



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 05:14 AM UTC

PDB ID : 5YT3 / pdb_00005yt3
Title : Structure of the Human Mitogen-Activated Protein Kinase Kinase 1 S218D and S222D mutant
Authors : Nakae, S.; Doko, K.; Tada, T.; Shirai, T.
Deposited on : 2017-11-16
Resolution : 2.90 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

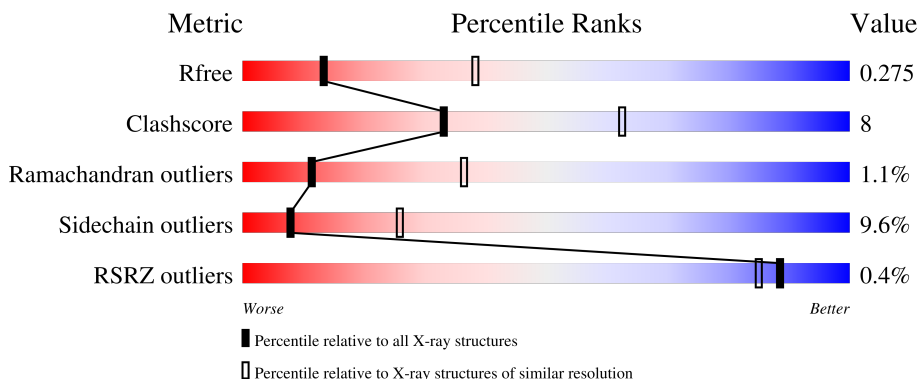
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	350	% 68% 14% • 15%
1	B	350	63% 22% • • 11%
1	C	350	% 62% 17% • 18%
1	D	350	65% 20% • 12%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9265 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 Mitogen-activated protein kinase kinase 1, isoform CRA_d.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	297	Total	C	N	O	S	0	0	1
			2277	1456	386	420	15			
1	B	311	Total	C	N	O	S	0	0	0
			2377	1515	407	440	15			
1	C	288	Total	C	N	O	S	0	0	2
			2099	1346	356	383	14			
1	D	309	Total	C	N	O	S	0	0	0
			2372	1513	408	436	15			

There are 40 discrepancies between the modelled and reference sequences:

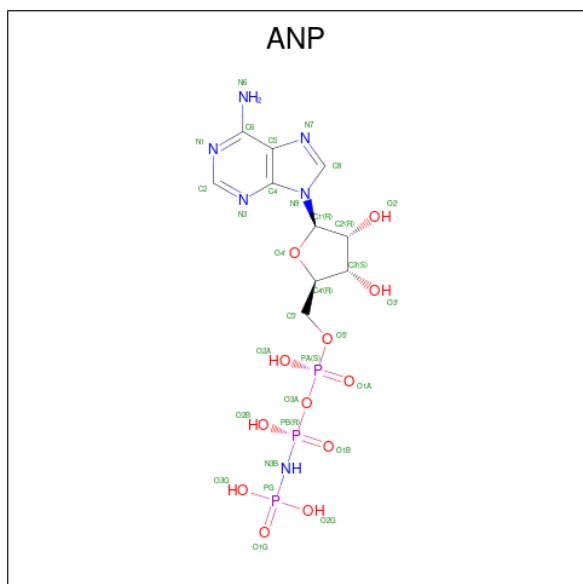
Chain	Residue	Modelled	Actual	Comment	Reference
A	218	ASP	SER	engineered mutation	UNP Q02750
A	222	ASP	SER	engineered mutation	UNP Q02750
A	292	ALA	THR	engineered mutation	UNP Q02750
A	298	ALA	SER	engineered mutation	UNP Q02750
A	383	HIS	-	expression tag	UNP Q02750
A	384	HIS	-	expression tag	UNP Q02750
A	385	HIS	-	expression tag	UNP Q02750
A	386	HIS	-	expression tag	UNP Q02750
A	387	HIS	-	expression tag	UNP Q02750
A	388	HIS	-	expression tag	UNP Q02750
B	218	ASP	SER	engineered mutation	UNP Q02750
B	222	ASP	SER	engineered mutation	UNP Q02750
B	292	ALA	THR	engineered mutation	UNP Q02750
B	298	ALA	SER	engineered mutation	UNP Q02750
B	383	HIS	-	expression tag	UNP Q02750
B	384	HIS	-	expression tag	UNP Q02750
B	385	HIS	-	expression tag	UNP Q02750
B	386	HIS	-	expression tag	UNP Q02750
B	387	HIS	-	expression tag	UNP Q02750
B	388	HIS	-	expression tag	UNP Q02750
C	218	ASP	SER	engineered mutation	UNP Q02750

