



# Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 09:14 am BST

PDB ID : 5XIJ  
Title : Crystal Structure of Toxoplasma gondii Prolyl-tRNA Synthetase (TgPRS) in complex with Inhibitor 9  
Authors : Jain, V.; Manickam, Y.; Sharma, A.  
Deposited on : 2017-04-26  
Resolution : 2.50 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

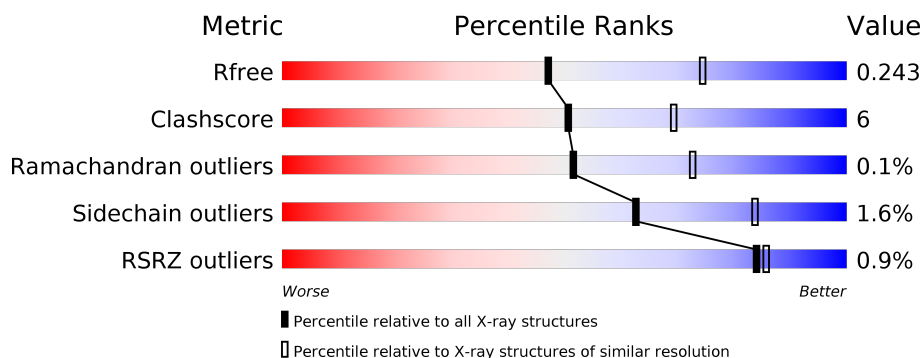
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	500	
1	B	500	
1	C	500	
1	D	500	

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 15971 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.

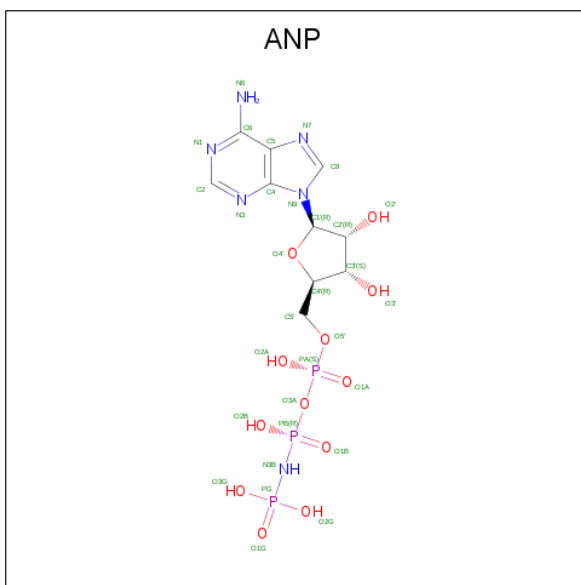
- Molecule 1 is a protein called Prolyl-tRNA synthetase (ProRS).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	482	Total	C	N	O	S	0	1	0
			3898	2505	663	708	22			
1	B	478	Total	C	N	O	S	0	0	0
			3831	2464	650	695	22			
1	C	477	Total	C	N	O	S	0	3	0
			3881	2496	665	698	22			
1	D	472	Total	C	N	O	S	0	2	0
			3807	2452	654	679	22			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	331	GLY	-	expression tag	UNP S8G8I1
A	332	ALA	-	expression tag	UNP S8G8I1
A	333	MET	-	expression tag	UNP S8G8I1
B	331	GLY	-	expression tag	UNP S8G8I1
B	332	ALA	-	expression tag	UNP S8G8I1
B	333	MET	-	expression tag	UNP S8G8I1
C	331	GLY	-	expression tag	UNP S8G8I1
C	332	ALA	-	expression tag	UNP S8G8I1
C	333	MET	-	expression tag	UNP S8G8I1
D	331	GLY	-	expression tag	UNP S8G8I1
D	332	ALA	-	expression tag	UNP S8G8I1
D	333	MET	-	expression tag	UNP S8G8I1

- Molecule 2 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>).

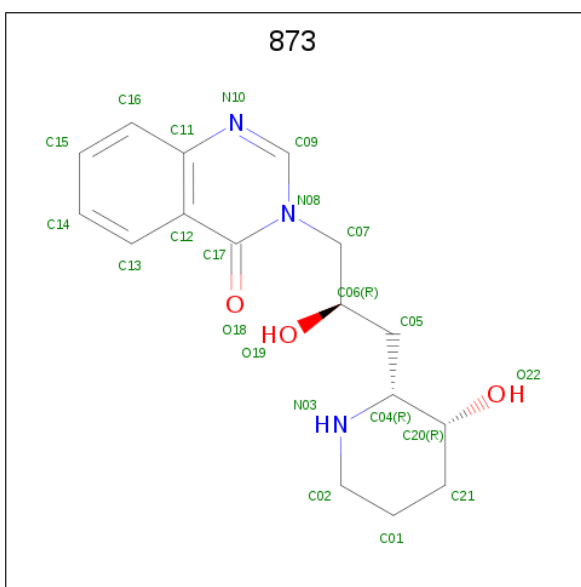


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 31	C 10	N 6	O 12	P 3	0	0
2	B	1	Total 31	C 10	N 6	O 12	P 3	0	0
2	C	1	Total 31	C 10	N 6	O 12	P 3	0	0
2	D	1	Total 31	C 10	N 6	O 12	P 3	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 4 is 3-[(2R)-2-oxidanyl-3-[(2R,3R)-3-oxidanylpiperidin-2-yl]propyl]quinazolin-4-one (three-letter code: 873) (formula: C<sub>16</sub>H<sub>21</sub>N<sub>3</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			22	16	3	3		
4	B	1	Total	C	N	O	0	0
			22	16	3	3		
4	C	1	Total	C	N	O	0	0
			22	16	3	3		
4	D	1	Total	C	N	O	0	0
			22	16	3	3		

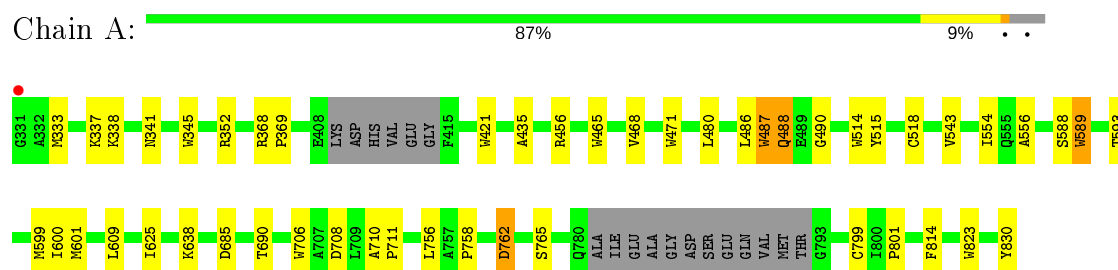
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	121	Total	O	0	0
			121	121		
5	B	66	Total	O	0	2
			68	68		
5	C	77	Total	O	0	0
			77	77		
5	D	67	Total	O	0	1
			68	68		

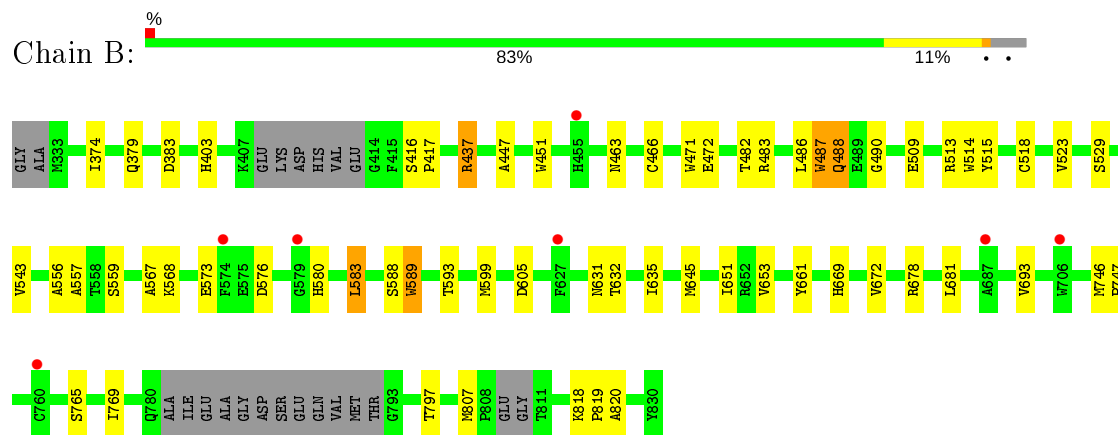
### 3 Residue-property plots

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.

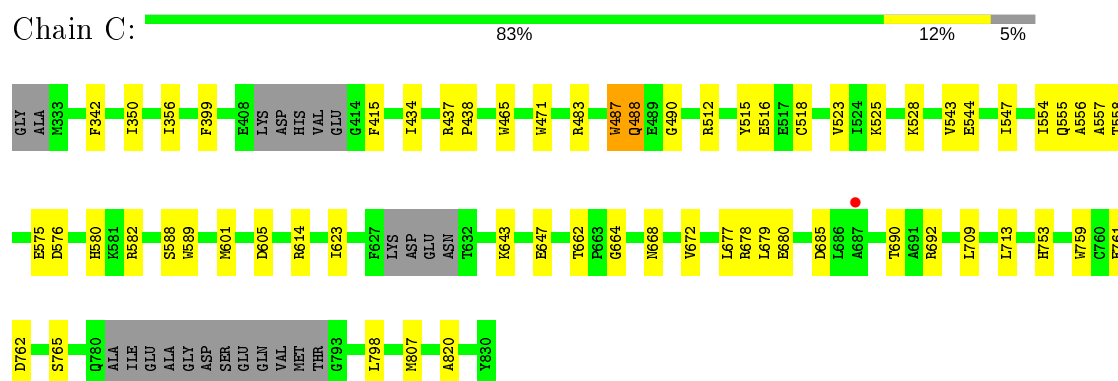
#### • Molecule 1: Prolyl-tRNA synthetase (ProRS)



