



Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 03:12 am BST

PDB ID : 3TII
Title : Tubulin tyrosine ligase
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Deposited on : 2011-08-20
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

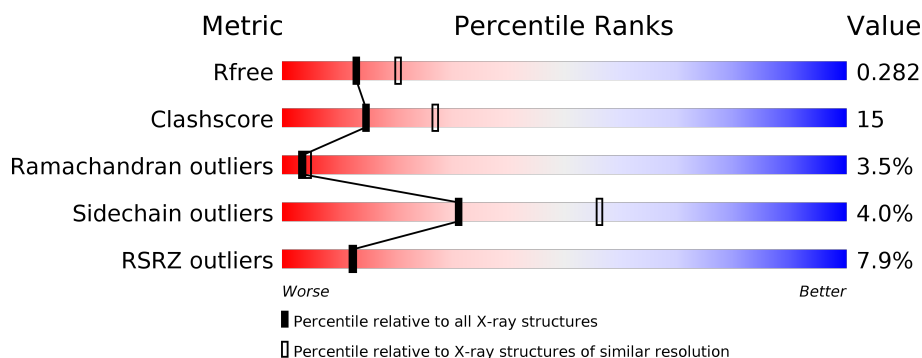
1 Overall quality at a glance

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 ≥ 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	380	<div> <div>7%</div> <div>54%</div> <div>23%</div> <div>18%</div> </div>
1	B	380	<div> <div>6%</div> <div>60%</div> <div>20%</div> <div>18%</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4949 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.

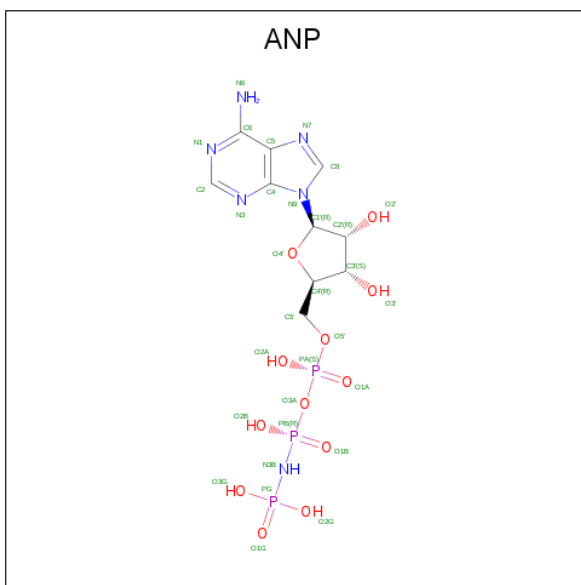
- Molecule 1 is a protein called Ttl protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	311	Total	C	N	O	S	0	0	0
			2396	1556	392	438	10			
1	B	313	Total	C	N	O	S	0	0	0
			2454	1593	404	447	10			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	EXPRESSION TAG	UNP A9ULH4
A	-1	SER	-	EXPRESSION TAG	UNP A9ULH4
A	0	PHE	-	EXPRESSION TAG	UNP A9ULH4
A	1	THR	-	EXPRESSION TAG	UNP A9ULH4
B	-2	GLY	-	EXPRESSION TAG	UNP A9ULH4
B	-1	SER	-	EXPRESSION TAG	UNP A9ULH4
B	0	PHE	-	EXPRESSION TAG	UNP A9ULH4
B	1	THR	-	EXPRESSION TAG	UNP A9ULH4

- Molecule 2 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: C₁₀H₁₇N₆O₁₂P₃).



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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	4	Total	Mg	0	0
			4	4		
3	A	3	Total	Mg	0	0
			3	3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	17	Total	O	0	0
			17	17		
4	B	13	Total	O	0	0
			13	13		

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	44.42Å 74.66Å 117.33Å 90.00° 90.11° 90.00°	Depositor
Resolution (Å)	29.38 – 2.50 29.38 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.8 (29.38-2.50) 98.8 (29.38-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.26 (at 2.51Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, R_{free}	0.254 , 0.285 0.249 , 0.282	Depositor DCC
R_{free} test set	1317 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	48.7	Xtriage
Anisotropy	0.608	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 57.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.027 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4949	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 69.57 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.6206e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.42	0/2450	0.61	0/3329
1	B	0.39	0/2509	0.62	0/3403
All	All	0.41	0/4959	0.62	0/6732

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

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	2396	0	2247	80	0
1	B	2454	0	2360	65	0
2	A	31	0	13	1	0
2	B	31	0	13	1	0
3	A	3	0	0	0	0
3	B	4	0	0	0	0
4	A	17	0	0	0	0
4	B	13	0	0	0	0
All	All	4949	0	4633	145	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 15.