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	222	ASP	SER	engineered mutation	UNP Q02750
C	292	ALA	THR	engineered mutation	UNP Q02750
C	298	ALA	SER	engineered mutation	UNP Q02750
C	383	HIS	-	expression tag	UNP Q02750
C	384	HIS	-	expression tag	UNP Q02750
C	385	HIS	-	expression tag	UNP Q02750
C	386	HIS	-	expression tag	UNP Q02750
C	387	HIS	-	expression tag	UNP Q02750
C	388	HIS	-	expression tag	UNP Q02750
D	218	ASP	SER	engineered mutation	UNP Q02750
D	222	ASP	SER	engineered mutation	UNP Q02750
D	292	ALA	THR	engineered mutation	UNP Q02750
D	298	ALA	SER	engineered mutation	UNP Q02750
D	383	HIS	-	expression tag	UNP Q02750
D	384	HIS	-	expression tag	UNP Q02750
D	385	HIS	-	expression tag	UNP Q02750
D	386	HIS	-	expression tag	UNP Q02750
D	387	HIS	-	expression tag	UNP Q02750
D	388	HIS	-	expression tag	UNP Q02750

- Molecule 2 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: C₁₀H₁₇N₆O₁₂P₃).



Continued from previous page...

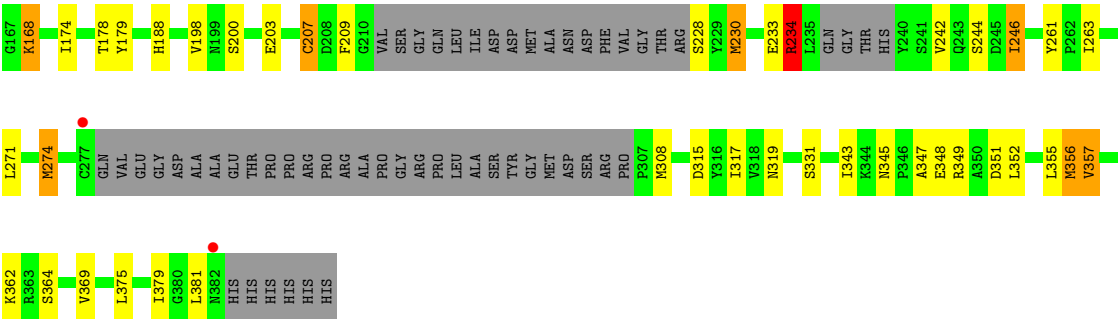
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
2	C	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
2	D	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

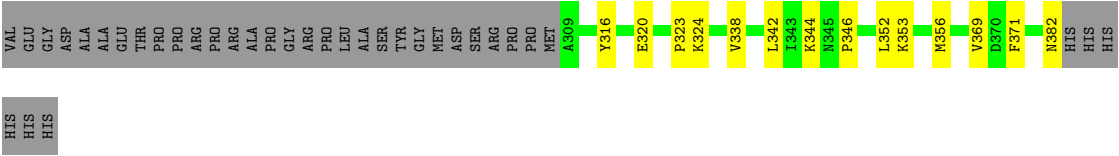
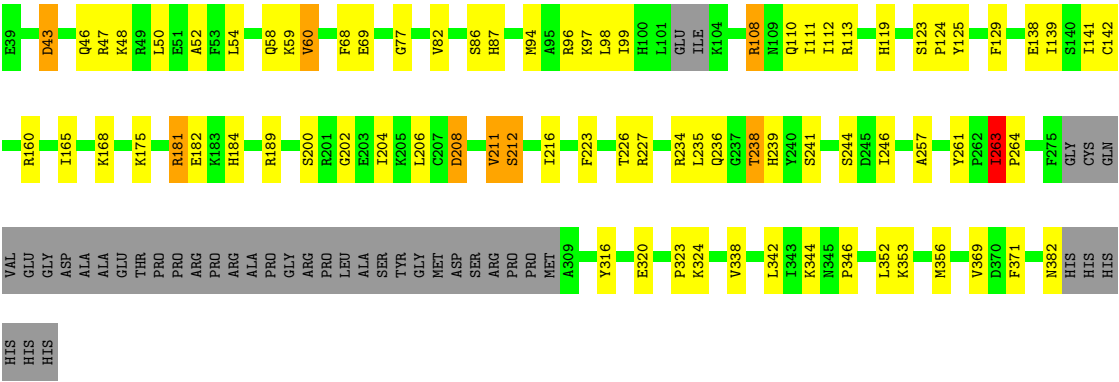
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	5	Total	O	0	0
			5	5		
4	B	2	Total	O	0	0
			2	2		
4	C	4	Total	O	0	0
			4	4		
4	D	3	Total	O	0	0
			3	3		