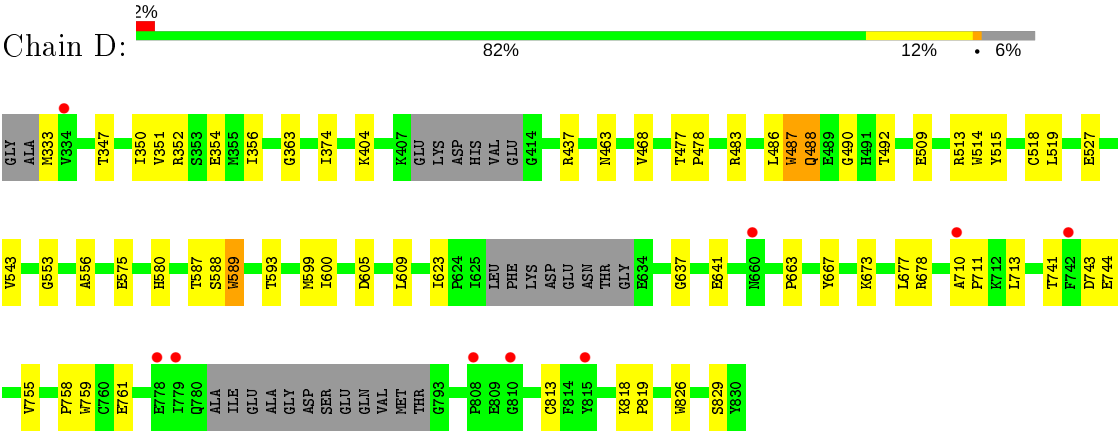
#### • Molecule 1: Prolyl-tRNA synthetase (ProRS)



#### • Molecule 1: Prolyl-tRNA synthetase (ProRS)



● Molecule 1: Prolyl-tRNA synthetase (ProRS)



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	76.85Å 93.16Å 91.01Å 89.81° 104.52° 99.60°	Depositor
Resolution (Å)	40.36 – 2.50 40.33 – 2.50	Depositor EDS
% Data completeness (in resolution range)	97.0 (40.36-2.50) 97.0 (40.33-2.50)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.50 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, $R_{free}$	0.180 , 0.240 0.190 , 0.243	Depositor DCC
$R_{free}$ test set	4043 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	37.3	Xtriage
Anisotropy	0.094	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 38.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	15971	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.84% 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: MG, ANP, 873

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	0.77	0/4007	0.81	0/5428
1	B	0.71	0/3935	0.82	0/5334
1	C	0.74	0/3994	0.83	0/5402
1	D	0.69	0/3917	0.80	0/5304
All	All	0.73	0/15853	0.82	0/21468

There are no bond length outliers.

There are no bond angle outliers.

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	3898	0	3798	34	0
1	B	3831	0	3698	47	0
1	C	3881	0	3816	42	0
1	D	3807	0	3713	38	0
2	A	31	0	13	2	0
2	B	31	0	13	7	0
2	C	31	0	13	1	0
2	D	31	0	13	2	0
3	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
4	A	22	0	0	1	0
4	B	22	0	0	4	0
4	C	22	0	0	2	0
4	D	22	0	0	2	0
5	A	121	0	0	1	0
5	B	68	0	0	1	0
5	C	77	0	0	3	0
5	D	68	0	0	2	0
All	All	15971	0	15077	174	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 6.

All (174) 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:C:547:ILE:HG21	1:C:601:MET:CE	2.02	0.89
1:C:547:ILE:HG21	1:C:601:MET:HE1	1.60	0.81
1:C:643:LYS:NZ	1:C:647:GLU:OE2	2.16	0.79
2:B:1001:ANP:O3A	2:B:1001:ANP:H3'	1.86	0.76
1:C:515:TYR:CZ	1:C:556:ALA:HB1	2.20	0.76
1:D:492:THR:OG1	1:D:587:THR:HB	1.88	0.74
1:B:567:ALA:HB1	1:B:583:LEU:HG	1.69	0.71
4:D:1004:873:N03	4:D:1004:873:O19	2.22	0.71
4:C:1004:873:O19	4:C:1004:873:N03	2.27	0.68
1:D:515:TYR:CZ	1:D:556:ALA:HB1	2.31	0.66
4:A:1004:873:O19	4:A:1004:873:N03	2.29	0.66
1:C:547:ILE:HG21	1:C:601:MET:HE2	1.76	0.66
1:B:567:ALA:CB	1:B:583:LEU:HG	2.26	0.65
1:D:350:ILE:HD12	1:D:356:ILE:HG12	1.80	0.64
1:A:710:ALA:N	1:A:711:PRO:HD2	2.13	0.64
1:D:486:LEU:HB2	1:D:593:THR:CG2	2.28	0.64
2:B:1001:ANP:O1A	4:B:1004:873:O22	2.17	0.62
1:D:437:ARG:HD3	5:D:1130:HOH:O	1.97	0.62
1:B:529:SER:HB3	1:B:797:THR:HG21	1.82	0.61
1:A:480:LEU:HD22	1:A:554:ILE:CD1	2.31	0.60
1:A:543:VAL:HG23	1:A:556:ALA:HB3	1.82	0.60
1:A:486:LEU:HB2	1:A:593:THR:HG23	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:463:ASN:OD1	1:B:488:GLN:HG2	2.02	0.60
1:A:486:LEU:HB2	1:A:593:THR:CG2	2.33	0.59
1:C:807:MET:CE	1:C:820:ALA:HB3	2.32	0.59
1:A:515:TYR:CZ	1:A:556:ALA:HB1	2.37	0.59
2:A:1001:ANP:O2G	5:A:1101:HOH:O	2.17	0.58
1:C:543:VAL:HG13	1:C:556:ALA:HB3	1.86	0.58
1:C:662:THR:HG22	1:C:664:GLY:N	2.19	0.57
1:D:486:LEU:HB2	1:D:593:THR:HG23	1.84	0.57
1:D:515:TYR:CE2	1:D:556:ALA:HB1	2.39	0.57
1:C:680:GLU:OE1	1:C:692:ARG:HD3	2.04	0.56
1:D:741:THR:HB	1:D:744:GLU:HG3	1.87	0.56
1:B:807:MET:HE3	1:B:820:ALA:HB3	1.88	0.56
1:C:512:ARG:HD3	1:C:525:LYS:HE3	1.87	0.56
2:A:1001:ANP:H3'	2:A:1001:ANP:O3A	2.07	0.55
1:B:568:LYS:HA	1:B:583:LEU:HD21	1.89	0.55
2:D:1001:ANP:O2A	4:D:1004:873:O22	2.25	0.55
1:B:669:HIS:O	1:B:672:VAL:HG12	2.06	0.54
1:A:708:ASP:O	1:A:711:PRO:HG2	2.08	0.54
2:B:1001:ANP:PA	4:B:1004:873:O22	2.66	0.54
1:C:523:VAL:CG2	1:C:543:VAL:HG22	2.38	0.53
1:B:543:VAL:CG1	1:B:557:ALA:HB3	2.38	0.53
1:B:635:ILE:HG23	1:B:681:LEU:HD23	1.91	0.53
1:B:514:TRP:O	1:B:518:CYS:HB2	2.09	0.53
1:B:437:ARG:O	1:B:437:ARG:HG2	2.08	0.52
1:D:818:LYS:HB3	1:D:819:PRO:CD	2.39	0.52
1:D:553:GLY:O	1:D:829:SER:HA	2.09	0.52
1:A:514:TRP:O	1:A:518:CYS:HB2	2.10	0.52
1:C:677:LEU:HD13	1:C:713:LEU:HD22	1.92	0.51
1:A:490:GLY:O	1:A:588:SER:HA	2.11	0.51
1:A:708:ASP:O	1:A:711:PRO:HD2	2.11	0.51
1:C:679:LEU:HD11	1:C:709:LEU:HD21	1.92	0.51
1:C:437:ARG:HD3	5:C:1132:HOH:O	2.10	0.51
1:D:543:VAL:HG23	1:D:556:ALA:HB3	1.92	0.50
1:C:528:LYS:NZ	1:C:544:GLU:OE2	2.38	0.50
1:D:490:GLY:O	1:D:588:SER:HA	2.11	0.50
1:A:515:TYR:CE2	1:A:556:ALA:HB1	2.46	0.50
1:D:741:THR:HG22	1:D:743:ASP:H	1.77	0.50
1:A:333:MET:O	1:A:352:ARG:NH1	2.45	0.49
1:B:573:GLU:HG2	1:B:583:LEU:CD1	2.42	0.49
1:D:637:GLY:O	1:D:641:GLU:HG3	2.12	0.49
1:D:600:ILE:HG23	1:D:609:LEU:CD2	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:575:GLU:HA	1:C:580:HIS:O	2.12	0.49
2:C:1001:ANP:H8	2:C:1001:ANP:O3A	2.13	0.49
1:D:519:LEU:HD22	1:D:599:MET:HE2	1.95	0.49
1:B:490:GLY:O	1:B:588:SER:HA	2.12	0.49
1:B:765:SER:O	1:B:769:ILE:HG13	2.13	0.48
1:B:472:GLU:O	1:B:483:ARG:NH1	2.32	0.48
1:D:333:MET:O	1:D:352:ARG:NH1	2.43	0.48
1:B:543:VAL:HG13	1:B:556:ALA:HB3	1.96	0.48
1:D:663:PRO:O	1:D:667:TYR:CD1	2.67	0.48
1:C:490:GLY:O	1:C:588:SER:HA	2.14	0.48
1:C:762:ASP:O	1:C:765:SER:OG	2.31	0.48
1:A:465:TRP:CE3	1:A:488:GLN:HB2	2.49	0.47
1:D:514:TRP:O	1:D:518:CYS:HB2	2.14	0.47
1:B:523:VAL:HG21	1:B:543:VAL:CG2	2.44	0.47
1:C:759:TRP:CZ3	1:C:761:GLU:HA	2.48	0.47
1:D:374:ILE:HG21	1:D:599:MET:HE3	1.96	0.47
1:A:338:LYS:HG3	1:A:345:TRP:CD2	2.49	0.47
1:C:415:PHE:HB3	4:C:1004:873:C15	2.45	0.47
1:B:482:THR:H	2:B:1001:ANP:HN62	1.63	0.46
1:C:753:HIS:NE2	5:C:1101:HOH:O	2.35	0.46
1:A:638:LYS:HE3	1:A:706:TRP:CZ3	2.50	0.46
1:A:480:LEU:HD11	1:A:601:MET:CE	2.45	0.46
1:A:710:ALA:N	1:A:711:PRO:CD	2.77	0.46
1:A:756:LEU:HD22	1:A:823:TRP:HB3	1.97	0.46
1:B:568:LYS:CA	1:B:583:LEU:HD21	2.45	0.46
1:C:342:PHE:HE2	1:C:601:MET:HE3	1.80	0.46
1:B:379:GLN:O	1:B:383:ASP:HB2	2.16	0.46
1:C:487:TRP:C	1:C:487:TRP:CD1	2.89	0.46
1:C:342:PHE:CE2	1:C:601:MET:HE3	2.51	0.46
1:B:437:ARG:NH2	1:B:466:CYS:HB2	2.31	0.46
1:A:625:ILE:HG22	1:A:625:ILE:O	2.16	0.45
1:A:685:ASP:HB3	1:A:690:THR:O	2.16	0.45
1:D:605:ASP:C	1:D:605:ASP:OD1	2.55	0.45
1:D:755:VAL:CG2	1:D:826:TRP:HB2	2.46	0.45
5:C:1123:HOH:O	1:D:404:LYS:HE2	2.16	0.45
1:B:631:ASN:O	1:B:632:THR:C	2.55	0.45
1:C:518:CYS:HA	1:C:614[B]:ARG:HG2	1.99	0.45
1:C:807:MET:HE1	1:C:820:ALA:HB3	1.98	0.45
1:C:662:THR:HG22	1:C:664:GLY:H	1.82	0.45
1:C:668:ASN:O	1:C:672:VAL:HG23	2.16	0.45
1:C:605:ASP:OD1	1:C:605:ASP:C	2.55	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:463:ASN:OD1	1:D:488:GLN:HG2	2.17	0.44
1:A:368:ARG:HB3	1:A:369:PRO:HD2	1.98	0.44
1:B:583:LEU:HD12	1:B:583:LEU:HA	1.77	0.44
1:C:576:ASP:OD2	1:C:582:ARG:NE	2.50	0.44
1:D:623:ILE:HD12	1:D:678:ARG:HD2	1.98	0.44
2:B:1001:ANP:O1B	5:B:1101:HOH:O	2.21	0.44
1:B:374:ILE:HG21	1:B:599:MET:CE	2.47	0.44
1:C:623:ILE:CD1	1:C:678:ARG:HG3	2.48	0.44
1:A:600:ILE:HG23	1:A:609:LEU:CD2	2.47	0.44
1:D:509:GLU:O	1:D:513:ARG:HG3	2.17	0.44
1:B:515:TYR:CE1	1:B:556:ALA:HB1	2.53	0.44
1:A:421:TRP:CZ3	1:A:435:ALA:HB2	2.53	0.44
1:B:523:VAL:CG2	1:B:543:VAL:HG22	2.47	0.44
1:C:350:ILE:HD12	1:C:356:ILE:HG12	1.98	0.44
1:D:587:THR:HG22	1:D:589:TRP:CD1	2.53	0.44
1:D:759:TRP:CZ3	1:D:761:GLU:HA	2.53	0.44
1:B:818:LYS:HB3	1:B:819:PRO:CD	2.48	0.44
1:C:556:ALA:O	1:C:557:ALA:HB2	2.18	0.44
1:A:762:ASP:O	1:A:765:SER:HB3	2.18	0.44
1:B:416:SER:HB2	1:B:417:PRO:HD3	2.00	0.44
1:C:399:PHE:CG	1:C:434:ILE:HD12	2.52	0.43
4:B:1004:873:O22	4:B:1004:873:C06	2.66	0.43
1:D:354:GLU:OE2	1:D:673:LYS:NZ	2.50	0.43
1:A:599:MET:HE2	1:A:600:ILE:N	2.33	0.43
1:B:515:TYR:CZ	1:B:556:ALA:HB1	2.53	0.43
1:B:576:ASP:OD1	1:B:580:HIS:N	2.52	0.43
1:C:465:TRP:CE3	1:C:488:GLN:HB2	2.52	0.43
1:B:482:THR:N	2:B:1001:ANP:HN62	2.16	0.43
1:B:374:ILE:HG21	1:B:599:MET:HE1	1.99	0.43
1:B:807:MET:CE	1:B:820:ALA:HB3	2.48	0.43
1:C:512:ARG:NH1	1:C:516:GLU:OE1	2.52	0.43
1:A:490:GLY:HA3	1:A:589:TRP:CZ3	2.52	0.43
1:A:337:LYS:HD3	1:A:337:LYS:HA	1.65	0.43
1:D:347:THR:O	1:D:351:VAL:HG23	2.18	0.43
1:D:363:GLY:HA3	1:D:483:ARG:HG3	2.00	0.43
1:D:818:LYS:HB3	1:D:819:PRO:HD2	2.01	0.43
1:A:758:PRO:HD3	1:A:823:TRP:CZ3	2.54	0.43
1:C:555:GLN:NE2	1:C:558:THR:HB	2.34	0.42
1:A:456:ARG:HD3	1:B:661:TYR:CE1	2.54	0.42
1:B:509:GLU:O	1:B:513:ARG:HG3	2.18	0.42
1:A:480:LEU:HD13	1:A:830:TYR:CE1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:605:ASP:C	1:B:605:ASP:OD1	2.58	0.42
1:D:677:LEU:HD13	1:D:713:LEU:HD22	2.02	0.42
1:B:523:VAL:HG21	1:B:543:VAL:HG22	2.02	0.42
1:B:651:ILE:O	1:B:653:VAL:HG23	2.20	0.42
2:D:1001:ANP:O2G	5:D:1101:HOH:O	2.21	0.41
1:B:746:MET:N	1:B:747:PRO:CD	2.83	0.41
1:D:710:ALA:HB3	1:D:711:PRO:CD	2.49	0.41
1:A:480:LEU:HD22	1:A:554:ILE:HD11	1.99	0.41
1:C:483:ARG:HG3	1:C:483:ARG:NH1	2.36	0.41
1:C:554:ILE:O	1:C:554:ILE:HG23	2.20	0.41
1:D:477:THR:O	1:D:478:PRO:C	2.59	0.41
1:B:543:VAL:HG12	1:B:557:ALA:HB3	2.00	0.41
1:B:588:SER:C	1:B:589:TRP:CD1	2.94	0.41
1:B:486:LEU:HB2	1:B:593:THR:HG23	2.02	0.41
1:A:799:CYS:O	1:A:801:PRO:HD3	2.21	0.41
1:B:447:ALA:HB1	1:B:451:TRP:CZ2	2.56	0.41
1:B:487:TRP:CD1	1:B:487:TRP:C	2.94	0.41
1:C:515:TYR:CE1	1:C:556:ALA:HB1	2.54	0.41
1:B:559:SER:HA	1:B:589:TRP:HB3	2.02	0.40
1:D:468:VAL:HG21	1:D:487:TRP:CE2	2.56	0.40
1:D:575:GLU:HA	1:D:580:HIS:O	2.21	0.40
1:A:468:VAL:HG21	1:A:487:TRP:CE2	2.57	0.40
2:B:1001:ANP:O2A	4:B:1004:873:C06	2.69	0.40
1:B:678:ARG:O	1:B:693:VAL:HA	2.20	0.40
1:C:685:ASP:HB3	1:C:690:THR:O	2.22	0.40
1:A:710:ALA:HB3	1:A:711:PRO:HD3	2.04	0.40
1:B:523:VAL:CG2	1:B:543:VAL:CG2	2.99	0.40
1:C:798:LEU:HA	1:C:798:LEU:HD23	1.87	0.40
1:D:588:SER:C	1:D:589:TRP:CD1	2.95	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	477/500 (95%)	457 (96%)	20 (4%)	0	100	100
1	B	470/500 (94%)	448 (95%)	22 (5%)	0	100	100
1	C	472/500 (94%)	461 (98%)	10 (2%)	1 (0%)	47	68
1	D	466/500 (93%)	448 (96%)	18 (4%)	0	100	100
All	All	1885/2000 (94%)	1814 (96%)	70 (4%)	1 (0%)	51	73