All (145) 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:71:LEU:HG	1:A:332:VAL:HG11	1.58	0.86
1:A:161:LEU:HD23	1:A:169:LEU:HD23	1.59	0.84
1:B:289:GLU:O	1:B:293:VAL:HG12	1.79	0.83
1:A:305:LYS:HD3	1:A:306:TYR:CE2	2.14	0.82
1:A:262:MET:HG3	1:A:266:GLU:OE2	1.80	0.80
1:A:173:ILE:HD12	1:A:180:HIS:HB2	1.64	0.79
1:A:289:GLU:CD	1:A:292:ARG:HH21	1.87	0.78
1:B:163:SER:HB3	1:B:169:LEU:HD13	1.65	0.78
1:A:264:PHE:HE2	1:A:284:LEU:HD21	1.49	0.77
1:A:289:GLU:O	1:A:293:VAL:HG12	1.84	0.77
1:A:373:VAL:HG13	1:A:374:PHE:HD2	1.50	0.76
1:A:86:GLU:O	1:A:90:THR:HG22	1.85	0.75
1:A:192:LEU:O	1:A:196:HIS:HA	1.87	0.74
1:B:339:ALA:HB3	1:B:342:LEU:HD22	1.74	0.69
1:A:72:CYS:HA	1:A:332:VAL:HG13	1.76	0.67
1:B:71:LEU:HD12	1:B:77:LEU:HD13	1.76	0.67
1:A:190:LEU:HD22	1:A:325:LEU:HD23	1.77	0.67
1:A:179:VAL:O	1:A:179:VAL:HG13	1.95	0.66
1:B:128:ARG:HH21	1:B:170:LEU:HD13	1.61	0.64
1:A:289:GLU:OE2	1:A:292:ARG:NH2	2.31	0.63
1:B:40:MET:HE3	1:B:47:LEU:HG	1.80	0.63
1:B:200:ASP:OD1	1:B:222:ARG:HB3	1.99	0.62
1:B:161:LEU:HD23	1:B:169:LEU:HD12	1.82	0.61
1:B:173:ILE:C	1:B:175:ASN:H	2.03	0.60
1:A:264:PHE:CE2	1:A:284:LEU:HD21	2.35	0.59
1:A:102:PRO:HG2	1:A:177:GLY:HA2	1.84	0.59
1:B:40:MET:HE1	1:B:47:LEU:HD21	1.85	0.59
1:B:179:VAL:O	1:B:179:VAL:HG13	2.02	0.58
1:A:331:GLU:HG2	1:A:332:VAL:N	2.19	0.57
1:B:98:TYR:HA	1:B:127:GLU:OE2	2.03	0.57
1:B:69:ASP:C	1:B:71:LEU:H	2.07	0.57
1:A:279:LEU:HD22	1:A:284:LEU:CD1	2.34	0.57
1:A:173:ILE:HD12	1:A:180:HIS:CB	2.34	0.57
1:A:372:ASN:O	1:A:374:PHE:N	2.38	0.56
1:B:320:MET:HG3	1:B:330:ILE:HD13	1.87	0.56
1:B:36:LYS:HA	1:B:58:LEU:HD11	1.88	0.55
1:A:280:GLU:HA	1:A:284:LEU:HB2	1.88	0.54
1:B:304:THR:HG21	1:B:311:SER:HB2	1.89	0.54
1:B:324:ASN:O	1:B:325:LEU:HB2	2.08	0.54
1:A:266:GLU:O	1:A:269:GLN:N	2.30	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:LEU:N	1:A:221:LEU:HD12	2.24	0.53
1:A:375:ILE:N	1:A:375:ILE:HD12	2.23	0.53
1:A:299:GLU:HB3	1:A:300:PRO:HD3	1.90	0.52
1:A:190:LEU:HB2	1:A:322:ASP:O	2.10	0.52
1:B:372:ASN:N	1:B:372:ASN:OD1	2.41	0.52
1:B:268:ASN:O	1:B:272:VAL:HG12	2.09	0.52
1:A:195:GLY:O	1:A:227:PRO:HB3	2.11	0.51
1:B:190:LEU:HA	1:B:323:LYS:HD3	1.91	0.51
1:B:102:PRO:HD3	1:B:179:VAL:HA	1.92	0.51
1:B:222:ARG:NH2	2:B:710:ANP:O3'	2.38	0.51
1:B:271:LEU:O	1:B:275:LEU:HB2	2.11	0.51
1:A:71:LEU:O	1:A:332:VAL:CG1	2.59	0.51
1:B:298:LEU:HG	1:B:302:ILE:HD13	1.93	0.51
1:A:280:GLU:O	1:A:285:CYS:SG	2.64	0.50
1:A:20:ILE:HD13	1:A:348:LYS:HA	1.94	0.49
1:B:348:LYS:O	1:B:351:VAL:HG22	2.12	0.49
1:A:36:LYS:HD2	1:A:55:GLU:HG2	1.95	0.49
1:A:266:GLU:O	1:A:269:GLN:HB2	2.12	0.49
1:A:205:VAL:CG2	1:A:291:ILE:HD13	2.43	0.48
1:A:74:LYS:HB2	1:A:152:SER:HA	1.95	0.48
1:A:8:ASP:HB2	1:A:43:GLU:HA	1.93	0.48
1:A:12:THR:HB	1:A:343:TYR:OH	2.12	0.48
1:B:148:ILE:HG22	1:B:183:GLN:O	2.13	0.48
1:B:304:THR:HA	1:B:307:LEU:HD12	1.95	0.48
1:B:283:ILE:HG23	1:B:327:VAL:CG2	2.44	0.48
1:A:150:LYS:HE3	2:A:700:ANP:O1A	2.14	0.47
1:B:170:LEU:C	1:B:172:PHE:H	2.16	0.47
1:A:17:VAL:HA	1:A:20:ILE:HG22	1.96	0.47
1:A:289:GLU:OE1	1:A:289:GLU:HA	2.14	0.47
1:A:320:MET:HG3	1:A:330:ILE:HD13	1.96	0.47
1:B:287:ILE:HG23	1:B:319:PHE:CE2	2.49	0.47
1:A:219:GLY:HA3	1:A:264:PHE:CE1	2.50	0.47
1:A:351:VAL:HG23	1:A:352:ASP:N	2.30	0.47