● Molecule 1: Mitogen-activated protein kinase kinase 1, isoform CRA_d



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	132.17Å 132.55Å 91.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	14.93 – 2.90 14.93 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.9 (14.93-2.90) 96.6 (14.93-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	16.10 (at 2.91Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.209 , 0.289 0.197 , 0.275	Depositor DCC
R_{free} test set	1771 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	62.1	Xtriage
Anisotropy	0.142	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 40.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.025 for k,h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9265	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.04% 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: 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	0.83	0/2320	1.13	1/3130 (0.0%)
1	B	0.82	0/2423	1.18	10/3273 (0.3%)
1	C	0.90	0/2138	1.19	7/2892 (0.2%)
1	D	0.85	0/2417	1.22	10/3262 (0.3%)
All	All	0.85	0/9298	1.18	28/12557 (0.2%)

There are no bond length outliers.

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	263	ILE	CA-C-N	-9.24	110.87	120.38
1	D	263	ILE	C-N-CA	-9.24	110.87	120.38
1	C	188	HIS	N-CA-C	8.27	120.07	111.14
1	B	338	VAL	N-CA-CB	7.55	119.39	110.55
1	D	236	GLN	N-CA-C	-7.18	99.18	109.96
1	B	263	ILE	CA-C-N	-7.12	113.05	120.38
1	B	263	ILE	C-N-CA	-7.12	113.05	120.38
1	D	181	ARG	N-CA-C	-6.25	103.18	111.24
1	B	265	PRO	N-CA-C	6.24	116.46	110.47
1	B	123	SER	CA-C-N	-6.17	113.60	120.45
1	B	123	SER	C-N-CA	-6.17	113.60	120.45
1	C	123	SER	CA-C-N	-6.10	113.53	119.87
1	C	123	SER	C-N-CA	-6.10	113.53	119.87
1	B	310	ILE	N-CA-C	6.05	116.69	110.82
1	C	93	VAL	N-CA-C	6.03	117.16	108.48
1	C	68	PHE	N-CA-C	5.79	118.34	108.90
1	C	319	ASN	N-CA-C	5.71	119.43	112.23
1	D	353	LYS	N-CA-C	-5.54	106.19	113.12
1	B	231	SER	CA-C-N	-5.54	113.32	119.19
1	B	231	SER	C-N-CA	-5.54	113.32	119.19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	212	SER	CA-C-N	5.46	126.16	119.99
1	D	212	SER	C-N-CA	5.46	126.16	119.99
1	D	204	ILE	N-CA-C	-5.42	100.67	108.48
1	D	263	ILE	N-CA-C	5.22	120.15	108.88
1	D	68	PHE	N-CA-C	5.18	117.41	109.07
1	A	199	ASN	N-CA-C	5.11	117.18	109.41
1	C	82	VAL	N-CA-C	-5.07	101.18	108.53
1	B	42	LEU	N-CA-C	5.06	117.01	108.96