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	438	PRO

### 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	408/436 (94%)	401 (98%)	7 (2%)	60	82
1	B	396/436 (91%)	388 (98%)	8 (2%)	55	79
1	C	408/436 (94%)	404 (99%)	4 (1%)	76	90
1	D	395/436 (91%)	389 (98%)	6 (2%)	65	85
All	All	1607/1744 (92%)	1582 (98%)	25 (2%)	62	84

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

Mol	Chain	Res	Type
1	A	341	ASN
1	A	471	TRP
1	A	487	TRP
1	A	488	GLN
1	A	589	TRP
1	A	762	ASP
1	A	814	PHE
1	B	403	HIS
1	B	437	ARG
1	B	471	TRP

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Mol	Chain	Res	Type
1	B	487	TRP
1	B	488	GLN
1	B	583	LEU
1	B	589	TRP
1	B	645	MET
1	C	471	TRP
1	C	487	TRP
1	C	488	GLN
1	C	589	TRP
1	D	487	TRP
1	D	488	GLN
1	D	527	GLU
1	D	589	TRP
1	D	758	PRO
1	D	813	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	555	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](#)

Of 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 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
4	873	A	1004	-	24,24,24	1.14	3 (12%)	23,33,33	0.97	1 (4%)
4	873	C	1004	-	24,24,24	1.92	6 (25%)	23,33,33	1.06	2 (8%)
2	ANP	A	1001	3	29,33,33	1.80	4 (13%)	31,52,52	1.07	2 (6%)
2	ANP	B	1001	3	29,33,33	1.65	3 (10%)	31,52,52	0.87	1 (3%)
2	ANP	D	1001	3	29,33,33	1.68	3 (10%)	31,52,52	0.95	1 (3%)
4	873	B	1004	-	24,24,24	1.80	3 (12%)	23,33,33	1.03	1 (4%)
4	873	D	1004	-	24,24,24	1.11	1 (4%)	23,33,33	1.12	2 (8%)
2	ANP	C	1001	3	29,33,33	2.17	5 (17%)	31,52,52	1.03	1 (3%)

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
4	873	A	1004	-	-	2/8/19/19	1/3/3/3
4	873	C	1004	-	-	3/8/19/19	1/3/3/3
2	ANP	A	1001	3	-	5/14/38/38	0/3/3/3
2	ANP	B	1001	3	-	4/14/38/38	0/3/3/3
2	ANP	D	1001	3	-	5/14/38/38	0/3/3/3
4	873	B	1004	-	-	2/8/19/19	1/3/3/3
4	873	D	1004	-	-	1/8/19/19	1/3/3/3
2	ANP	C	1001	3	-	8/14/38/38	0/3/3/3