1:B:272:VAL:HG13	1:B:273:THR:N	2.29	0.47
1:B:55:GLU:HG2	1:B:58:LEU:HD12	1.96	0.47
1:B:99:VAL:N	1:B:127:GLU:OE2	2.39	0.47
1:B:289:GLU:O	1:B:293:VAL:CG1	2.58	0.47
1:B:64:TYR:O	1:B:311:SER:OG	2.32	0.47
1:A:202:ARG:HA	1:A:317:PHE:O	2.13	0.47
1:B:321:VAL:HG22	1:B:327:VAL:HG22	1.97	0.47
1:A:205:VAL:HG21	1:A:291:ILE:HD13	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:ALA:HB1	1:A:173:ILE:HD11	1.97	0.46
1:B:100:ILE:HA	1:B:126:ASP:CB	2.45	0.46
1:A:198:LYS:NZ	1:A:320:MET:CE	2.79	0.46
1:A:348:LYS:HA	1:A:351:VAL:HG22	1.98	0.46
1:A:373:VAL:HG13	1:A:374:PHE:CD2	2.40	0.45
1:A:130:GLU:N	1:A:130:GLU:OE1	2.49	0.45
1:A:189:PRO:HA	1:A:322:ASP:HA	1.99	0.45
1:B:283:ILE:HG23	1:B:327:VAL:HG21	1.98	0.45
1:A:340:GLN:HA	1:A:343:TYR:HD2	1.82	0.44
1:A:283:ILE:HG23	1:A:327:VAL:HG11	1.99	0.44
1:B:173:ILE:C	1:B:175:ASN:N	2.70	0.44
1:A:19:LYS:O	1:A:21:LEU:N	2.50	0.44
1:A:342:LEU:O	1:A:344:ALA:N	2.51	0.44
1:A:178:GLN:O	1:A:179:VAL:C	2.57	0.43
1:B:9:GLU:OE2	1:B:9:GLU:N	2.49	0.43
1:A:279:LEU:HD22	1:A:284:LEU:HG	1.99	0.43
1:B:198:LYS:HE2	1:B:320:MET:HE3	1.99	0.43
1:A:332:VAL:HG13	1:A:332:VAL:O	2.18	0.43
1:A:4:PHE:CZ	1:A:29:ARG:HB2	2.54	0.43
1:B:163:SER:OG	1:B:164:SER:N	2.52	0.43
1:B:100:ILE:HA	1:B:126:ASP:HB2	2.01	0.43
1:A:220:VAL:HG23	1:A:263:PHE:CD1	2.54	0.43
1:B:136:ASN:O	1:B:139:LYS:HB3	2.19	0.43
1:A:192:LEU:HD12	1:A:223:THR:HG22	2.00	0.42
1:A:287:ILE:HG23	1:A:319:PHE:CE2	2.54	0.42
1:A:74:LYS:HB3	1:A:181:VAL:HG21	2.01	0.42
1:A:214:TYR:HB3	1:A:374:PHE:HD1	1.84	0.42
1:B:166:ALA:O	1:B:170:LEU:HG	2.19	0.42
1:B:173:ILE:O	1:B:175:ASN:N	2.52	0.42
1:A:34:ASN:HA	1:A:35:PRO:HD3	1.91	0.42
1:B:73:ARG:HB3	1:B:73:ARG:HH11	1.84	0.42
1:A:198:LYS:NZ	1:A:320:MET:HE3	2.35	0.42
1:B:223:THR:O	1:B:260:ASN:OD1	2.38	0.42
1:A:188:SER:O	1:A:322:ASP:HB2	2.19	0.42
1:B:272:VAL:HA	1:B:277:ILE:H	1.84	0.42
1:B:40:MET:HE3	1:B:47:LEU:CG	2.47	0.42
1:B:40:MET:CE	1:B:47:LEU:HD21	2.48	0.42
1:A:100:ILE:HD12	1:A:128:ARG:CB	2.50	0.42
1:A:190:LEU:HD22	1:A:325:LEU:CD2	2.46	0.42
1:B:272:VAL:HG13	1:B:273:THR:H	1.84	0.42
1:B:325:LEU:HA	1:B:325:LEU:HD23	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:263:PHE:CZ	1:B:341:LYS:HE2	2.55	0.42
1:A:193:GLU:HA	1:A:194:PRO:C	2.40	0.42
1:B:70:LYS:CG	1:B:70:LYS:O	2.68	0.41
1:A:19:LYS:C	1:A:21:LEU:N	2.74	0.41
1:A:47:LEU:C	1:A:47:LEU:HD23	2.41	0.41
1:B:192:LEU:O	1:B:196:HIS:HA	2.20	0.41
1:B:304:THR:HG22	1:B:307:LEU:HD12	2.01	0.41
1:A:48:PRO:O	1:A:51:ARG:HG2	2.19	0.41
1:B:289:GLU:HA	1:B:289:GLU:OE1	2.19	0.41
1:B:205:VAL:CG2	1:B:291:ILE:HD13	2.50	0.41
1:A:318:ASP:O	1:A:330:ILE:HG12	2.21	0.41
1:B:71:LEU:O	1:B:71:LEU:HG	2.20	0.41
1:B:178:GLN:O	1:B:179:VAL:C	2.59	0.41
1:A:199:PHE:CD1	1:A:200:ASP:N	2.88	0.41
1:B:349:GLY:HA3	1:B:374:PHE:CE2	2.55	0.41
1:A:49:PHE:HB2	1:A:66:ARG:HE	1.86	0.41
1:A:283:ILE:HG23	1:A:327:VAL:CG1	2.51	0.41
1:B:202:ARG:HH11	1:B:202:ARG:HG3	1.86	0.41
1:B:173:ILE:HG13	1:B:174:ASP:N	2.36	0.40
1:A:100:ILE:HD12	1:A:128:ARG:HB3	2.02	0.40
1:A:20:ILE:CD1	1:A:348:LYS:HA	2.52	0.40
1:B:287:ILE:O	1:B:291:ILE:HG13	2.21	0.40
1:A:321:VAL:HG12	1:A:325:LEU:HA	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	299/380 (79%)	247 (83%)	37 (12%)	15 (5%)	2	2
1	B	303/380 (80%)	269 (89%)	28 (9%)	6 (2%)	7	12