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	2277	0	2246	30	0
1	B	2377	0	2342	45	0
1	C	2099	0	2005	33	0
1	D	2372	0	2340	38	0
2	A	31	0	13	0	0
2	B	31	0	13	1	0
2	C	31	0	13	0	0
2	D	31	0	13	3	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
4	A	5	0	0	0	0
4	B	2	0	0	0	0
4	C	4	0	0	0	0
4	D	3	0	0	0	0
All	All	9265	0	8985	142	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (142) 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:260:ARG:HD3	1:A:274:MET:HE1	1.47	0.96
1:A:346:PRO:HG3	1:B:233:GLU:HG2	1.61	0.80
1:A:231:SER:OG	1:A:233:GLU:HG3	1.88	0.73
1:C:234:ARG:O	1:C:234:ARG:HD2	1.88	0.72
1:B:161:ILE:HD12	1:B:256:MET:HG2	1.73	0.69
1:D:246:ILE:HD11	1:D:352:LEU:HD23	1.77	0.67
1:C:127:VAL:HG11	1:C:207:CYS:HB2	1.79	0.65
1:A:255:GLU:HG3	1:A:261:TYR:HA	1.79	0.63
1:B:261:TYR:CE2	1:B:263:ILE:HB	2.34	0.62
1:B:51:GLU:O	1:B:55:THR:HG23	2.00	0.61
1:D:141:ILE:HD11	1:D:211:VAL:HG21	1.83	0.60
1:B:189:ARG:HD3	1:B:190:ASP:O	2.01	0.60
1:D:125:TYR:CZ	1:D:175:LYS:HD2	2.37	0.60
1:A:70:LYS:HA	1:A:85:VAL:HG12	1.82	0.60
1:B:141:ILE:HD11	1:B:211:VAL:HG21	1.83	0.59
1:A:94:MET:HE3	1:A:142:CYS:HB3	1.85	0.59
1:A:260:ARG:HD3	1:A:274:MET:CE	2.28	0.56
1:A:199:ASN:HD21	1:A:203:GLU:HG3	1.70	0.56
1:B:175:LYS:HD2	1:B:356:MET:HE1	1.86	0.56
1:C:174:ILE:HG23	1:C:352:LEU:HD22	1.88	0.56
1:A:98:LEU:HD23	1:A:140:SER:HB3	1.88	0.56
1:C:343:ILE:HG21	1:C:348:GLU:HB2	1.87	0.56
1:D:160:ARG:HD3	1:D:257:ALA:O	2.06	0.56
1:D:60:VAL:HG22	1:D:87:HIS:CE1	2.41	0.55
1:A:199:ASN:ND2	1:A:203:GLU:HG3	2.21	0.55
1:C:168:LYS:NZ	1:C:364:SER:O	2.40	0.55
1:D:202:GLY:HA2	1:D:371:PHE:HD1	1.72	0.55
1:C:198:VAL:HA	1:C:203:GLU:O	2.08	0.54
1:D:235:LEU:O	1:D:238:THR:HG22	2.08	0.54
1:A:68:PHE:CE1	1:A:94:MET:HE2	2.43	0.53
1:B:320:GLU:HB3	1:B:321:PRO:HD2	1.91	0.53
1:D:212:SER:O	1:D:216:ILE:HG12	2.10	0.52
1:A:322:PRO:HG3	1:A:344:LYS:HG2	1.92	0.52
1:C:94:MET:CE	1:C:142:CYS:HB3	2.40	0.52
1:D:119:HIS:ND1	1:D:208:ASP:OD2	2.29	0.52
1:A:325:LEU:HG	1:A:338:VAL:HG21	1.91	0.51
1:C:209:PHE:H	1:C:209:PHE:HD1	1.57	0.51
1:D:97:LYS:HD2	2:D:401:ANP:O1B	2.11	0.51
1:D:168:LYS:HE2	1:D:369:VAL:HG12	1.90	0.51
1:B:352:LEU:O	1:B:356:MET:HB2	2.10	0.51
1:D:261:TYR:CE2	1:D:263:ILE:HB	2.45	0.51
1:B:107:ILE:HB	1:B:223:PHE:HE2	1.75	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:260:ARG:NH2	1:B:264:PRO:O	2.44	0.51
