



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 07:08 AM UTC

PDB ID : 4A59 / pdb_00004a59
Title : Crystal structure of Toxoplasma gondii nucleoside triphosphate diphosphohydrolase 3 (NTPDase3) in complex with AMP
Authors : Krug, U.; Zebisch, M.; Straeter, N.
Deposited on : 2011-10-24
Resolution : 2.20 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

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>.

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

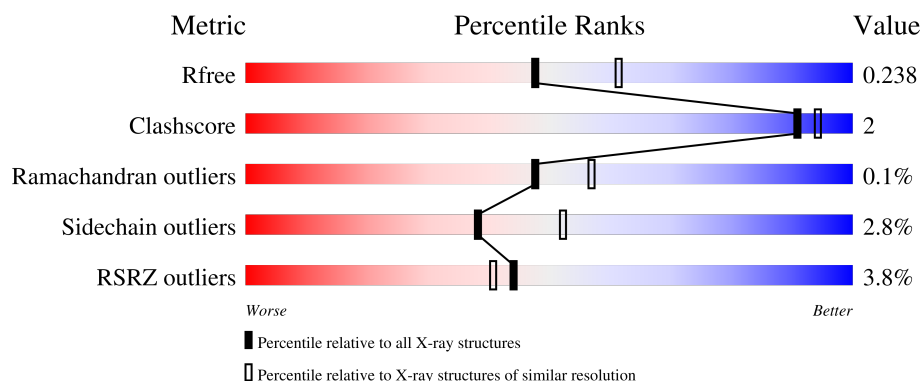
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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 ≥ 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	611	4% 89% 8% .
1	B	611	6% 89% 8% .
1	C	611	2% 87% 9% ..
1	D	611	3% 88% 9% ..

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 19482 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 NUCLEOSIDE-TRIPHOSPHATASE 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	593	Total	C	N	O	S	0	7	0
			4650	2923	825	875	27			
1	B	593	Total	C	N	O	S	0	2	0
			4612	2899	818	868	27			
1	C	590	Total	C	N	O	S	0	1	0
			4584	2883	812	862	27			
1	D	595	Total	C	N	O	S	0	3	0
			4629	2910	820	872	27			

There are 32 discrepancies between the modelled and reference sequences:

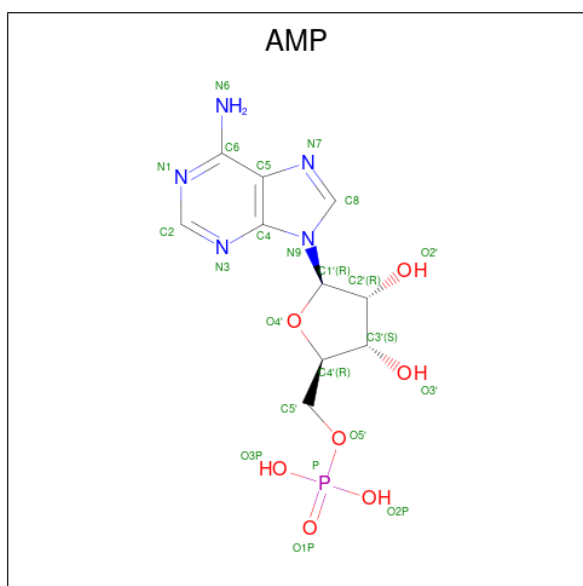
Chain	Residue	Modelled	Actual	Comment	Reference
A	25	MET	-	expression tag	UNP Q27893
A	629	GLU	-	expression tag	UNP Q27893
A	630	HIS	-	expression tag	UNP Q27893
A	631	HIS	-	expression tag	UNP Q27893
A	632	HIS	-	expression tag	UNP Q27893
A	633	HIS	-	expression tag	UNP Q27893
A	634	HIS	-	expression tag	UNP Q27893
A	635	HIS	-	expression tag	UNP Q27893
B	25	MET	-	expression tag	UNP Q27893
B	629	GLU	-	expression tag	UNP Q27893
B	630	HIS	-	expression tag	UNP Q27893
B	631	HIS	-	expression tag	UNP Q27893
B	632	HIS	-	expression tag	UNP Q27893
B	633	HIS	-	expression tag	UNP Q27893
B	634	HIS	-	expression tag	UNP Q27893
B	635	HIS	-	expression tag	UNP Q27893
C	25	MET	-	expression tag	UNP Q27893
C	629	GLU	-	expression tag	UNP Q27893
C	630	HIS	-	expression tag	UNP Q27893
C	631	HIS	-	expression tag	UNP Q27893
C	632	HIS	-	expression tag	UNP Q27893

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Chain	Residue	Modelled	Actual	Comment	Reference
C	633	HIS	-	expression tag	UNP Q27893
C	634	HIS	-	expression tag	UNP Q27893
C	635	HIS	-	expression tag	UNP Q27893
D	25	MET	-	expression tag	UNP Q27893
D	629	GLU	-	expression tag	UNP Q27893
D	630	HIS	-	expression tag	UNP Q27893
D	631	HIS	-	expression tag	UNP Q27893
D	632	HIS	-	expression tag	UNP Q27893
D	633	HIS	-	expression tag	UNP Q27893
D	634	HIS	-	expression tag	UNP Q27893
D	635	HIS	-	expression tag	UNP Q27893

- Molecule 2 is ADENOSINE MONOPHOSPHATE (CCD ID: AMP) (formula: $C_{10}H_{14}N_5O_7P$).



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

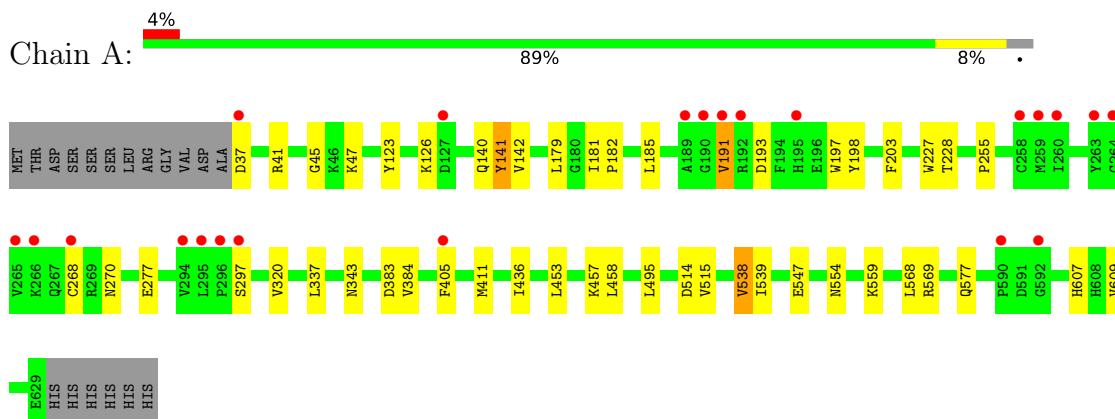
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	307	Total 310	O 310	0	3
3	B	166	Total 169	O 169	0	3
3	C	225	Total 226	O 226	0	1
3	D	186	Total 187	O 187	0	1

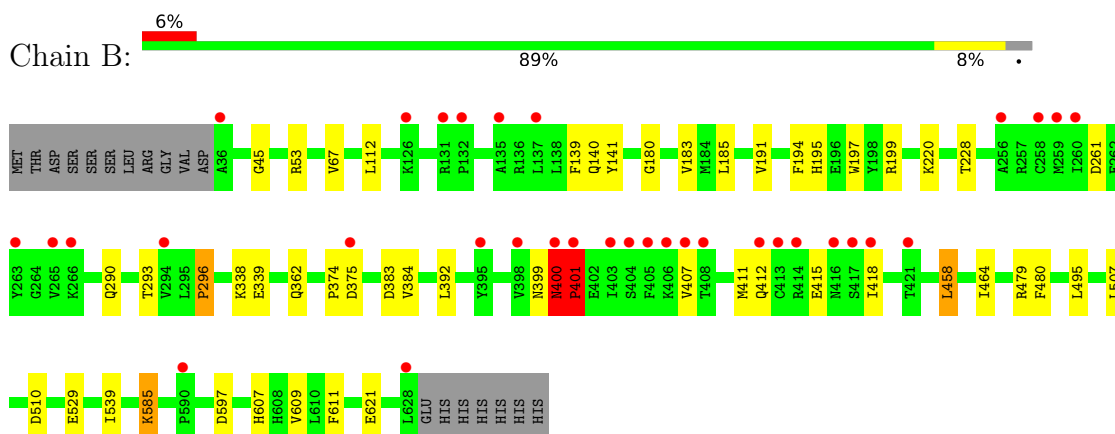
3 Residue-property plots [i](#)

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.