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	602/760 (79%)	516 (86%)	65 (11%)	21 (4%)	3 4

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	178	GLN
1	A	179	VAL
1	A	274	SER
1	A	373	VAL
1	B	179	VAL
1	B	280	GLU
1	A	32	ARG
1	A	284	LEU
1	A	343	TYR
1	A	281	ASN
1	B	174	ASP
1	B	211	TYR
1	B	282	SER
1	A	225	SER
1	A	20	ILE
1	A	261	GLU
1	A	102	PRO
1	A	267	PHE
1	A	347	CYS
1	A	283	ILE
1	B	85	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	242/342 (71%)	233 (96%)	9 (4%)	34 60
1	B	256/342 (75%)	245 (96%)	11 (4%)	29 53
All	All	498/684 (73%)	478 (96%)	20 (4%)	31 56

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	196	HIS
1	A	200	ASP
1	A	202	ARG
1	A	220	VAL
1	A	279	LEU
1	A	293	VAL
1	A	318	ASP
1	A	352	ASP
1	A	372	ASN
1	B	12	THR
1	B	22	LEU
1	B	31	LYS
1	B	181	VAL
1	B	196	HIS
1	B	260	ASN
1	B	293	VAL
1	B	311	SER
1	B	323	LYS
1	B	330	ILE
1	B	342	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	210	GLN
1	B	286	GLN
1	B	372	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 9 ligands modelled in this entry, 7 are monoatomic - leaving 2 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
2	ANP	A	700	3	29,33,33	1.97	8 (27%)	31,52,52	1.52	5 (16%)
2	ANP	B	710	3	29,33,33	2.05	8 (27%)	31,52,52	1.51	5 (16%)