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1001	ANP	PB-O1B	6.47	1.56	1.46
2	C	1001	ANP	PB-O1B	6.47	1.56	1.46
2	C	1001	ANP	PG-O1G	6.44	1.56	1.46
2	A	1001	ANP	PG-O1G	6.42	1.56	1.46
2	D	1001	ANP	PG-O1G	6.40	1.56	1.46
4	B	1004	873	C20-C04	6.13	1.58	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	1004	873	C20-C04	4.70	1.57	1.52
4	C	1004	873	C07-N08	-4.40	1.43	1.48
2	C	1001	ANP	PG-O3G	-3.88	1.46	1.56
2	D	1001	ANP	PG-O3G	-3.86	1.46	1.56
2	A	1001	ANP	PG-O3G	-3.85	1.46	1.56
2	B	1001	ANP	PB-O2B	-3.85	1.46	1.56
2	C	1001	ANP	PB-O2B	-3.84	1.46	1.56
2	A	1001	ANP	PB-O3A	3.73	1.63	1.59
2	A	1001	ANP	O4'-C1'	3.72	1.46	1.41
2	D	1001	ANP	O4'-C1'	3.70	1.46	1.41
4	C	1004	873	C04-N03	-3.69	1.42	1.47
4	D	1004	873	C17-C12	3.58	1.48	1.41
4	B	1004	873	C17-C12	3.55	1.48	1.41
2	C	1001	ANP	O4'-C1'	3.21	1.45	1.41
2	B	1001	ANP	O4'-C1'	3.13	1.45	1.41
4	B	1004	873	C01-C21	2.79	1.60	1.53
4	C	1004	873	C17-C12	2.74	1.46	1.41
4	C	1004	873	C16-C11	-2.59	1.37	1.41
4	A	1004	873	O18-C17	-2.45	1.18	1.24
4	A	1004	873	C15-C16	2.15	1.41	1.36
4	A	1004	873	C14-C13	2.12	1.41	1.36
4	C	1004	873	C05-C04	2.11	1.56	1.52

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1001	ANP	O2G-PG-O1G	-3.15	105.54	113.45
2	A	1001	ANP	O2G-PG-O1G	-3.14	105.55	113.45
2	D	1001	ANP	O2G-PG-O1G	-3.12	105.60	113.45
4	D	1004	873	C09-N10-C11	2.96	119.24	116.69
4	D	1004	873	C06-C05-C04	-2.85	109.49	115.22
4	B	1004	873	C09-N10-C11	2.81	119.12	116.69
4	C	1004	873	C09-N10-C11	2.78	119.09	116.69
2	A	1001	ANP	C5'-C4'-C3'	-2.70	105.06	115.18
2	B	1001	ANP	O1G-PG-N3B	-2.55	108.02	111.77
4	C	1004	873	C06-C05-C04	-2.32	110.55	115.22
4	A	1004	873	C13-C12-C11	2.02	120.49	117.55

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1004	873	N03-C04-C05-C06
4	C	1004	873	N03-C04-C05-C06
2	A	1001	ANP	PB-N3B-PG-O1G
2	B	1001	ANP	PG-N3B-PB-O1B
2	D	1001	ANP	PB-N3B-PG-O1G
2	D	1001	ANP	C5'-O5'-PA-O2A
4	B	1004	873	C05-C06-C07-N08
4	D	1004	873	N03-C04-C05-C06
2	C	1001	ANP	PB-N3B-PG-O1G
2	C	1001	ANP	PG-N3B-PB-O1B
2	C	1001	ANP	PG-N3B-PB-O3A
2	C	1001	ANP	O4'-C4'-C5'-O5'
4	B	1004	873	O19-C06-C07-N08
2	A	1001	ANP	O4'-C4'-C5'-O5'
2	A	1001	ANP	C4'-C5'-O5'-PA
2	B	1001	ANP	C4'-C5'-O5'-PA
2	D	1001	ANP	C5'-O5'-PA-O3A
2	D	1001	ANP	C5'-O5'-PA-O1A
2	C	1001	ANP	C5'-O5'-PA-O1A
2	C	1001	ANP	C4'-C5'-O5'-PA
2	C	1001	ANP	C3'-C4'-C5'-O5'
4	A	1004	873	C20-C04-C05-C06
4	C	1004	873	C20-C04-C05-C06
2	A	1001	ANP	C5'-O5'-PA-O3A
2	B	1001	ANP	C5'-O5'-PA-O3A
2	C	1001	ANP	C5'-O5'-PA-O3A
4	C	1004	873	O19-C06-C07-N08
2	A	1001	ANP	C5'-O5'-PA-O1A
2	B	1001	ANP	C5'-O5'-PA-O1A
2	D	1001	ANP	C4'-C5'-O5'-PA

All (4) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1004	873	C01-C02-C04-C20-C21-N03
4	C	1004	873	C01-C02-C04-C20-C21-N03
4	D	1004	873	C01-C02-C04-C20-C21-N03
4	A	1004	873	C01-C02-C04-C20-C21-N03

8 monomers are involved in 17 short contacts:

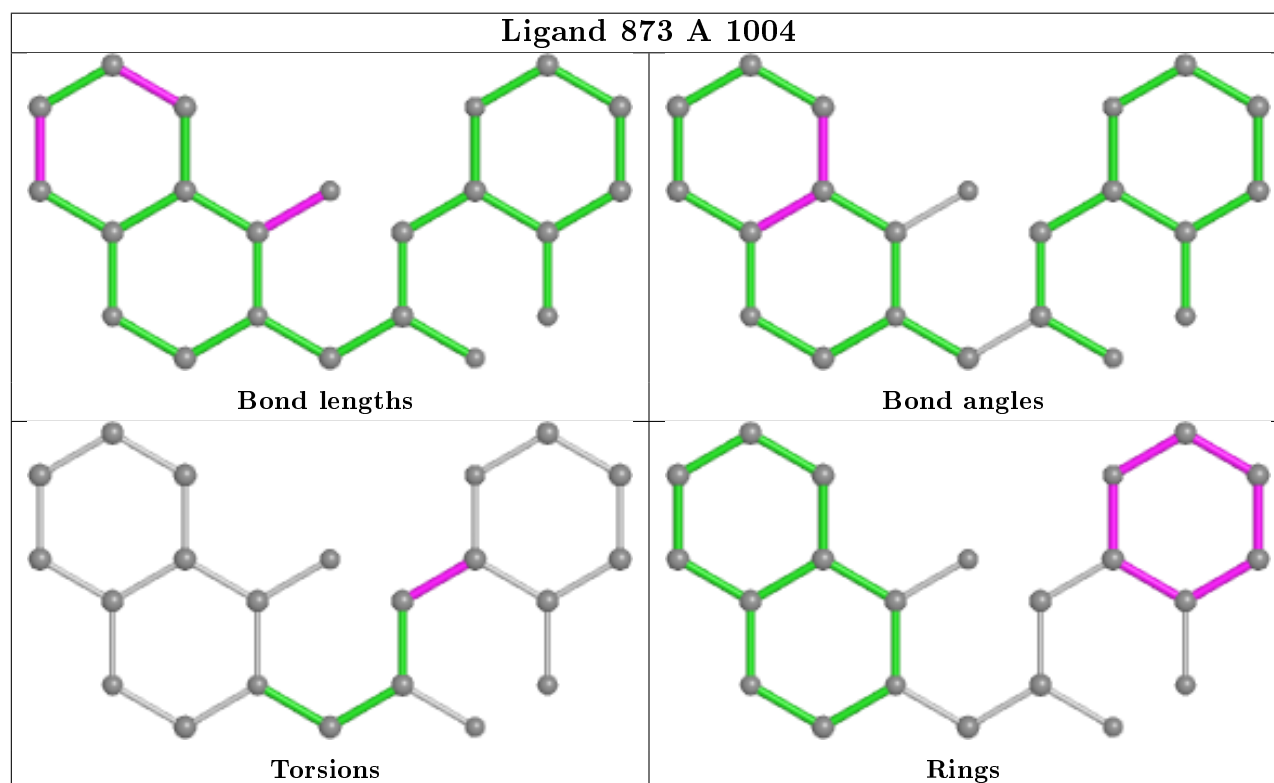
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1004	873	1	0

