096:HOH:O	2.20	0.73
1:A:190[A]:GLU:OE2	6:A:2096:HOH:O	2.08	0.72
1:C:13:GLN:NE2	1:C:15:ASN:OD1	2.22	0.72
1:B:246:TYR:O	4:B:1315:ANP:H2	1.90	0.72
1:B:183:ILE:HB	6:B:2104:HOH:O	1.89	0.71
1:B:190:GLU:HG3	1:B:221:LYS:HE2	1.72	0.71
1:B:238[A]:ASN:OD1	6:B:2125:HOH:O	2.10	0.70
1:C:63[A]:LYS:CE	6:C:2029:HOH:O	2.06	0.69
1:A:226:LYS:HB3	4:A:1315:ANP:O1A	1.94	0.68
1:A:94:ARG:CZ	6:A:2042:HOH:O	2.20	0.67
1:C:175[A]:LYS:HE2	6:C:2032:HOH:O	1.96	0.64
1:B:238[A]:ASN:ND2	6:B:2124:HOH:O	2.30	0.64
1:A:246:TYR:O	4:A:1315:ANP:H2	1.99	0.63
1:C:119[A]:GLU:HB2	6:C:2067:HOH:O	2.00	0.62
1:A:6:ALA:HB1	6:A:2067:HOH:O	2.00	0.61
1:A:185:LYS:HD2	6:A:2092:HOH:O	2.01	0.60
1:B:210[A]:GLU:OE2	1:B:213:ARG:NH2	2.35	0.60
1:C:253:PRO:HA	1:C:289:ILE:HG22	1.84	0.59
1:B:226:LYS:HB3	5:B:1316:AMP:O2P	2.02	0.59
1:C:293:GLY:N	6:C:2139:HOH:O	1.90	0.59
1:B:238[A]:ASN:CG	6:B:2125:HOH:O	2.45	0.59
1:B:180:ILE:HA	6:B:2104:HOH:O	2.02	0.59
1:B:15:ASN:HD21	1:B:94:ARG:HD3	1.68	0.58
1:A:218:LEU:O	6:A:2107:HOH:O	2.17	0.57
1:B:221:LYS:HE3	1:B:268:TYR:OH	2.05	0.56
1:A:84:GLU:HG3	6:A:2037:HOH:O	2.05	0.56
1:B:71:ALA:HB2	1:C:71:ALA:HB2	1.87	0.56
1:B:186:LYS:HD2	1:B:187:TYR:CE1	2.40	0.56
1:C:206[A]:THR:CG2	6:C:2103:HOH:O	2.40	0.55
1:A:186:LYS:HD2	1:A:187:TYR:CE1	2.43	0.54
1:A:25:VAL:O	1:B:30:LYS:HE2	2.09	0.53
1:B:195:ASP:HB2	1:B:196:PRO:HD2	1.90	0.53
1:C:221[A]:LYS:HD3	6:C:2110:HOH:O	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:ASN:HB3	6:C:2059:HOH:O	2.10	0.51
1:C:291:VAL:HG21	1:C:297:LEU:HD13	1.92	0.51
1:C:224:LEU:HD21	1:C:260:MET:HG2	1.93	0.51
1:A:15:ASN:HD21	1:A:94:ARG:CD	2.17	0.51
1:B:92:ILE:HG12	1:B:104:LEU:HD22	1.93	0.50
1:C:301:LEU:C	1:C:301:LEU:HD23	2.36	0.50
1:C:123[A]:GLU:HG3	6:C:2085:HOH:O	2.11	0.50
1:A:159:ARG:HD2	1:A:188:ASP:O	2.11	0.49
1:A:312:LYS:HA	6:A:2135:HOH:O	2.11	0.49
1:A:36[A]:GLU:HG2	6:A:2067:HOH:O	2.13	0.49
1:C:12:ILE:HG13	1:C:61:PHE:HB3	1.95	0.49
1:C:109[A]:LYS:HG3	6:C:2016:HOH:O	2.11	0.49
1:B:34:GLY:HA2	2:B:1313:KDG:O5	2.12	0.49
1:C:243:LYS:HG2	1:C:282:ILE:HG13	1.94	0.49
1:C:80[A]:LYS:HE2	6:C:2037:HOH:O	2.13	0.48
1:A:80:LYS:HG3	6:A:2032:HOH:O	2.12	0.48
1:B:140:ALA:HB2	1:B:170:TRP:CE2	2.48	0.48
1:B:146:LYS:HD2	1:B:179:THR:HG23	1.96	0.48
1:A:285:SER:HB3	5:A:1316:AMP:O4'	2.13	0.48
1:B:285:SER:O	1:B:289:ILE:HG23	2.14	0.48
1:C:221[A]:LYS:HE3	6:C:2112:HOH:O	2.14	0.47
1:C:124[A]:ASN:HB2	6:C:2071:HOH:O	2.14	0.47
1:A:186:LYS:HD2	1:A:187:TYR:CZ	2.50	0.46
1:C:246:TYR:O	4:C:1315:ANP:H2	2.15	0.46
1:C:260:MET:HE1	5:C:1316:AMP:O3'	2.15	0.46
1:B:150:ILE:HG12	1:B:183:ILE:HD11	1.96	0.46
1:A:127[A]:ARG:HD2	6:A:2061:HOH:O	2.15	0.46
1:A:226:LYS:CB	4:A:1315:ANP:O1A	2.64	0.46
1:C:16:SER:HB2	6:C:2043:HOH:O	2.15	0.46
1:B:257:GLY:CA	4:B:1315:ANP:HNB1	2.30	0.45
1:B:253:PRO:HA	1:B:289:ILE:HG22	1.98	0.45
1:C:100:MET:HE2	1:C:100:MET:HB2	1.87	0.45
1:A:181:LEU:O	1:A:185:LYS:HG3	2.18	0.44
1:A:253:PRO:HA	1:A:289:ILE:HG22	1.99	0.44
1:A:312:LYS:HD3	6:A:2135:HOH:O	2.17	0.44
1:A:92:ILE:HG12	1:A:104:LEU:HD22	1.99	0.44
1:B:224:LEU:HD21	1:B:260:MET:HG2	1.98	0.44
1:A:255:GLY:HA2	2:A:1313:KDG:H1C1	1.99	0.43
1:C:226:LYS:HE3	1:C:226:LYS:HB2	1.86	0.43
1:A:166[A]:ARG:NH2	2:A:1313:KDG:O1B	2.51	0.43
1:B:127:ARG:O	1:B:157:LYS:HE3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:307:PHE:CD1	1:B:307:PHE:C	2.97	0.43
1:A:41:ILE:HD13	1:A:74:ILE:HD11	1.99	0.43
1:A:140:ALA:HB2	1:A:170:TRP:CE2	2.53	0.43
1:B:12:ILE:HB	1:B:89:ILE:HG22	2.00	0.43
1:A:18:ASN:HB2	1:A:19:PRO:CD	2.50	0.42
1:B:221:LYS:HE3	1:B:268:TYR:HH	1.83	0.42
1:B:140:ALA:HB2	1:B:170:TRP:CZ2	2.54	0.42
1:C:226:LYS:NZ	4:C:1315:ANP:O1B	2.47	0.42
1:A:16:SER:HB2	1:A:25:VAL:HG11	2.02	0.42
1:A:255:GLY:N	2:A:1313:KDG:H1C1	2.35	0.42
1:C:140:ALA:HB2	1:C:170:TRP:CE2	2.55	0.42
1:C:221[A]:LYS:CD	6:C:2110:HOH:O	2.66	0.42
1:A:31:HIS:ND1	1:A:296[A]:GLU:OE1	2.44	0.41
1:C:212:TYR:CZ	1:C:216:LYS:HD3	2.55	0.41
1:A:195:ASP:HB2	1:A:196:PRO:HD2	2.02	0.41
1:A:280:HIS:CE1	1:A:305[A]:GLU:HG2	2.56	0.41
1:C:292:ARG:CA	6:C:2139:HOH:O	2.69	0.40
1:C:63[A]:LYS:NZ	6:C:2029:HOH:O	2.36	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	313/313 (100%)	306 (98%)	7 (2%)	0	100	100
1	B	312/313 (100%)	304 (97%)	8 (3%)	0	100	100
1	C	309/313 (99%)	302 (98%)	7 (2%)	0	100	100
All	All	934/939 (100%)	912 (98%)	22 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	271/269 (101%)	263 (97%)	8 (3%)	36	41
1	B	270/269 (100%)	263 (97%)	7 (3%)	40	46
1	C	267/269 (99%)	257 (96%)	10 (4%)	30	33
All	All	808/807 (100%)	783 (97%)	25 (3%)	35	39