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	ANP	A	700	3	-	3/14/38/38	0/3/3/3
2	ANP	B	710	3	-	4/14/38/38	0/3/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	710	ANP	PB-N3B	-5.84	1.48	1.63
2	A	700	ANP	PB-N3B	-5.79	1.48	1.63
2	B	710	ANP	O4'-C1'	4.87	1.47	1.41
2	A	700	ANP	O4'-C1'	4.38	1.47	1.41
2	A	700	ANP	PG-O1G	3.64	1.51	1.46
2	B	710	ANP	PG-O1G	3.51	1.51	1.46
2	B	710	ANP	PB-O2B	-2.80	1.49	1.56
2	B	710	ANP	PB-O3A	-2.79	1.55	1.59
2	A	700	ANP	O2'-C2'	2.48	1.48	1.43
2	B	710	ANP	O2'-C2'	2.46	1.48	1.43
2	A	700	ANP	PB-O2B	-2.45	1.50	1.56
2	A	700	ANP	PB-O1B	2.40	1.50	1.46
2	A	700	ANP	C2-N3	2.15	1.35	1.32
2	B	710	ANP	C8-N7	-2.13	1.30	1.34
2	B	710	ANP	PB-O1B	2.12	1.49	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	700	ANP	C8-N7	-2.01	1.31	1.34

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	700	ANP	C3'-C2'-C1'	4.20	107.30	100.98
2	B	710	ANP	C3'-C2'-C1'	4.04	107.06	100.98
2	B	710	ANP	O2'-C2'-C3'	-3.51	100.48	111.82
2	A	700	ANP	O2'-C2'-C3'	-3.18	101.55	111.82
2	A	700	ANP	O2B-PB-O3A	2.95	114.49	104.64
2	B	710	ANP	O1G-PG-N3B	-2.94	107.44	111.77
2	B	710	ANP	O2B-PB-O3A	2.66	113.52	104.64
2	A	700	ANP	O1G-PG-N3B	-2.62	107.92	111.77
2	A	700	ANP	PA-O3A-PB	2.52	141.47	132.62
2	B	710	ANP	PA-O3A-PB	2.35	140.90	132.62

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	700	ANP	PB-N3B-PG-O1G
2	A	700	ANP	PA-O3A-PB-O1B
2	A	700	ANP	PA-O3A-PB-O2B
2	B	710	ANP	PG-N3B-PB-O1B
2	B	710	ANP	PG-N3B-PB-O3A
2	B	710	ANP	PA-O3A-PB-O1B
2	B	710	ANP	PA-O3A-PB-O2B

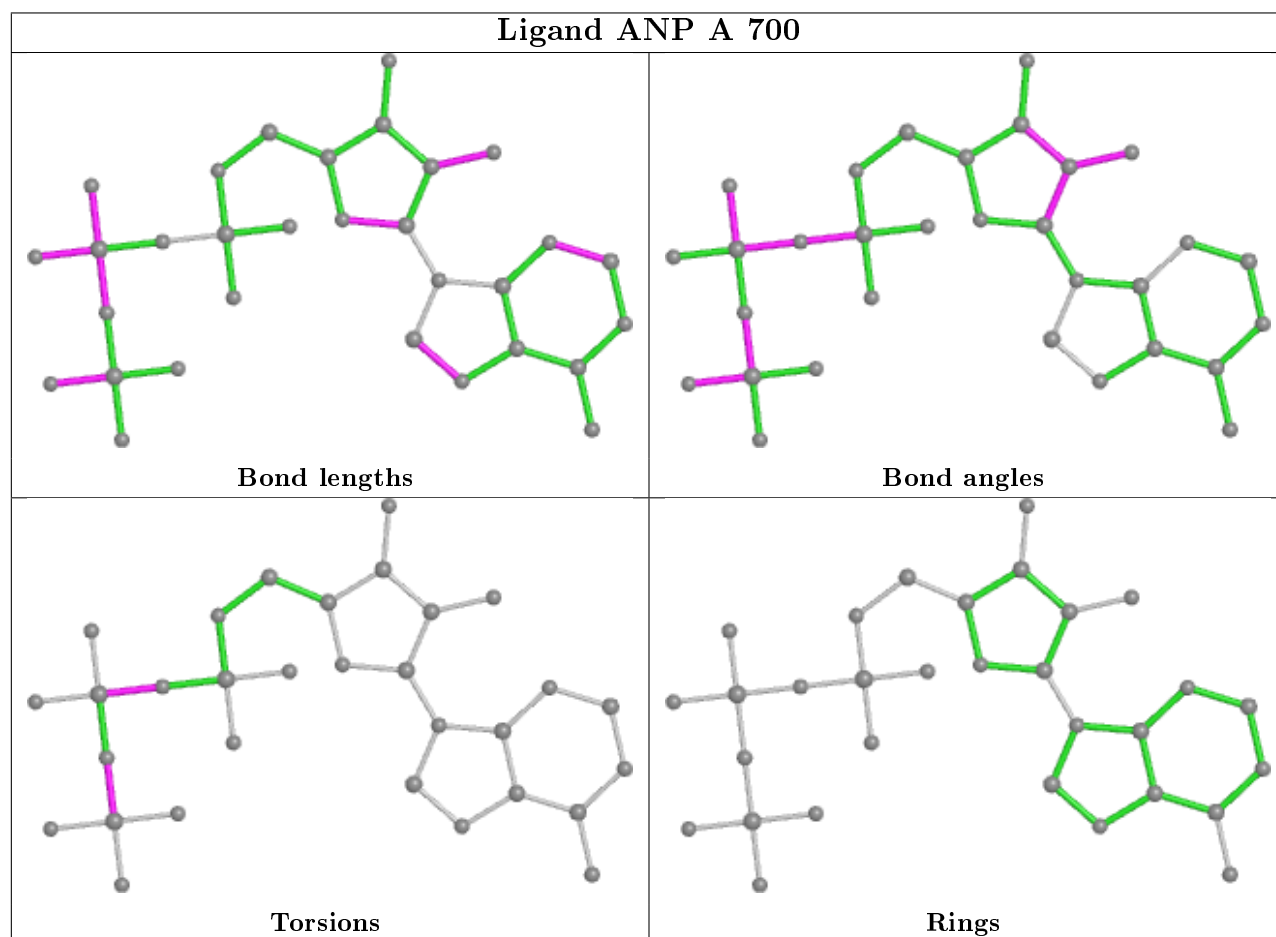
There are no ring outliers.