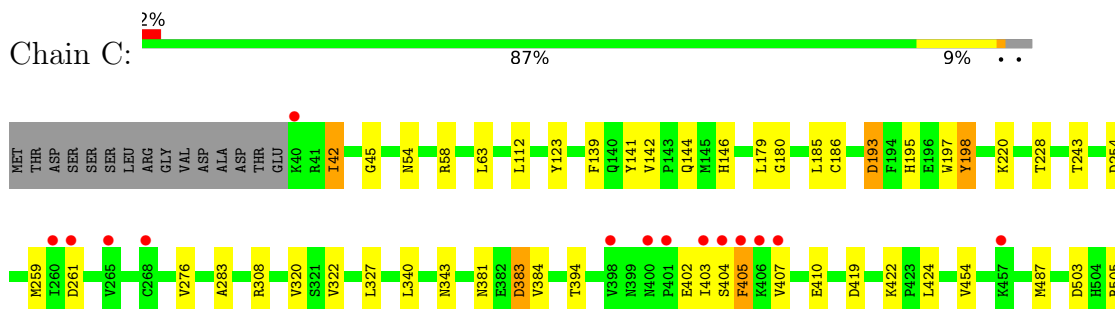
• Molecule 1: NUCLEOSIDE-TRIPHOSPHATASE 1



• Molecule 1: NUCLEOSIDE-TRIPHOSPHATASE 1



• Molecule 1: NUCLEOSIDE-TRIPHOSPHATASE 1





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	89.17Å 166.03Å 97.94Å 90.00° 97.15° 90.00°	Depositor
Resolution (Å)	42.30 – 2.20 42.30 – 2.20	Depositor EDS
% Data completeness (in resolution range)	(Not available) (42.30-2.20) 99.7 (42.30-2.20)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.03 (at 2.20Å)	Xtriage
Refinement program	BUSTER 2.8.0	Depositor
R, R_{free}	0.180 , 0.228 0.189 , 0.238	Depositor DCC
R_{free} test set	1399 reflections (0.98%)	wwPDB-VP
Wilson B-factor (Å ²)	30.7	Xtriage
Anisotropy	0.156	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 45.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	19482	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.30% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: AMP

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	0.87	1/4760 (0.0%)	1.31	22/6439 (0.3%)
1	B	0.81	0/4707	1.36	27/6369 (0.4%)
1	C	0.85	1/4676 (0.0%)	1.33	23/6327 (0.4%)
1	D	0.83	0/4727	1.32	22/6397 (0.3%)
All	All	0.84	2/18870 (0.0%)	1.33	94/25532 (0.4%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	142	VAL	CA-C	6.40	1.58	1.52
1	C	142	VAL	CA-C	5.53	1.57	1.52

All (94) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	193	ASP	N-CA-C	7.91	122.24	112.59
1	D	198	TYR	N-CA-C	7.47	119.06	111.07
1	A	141	TYR	CA-C-N	7.30	124.84	120.24
1	A	141	TYR	C-N-CA	7.30	124.84	120.24
1	A	383	ASP	CA-CB-CG	7.00	119.60	112.60
1	C	198	TYR	N-CA-C	6.97	119.48	111.11
1	A	179	LEU	N-CA-C	6.88	119.80	111.82
1	C	261	ASP	CA-CB-CG	6.70	119.30	112.60
1	B	112	LEU	CA-C-N	6.46	129.23	120.38
1	B	112	LEU	C-N-CA	6.46	129.23	120.38
1	B	375	ASP	CA-CB-CG	6.45	119.05	112.60
1	C	193	ASP	N-CA-C	6.35	120.73	112.92
1	B	141	TYR	CA-C-N	6.33	125.40	120.33
1	B	141	TYR	C-N-CA	6.33	125.40	120.33
1	B	401	PRO	CA-C-N	6.27	132.66	120.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	401	PRO	C-N-CA	6.27	132.66	120.99
1	C	112	LEU	CA-C-N	6.21	128.89	120.38
1	C	112	LEU	C-N-CA	6.21	128.89	120.38
1	B	261	ASP	CA-CB-CG	6.14	118.74	112.60
1	A	198	TYR	N-CA-C	6.14	118.51	111.02
1	B	383	ASP	CA-CB-CG	6.13	118.73	112.60
1	A	181	ILE	N-CA-C	6.13	114.22	108.15
1	D	194	PHE	N-CA-C	6.12	118.04	111.36
1	A	320	VAL	N-CA-C	-5.93	100.04	108.58
1	A	383	ASP	CA-C-N	5.92	128.57	120.46
1	A	383	ASP	C-N-CA	5.92	128.57	120.46
1	B	194	PHE	N-CA-C	5.91	118.96	111.69
1	D	608	HIS	CA-C-N	5.90	129.80	120.47
1	D	608	HIS	C-N-CA	5.90	129.80	120.47
1	C	146	HIS	CA-C-N	5.83	128.09	120.28
1	C	146	HIS	C-N-CA	5.83	128.09	120.28
1	B	195	HIS	N-CA-C	5.81	119.58	111.74
1	A	270	ASN	CA-CB-CG	5.79	118.39	112.60
1	C	611	PHE	CA-C-N	5.78	130.37	121.19
1	C	611	PHE	C-N-CA	5.78	130.37	121.19
1	D	195	HIS	N-CA-C	5.71	119.82	112.86
1	A	126	LYS	N-CA-C	5.65	118.98	111.75
1	C	343	ASN	CA-C-N	5.64	128.62	120.38
1	C	343	ASN	C-N-CA	5.64	128.62	120.38
1	D	215	PRO	CA-C-N	5.62	128.09	120.38
1	D	215	PRO	C-N-CA	5.62	128.09	120.38
1	A	453	LEU	N-CA-C	5.60	120.13	112.68
1	C	503	ASP	CA-CB-CG	5.60	118.20	112.60
1	B	400	ASN	N-CA-C	5.57	122.12	109.81
1	D	179	LEU	N-CA-C	5.53	119.75	112.89
1	B	374	PRO	CA-C-N	5.52	128.44	120.38
1	B	374	PRO	C-N-CA	5.52	128.44	120.38
1	C	141	TYR	CA-C-N	5.52	123.72	120.24
1	C	141	TYR	C-N-CA	5.52	123.72	120.24
1	B	296	PRO	CA-C-N	5.51	127.93	120.38
1	B	296	PRO	C-N-CA	5.51	127.93	120.38
1	A	514	ASP	CA-C-N	5.50	127.50	120.56
1	A	514	ASP	C-N-CA	5.50	127.50	120.56
1	C	197	TRP	CA-C-N	5.42	127.86	120.54
1	C	197	TRP	C-N-CA	5.42	127.86	120.54
1	C	601	GLN	N-CA-C	5.42	116.87	111.07
1	A	539	ILE	N-CA-C	-5.42	99.44	107.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	320	VAL	N-CA-C	-5.41	99.95	108.23
1	D	533	ARG	CA-C-N	5.38	127.43	120.44
1	D	533	ARG	C-N-CA	5.38	127.43	120.44
1	B	585	LYS	N-CA-C	-5.35	106.88	113.41
1	C	195	HIS	N-CA-C	5.34	118.81	111.54
1	B	611	PHE	CA-C-N	5.29	129.61	121.19
1	B	611	PHE	C-N-CA	5.29	129.61	121.19
1	D	112	LEU	CA-C-N	5.29	127.63	120.38
1	D	112	LEU	C-N-CA	5.29	127.63	120.38
1	C	320	VAL	N-CA-C	-5.25	100.19	108.23
1	C	405	PHE	CA-CB-CG	5.25	119.05	113.80
1	D	514	ASP	CA-C-N	5.22	127.61	120.77
1	D	514	ASP	C-N-CA	5.22	127.61	120.77
1	B	401	PRO	N-CA-C	5.22	123.22	112.47
1	C	179	LEU	N-CA-C	5.21	118.90	112.54
1	D	261	ASP	CA-CB-CG	5.19	117.79	112.60
1	B	510	ASP	CA-CB-CG	5.18	117.78	112.60
1	C	454	VAL	N-CA-C	5.16	116.57	111.67
1	D	123	TYR	N-CA-C	5.15	119.65	112.90
1	D	188	THR	CB-CA-C	5.13	120.63	110.42
1	A	197	TRP	CA-C-N	5.10	127.89	120.79
1	A	197	TRP	C-N-CA	5.10	127.89	120.79
1	D	454	VAL	N-CA-C	5.10	115.77	110.82
1	A	203	PHE	CA-CB-CG	-5.10	108.70	113.80
1	B	539	ILE	N-CA-C	-5.07	99.83	107.73
1	D	410	GLU	CA-C-N	5.06	127.37	120.54
1	D	410	GLU	C-N-CA	5.06	127.37	120.54
1	D	463	ASN	CA-CB-CG	5.06	117.66	112.60
1	B	383	ASP	CA-C-N	5.04	127.63	120.53
1	B	383	ASP	C-N-CA	5.04	127.63	120.53
1	A	343	ASN	CA-C-N	5.02	127.51	120.28
1	A	343	ASN	C-N-CA	5.02	127.51	120.28
1	B	197	TRP	CA-C-N	5.02	127.32	120.54
1	B	197	TRP	C-N-CA	5.02	127.32	120.54
1	C	424	LEU	N-CA-C	5.01	119.64	111.37
1	A	554	ASN	CA-CB-CG	5.01	117.61	112.60
1	B	464	ILE	N-CA-C	5.01	116.98	111.77