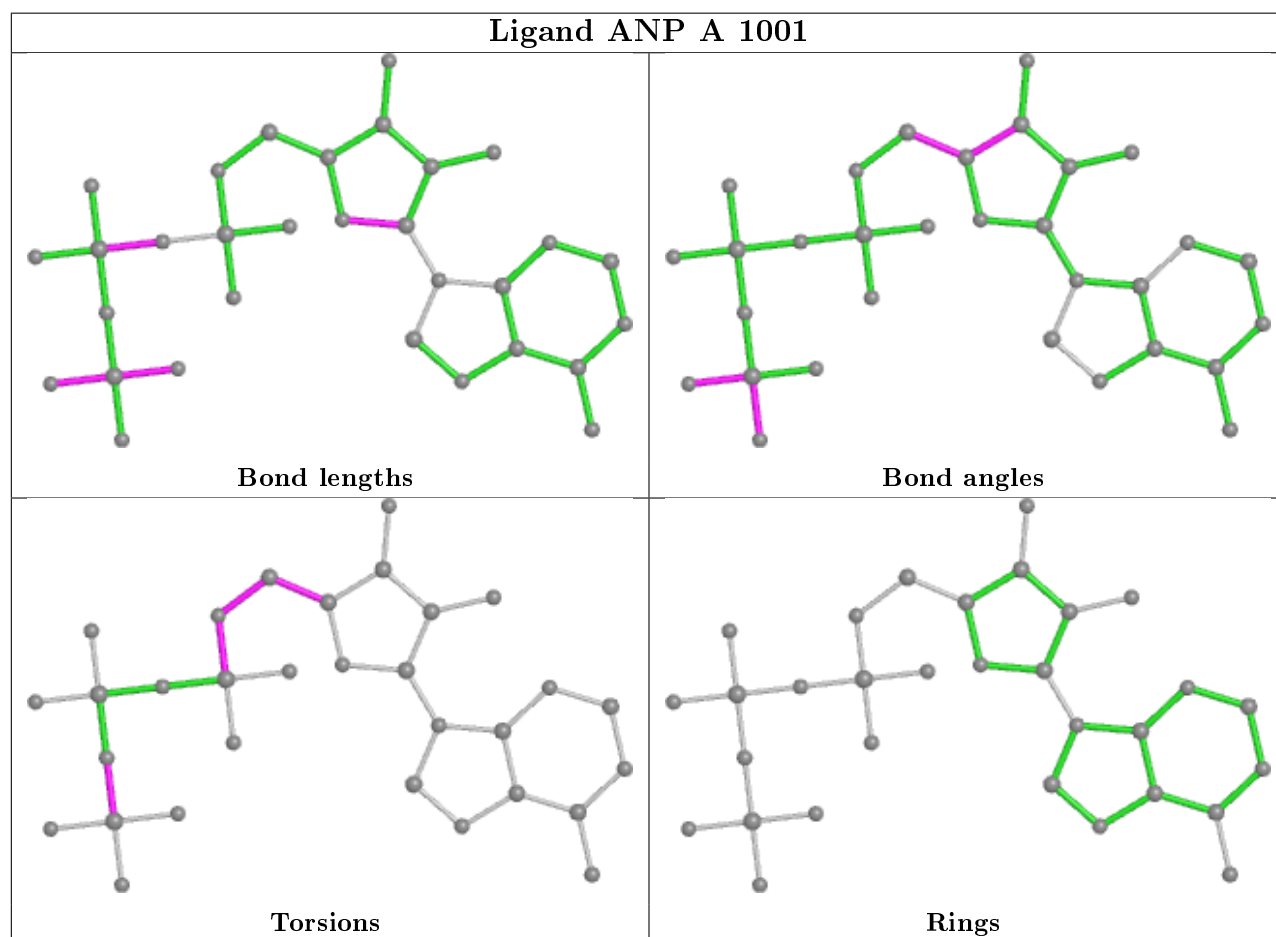
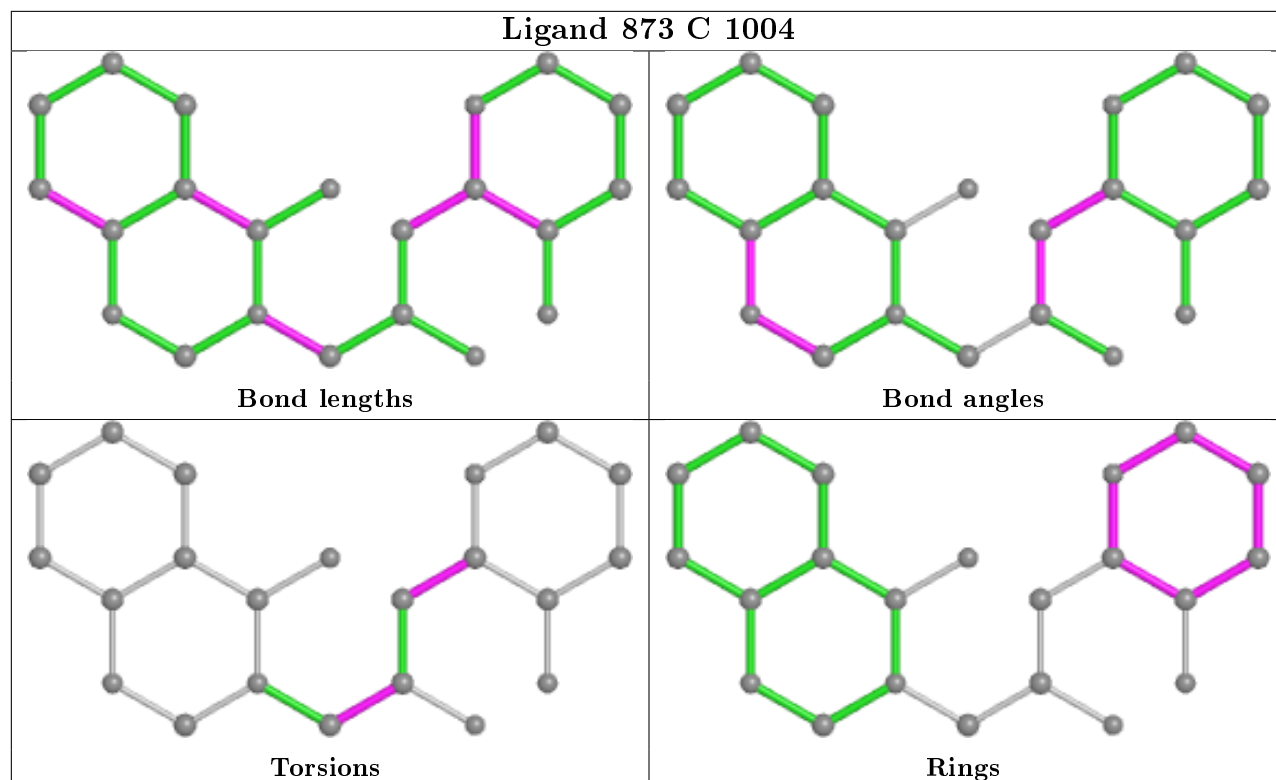
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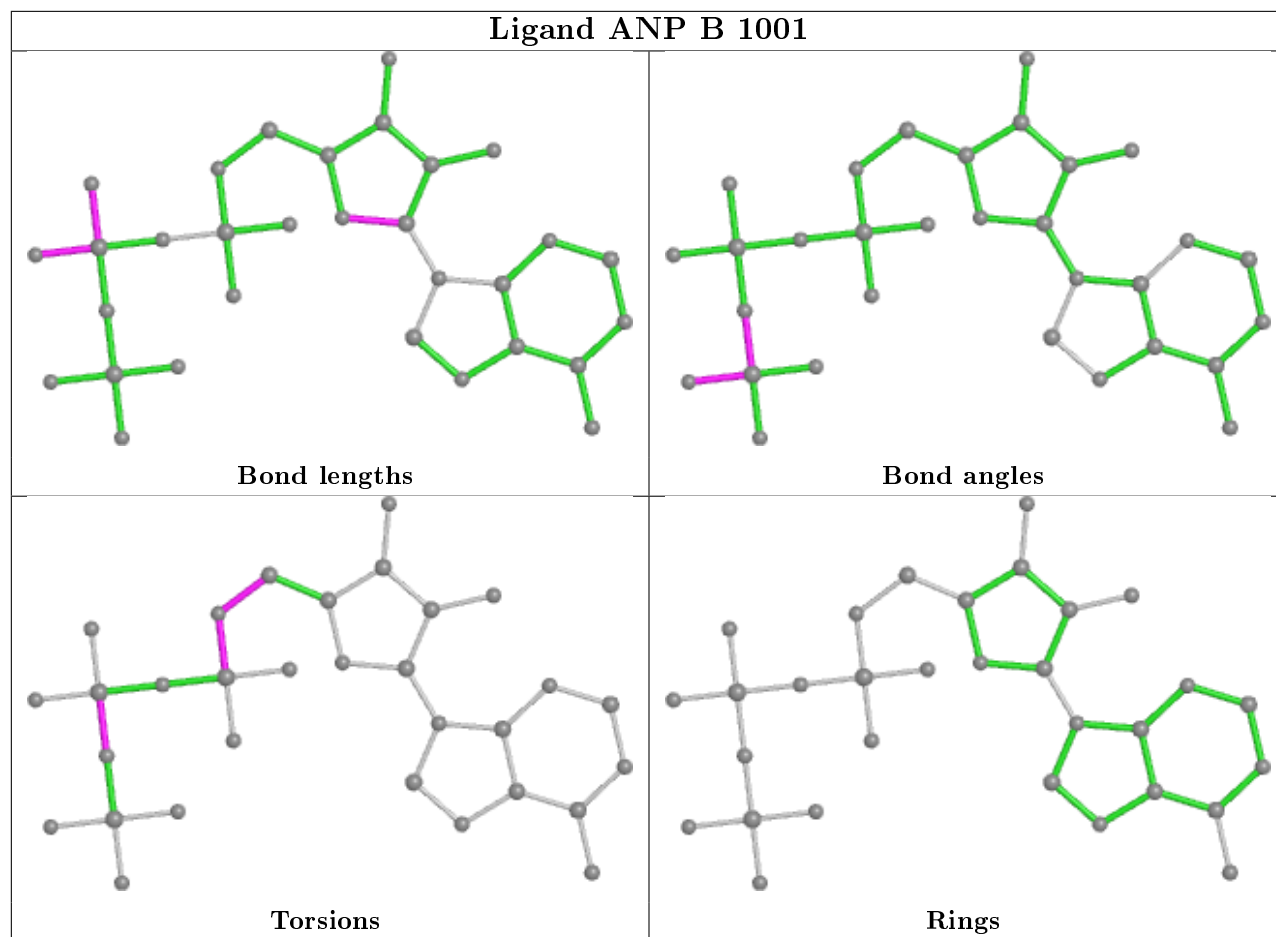
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	1004	873	2	0
2	A	1001	ANP	2	0
2	B	1001	ANP	7	0
2	D	1001	ANP	2	0
4	B	1004	873	4	0
4	D	1004	873	2	0
2	C	1001	ANP	1	0

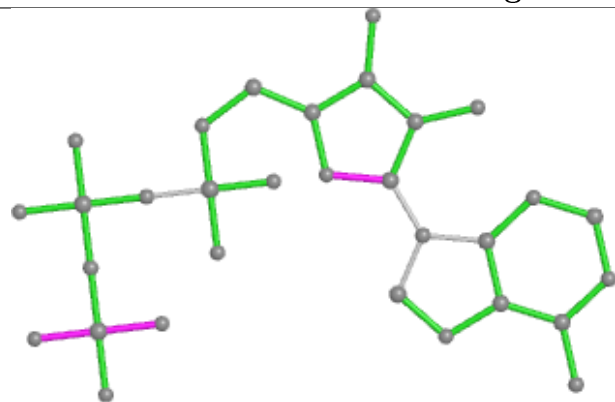
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