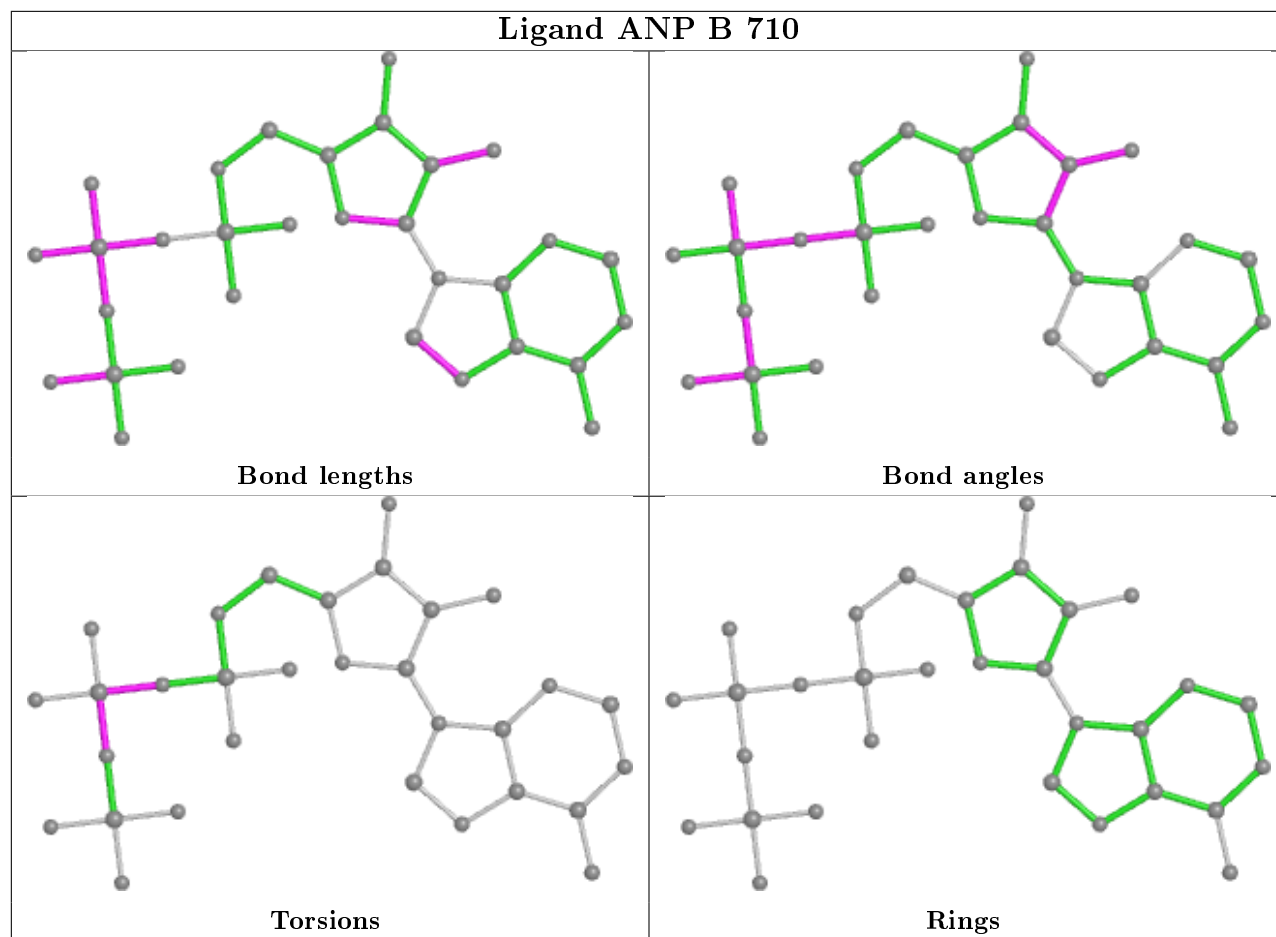
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	700	ANP	1	0
2	B	710	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.