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4650	0	4644	16	0
1	B	4612	0	4597	18	0
1	C	4584	0	4568	17	0
1	D	4629	0	4612	20	0
2	A	23	0	12	0	0
2	B	23	0	12	0	0
2	C	23	0	12	0	0
2	D	46	0	24	0	0
3	A	310	0	0	2	0
3	B	169	0	0	0	0
3	C	226	0	0	0	0
3	D	187	0	0	2	0
All	All	19482	0	18481	63	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 2.

All (63) 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:277[B]:GLU:OE1	3:A:2106[B]:HOH:O	1.54	1.23
1:B:191:VAL:HG12	1:B:199:ARG:HG3	1.71	0.71
1:B:185:LEU:HB3	1:B:228:THR:HG23	1.82	0.61
1:D:287:PHE:CB	1:D:487:MET:HE1	2.31	0.60
1:B:180:GLY:HA2	1:B:220:LYS:HB2	1.84	0.59
1:A:185:LEU:HB3	1:A:228:THR:HG23	1.85	0.59
1:C:185:LEU:HB3	1:C:228:THR:HG23	1.85	0.58
1:A:337:LEU:HD22	1:A:436:ILE:HD13	1.86	0.58
1:D:410:GLU:HG2	1:D:414:ARG:HE	1.69	0.57
1:D:392:LEU:HG	3:D:2138:HOH:O	2.04	0.56
1:A:515:VAL:HG11	1:A:569:ARG:HG3	1.87	0.56
1:B:400:ASN:HB3	1:B:401:PRO:HD3	1.88	0.56
1:A:45:GLY:HA3	1:D:139:PHE:O	2.06	0.55
1:C:381:ASN:OD1	1:C:383:ASP:HB2	2.07	0.55
1:C:402:GLU:HA	1:C:405:PHE:CE2	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:457:LYS:O	1:B:407:VAL:HG21	2.06	0.54
1:A:191:VAL:HG23	3:A:2030:HOH:O	2.08	0.54
1:D:47:LYS:O	1:D:51:THR:HG23	2.08	0.53
1:D:287:PHE:HB3	1:D:487:MET:HE1	1.90	0.53
1:A:411:MET:HE3	1:A:458:LEU:HD21	1.91	0.53
1:B:45:GLY:HA3	1:C:139:PHE:O	2.08	0.52
1:D:259:MET:HE2	1:D:291:GLU:HG2	1.90	0.52
1:C:123:TYR:OH	1:C:144:GLN:HG2	2.09	0.52
1:B:338:LYS:HE2	1:B:418:ILE:HG13	1.92	0.51
1:D:415:GLU:HG3	1:D:458:LEU:HD12	1.93	0.49
1:A:515:VAL:HG22	1:A:568:LEU:HB3	1.96	0.48
1:D:77:ARG:HE	1:D:105:ALA:HB1	1.79	0.48
1:C:276:VAL:HG23	1:C:487:MET:HE3	1.96	0.47
1:A:405:PHE:CE1	1:B:296:PRO:HG2	2.50	0.47
1:C:419:ASP:HB3	1:C:422:LYS:HD2	1.96	0.46
1:A:123:TYR:HB3	1:A:141:TYR:CD2	2.51	0.46
1:D:322[A]:VAL:HG23	3:D:2117:HOH:O	2.16	0.46
1:B:479:ARG:HD2	1:B:480:PHE:CE1	2.51	0.46
1:A:255:PRO:HB3	1:A:268:CYS:HB3	1.98	0.46
1:C:243:THR:HG23	1:C:602:VAL:HB	1.98	0.46
1:C:193:ASP:HB2	1:C:394:THR:HG21	1.98	0.45
1:C:186:CYS:HB2	1:C:600:TRP:CH2	2.51	0.45
1:D:287:PHE:HB2	1:D:487:MET:HE1	1.99	0.45
1:B:495:LEU:HD22	1:B:585:LYS:HB3	1.98	0.45
1:D:41:ARG:HA	1:D:44:VAL:HG22	1.99	0.44
1:D:272:LEU:HB2	1:D:288:PRO:HG3	2.00	0.44
1:D:514:ASP:OD2	1:D:517:GLU:HB2	2.18	0.44
1:B:412:GLN:HG3	1:B:458:LEU:HD23	2.00	0.43
1:B:67:VAL:HB	1:B:183:VAL:HG22	2.01	0.43
1:C:54:ASN:HB3	1:C:58:ARG:HE	1.83	0.43
1:A:538:VAL:HG13	1:A:547:GLU:HB2	2.01	0.43
1:D:341:CYS:HB2	1:D:430:ILE:HG21	2.01	0.43
1:D:285:ILE:HB	1:D:322[B]:VAL:HG22	2.02	0.42
1:B:290:GLN:O	1:B:293:THR:HB	2.20	0.41
1:A:182:PRO:HB3	1:A:227:TRP:CZ3	2.55	0.41
1:B:621:GLU:HG2	1:C:620:TYR:HB2	2.01	0.41
1:B:507:LEU:HD23	1:B:507:LEU:HA	1.95	0.41
1:D:243:THR:HG23	1:D:602:VAL:HB	2.02	0.41
1:D:338:LYS:HD3	1:D:389:LEU:HD11	2.02	0.41
1:D:185:LEU:HB3	1:D:228:THR:HG23	2.02	0.41
1:B:411:MET:O	1:B:415:GLU:HG2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:ASP:HB2	1:A:41:ARG:HH12	1.85	0.41
1:B:139:PHE:O	1:C:45:GLY:HA3	2.20	0.41
1:C:308:ARG:HD2	1:C:611:PHE:CE2	2.56	0.40
1:A:140:GLN:HB2	1:D:41:ARG:HB3	2.04	0.40
1:C:283:ALA:HB3	1:C:327:LEU:HB2	2.03	0.40
1:B:140:GLN:HG3	1:C:42:ILE:HG22	2.03	0.40
1:C:180:GLY:HA2	1:C:220:LYS:HB2	2.04	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	598/611 (98%)	585 (98%)	12 (2%)	1 (0%)	43	51
1	B	593/611 (97%)	583 (98%)	8 (1%)	2 (0%)	36	42
1	C	589/611 (96%)	584 (99%)	5 (1%)	0	100	100
1	D	596/611 (98%)	584 (98%)	12 (2%)	0	100	100
All	All	2376/2444 (97%)	2336 (98%)	37 (2%)	3 (0%)	48	57