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	ASN
1	A	18	ASN
1	A	161	LEU
1	A	173	LEU
1	A	182	SER
1	A	218	LEU
1	A	269	LEU
1	A	301	LEU
1	B	15	ASN
1	B	83[A]	ASN
1	B	161	LEU
1	B	173	LEU
1	B	183	ILE
1	B	218	LEU
1	B	269	LEU
1	C	2	VAL
1	C	80[A]	LYS
1	C	100	MET
1	C	101	LYS
1	C	155	LEU
1	C	161	LEU
1	C	173	LEU
1	C	206[A]	THR
1	C	218	LEU
1	C	247[A]	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	GLN
1	A	15	ASN
1	A	58	ASN
1	A	122	ASN
1	B	13	GLN
1	B	15	ASN
1	B	83[A]	ASN
1	C	46	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 oligosaccharides in this entry.

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

12 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	KDF	C	1314	-	12,12,12	1.35	2 (16%)	10,18,18	1.57	1 (10%)
3	KDF	A	1314	-	12,12,12	1.71	1 (8%)	10,18,18	2.14	2 (20%)
2	KDG	A	1313	-	11,11,11	1.17	1 (9%)	13,14,14	1.30	1 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	ANP	B	1315	-	33,33,33	2.67	11 (33%)	45,52,52	2.99	12 (26%)
3	KDF	B	1314	-	12,12,12	1.46	2 (16%)	10,18,18	2.05	2 (20%)
5	AMP	A	1316	-	25,25,25	1.51	3 (12%)	37,38,38	1.98	11 (29%)
4	ANP	A	1315	-	33,33,33	2.75	8 (24%)	45,52,52	2.34	16 (35%)
5	AMP	B	1316	-	25,25,25	1.51	4 (16%)	37,38,38	1.84	10 (27%)
5	AMP	C	1316	-	25,25,25	1.51	4 (16%)	37,38,38	1.95	8 (21%)
4	ANP	C	1315	-	33,33,33	3.38	8 (24%)	45,52,52	2.06	13 (28%)
2	KDG	B	1313	-	11,11,11	1.03	1 (9%)	13,14,14	1.82	3 (23%)
2	KDG	C	1313	-	11,11,11	1.19	1 (9%)	13,14,14	1.46	2 (15%)

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	KDF	C	1314	-	-	0/8/22/22	0/1/1/1
3	KDF	A	1314	-	-	0/8/22/22	0/1/1/1
2	KDG	A	1313	-	-	6/14/14/14	-
4	ANP	B	1315	-	-	5/18/38/38	0/3/3/3
3	KDF	B	1314	-	-	0/8/22/22	0/1/1/1
5	AMP	A	1316	-	-	0/10/26/26	0/3/3/3
4	ANP	A	1315	-	-	7/18/38/38	0/3/3/3
5	AMP	B	1316	-	-	0/10/26/26	0/3/3/3
5	AMP	C	1316	-	-	2/10/26/26	0/3/3/3
4	ANP	C	1315	-	-	3/18/38/38	0/3/3/3
2	KDG	B	1313	-	-	4/14/14/14	-
2	KDG	C	1313	-	-	5/14/14/14	-

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	1315	ANP	PG-O1G	14.83	1.68	1.46
4	A	1315	ANP	PB-O1B	11.30	1.63	1.46
4	C	1315	ANP	PB-O1B	10.17	1.61	1.46
4	A	1315	ANP	PG-O1G	7.94	1.58	1.46
4	B	1315	ANP	PG-O1G	7.90	1.58	1.46
4	B	1315	ANP	PB-O1B	6.96	1.56	1.46
4	B	1315	ANP	PA-O3A	6.72	1.66	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1316	AMP	C5-C4	5.21	1.48	1.39
5	C	1316	AMP	C5-C4	5.07	1.48	1.39
5	A	1316	AMP	C5-C4	4.92	1.47	1.39
3	A	1314	KDF	O2-C2	4.73	1.46	1.39
4	B	1315	ANP	PA-O1A	4.02	1.64	1.50
5	A	1316	AMP	C5-C6	3.33	1.50	1.41
4	B	1315	ANP	PB-O3A	3.31	1.63	1.59
3	B	1314	KDF	O2-C2	3.23	1.44	1.39
4	B	1315	ANP	PG-O2G	3.18	1.65	1.56
4	A	1315	ANP	PG-O2G	3.15	1.65	1.56
4	C	1315	ANP	PA-O1A	3.02	1.61	1.50
3	C	1314	KDF	O2-C2	3.00	1.43	1.39
4	A	1315	ANP	C5-N7	-2.98	1.33	1.39
5	C	1316	AMP	C5-C6	2.97	1.49	1.41
4	B	1315	ANP	C5-N7	-2.92	1.33	1.39
5	B	1316	AMP	C5-C6	2.84	1.48	1.41
3	B	1314	KDF	C3-C2	2.70	1.56	1.52
2	C	1313	KDG	C4-C5	2.70	1.55	1.51
3	C	1314	KDF	C3-C2	2.65	1.56	1.52
4	C	1315	ANP	C5-N7	-2.59	1.34	1.39
5	B	1316	AMP	C8-N7	2.47	1.36	1.31
5	C	1316	AMP	C8-N7	2.44	1.36	1.31
4	C	1315	ANP	PG-O3G	-2.36	1.50	1.56
4	C	1315	ANP	PB-O2B	-2.34	1.50	1.56
4	A	1315	ANP	PA-O3A	2.31	1.62	1.59
4	A	1315	ANP	PA-O1A	2.24	1.58	1.50
2	A	1313	KDG	C4-C5	2.23	1.55	1.51
4	C	1315	ANP	C4-N9	-2.23	1.33	1.37
4	B	1315	ANP	PB-N3B	-2.18	1.57	1.63
4	B	1315	ANP	PB-O2B	-2.18	1.51	1.56
4	B	1315	ANP	C4-N9	-2.12	1.33	1.37
4	C	1315	ANP	PA-O3A	2.12	1.61	1.59
5	C	1316	AMP	C5-N7	-2.12	1.35	1.39
4	B	1315	ANP	O4'-C1'	2.12	1.46	1.42
5	A	1316	AMP	C8-N7	2.11	1.35	1.31
2	B	1313	KDG	C4-C5	2.08	1.54	1.51
5	B	1316	AMP	C5-N7	-2.07	1.35	1.39
4	A	1315	ANP	O4'-C1'	2.05	1.46	1.42
4	A	1315	ANP	PB-O2B	-2.03	1.51	1.56