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	311/380 (81%)	0.44	26 (8%) 11 11	28, 66, 111, 137	0
1	B	313/380 (82%)	0.25	23 (7%) 15 15	26, 62, 106, 137	0
All	All	624/760 (82%)	0.34	49 (7%) 12 12	26, 64, 110, 137	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	194	PRO	6.8
1	B	88	THR	4.4
1	A	277	ILE	4.2
1	A	272	VAL	4.2
1	A	270	TYR	4.2
1	A	276	ASN	3.9
1	B	161	LEU	3.8
1	B	177	GLY	3.6
1	A	153	SER	3.3
1	A	103	THR	3.3
1	A	228	TYR	3.0
1	B	169	LEU	3.0
1	B	330	ILE	3.0
1	A	202	ARG	2.9
1	B	-2	GLY	2.8
1	A	316	GLY	2.8
1	B	172	PHE	2.7
1	B	194	PRO	2.7
1	A	101	TYR	2.7
1	B	281	ASN	2.6
1	B	225	SER	2.6
1	B	203	SER	2.6
1	A	203	SER	2.5
1	B	222	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	373	VAL	2.5
1	A	282	SER	2.5
1	A	267	PHE	2.5
1	B	329	LEU	2.4
1	B	318	ASP	2.4
1	B	270	TYR	2.4
1	B	316	GLY	2.4
1	B	277	ILE	2.4
1	A	343	TYR	2.3
1	A	85	PRO	2.3
1	A	172	PHE	2.3
1	A	278	ASN	2.2
1	A	281	ASN	2.2
1	B	202	ARG	2.2
1	B	101	TYR	2.2
1	A	15	ALA	2.2
1	B	317	PHE	2.2
1	A	268	ASN	2.1
1	B	179	VAL	2.1
1	B	102	PRO	2.1
1	A	225	SER	2.1
1	A	192	LEU	2.1
1	A	271	LEU	2.1
1	A	73	ARG	2.1
1	A	330	ILE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

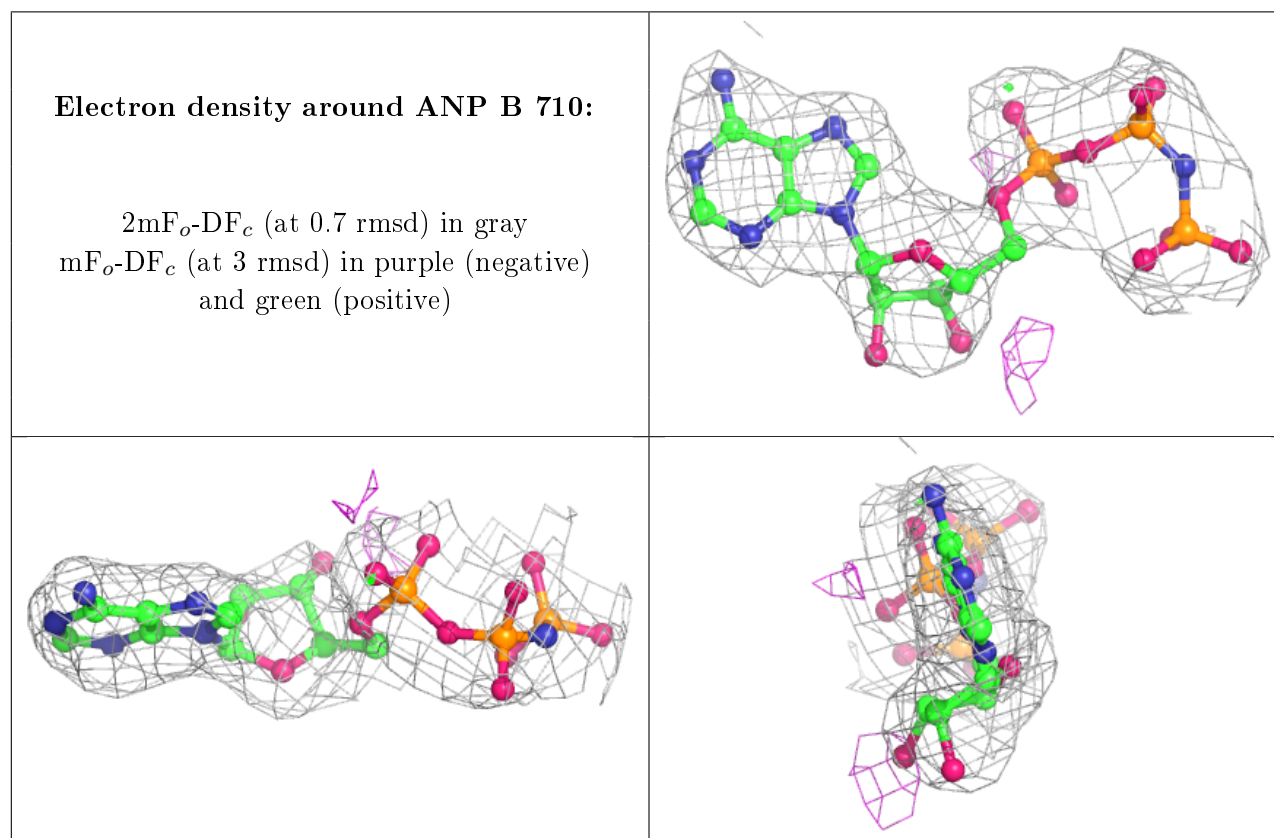
There are no carbohydrates in this entry.