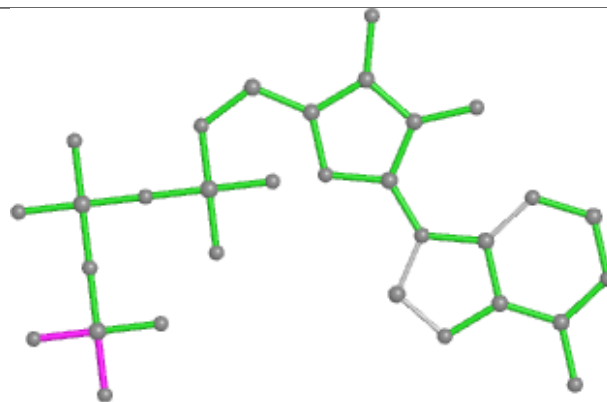




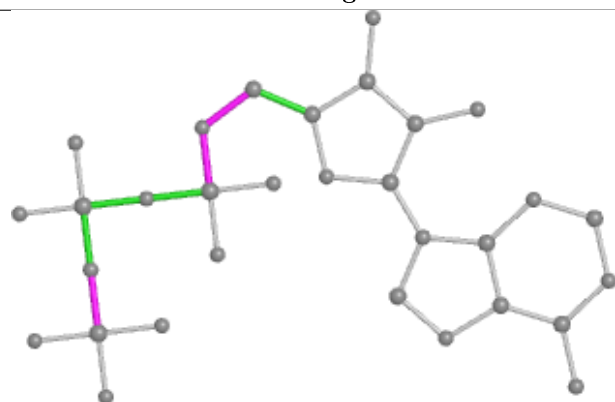
## Ligand ANP D 1001



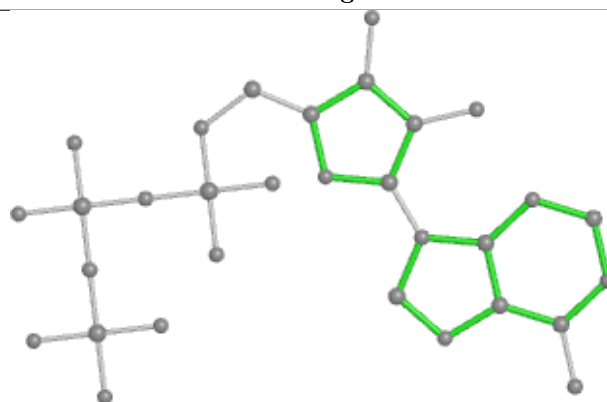
Bond lengths



Bond angles

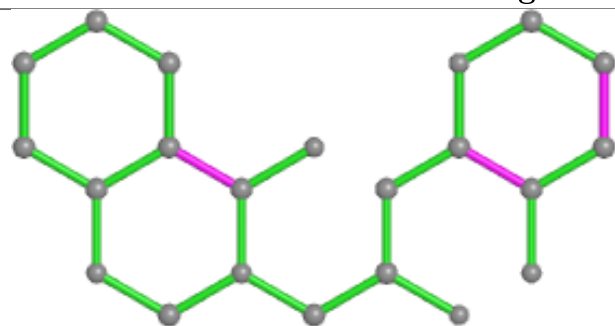


Torsions

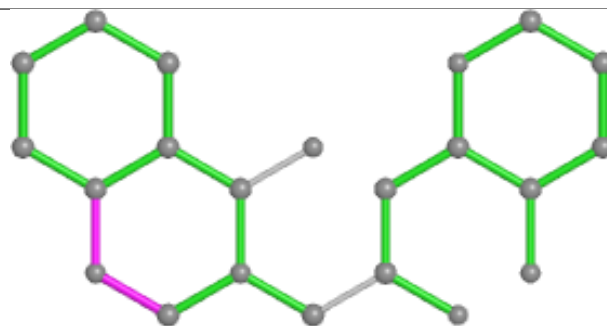


Rings

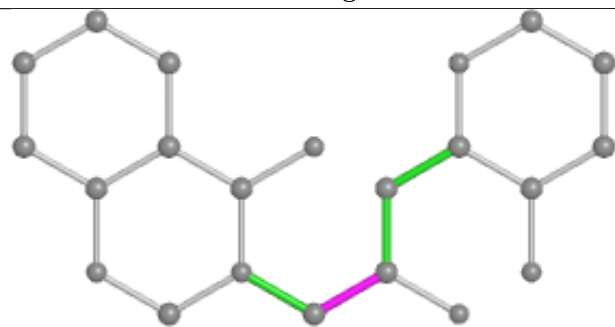
## Ligand 873 B 1004



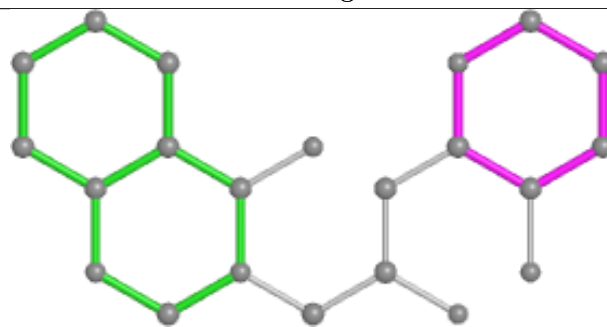
Bond lengths



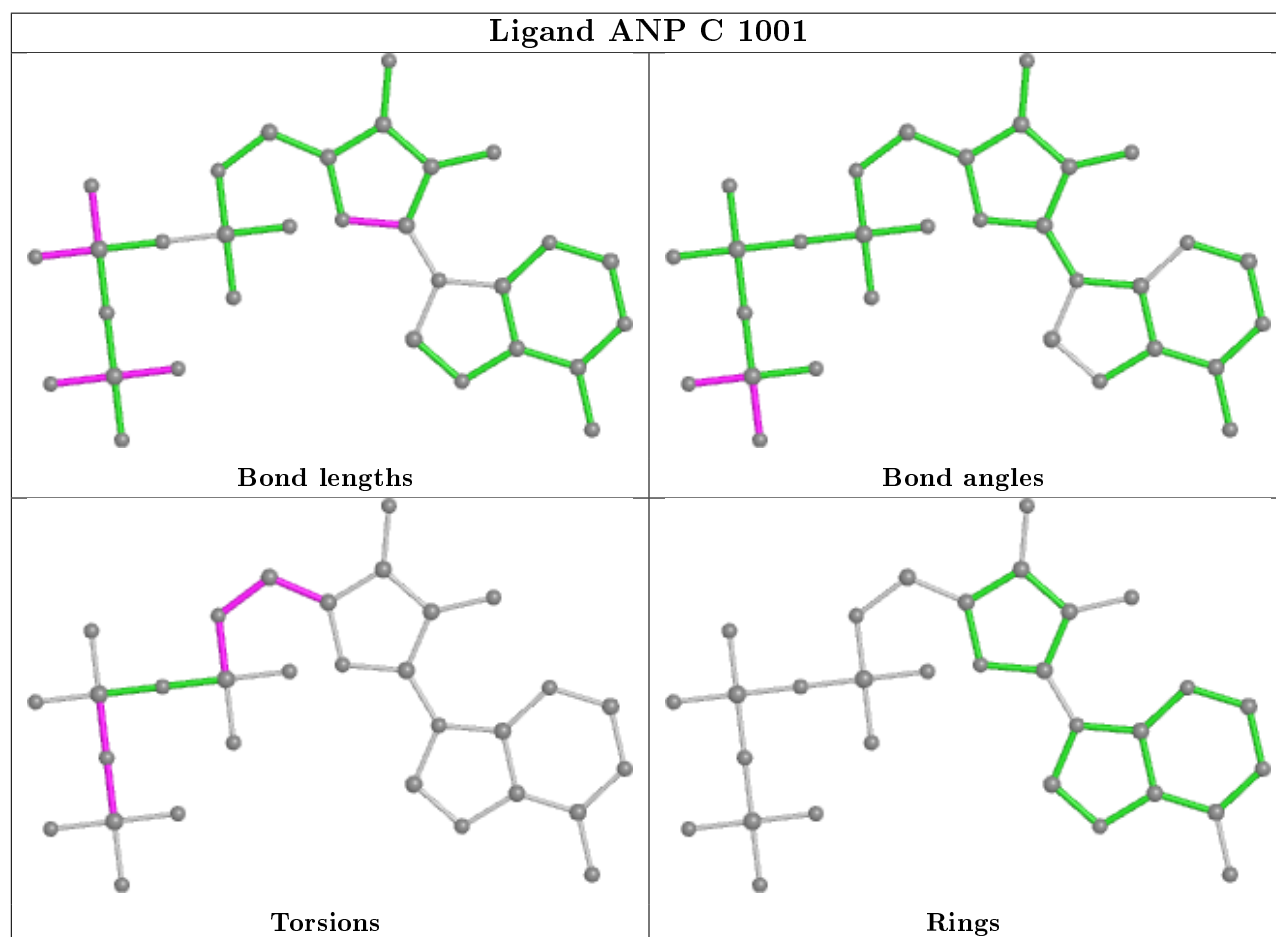
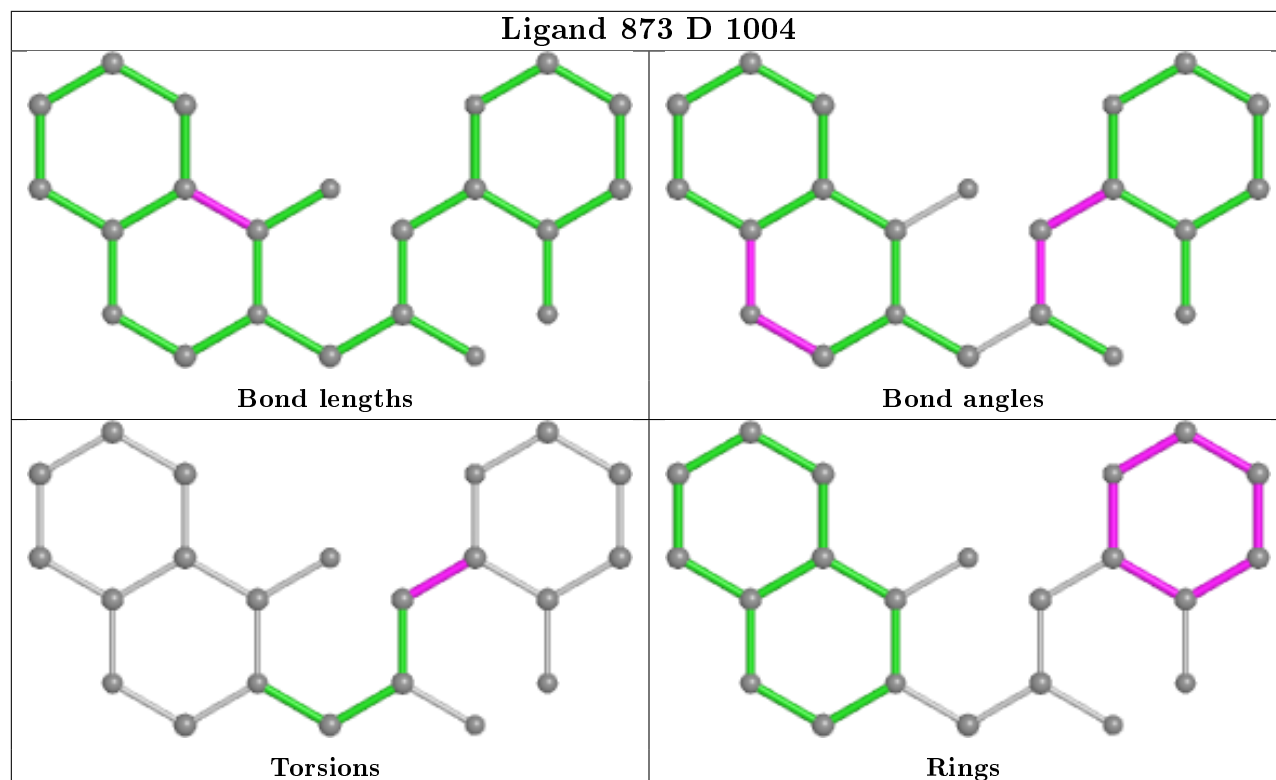
Bond angles