All (81) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1315	ANP	O1G-PG-N3B	-15.55	88.87	111.77
4	A	1315	ANP	O2G-PG-O1G	-6.45	97.28	113.45
5	C	1316	AMP	C5-C4-N3	-5.96	118.51	126.72
3	B	1314	KDF	O1A-C1-C2	-5.44	114.78	123.85
5	A	1316	AMP	C5-C4-N3	-5.38	119.30	126.72
4	A	1315	ANP	O1G-PG-N3B	-5.26	104.02	111.77
4	A	1315	ANP	C5-C4-N3	-5.24	119.50	126.72
4	C	1315	ANP	N3-C2-N1	-4.83	121.28	128.58
4	B	1315	ANP	N3-C2-N1	-4.80	121.32	128.58
4	C	1315	ANP	O1G-PG-N3B	-4.79	104.72	111.77
5	B	1316	AMP	C5-C4-N3	-4.77	120.15	126.72
3	A	1314	KDF	O1A-C1-C2	-4.69	116.02	123.85
4	C	1315	ANP	C5-C4-N3	-4.67	120.28	126.72
5	C	1316	AMP	N3-C4-N9	4.62	135.03	127.17
4	B	1315	ANP	C5-C4-N3	-4.49	120.53	126.72
2	B	1313	KDG	O6B-C6-C5	-4.48	116.24	121.81
4	A	1315	ANP	N3-C2-N1	-4.42	121.90	128.58
5	A	1316	AMP	N3-C4-N9	4.30	134.48	127.17
4	B	1315	ANP	O2G-PG-O1G	-4.22	102.86	113.45
3	A	1314	KDF	O2-C2-O5	4.18	115.46	109.40
5	A	1316	AMP	C4-C5-N7	-4.08	105.92	110.58
5	B	1316	AMP	N3-C4-N9	4.06	134.08	127.17
3	C	1314	KDF	O1A-C1-C2	-4.03	117.13	123.85
4	C	1315	ANP	O2B-PB-O3A	3.92	117.71	104.64
5	B	1316	AMP	N3-C2-N1	-3.91	122.66	128.58
4	A	1315	ANP	N3-C4-N9	3.87	133.75	127.17
5	C	1316	AMP	C2-N3-C4	3.82	121.16	111.83
5	A	1316	AMP	C2-N3-C4	3.77	121.03	111.83
4	C	1315	ANP	N9-C8-N7	-3.69	108.69	113.94
5	A	1316	AMP	N3-C2-N1	-3.63	123.09	128.58
5	C	1316	AMP	C4-C5-N7	-3.60	106.46	110.58
4	C	1315	ANP	N3-C4-N9	3.57	133.25	127.17
4	A	1315	ANP	N9-C8-N7	-3.52	108.94	113.94
5	B	1316	AMP	C2-N3-C4	3.50	120.37	111.83
2	C	1313	KDG	O6B-C6-C5	-3.47	117.49	121.81
4	A	1315	ANP	C2-N3-C4	3.44	120.24	111.83
4	B	1315	ANP	N3-C4-N9	3.40	132.96	127.17
4	C	1315	ANP	C2-N3-C4	3.37	120.05	111.83
4	A	1315	ANP	O1B-PB-N3B	-3.35	106.84	111.77
5	C	1316	AMP	N3-C2-N1	-3.34	123.53	128.58
4	B	1315	ANP	O2B-PB-O1B	3.30	116.94	109.87
4	B	1315	ANP	C2-N3-C4	3.27	119.82	111.83
4	A	1315	ANP	O2B-PB-O3A	3.23	115.42	104.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	1315	ANP	C4-N9-C8	3.20	109.10	105.74
4	A	1315	ANP	O2A-PA-O3A	3.11	115.68	107.27
4	B	1315	ANP	N9-C8-N7	-3.11	109.53	113.94
4	A	1315	ANP	C5-N7-C8	3.03	108.21	103.45
4	C	1315	ANP	O2A-PA-O3A	3.03	115.46	107.27
5	A	1316	AMP	C4-N9-C8	3.00	108.89	105.74
2	A	1313	KDG	O6B-C6-C5	-3.00	118.08	121.81
5	A	1316	AMP	C5-N7-C8	2.98	108.13	103.45
5	B	1316	AMP	C4-N9-C8	2.92	108.81	105.74
5	B	1316	AMP	C4-C5-N7	-2.90	107.27	110.58
5	B	1316	AMP	C2-N1-C6	2.87	123.44	118.73
5	A	1316	AMP	C6-C5-N7	2.76	137.41	132.09
4	C	1315	ANP	O1B-PB-N3B	-2.75	107.72	111.77
2	B	1313	KDG	C4-C5-C6	2.74	120.78	115.89
4	B	1315	ANP	O2B-PB-O3A	2.67	113.54	104.64
3	B	1314	KDF	C6-C5-C4	-2.65	108.23	114.82
4	A	1315	ANP	C4-N9-C8	2.64	108.51	105.74
4	A	1315	ANP	C4-C5-N7	-2.63	107.58	110.58
4	A	1315	ANP	O3A-PA-O1A	-2.63	102.80	110.70
5	C	1316	AMP	C5-N7-C8	2.63	107.58	103.45
4	C	1315	ANP	C5-N7-C8	2.62	107.56	103.45
4	B	1315	ANP	C4-N9-C8	2.48	108.34	105.74
4	B	1315	ANP	C5-N7-C8	2.41	107.24	103.45
4	B	1315	ANP	O1B-PB-N3B	2.40	115.31	111.77
5	B	1316	AMP	C6-C5-N7	2.40	136.72	132.09
4	C	1315	ANP	O2G-PG-O1G	-2.40	107.44	113.45
5	B	1316	AMP	C5-N7-C8	2.38	107.19	103.45
2	C	1313	KDG	C4-C5-C6	2.33	120.04	115.89
5	C	1316	AMP	C6-C5-N7	2.31	136.54	132.09
5	C	1316	AMP	C4-N9-C8	2.22	108.06	105.74
5	A	1316	AMP	N9-C8-N7	-2.18	110.85	113.94
4	C	1315	ANP	C4-C5-N7	-2.10	108.18	110.58
5	B	1316	AMP	N9-C8-N7	-2.08	110.98	113.94
5	A	1316	AMP	C2-N1-C6	2.07	122.12	118.73
2	B	1313	KDG	O6A-C6-C5	2.05	119.29	113.59
4	A	1315	ANP	O2B-PB-O1B	2.05	114.27	109.87
4	A	1315	ANP	O4'-C4'-C3'	-2.05	101.08	105.15
5	A	1316	AMP	O4'-C1'-N9	2.03	111.99	108.09

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1313	KDG	C1-C2-C3-O3
2	A	1313	KDG	C1-C2-C3-C4
2	A	1313	KDG	O2-C2-C3-O3
2	A	1313	KDG	O2-C2-C3-C4
2	B	1313	KDG	C1-C2-C3-O3
2	B	1313	KDG	C1-C2-C3-C4
2	B	1313	KDG	O2-C2-C3-O3
2	B	1313	KDG	O2-C2-C3-C4
2	C	1313	KDG	O2-C2-C3-C4
4	A	1315	ANP	PB-N3B-PG-O1G
4	A	1315	ANP	PG-N3B-PB-O1B
4	A	1315	ANP	PA-O3A-PB-O2B
4	B	1315	ANP	PG-N3B-PB-O1B
4	B	1315	ANP	PG-N3B-PB-O3A
4	B	1315	ANP	C5'-O5'-PA-O1A
4	B	1315	ANP	C5'-O5'-PA-O2A
4	B	1315	ANP	C5'-O5'-PA-O3A
4	C	1315	ANP	PB-N3B-PG-O1G
4	C	1315	ANP	PA-O3A-PB-O2B
2	A	1313	KDG	O1B-C1-C2-O2
5	C	1316	AMP	O4'-C4'-C5'-O5'
2	C	1313	KDG	O2-C2-C3-O3
4	A	1315	ANP	O4'-C4'-C5'-O5'
2	A	1313	KDG	O1B-C1-C2-C3
2	C	1313	KDG	C2-C3-C4-C5
2	C	1313	KDG	C3-C4-C5-O5
2	C	1313	KDG	C3-C4-C5-C6
4	C	1315	ANP	C5'-O5'-PA-O1A
4	A	1315	ANP	PB-O3A-PA-O2A
5	C	1316	AMP	C3'-C4'-C5'-O5'
4	A	1315	ANP	PB-O3A-PA-O1A
4	A	1315	ANP	PA-O3A-PB-O1B

There are no ring outliers.