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	401	PRO
1	B	400	ASN
1	A	297	SER

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	512/521 (98%)	503 (98%)	9 (2%)	51	68
1	B	506/521 (97%)	495 (98%)	11 (2%)	45	61
1	C	503/521 (96%)	485 (96%)	18 (4%)	31	42
1	D	508/521 (98%)	488 (96%)	20 (4%)	28	39
All	All	2029/2084 (97%)	1971 (97%)	58 (3%)	38	51

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	LYS
1	A	191	VAL
1	A	384	VAL
1	A	495	LEU
1	A	538	VAL
1	A	559	LYS
1	A	577	GLN
1	A	607	HIS
1	A	609	VAL
1	B	53	ARG
1	B	339	GLU
1	B	362	GLN
1	B	384	VAL
1	B	392	LEU
1	B	399	ASN
1	B	458	LEU
1	B	529	GLU
1	B	597	ASP
1	B	607	HIS
1	B	609	VAL
1	C	42	ILE
1	C	63	LEU
1	C	198	TYR
1	C	254	ASP
1	C	259	MET
1	C	322	VAL
1	C	340	LEU
1	C	383	ASP

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Mol	Chain	Res	Type
1	C	384	VAL
1	C	403	ILE
1	C	404	SER
1	C	407	VAL
1	C	410	GLU
1	C	505	ARG
1	C	531	ILE
1	C	535	ASP
1	C	559	LYS
1	C	607	HIS
1	D	51	THR
1	D	58	ARG
1	D	63	LEU
1	D	191	VAL
1	D	259	MET
1	D	322[A]	VAL
1	D	322[B]	VAL
1	D	339	GLU
1	D	371	GLU
1	D	384	VAL
1	D	388	ARG
1	D	403	ILE
1	D	435	ILE
1	D	495	LEU
1	D	529	GLU
1	D	543	ASN
1	D	559	LYS
1	D	591	ASP
1	D	607	HIS
1	D	609	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	48	HIS
1	A	175	GLN
1	A	270	ASN
1	A	399	ASN
1	A	400	ASN
1	B	43	ASN
1	B	48	HIS
1	B	50	GLN

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Mol	Chain	Res	Type
1	B	54	ASN
1	B	195	HIS
1	B	270	ASN
1	B	400	ASN
1	B	540	GLN
1	C	54	ASN
1	C	267	GLN
1	C	540	GLN
1	D	43	ASN
1	D	154	GLN
1	D	270	ASN
1	D	363	GLN
1	D	400	ASN
1	D	504	HIS
1	D	540	GLN
1	D	548	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

5 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
2	AMP	D	700	-	25,25,25	1.24	2 (8%)	37,38,38	1.06	1 (2%)
2	AMP	B	700	-	25,25,25	1.27	3 (12%)	37,38,38	0.86	2 (5%)
2	AMP	A	700	-	25,25,25	1.32	3 (12%)	37,38,38	1.15	5 (13%)
2	AMP	D	701	-	25,25,25	1.17	3 (12%)	37,38,38	1.21	2 (5%)
2	AMP	C	700	-	25,25,25	1.17	1 (4%)	37,38,38	0.96	1 (2%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	AMP	D	700	-	-	1/10/26/26	0/3/3/3
2	AMP	B	700	-	-	0/10/26/26	0/3/3/3
2	AMP	A	700	-	-	0/10/26/26	0/3/3/3
2	AMP	D	701	-	-	3/10/26/26	0/3/3/3
2	AMP	C	700	-	-	0/10/26/26	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	700	AMP	C2-N3	2.97	1.39	1.33
2	B	700	AMP	O4'-C1'	2.93	1.48	1.42
2	B	700	AMP	C2-N3	2.80	1.38	1.33
2	A	700	AMP	O4'-C1'	2.79	1.48	1.42
2	A	700	AMP	C8-N7	2.57	1.36	1.31
2	D	701	AMP	O4'-C1'	2.49	1.47	1.42
2	C	700	AMP	C2-N1	2.47	1.38	1.33
2	D	701	AMP	C2-N1	2.45	1.38	1.33
2	D	700	AMP	C5-N7	2.16	1.43	1.39
2	B	700	AMP	C8-N9	2.15	1.41	1.37
2	D	700	AMP	C8-N9	2.14	1.41	1.37
2	D	701	AMP	C4-N3	2.00	1.38	1.34

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	701	AMP	O4'-C1'-N9	3.36	114.54	108.09
2	D	701	AMP	C2'-C1'-N9	2.94	120.60	113.30
2	D	700	AMP	O5'-P-O1P	2.79	113.99	106.44
2	A	700	AMP	C4-N9-C8	2.60	108.46	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	700	AMP	C4-N9-C1'	-2.45	120.89	126.63
2	B	700	AMP	C4-N9-C8	2.36	108.21	105.74
2	A	700	AMP	N3-C2-N1	-2.23	125.20	128.58
2	C	700	AMP	O5'-P-O1P	-2.12	100.70	106.44
2	B	700	AMP	N9-C8-N7	-2.12	110.92	113.94
2	A	700	AMP	O2'-C2'-C1'	-2.05	103.06	110.10
2	A	700	AMP	C6-C5-C4	-2.01	114.44	117.18

There are no chirality outliers.