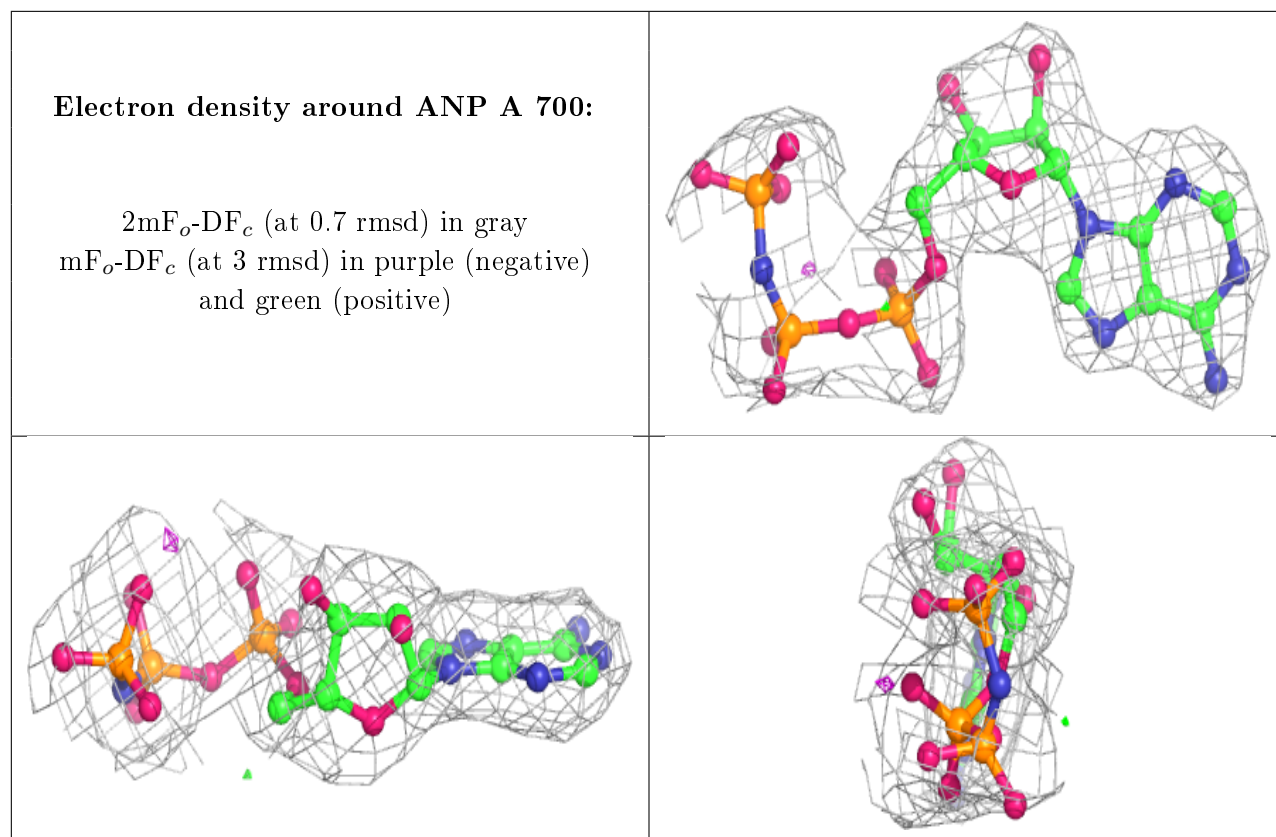
6.4 Ligands ⓘ

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(\AA^2)	Q<0.9
2	ANP	B	710	31/31	0.87	0.16	72,88,104,104	0
2	ANP	A	700	31/31	0.88	0.16	69,82,107,107	0
3	MG	B	384	1/1	0.89	0.20	39,39,39,39	0
3	MG	A	382	1/1	0.94	0.38	39,39,39,39	0
3	MG	B	383	1/1	0.95	0.06	68,68,68,68	0
3	MG	A	381	1/1	0.96	0.08	32,32,32,32	0
3	MG	B	382	1/1	0.98	0.25	36,36,36,36	0
3	MG	A	383	1/1	0.98	0.06	49,49,49,49	0
3	MG	B	381	1/1	0.98	0.13	35,35,35,35	0

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





6.5 Other polymers [i](#)

There are no such residues in this entry.