1:D:316:TYR:CE1	1:D:320:GLU:HB3	2.45	0.51
1:A:272:GLU:HG3	1:A:276:GLY:HA2	1.93	0.51
1:B:70:LYS:HA	1:B:85:VAL:HG12	1.92	0.50
1:A:68:PHE:HE1	1:A:94:MET:HE2	1.76	0.50
1:C:160:ARG:NH2	1:C:274:MET:HB2	2.26	0.49
1:B:151:LEU:HD13	1:B:256:MET:CE	2.42	0.49
1:A:105:PRO:HA	1:A:108:ARG:HD3	1.94	0.49
1:B:246:ILE:HD11	1:B:352:LEU:HD23	1.95	0.49
1:B:179:TYR:C	1:B:179:TYR:CD1	2.90	0.49
1:C:233:GLU:CD	1:D:346:PRO:HG3	2.38	0.49
1:C:164:GLN:HB3	1:C:369:VAL:HG21	1.94	0.49
1:B:187:MET:HE2	1:B:239:HIS:HB2	1.95	0.48
1:B:116:GLN:O	1:B:120:GLU:HG2	2.11	0.48
1:D:77:GLY:N	2:D:401:ANP:H5'1	2.27	0.48
1:D:323:PRO:HG2	1:D:342:LEU:HD13	1.96	0.48
1:C:263:ILE:HD13	1:C:317:ILE:HG12	1.95	0.48
1:C:121:CYS:HA	1:C:179:TYR:OH	2.14	0.48
1:C:124:PRO:HG2	1:C:125:TYR:CE1	2.48	0.48
1:C:355:LEU:C	1:C:357:VAL:H	2.22	0.48
1:A:340:LYS:HB3	1:A:350:ALA:HB2	1.96	0.48
1:A:173:VAL:HG22	1:A:249:MET:SD	2.53	0.47
1:B:343:ILE:HD12	1:B:349:ARG:HA	1.96	0.47
1:B:111:ILE:HG22	1:B:223:PHE:CZ	2.49	0.47
2:B:401:ANP:H5'1	2:B:401:ANP:H8	1.95	0.47
1:D:96:ARG:HH21	1:D:98:LEU:HD21	1.79	0.47
1:B:90:SER:HB3	1:B:92:LEU:HD12	1.97	0.47
1:B:103:ILE:HD11	1:B:139:ILE:HD11	1.95	0.47
1:B:151:LEU:HD13	1:B:256:MET:HE1	1.96	0.47
1:D:43:ASP:OD2	1:D:46:GLN:HG3	2.14	0.47
1:B:160:ARG:HD2	1:B:257:ALA:O	2.16	0.46
1:D:189:ARG:HD3	1:D:206:LEU:HD13	1.96	0.46
1:C:168:LYS:HE3	1:C:369:VAL:HB	1.98	0.46
1:D:263:ILE:HG22	1:D:264:PRO:HD3	1.98	0.46
1:B:158:ALA:HB2	1:B:378:THR:CG2	2.45	0.46
1:D:263:ILE:HD12	1:D:263:ILE:HA	1.79	0.46
1:B:88:LYS:HB2	1:B:89:PRO:HD3	1.97	0.46
1:B:101:LEU:HD23	1:B:215:LEU:HD12	1.98	0.46
1:A:325:LEU:HD12	1:A:335:GLN:HA	1.97	0.45
1:A:51:GLU:O	1:A:55:THR:HG23	2.16	0.45
1:D:58:GLN:C	1:D:60:VAL:H	2.24	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:209:PHE:CD1	1:A:209:PHE:N	2.82	0.45
1:B:325:LEU:HD12	1:B:335:GLN:HA	1.98	0.45
1:C:147:ASP:OD1	1:C:200:SER:N	2.45	0.45
1:C:315:ASP:CG	1:D:184:HIS:HB3	2.41	0.45
1:B:43:ASP:HB3	1:B:46:GLN:HB2	1.99	0.45
1:C:40:LEU:HA	1:C:356:MET:HE2	1.98	0.45
1:A:178:THR:O	1:A:182:GLU:HG3	2.16	0.44
1:A:174:ILE:HD11	1:A:337:PHE:HZ	1.82	0.44
1:B:189:ARG:NH2	1:B:208:ASP:O	2.50	0.44
1:A:125:TYR:CZ	1:A:175:LYS:HD2	2.53	0.44
1:D:94:MET:CE	1:D:142:CYS:HB3	2.47	0.44
1:D:238:THR:HG23	1:D:239:HIS:ND1	2.33	0.44
1:B:129:PHE:HE1	1:B:141:ILE:HG23	1.82	0.44