8 monomers are involved in 16 short contacts:

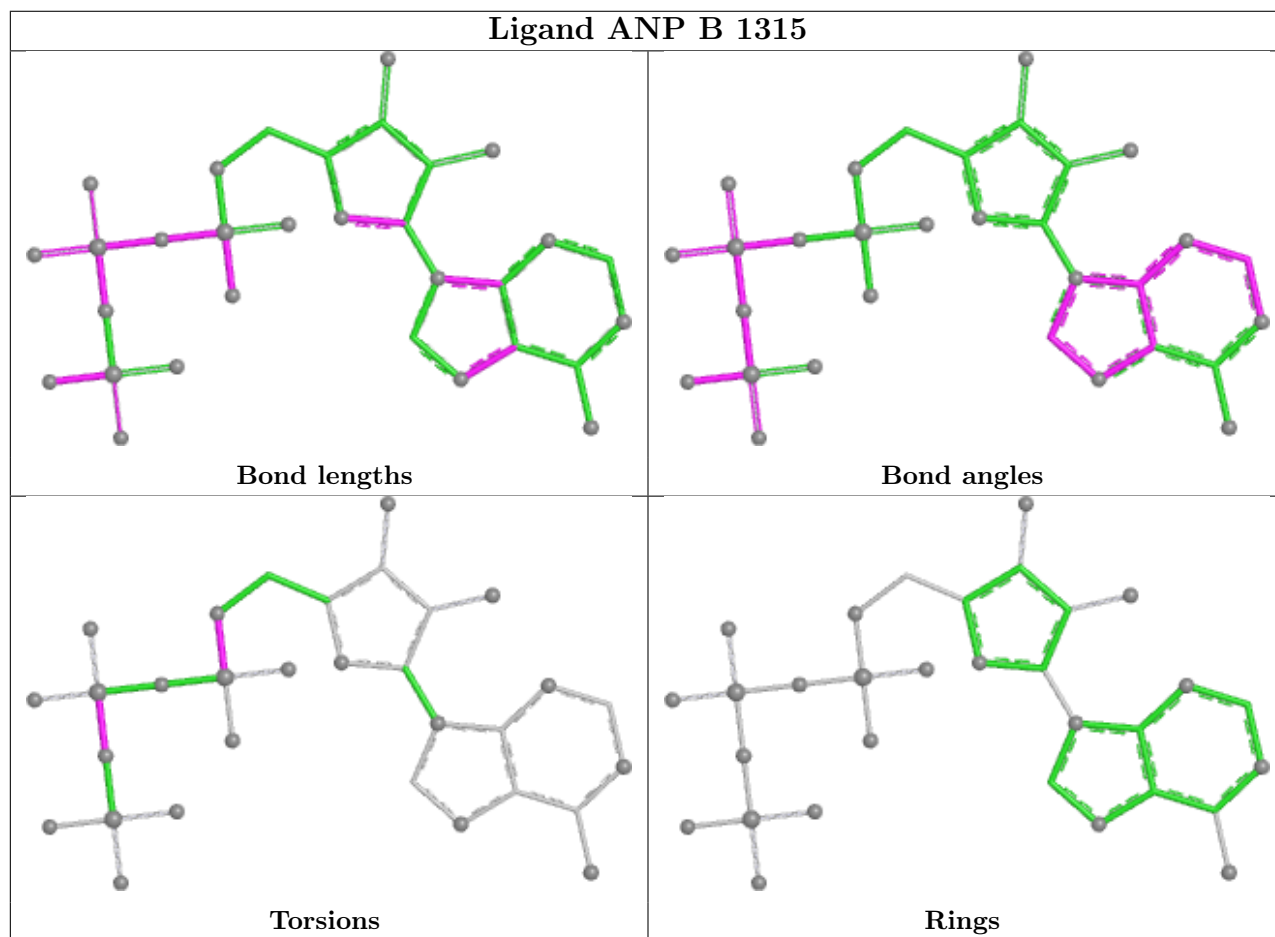
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1313	KDG	3	0
4	B	1315	ANP	4	0
5	A	1316	AMP	1	0
4	A	1315	ANP	3	0
5	B	1316	AMP	1	0
5	C	1316	AMP	1	0