Torsions



Rings



## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<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	482/500 (96%)	-0.33	1 (0%) 95 95	17, 29, 54, 91	2 (0%)
1	B	478/500 (95%)	-0.10	7 (1%) 73 75	21, 37, 70, 95	1 (0%)
1	C	477/500 (95%)	-0.14	1 (0%) 95 95	17, 34, 62, 80	1 (0%)
1	D	472/500 (94%)	-0.05	9 (1%) 66 69	17, 38, 69, 98	0
All	All	1909/2000 (95%)	-0.16	18 (0%) 84 86	17, 34, 66, 98	4 (0%)

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	810	GLY	5.5
1	A	331	GLY	3.8
1	B	687	ALA	3.5
1	D	808	PRO	2.8
1	C	687	ALA	2.7
1	B	455	HIS	2.4
1	B	574	PHE	2.4
1	B	627	PHE	2.4
1	B	760	CYS	2.3
1	D	778	GLU	2.2
1	D	779	ILE	2.2
1	D	660	ASN	2.1
1	D	710	ALA	2.1
1	B	706	TRP	2.1
1	D	815	TYR	2.1
1	D	334	VAL	2.0
1	D	742	PHE	2.0
1	B	579	GLY	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](#)

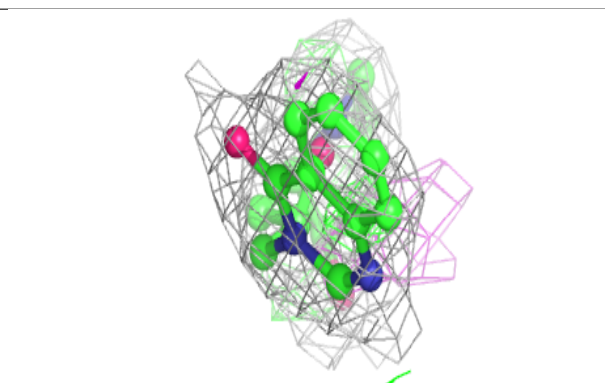
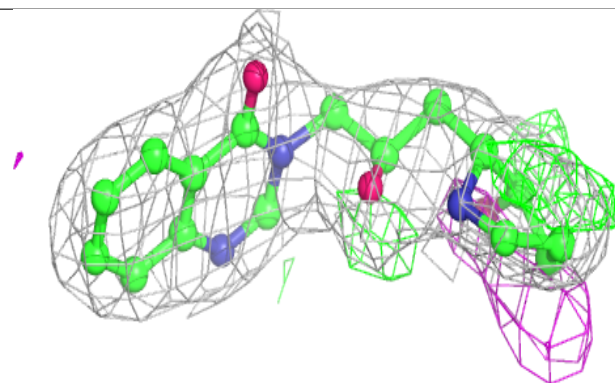
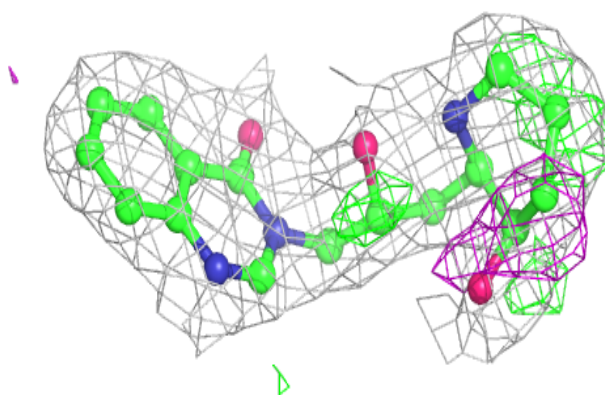
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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	MG	A	1002	1/1	0.79	0.08	21,21,21,21	0
3	MG	A	1003	1/1	0.88	0.06	37,37,37,37	0
4	873	D	1004	22/22	0.89	0.19	24,26,30,34	0
3	MG	D	1002	1/1	0.89	0.09	22,22,22,22	0
4	873	C	1004	22/22	0.90	0.16	26,28,32,32	0
4	873	A	1004	22/22	0.92	0.16	23,27,28,29	0
3	MG	B	1003	1/1	0.93	0.06	38,38,38,38	0
2	ANP	A	1001	31/31	0.93	0.17	17,19,21,22	0
2	ANP	B	1001	31/31	0.94	0.18	20,23,26,30	0
4	873	B	1004	22/22	0.94	0.16	20,24,27,31	0
2	ANP	D	1001	31/31	0.95	0.16	23,25,30,34	0
2	ANP	C	1001	31/31	0.96	0.14	22,24,28,31	0
3	MG	C	1002	1/1	0.97	0.04	23,23,23,23	0
3	MG	C	1003	1/1	0.97	0.04	42,42,42,42	0
3	MG	D	1003	1/1	0.97	0.10	38,38,38,38	0
3	MG	B	1002	1/1	0.98	0.10	24,24,24,24	0

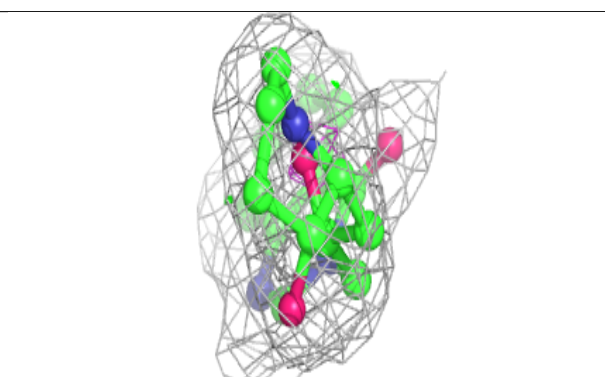
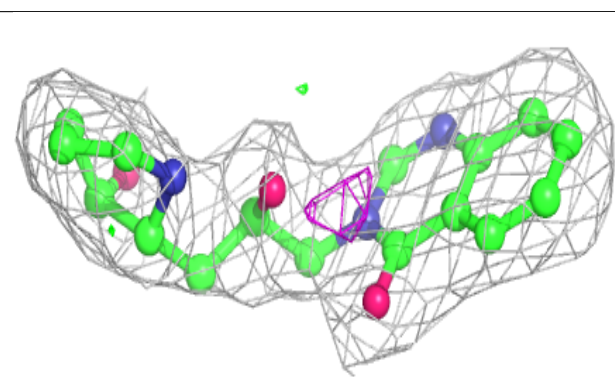
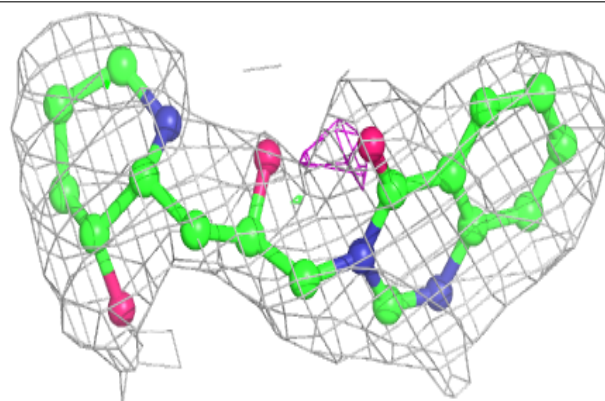
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around 873 D 1004:**

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

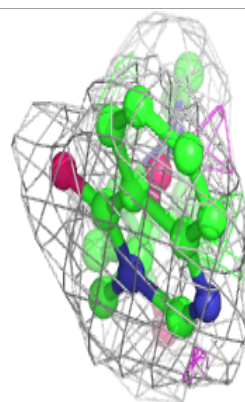
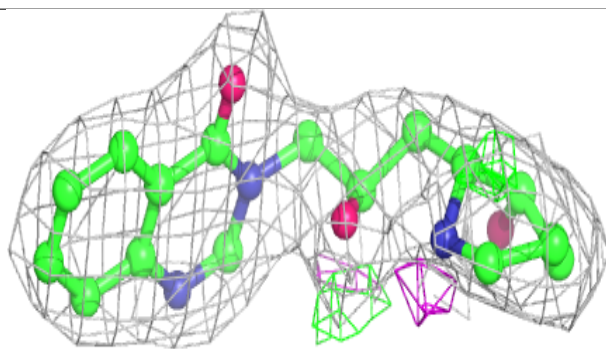
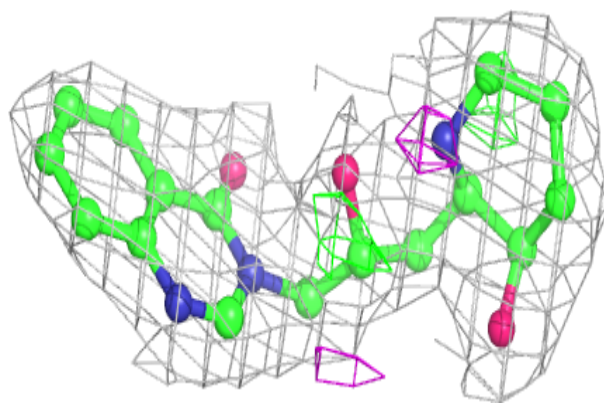
**Electron density around 873 C 1004:**