1:C:118:LEU:HA	1:C:121:CYS:SG	2.57	0.44
1:C:375:LEU:O	1:C:379:ILE:HG12	2.17	0.44
1:A:315:ASP:CG	1:B:184:HIS:HB3	2.43	0.44
1:B:191:VAL:O	1:B:248:SER:HB3	2.17	0.44
1:A:112:ILE:HD11	1:A:139:ILE:HG12	1.99	0.43
1:C:127:VAL:CG1	1:C:207:CYS:HB2	2.47	0.43
1:C:94:MET:HG2	1:C:130:TYR:CD2	2.54	0.43
1:C:357:VAL:CG1	1:C:357:VAL:O	2.66	0.43
1:D:82:VAL:HG21	2:D:401:ANP:C8	2.49	0.43
1:B:80:GLY:HA3	1:B:98:LEU:O	2.18	0.43
1:B:247:TRP:CD1	1:B:247:TRP:C	2.97	0.43
1:D:110:GLN:HG3	1:D:223:PHE:CE1	2.53	0.43
1:B:47:ARG:O	1:B:51:GLU:HB2	2.18	0.43
1:B:246:ILE:HD11	1:B:352:LEU:CD2	2.49	0.43
1:C:261:TYR:HB2	1:D:227:ARG:HD2	2.01	0.43
1:D:47:ARG:HA	1:D:50:LEU:HB2	2.00	0.43
1:A:42:LEU:HD21	1:A:50:LEU:HD13	2.01	0.42
1:C:82:VAL:HG22	1:C:97:LYS:HG3	2.02	0.42
1:C:356:MET:HG3	1:C:356:MET:O	2.20	0.42
1:D:238:THR:HG23	1:D:239:HIS:CE1	2.54	0.42
1:A:181:ARG:O	1:A:185:LYS:HA	2.20	0.42
1:D:94:MET:HE3	1:D:142:CYS:HB3	2.01	0.42
1:D:238:THR:CG2	1:D:239:HIS:ND1	2.83	0.42
1:A:231:SER:HB3	1:A:234:ARG:HB3	2.01	0.42
1:A:272:GLU:C	1:A:274:MET:H	2.28	0.42
1:D:123:SER:HA	1:D:124:PRO:HD3	1.87	0.42
1:B:249:MET:HE2	1:B:249:MET:HB3	1.88	0.42
1:D:234:ARG:O	1:D:238:THR:HB	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:105:PRO:HA	1:B:108:ARG:HG3	2.01	0.41
1:C:166:LEU:HD23	1:C:166:LEU:HA	1.63	0.41
1:B:56:GLN:HE21	1:B:92:LEU:HD21	1.86	0.41
1:B:141:ILE:HD11	1:B:211:VAL:CG2	2.50	0.41
1:B:190:ASP:HB3	1:B:240:TYR:CE1	2.55	0.41
1:C:163:GLU:OE1	1:C:331:SER:N	2.52	0.41
1:B:60:VAL:HG23	1:B:87:HIS:NE2	2.35	0.41
1:C:178:THR:O	1:C:179:TYR:C	2.64	0.41
1:D:165:ILE:HG23	1:D:371:PHE:CD2	2.56	0.41
1:B:155:LEU:HD22	1:B:256:MET:HG3	2.03	0.41
1:D:48:LYS:O	1:D:52:ALA:HB2	2.20	0.41
1:D:60:VAL:HG22	1:D:87:HIS:ND1	2.35	0.41
1:C:230:MET:HE3	1:C:234:ARG:HG3	2.02	0.41
1:D:129:PHE:HE1	1:D:141:ILE:HG23	1.86	0.41
1:B:222:ASP:OD2	1:B:227:ARG:NH1	2.48	0.41
1:C:345:ASN:OD1	1:C:347:ALA:HB3	2.21	0.40
1:B:107:ILE:HB	1:B:223:PHE:CE2	2.55	0.40
1:C:246:ILE:HG22	1:C:349:ARG:HD3	2.03	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	289/350 (83%)	264 (91%)	22 (8%)	3 (1%)	12	39
1	B	307/350 (88%)	270 (88%)	33 (11%)	4 (1%)	9	32
1	C	278/350 (79%)	242 (87%)	34 (12%)	2 (1%)	18	48
1	D	303/350 (87%)	271 (89%)	28 (9%)	4 (1%)	9	32
All	All	1177/1400 (84%)	1047 (89%)	117 (10%)	13 (1%)	11	36