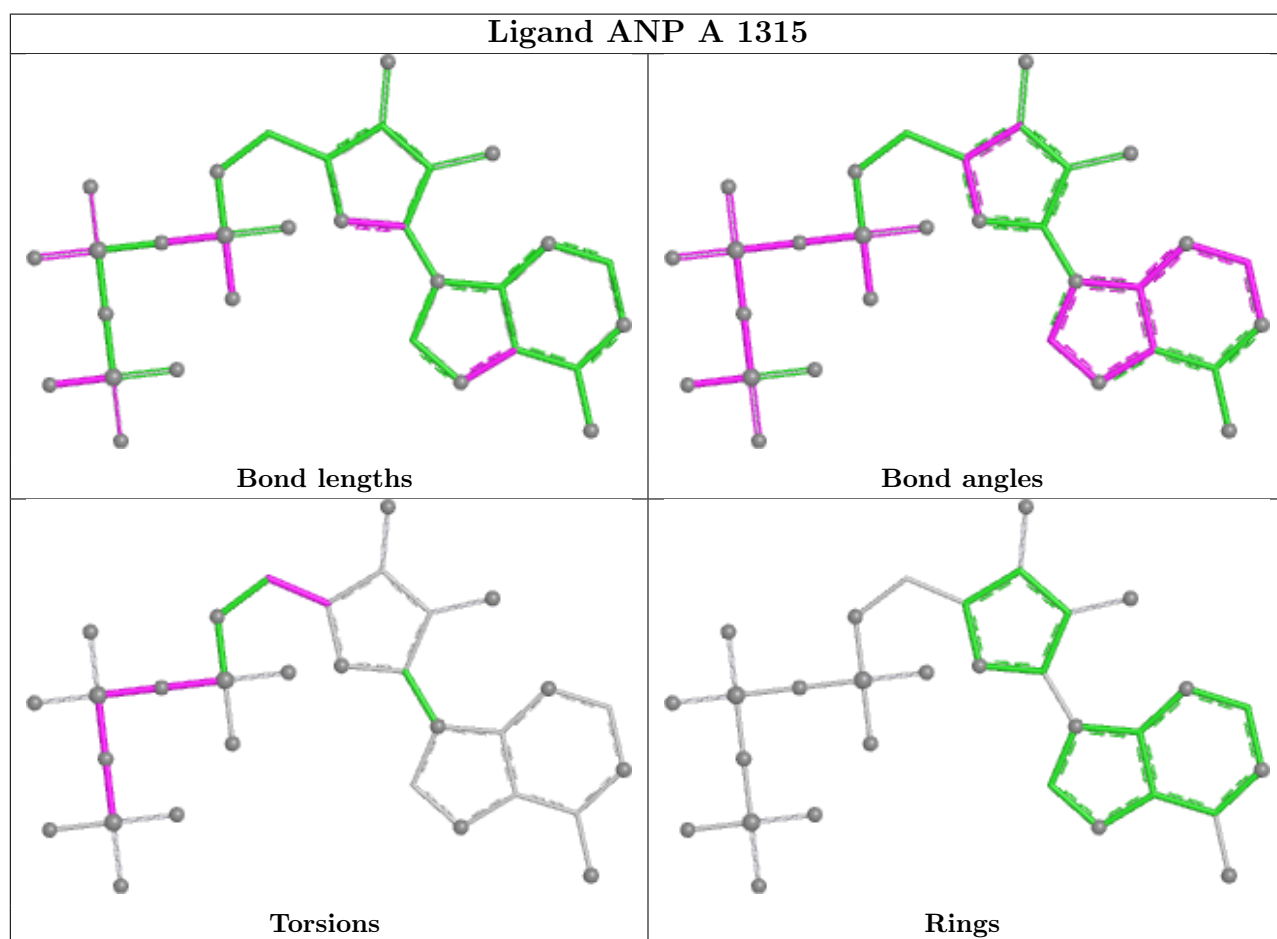
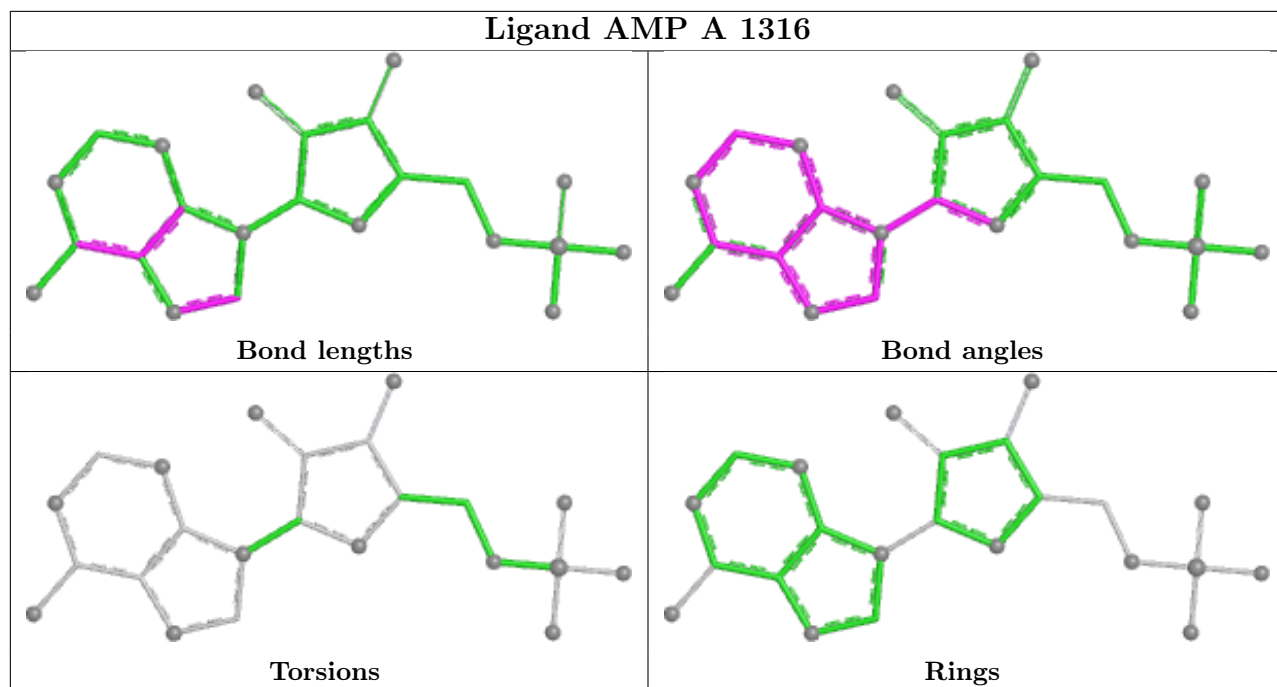
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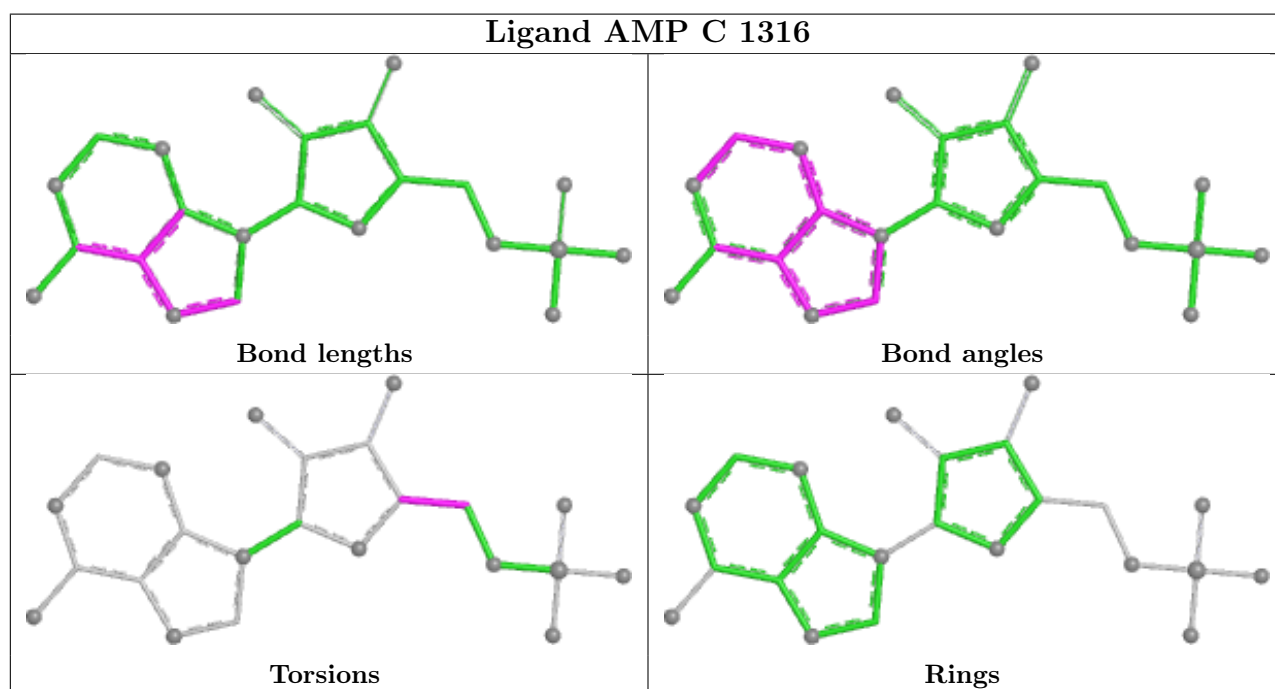
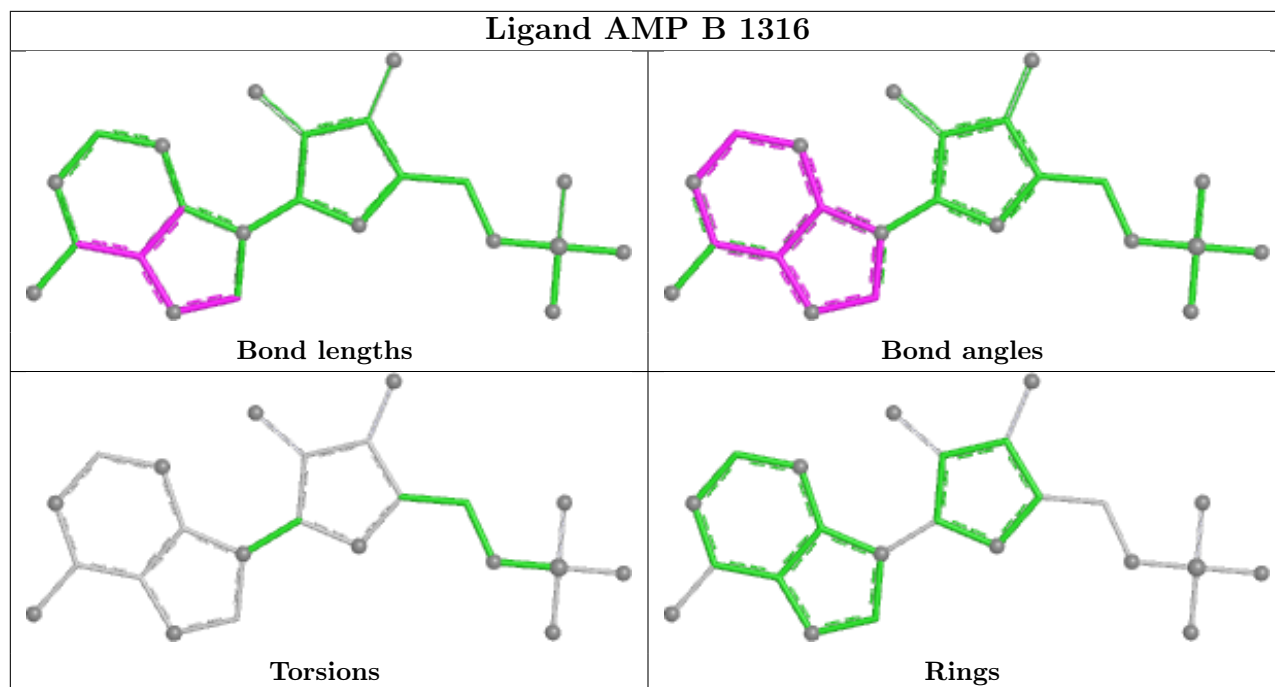
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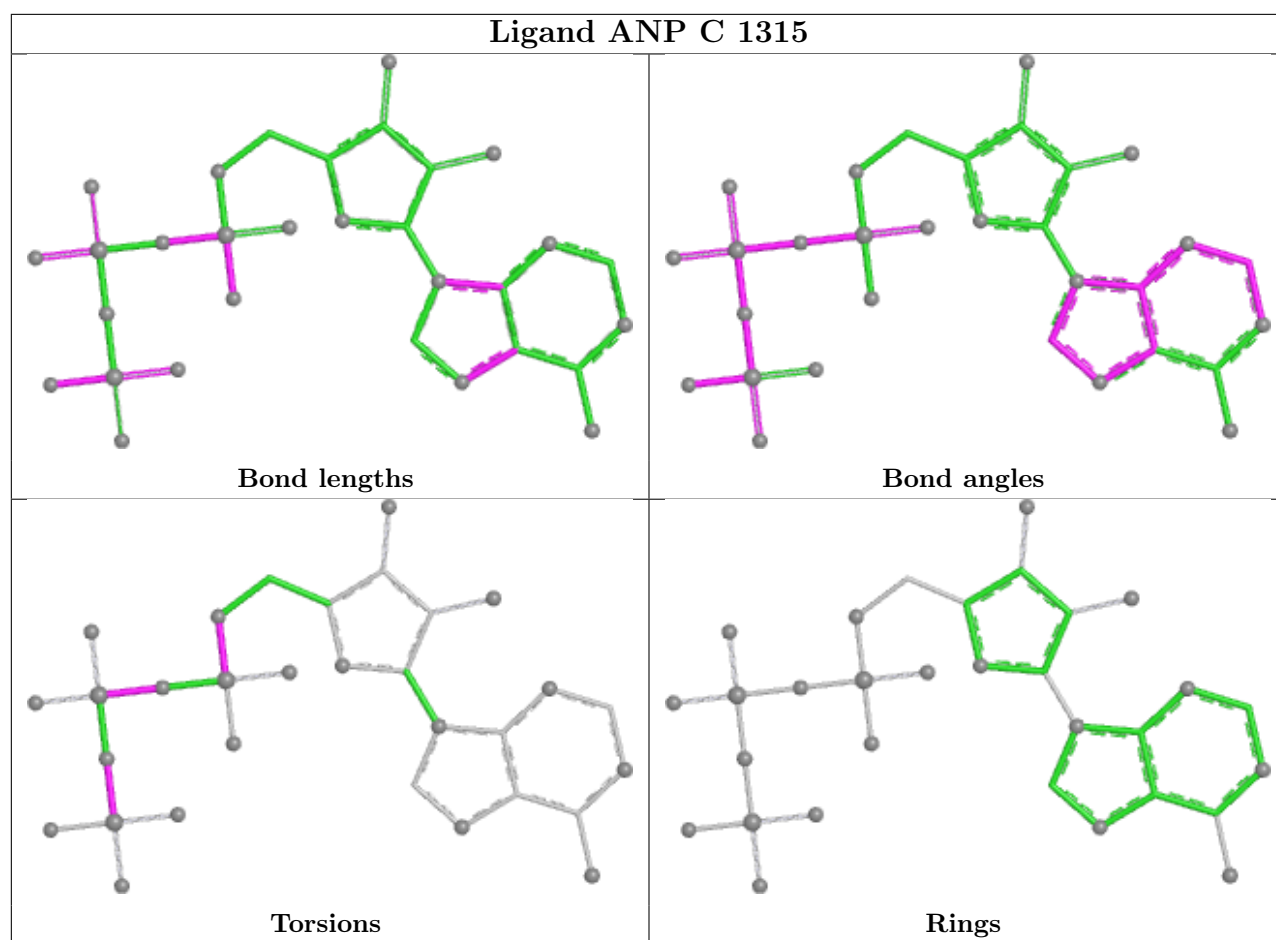
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	1315	ANP	2	0
2	B	1313	KDG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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	311/313 (99%)	-0.42	3 (0%) 79 81	11, 20, 31, 37	14 (4%)
1	B	311/313 (99%)	-0.47	1 (0%) 90 91	11, 19, 30, 39	15 (4%)
1	C	311/313 (99%)	-0.30	0 100 100	14, 24, 33, 44	13 (4%)
All	All	933/939 (99%)	-0.40	4 (0%) 88 90	11, 21, 32, 44	42 (4%)