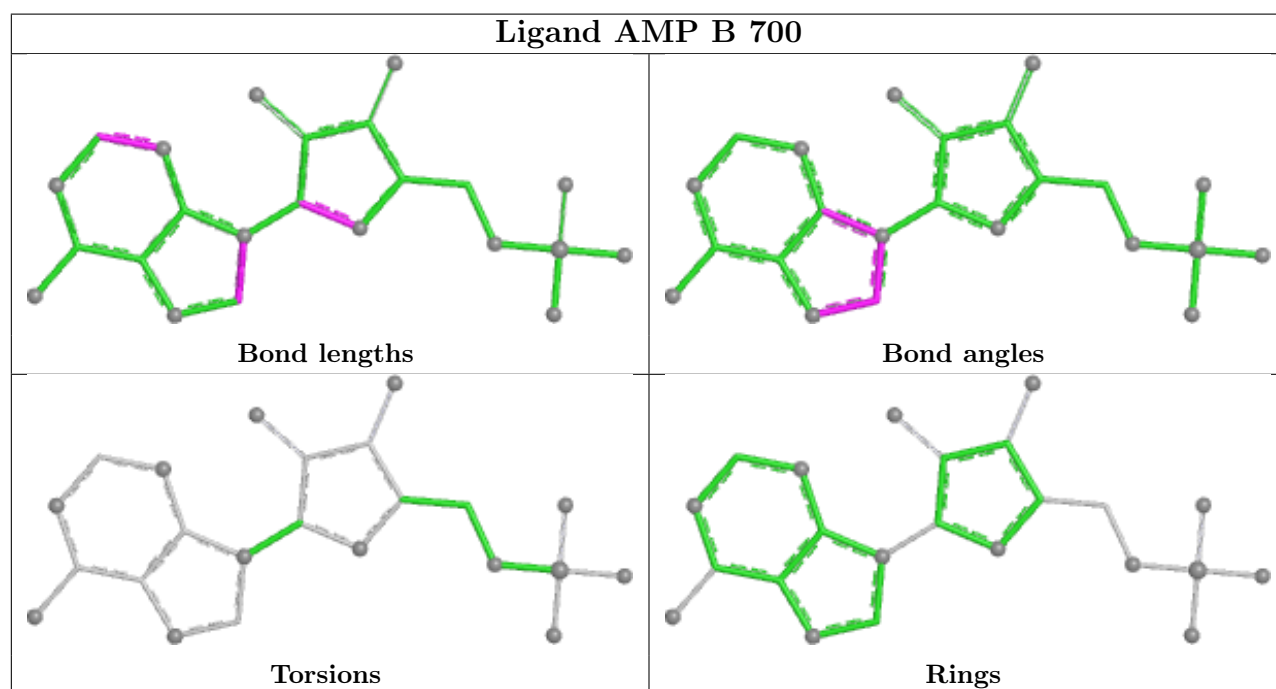
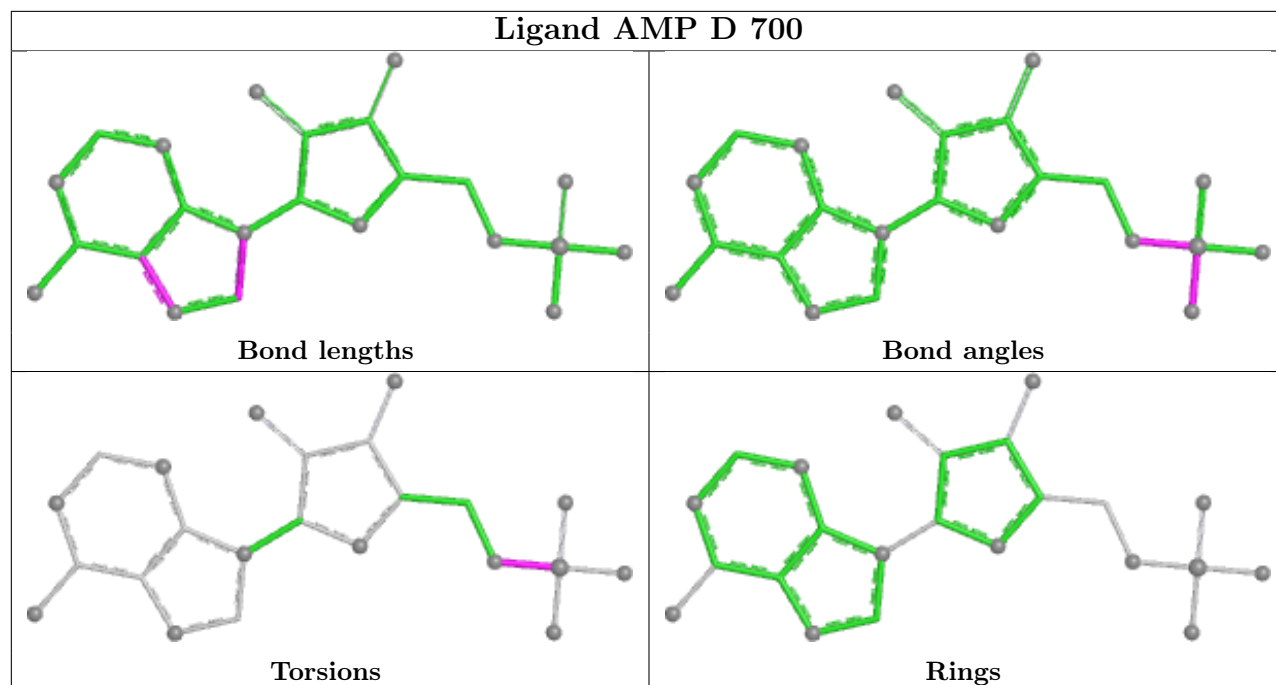
All (4) torsion outliers are listed below:

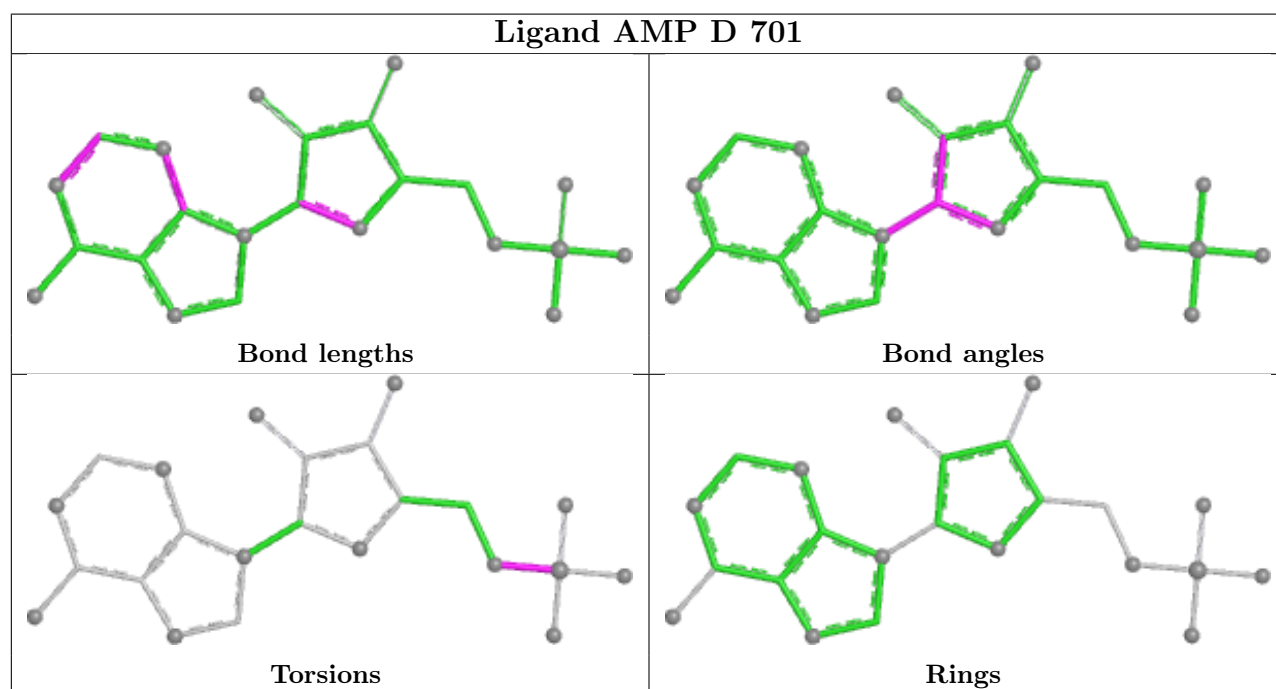
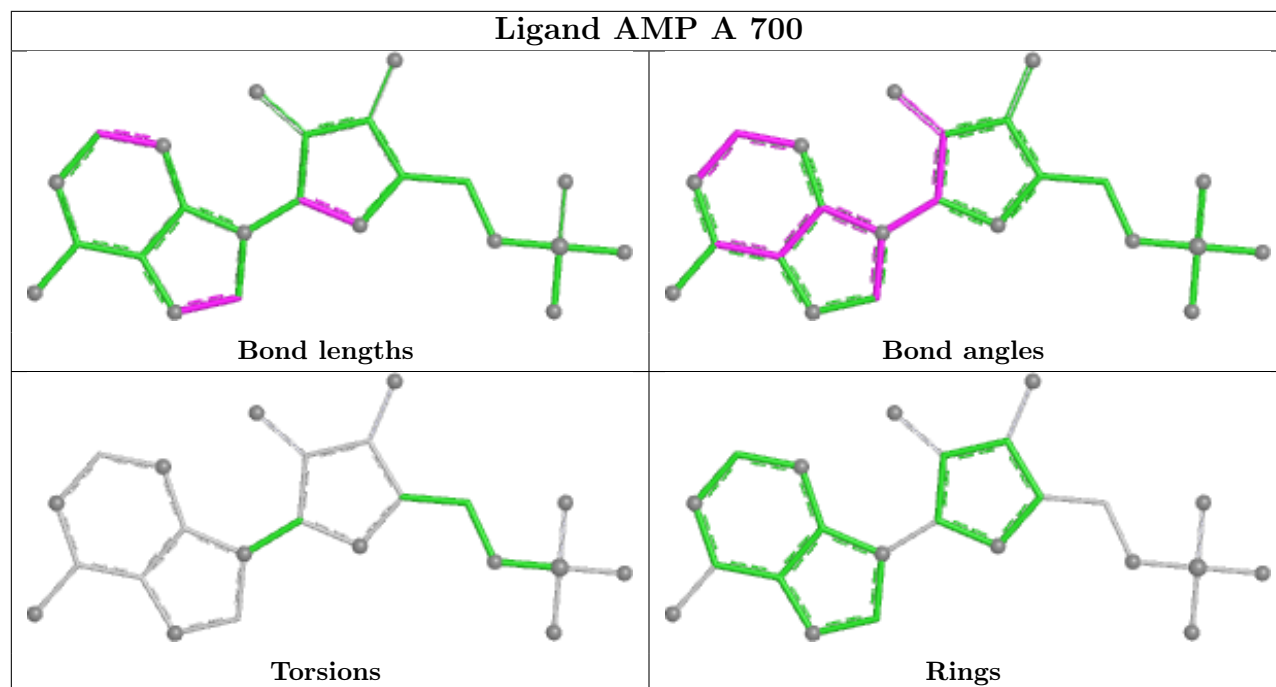
Mol	Chain	Res	Type	Atoms
2	D	700	AMP	C5'-O5'-P-O3P
2	D	701	AMP	C5'-O5'-P-O2P
2	D	701	AMP	C5'-O5'-P-O3P
2	D	701	AMP	C5'-O5'-P-O1P

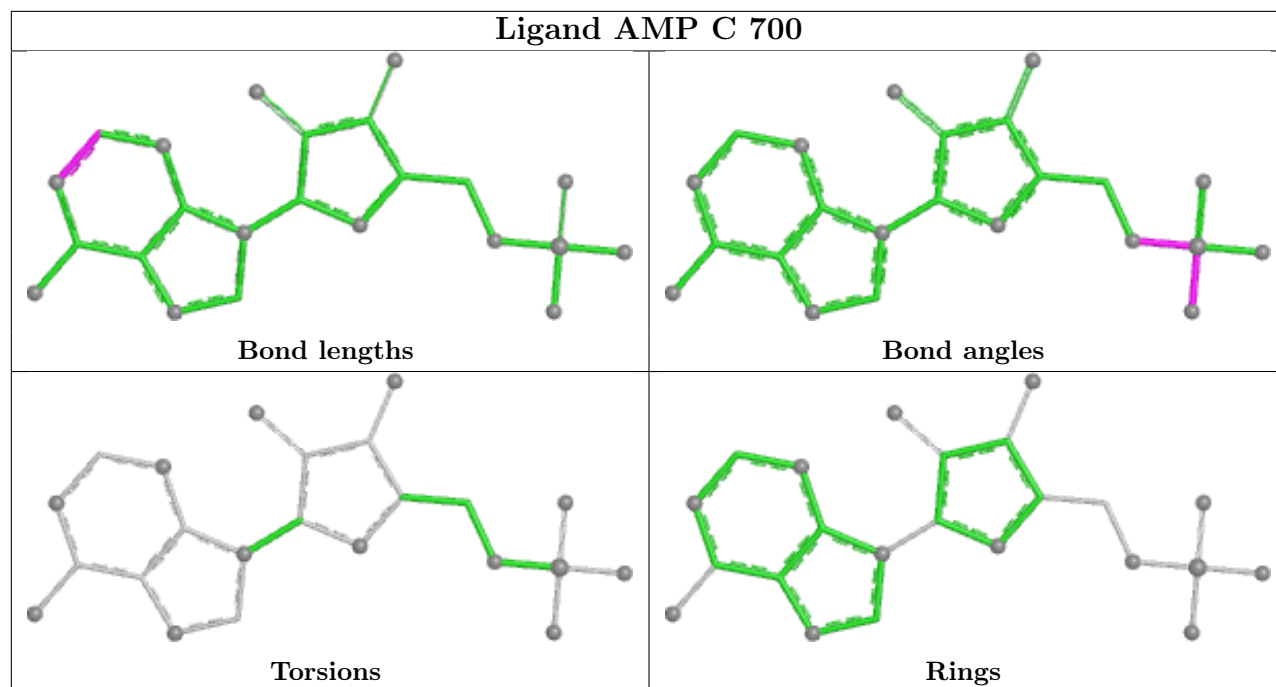
There are no ring outliers.

No monomer is involved in short contacts.

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







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th 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 ²)	Q<0.9
1	A	593/611 (97%)	-0.26	22 (3%) 45 42	15, 30, 64, 98	7 (1%)
1	B	593/611 (97%)	0.23	34 (5%) 29 26	17, 42, 80, 141	2 (0%)
1	C	590/611 (96%)	-0.12	15 (2%) 58 55	21, 36, 64, 108	1 (0%)
1	D	595/611 (97%)	0.06	20 (3%) 48 45	19, 40, 76, 106	3 (0%)
All	All	2371/2444 (97%)	-0.02	91 (3%) 44 41	15, 37, 74, 141	13 (0%)

All (91) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	628	LEU	6.7
1	B	407	VAL	6.2
1	C	405	PHE	5.6
1	B	36	ALA	5.0
1	A	265	VAL	4.9
1	B	401	PRO	4.6
1	D	534	THR	4.3
1	C	403	ILE	4.3
1	B	395	TYR	4.3
1	D	263	TYR	4.1
1	C	407	VAL	4.1
1	B	137	LEU	4.0
1	B	400	ASN	3.9
1	B	408	THR	3.9
1	B	406	LYS	3.8
1	D	260	ILE	3.8
1	C	406	LYS	3.7
1	B	398	VAL	3.7
1	D	265	VAL	3.7
1	A	263	TYR	3.5
1	B	405	PHE	3.5