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	356	MET
1	A	185	LYS
1	B	182	GLU
1	B	349	ARG
1	C	234	ARG
1	D	200	SER
1	A	136	ASP
1	B	57	LYS
1	D	108	ARG
1	A	42	LEU
1	D	54	LEU
1	D	59	LYS
1	B	237	GLY

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	242/302 (80%)	226 (93%)	16 (7%)	15	43
1	B	252/302 (83%)	228 (90%)	24 (10%)	8	26
1	C	209/302 (69%)	182 (87%)	27 (13%)	4	13
1	D	251/302 (83%)	226 (90%)	25 (10%)	7	24
All	All	954/1208 (79%)	862 (90%)	92 (10%)	8	26

All (92) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	LEU
1	A	43	ASP
1	A	45	GLN
1	A	50	LEU
1	A	63	LEU
1	A	69	GLU
1	A	93	VAL
1	A	108	ARG
1	A	173	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	209	PHE
1	A	242	VAL
1	A	253	LEU
1	A	272	GLU
1	A	310	ILE
1	A	329	VAL
1	A	343	ILE
1	B	43	ASP
1	B	51	GLU
1	B	54	LEU
1	B	58	GLN
1	B	63	LEU
1	B	86	SER
1	B	93	VAL
1	B	97	LYS
1	B	107	ILE
1	B	111	ILE
1	B	174	ILE
1	B	175	LYS
1	B	178	THR
1	B	182	GLU
1	B	212	SER
1	B	219	MET
1	B	227	ARG
1	B	233	GLU
1	B	256	MET
1	B	263	ILE
1	B	273	LEU
1	B	327	SER
1	B	349	ARG
1	B	353	LYS
1	C	54	LEU
1	C	58	GLN
1	C	60	VAL
1	C	63	LEU
1	C	70	LYS
1	C	93	VAL
1	C	98	LEU
1	C	121	CYS
1	C	139	ILE
1	C	156	LYS
1	C	161	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	164	GLN
1	C	168	LYS
1	C	207	CYS
1	C	228	SER
1	C	230	MET
1	C	234	ARG
1	C	242	VAL
1	C	244	SER
1	C	246	ILE
1	C	271	LEU
1	C	274	MET
1	C	308	MET
1	C	351	ASP
1	C	357	VAL
1	C	362	LYS
1	C	381	LEU
1	D	43	ASP
1	D	60	VAL
1	D	69	GLU
1	D	86	SER
1	D	99	ILE
1	D	108	ARG
1	D	111	ILE
1	D	112	ILE
1	D	113	ARG
1	D	138	GLU
1	D	139	ILE
1	D	181	ARG
1	D	182	GLU
1	D	208	ASP
1	D	211	VAL
1	D	226	THR
1	D	238	THR
1	D	241	SER
1	D	244	SER
1	D	263	ILE
1	D	324	LYS
1	D	338	VAL
1	D	344	LYS
1	D	356	MET
1	D	382	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	45	GLN
1	A	78	ASN
1	A	109	ASN
1	A	116	GLN
1	A	184	HIS
1	A	335	GLN
1	B	56	GLN
1	B	58	GLN
1	B	122	ASN
1	B	335	GLN
1	B	339	ASN
1	C	164	GLN
1	D	122	ASN
1	D	236	GLN
1	D	243	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](#)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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	B	401	-	33,33,33	1.82	8 (24%)	45,52,52	2.35	15 (33%)
2	ANP	C	401	3	33,33,33	1.90	9 (27%)	45,52,52	2.58	13 (28%)
2	ANP	A	401	3	33,33,33	2.02	11 (33%)	45,52,52	2.61	13 (28%)
2	ANP	D	401	-	33,33,33	2.11	11 (33%)	45,52,52	2.19	13 (28%)

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	B	401	-	-	6/18/38/38	0/3/3/3
2	ANP	C	401	3	-	4/18/38/38	0/3/3/3
2	ANP	A	401	3	-	1/18/38/38	0/3/3/3
2	ANP	D	401	-	-	0/18/38/38	0/3/3/3

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	401	ANP	C5-C4	4.53	1.47	1.39
2	B	401	ANP	PB-N3B	4.51	1.75	1.63
2	C	401	ANP	PG-N3B	4.50	1.75	1.63
2	D	401	ANP	PG-N3B	4.40	1.74	1.63
2	A	401	ANP	PG-N3B	4.31	1.74	1.63
2	A	401	ANP	PG-O1G	4.29	1.52	1.46
2	A	401	ANP	C5-C4	4.26	1.46	1.39
2	D	401	ANP	PB-N3B	4.25	1.74	1.63
2	D	401	ANP	PB-O1B	4.22	1.52	1.46
2	B	401	ANP	PB-O1B	3.95	1.52	1.46
2	D	401	ANP	PG-O1G	3.91	1.52	1.46
2	C	401	ANP	PB-N3B	3.90	1.73	1.63
2	C	401	ANP	C5-C4	3.90	1.46	1.39
2	B	401	ANP	PG-N3B	3.88	1.73	1.63
2	A	401	ANP	PB-O1B	3.71	1.51	1.46
2	A	401	ANP	PB-N3B	3.71	1.73	1.63
2	C	401	ANP	PG-O1G	3.64	1.51	1.46
2	C	401	ANP	C5-N7	-3.64	1.32	1.39
2	B	401	ANP	PG-O1G	3.47	1.51	1.46
2	D	401	ANP	C8-N7	3.21	1.37	1.31
2	B	401	ANP	C5-C4	3.11	1.44	1.39
2	D	401	ANP	C5-N7	-3.08	1.33	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	ANP	C5-N7	-2.97	1.33	1.39
2	B	401	ANP	C5-N7	-2.64	1.34	1.39
2	D	401	ANP	PA-O3A	2.38	1.62	1.59
2	D	401	ANP	PB-O3A	2.38	1.62	1.59
2	B	401	ANP	PG-O2G	-2.37	1.50	1.56
2	A	401	ANP	C8-N9	-2.37	1.33	1.37
2	A	401	ANP	PB-O3A	2.34	1.62	1.59
2	C	401	ANP	PB-O2B	-2.33	1.50	1.56
2	A	401	ANP	C8-N7	2.32	1.36	1.31
2	A	401	ANP	C5-C6	2.28	1.47	1.41
2	D	401	ANP	PB-O2B	-2.25	1.50	1.56
2	C	401	ANP	C8-N7	2.21	1.35	1.31
2	A	401	ANP	C4-N9	-2.12	1.33	1.37
2	B	401	ANP	C4-N9	-2.08	1.33	1.37
2	D	401	ANP	PG-O2G	-2.08	1.51	1.56
2	C	401	ANP	PB-O1B	2.08	1.49	1.46
2	C	401	ANP	C5-C6	2.01	1.46	1.41