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	128	ASN	2.7
1	A	123[A]	GLU	2.3
1	A	124[A]	ASN	2.1
1	A	18	ASN	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](#)

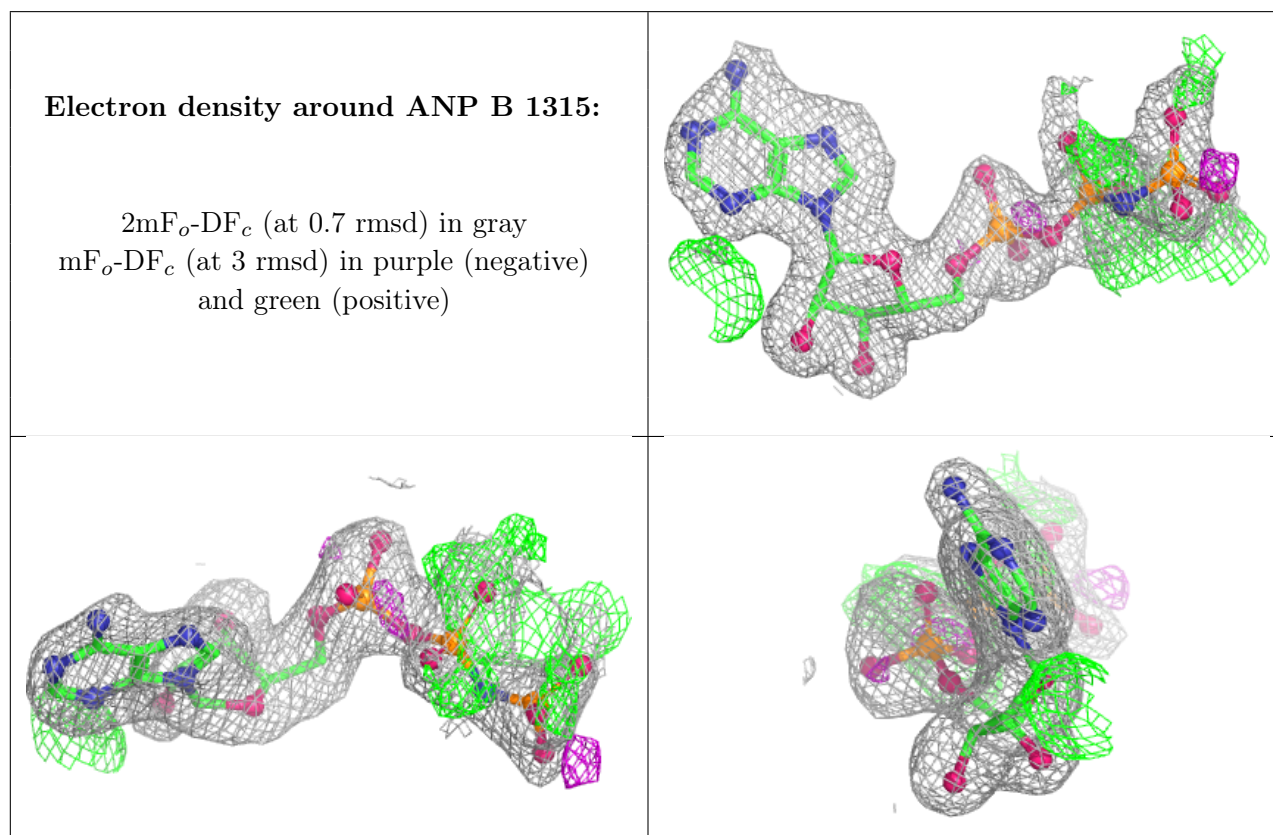
There are no oligosaccharides in this entry.

### 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.

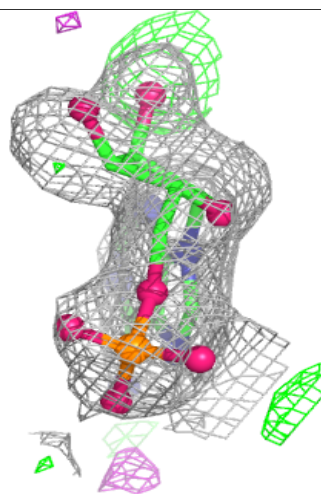
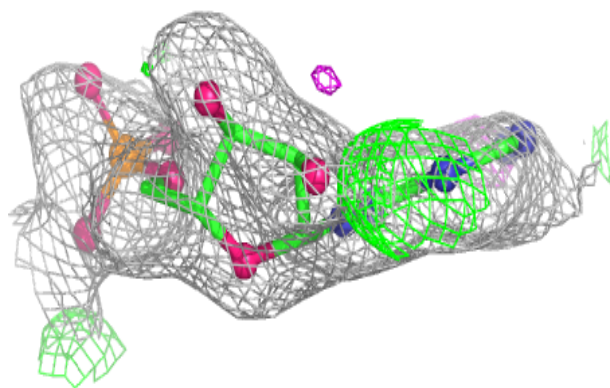
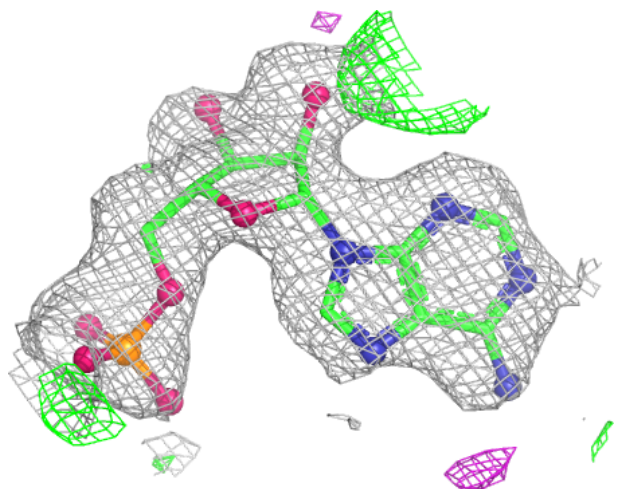
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	ANP	B	1315	31/31	0.82	0.15	19,38,41,42	31
5	AMP	C	1316	23/23	0.82	0.24	97,98,99,99	23
4	ANP	A	1315	31/31	0.87	0.13	17,27,31,33	31
4	ANP	C	1315	31/31	0.92	0.09	14,17,24,24	31
5	AMP	A	1316	23/23	0.92	0.09	24,26,31,32	23
2	KDG	C	1313	12/12	0.92	0.14	45,46,48,48	12
2	KDG	B	1313	12/12	0.94	0.15	63,64,64,65	12
5	AMP	B	1316	23/23	0.95	0.08	19,22,26,28	23
2	KDG	A	1313	12/12	0.95	0.14	52,53,54,55	12
3	KDF	A	1314	12/12	0.97	0.06	6,8,9,10	12
3	KDF	C	1314	12/12	0.97	0.06	10,13,14,17	12
3	KDF	B	1314	12/12	0.99	0.04	3,6,8,9	12

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.



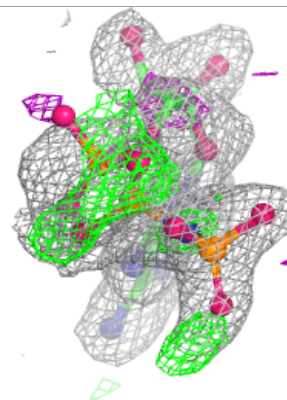
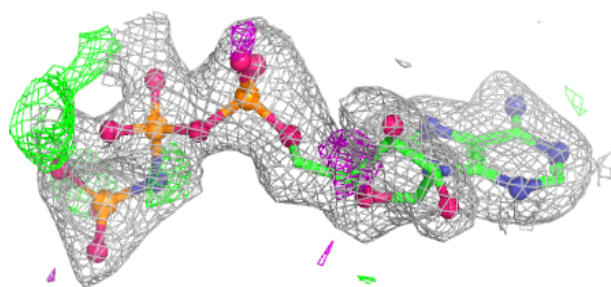
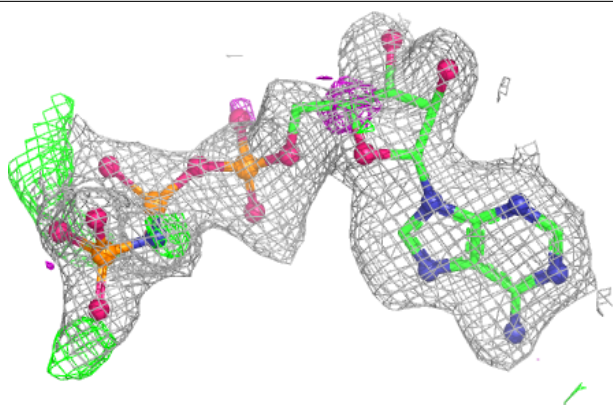
**Electron density around AMP C 1316:**