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Mol	Chain	Res	Type	RSRZ
1	D	258	CYS	3.5
1	A	260	ILE	3.5
1	A	405	PHE	3.4
1	B	260	ILE	3.3
1	B	403	ILE	3.2
1	A	592	GLY	3.2
1	C	40	LYS	3.1
1	D	629	GLU	3.1
1	A	296	PRO	3.1
1	C	629	GLU	3.0
1	B	258	CYS	3.0
1	D	535	ASP	3.0
1	B	132	PRO	3.0
1	B	421	THR	3.0
1	C	265	VAL	2.9
1	B	418	ILE	2.9
1	A	190	GLY	2.9
1	A	259	MET	2.9
1	B	131	ARG	2.8
1	C	260	ILE	2.8
1	A	294	VAL	2.7
1	C	400	ASN	2.7
1	A	268	CYS	2.7
1	A	191	VAL	2.6
1	B	404	SER	2.6
1	A	195	HIS	2.6
1	D	262	GLU	2.6
1	A	590	PRO	2.6
1	B	266	LYS	2.6
1	D	392	LEU	2.5
1	B	259	MET	2.5
1	D	256	ALA	2.5
1	C	457	LYS	2.5
1	B	412	GLN	2.5
1	D	266	LYS	2.5
1	B	135	ALA	2.5
1	B	413	CYS	2.4
1	A	192	ARG	2.4
1	A	264	GLY	2.4
1	B	417	SER	2.4
1	A	295	LEU	2.4
1	C	261	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	189	ALA	2.3
1	A	127	ASP	2.3
1	C	268	CYS	2.3
1	B	416	ASN	2.3
1	C	401	PRO	2.3
1	D	408	THR	2.3
1	B	126	LYS	2.2
1	B	414[A]	ARG	2.2
1	D	36	ALA	2.2
1	C	404	SER	2.2
1	D	417	SER	2.2
1	B	263	TYR	2.2
1	B	265	VAL	2.2
1	A	297	SER	2.2
1	D	191	VAL	2.1
1	B	590	PRO	2.1
1	D	524	GLU	2.1
1	A	266	LYS	2.1
1	A	37	ASP	2.1
1	B	375	ASP	2.1
1	C	398	VAL	2.1
1	D	300[A]	ARG	2.1
1	D	407	VAL	2.1
1	A	258	CYS	2.0
1	B	256	ALA	2.0
1	D	374	PRO	2.0
1	B	294	VAL	2.0
1	D	526	CYS	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.

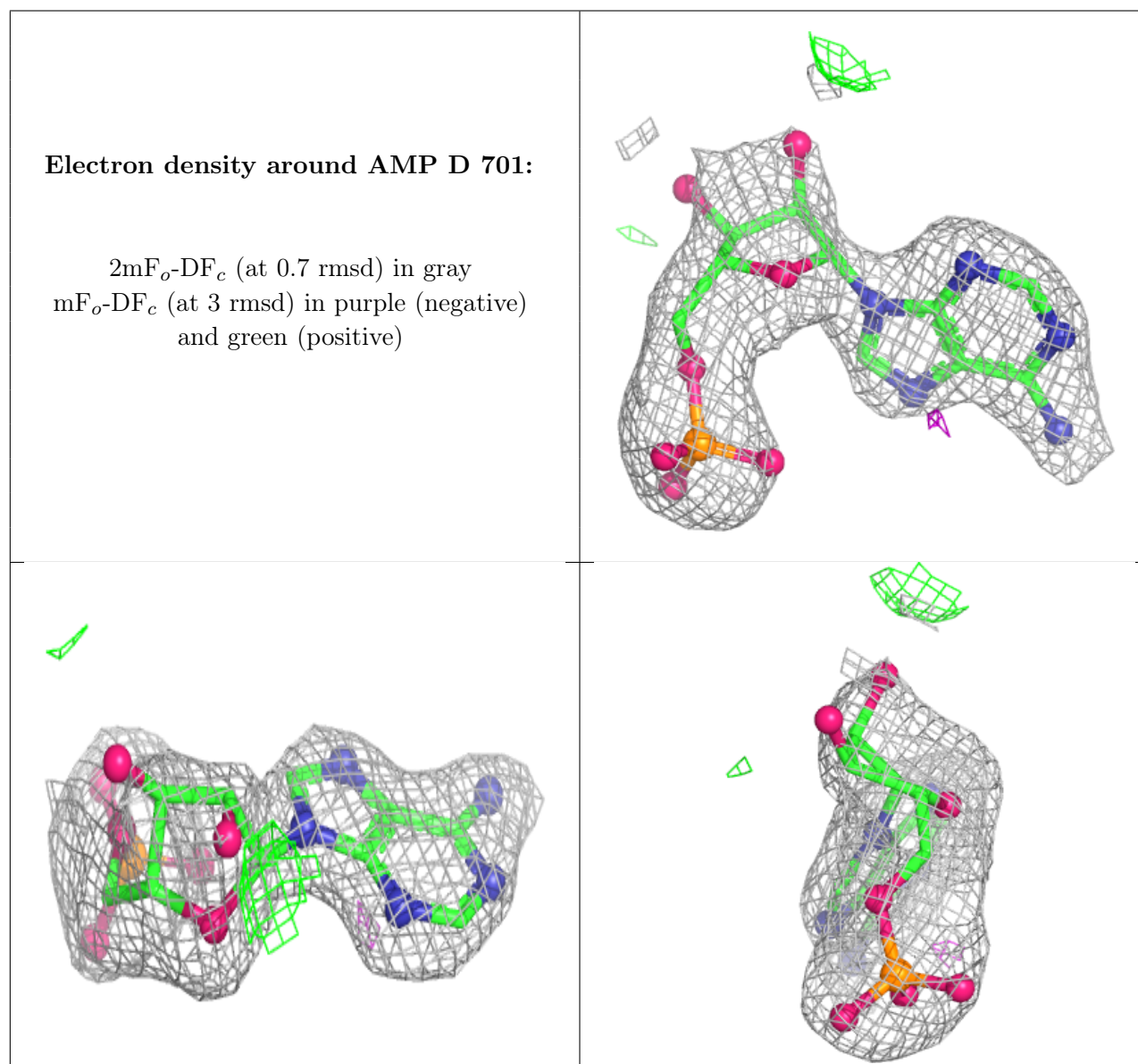
6.4 Ligands [i](#)

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, 95th 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.

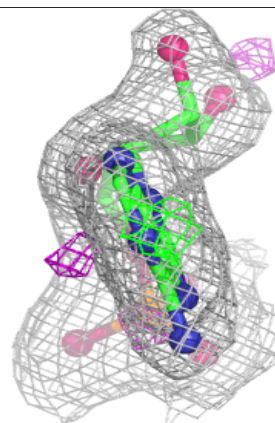
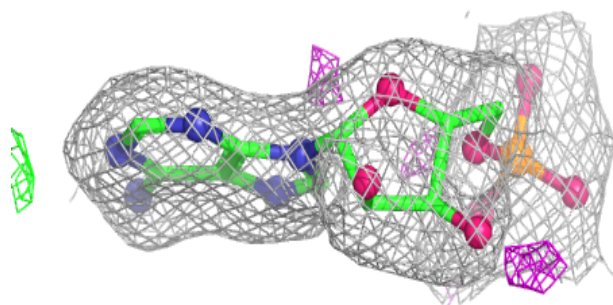
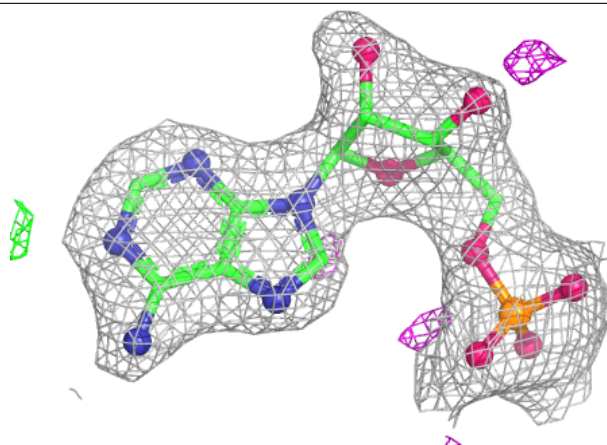
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	AMP	D	701	23/23	0.78	0.12	57,75,88,90	0
2	AMP	C	700	23/23	0.93	0.08	29,35,47,48	0
2	AMP	D	700	23/23	0.94	0.08	36,45,50,53	0
2	AMP	B	700	23/23	0.94	0.08	28,43,57,58	0
2	AMP	A	700	23/23	0.98	0.05	23,30,38,40	0

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.