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



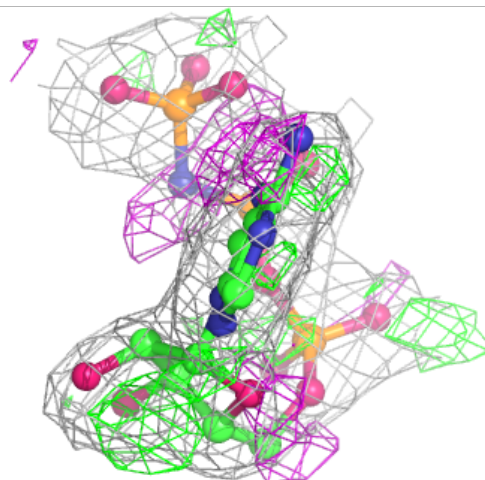
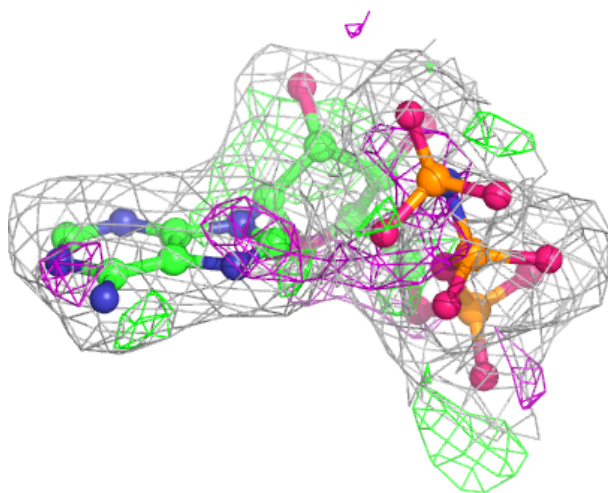
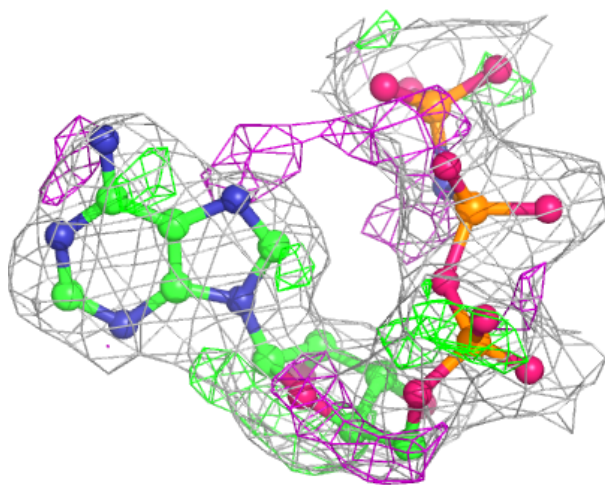
**Electron density around 873 A 1004:**

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



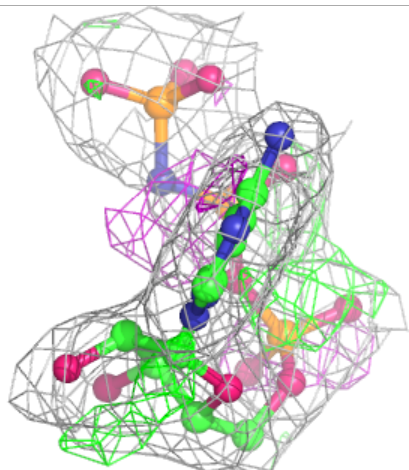
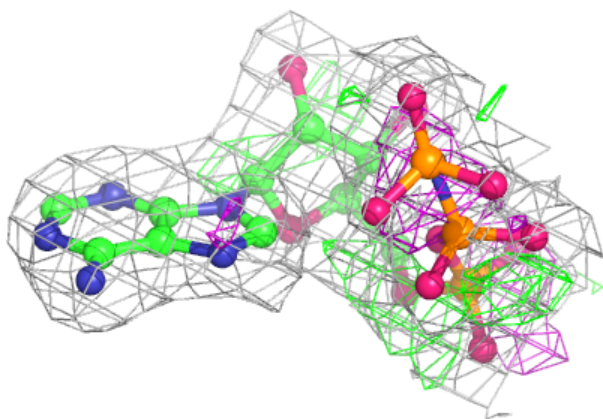
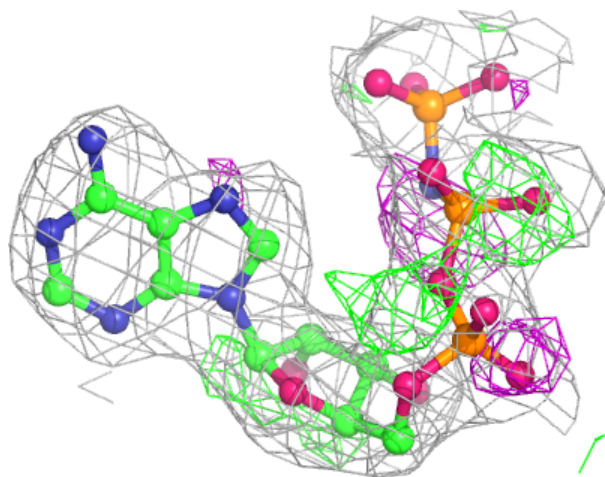
**Electron density around ANP A 1001:**

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



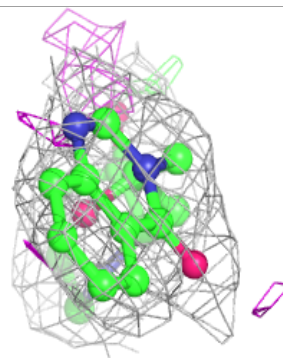
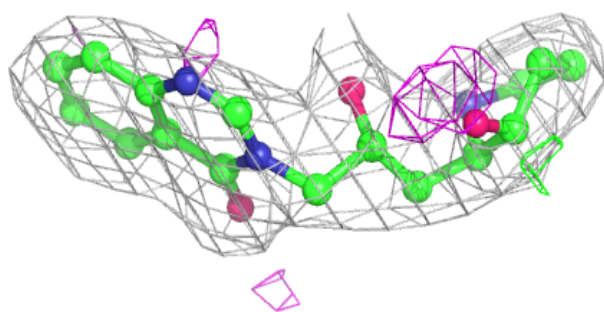
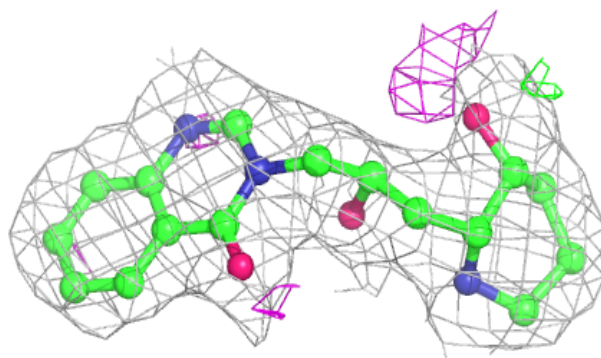
**Electron density around ANP B 1001:**

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



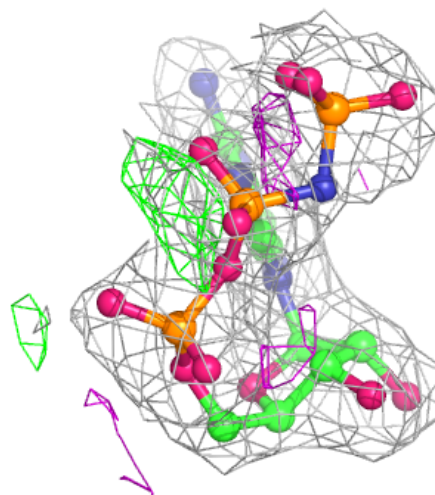
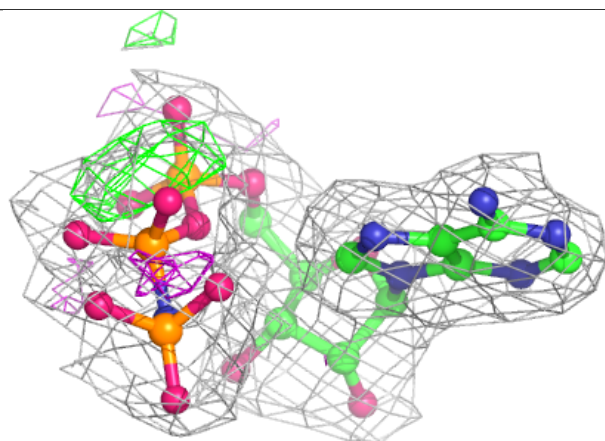
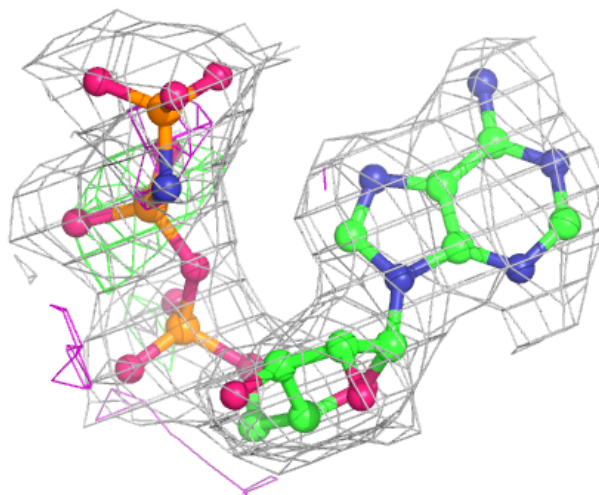
**Electron density around 873 B 1004:**

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



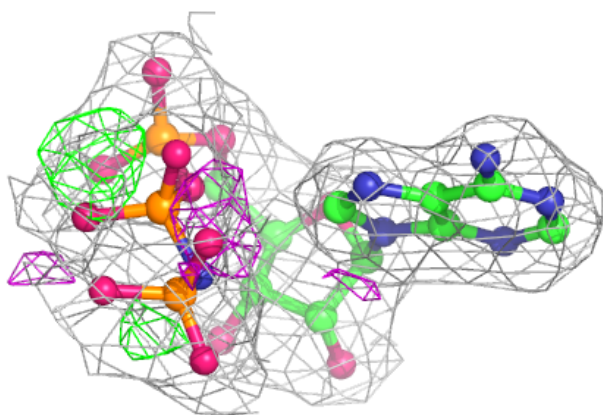
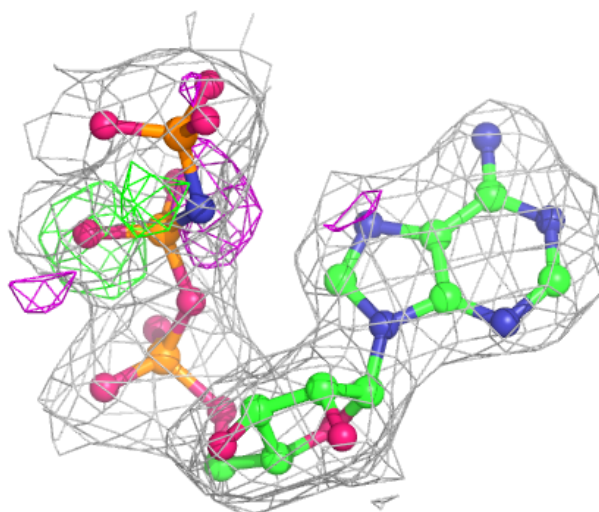
**Electron density around ANP D 1001:**

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



**Electron density around ANP C 1001:**

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



## 6.5 Other polymers ⓘ

There are no such residues in this entry.