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

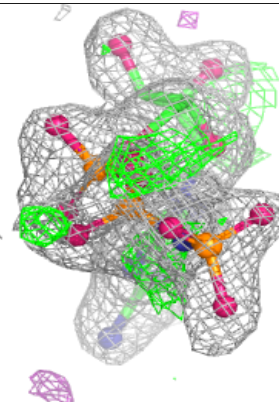
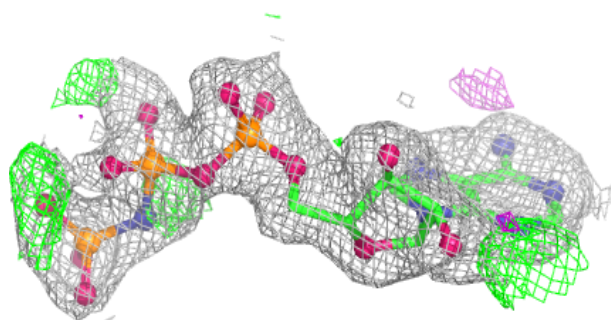
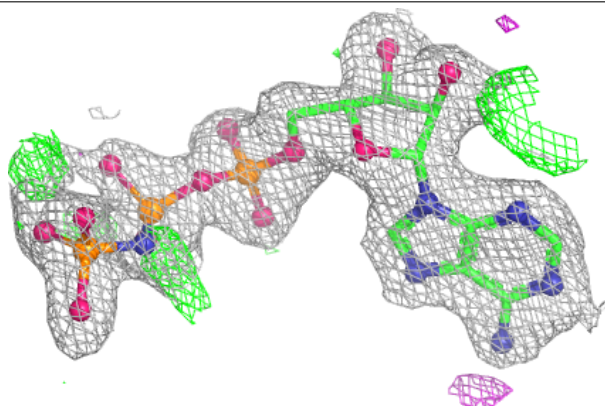


**Electron density around ANP A 1315:**

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

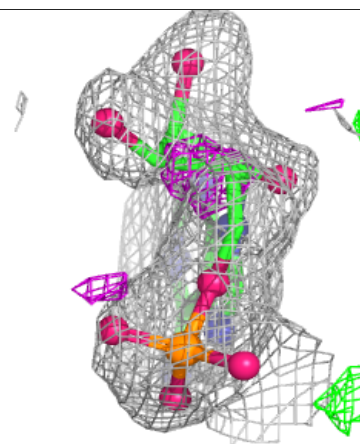
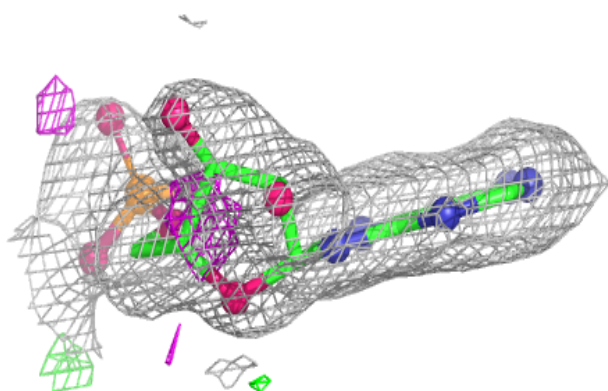
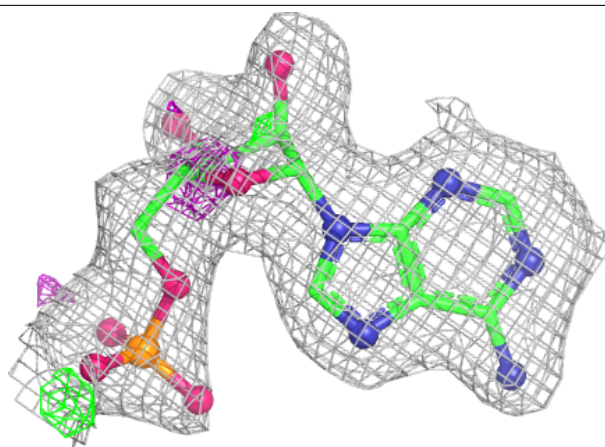
**Electron density around ANP C 1315:**

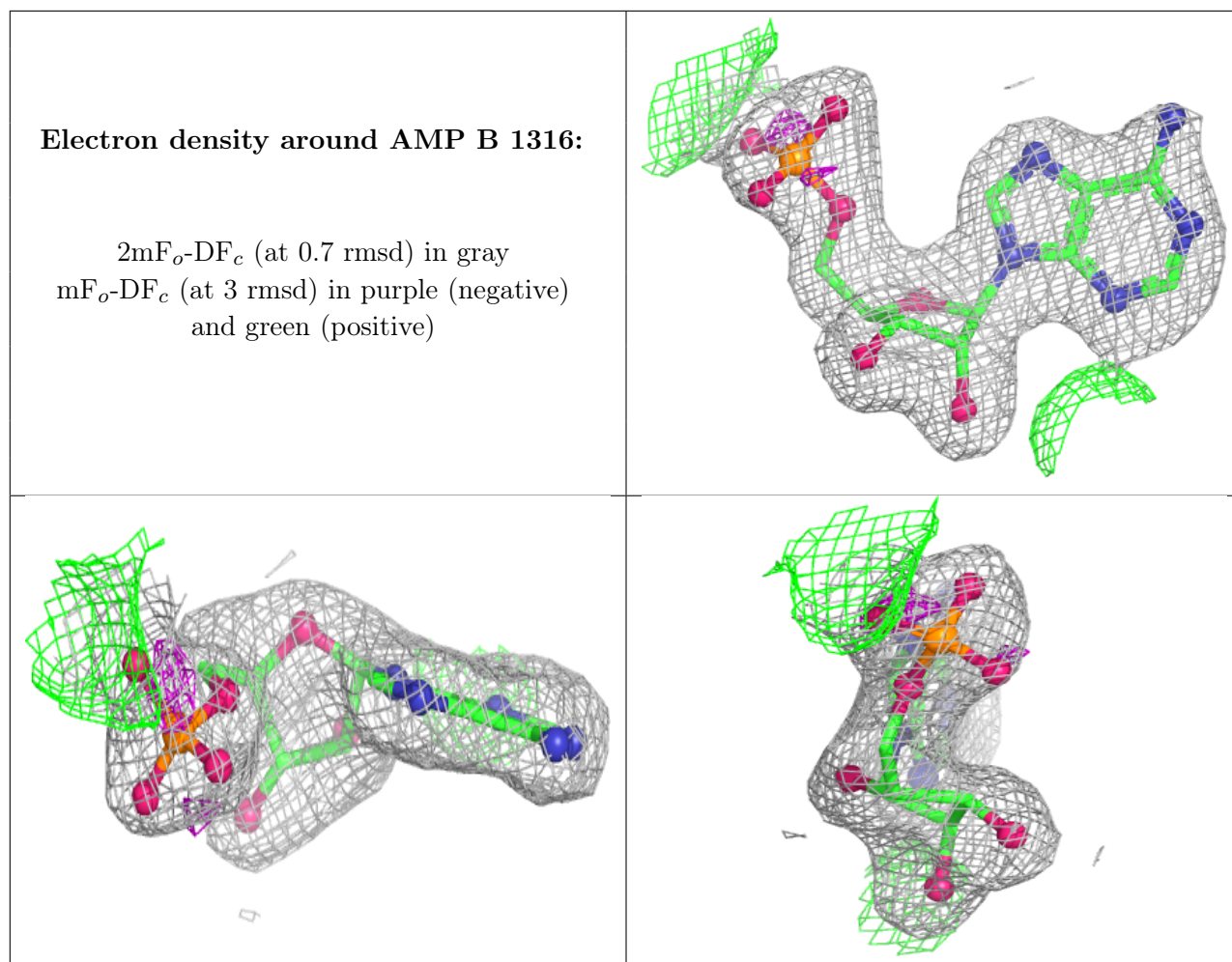
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around AMP A 1316:**

$2mF_o-DF_c$  (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.