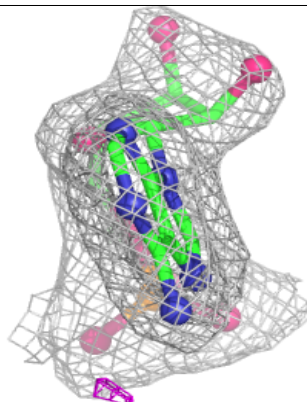
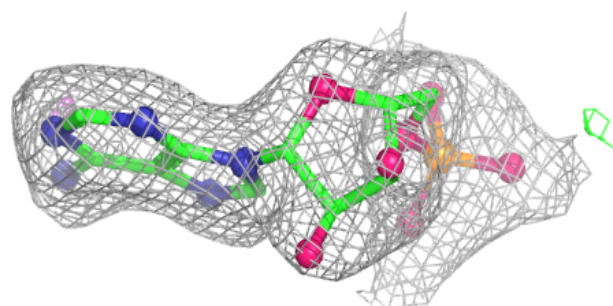
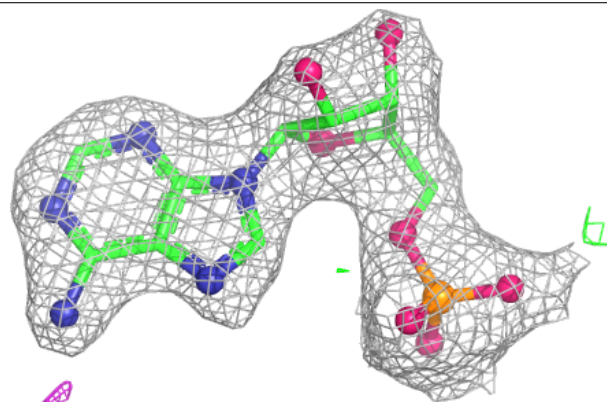


Electron density around AMP C 700:

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

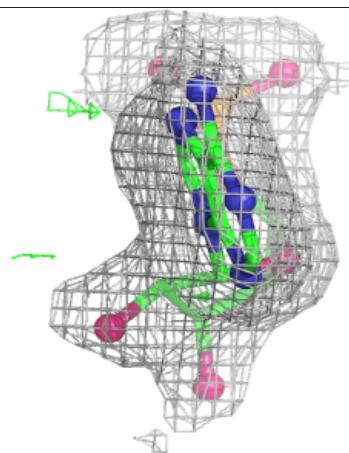
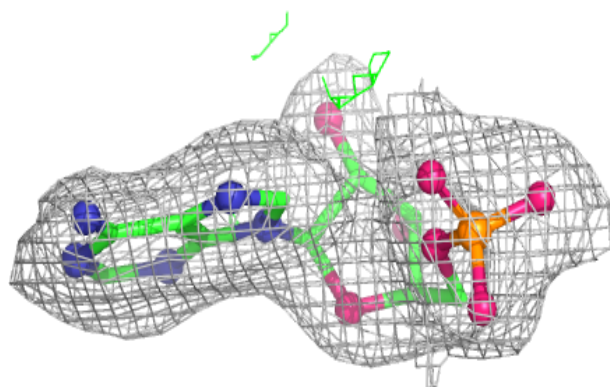
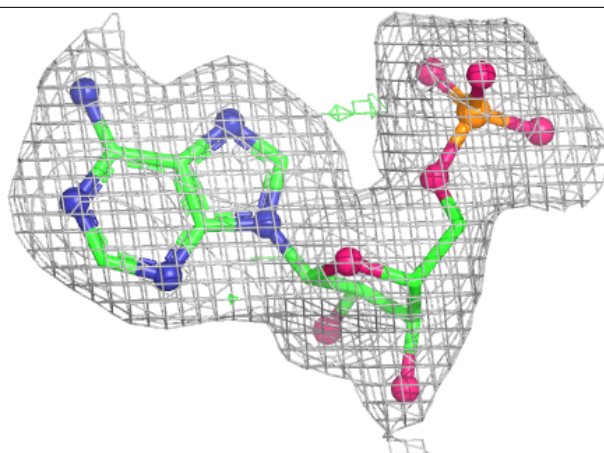
**Electron density around AMP D 700:**

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



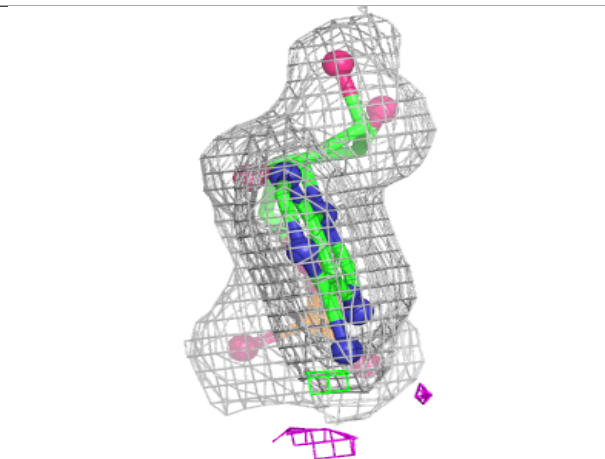
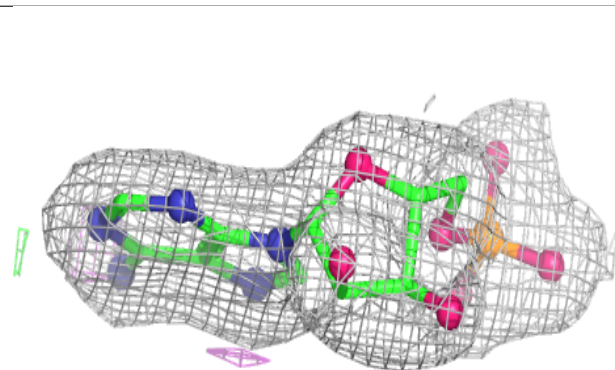
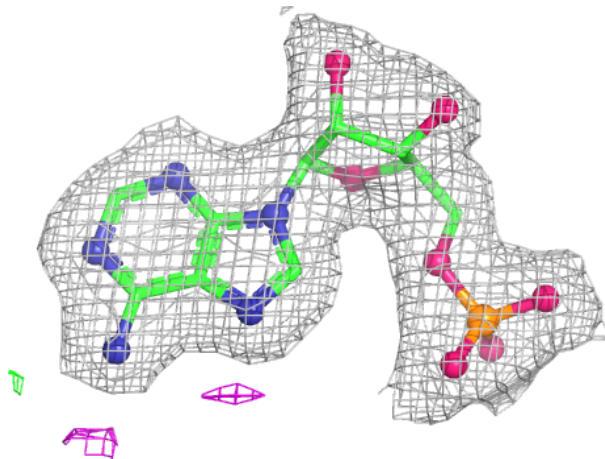
Electron density around AMP B 700:

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



Electron density around AMP A 700:

$2mF_o-DF_c$ (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.