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	ANP	O1G-PG-N3B	-10.71	96.00	111.77
2	C	401	ANP	O1G-PG-N3B	-9.33	98.03	111.77
2	D	401	ANP	O1G-PG-N3B	-6.96	101.52	111.77
2	C	401	ANP	C5-C4-N3	-6.17	118.23	126.72
2	A	401	ANP	C5-C4-N3	-5.91	118.58	126.72
2	B	401	ANP	C5-C4-N3	-5.45	119.22	126.72
2	B	401	ANP	N3-C2-N1	-5.26	120.61	128.58
2	D	401	ANP	C5-C4-N3	-5.21	119.54	126.72
2	A	401	ANP	N3-C4-N9	4.97	135.62	127.17
2	D	401	ANP	N3-C2-N1	-4.88	121.19	128.58
2	C	401	ANP	N3-C4-N9	4.84	135.40	127.17
2	B	401	ANP	O2B-PB-O1B	4.69	119.93	109.87
2	B	401	ANP	N3-C4-N9	4.60	135.00	127.17
2	D	401	ANP	O2B-PB-O1B	4.48	119.48	109.87
2	C	401	ANP	O2B-PB-O1B	4.42	119.36	109.87
2	B	401	ANP	O1G-PG-N3B	-4.42	105.26	111.77
2	B	401	ANP	C2-N3-C4	4.41	122.59	111.83
2	C	401	ANP	O2A-PA-O3A	-4.18	95.98	107.27
2	C	401	ANP	C2-N3-C4	4.16	121.99	111.83
2	D	401	ANP	C2-N3-C4	3.94	121.45	111.83
2	D	401	ANP	N3-C4-N9	3.92	133.83	127.17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	401	ANP	N3-C2-N1	-3.88	122.71	128.58
2	A	401	ANP	C4-N9-C8	3.69	109.61	105.74
2	A	401	ANP	C2-N3-C4	3.66	120.77	111.83
2	B	401	ANP	O1B-PB-N3B	-3.64	106.41	111.77
2	B	401	ANP	C4-N9-C8	3.64	109.56	105.74
2	A	401	ANP	C4-C5-N7	-3.62	106.45	110.58
2	C	401	ANP	C2'-C1'-N9	-3.56	104.47	113.30
2	A	401	ANP	N3-C2-N1	-3.33	123.55	128.58
2	B	401	ANP	N9-C8-N7	-3.32	109.23	113.94
2	A	401	ANP	C2'-C1'-N9	-3.26	105.19	113.30
2	A	401	ANP	O2B-PB-O1B	3.25	116.83	109.87
2	B	401	ANP	C5-N7-C8	3.06	108.26	103.45
2	A	401	ANP	C5-N7-C8	3.02	108.20	103.45
2	B	401	ANP	C4-C5-N7	-2.99	107.16	110.58
2	A	401	ANP	N9-C8-N7	-2.81	109.95	113.94
2	D	401	ANP	C4-C5-N7	-2.54	107.68	110.58
2	C	401	ANP	C4-C5-N7	-2.51	107.71	110.58
2	B	401	ANP	C2-N1-C6	2.44	122.74	118.73
2	C	401	ANP	C3'-C2'-C1'	2.44	106.08	101.46
2	D	401	ANP	C2-N1-C6	2.43	122.72	118.73
2	C	401	ANP	O2A-PA-O1A	2.42	123.70	112.44
2	A	401	ANP	O1B-PB-N3B	-2.30	108.39	111.77
2	C	401	ANP	C5-N7-C8	2.24	106.97	103.45
2	B	401	ANP	C6-C5-N7	2.23	136.39	132.09
2	B	401	ANP	O5'-C5'-C4'	2.21	116.52	108.99
2	D	401	ANP	C5-N7-C8	2.17	106.86	103.45
2	A	401	ANP	C6-C5-N7	2.11	136.16	132.09
2	D	401	ANP	C4'-O4'-C1'	2.10	114.10	109.47
2	C	401	ANP	O1B-PB-N3B	-2.10	108.68	111.77
2	D	401	ANP	C6-C5-N7	2.10	136.13	132.09
2	D	401	ANP	O2G-PG-O3G	2.07	113.16	107.59
2	B	401	ANP	O4'-C4'-C5'	-2.06	102.74	109.33
2	D	401	ANP	N9-C8-N7	-2.04	111.04	113.94

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	ANP	PB-N3B-PG-O1G
2	B	401	ANP	PB-N3B-PG-O1G
2	B	401	ANP	C5'-O5'-PA-O1A
2	B	401	ANP	C5'-O5'-PA-O2A

Continued on next page...

Continued from previous page...

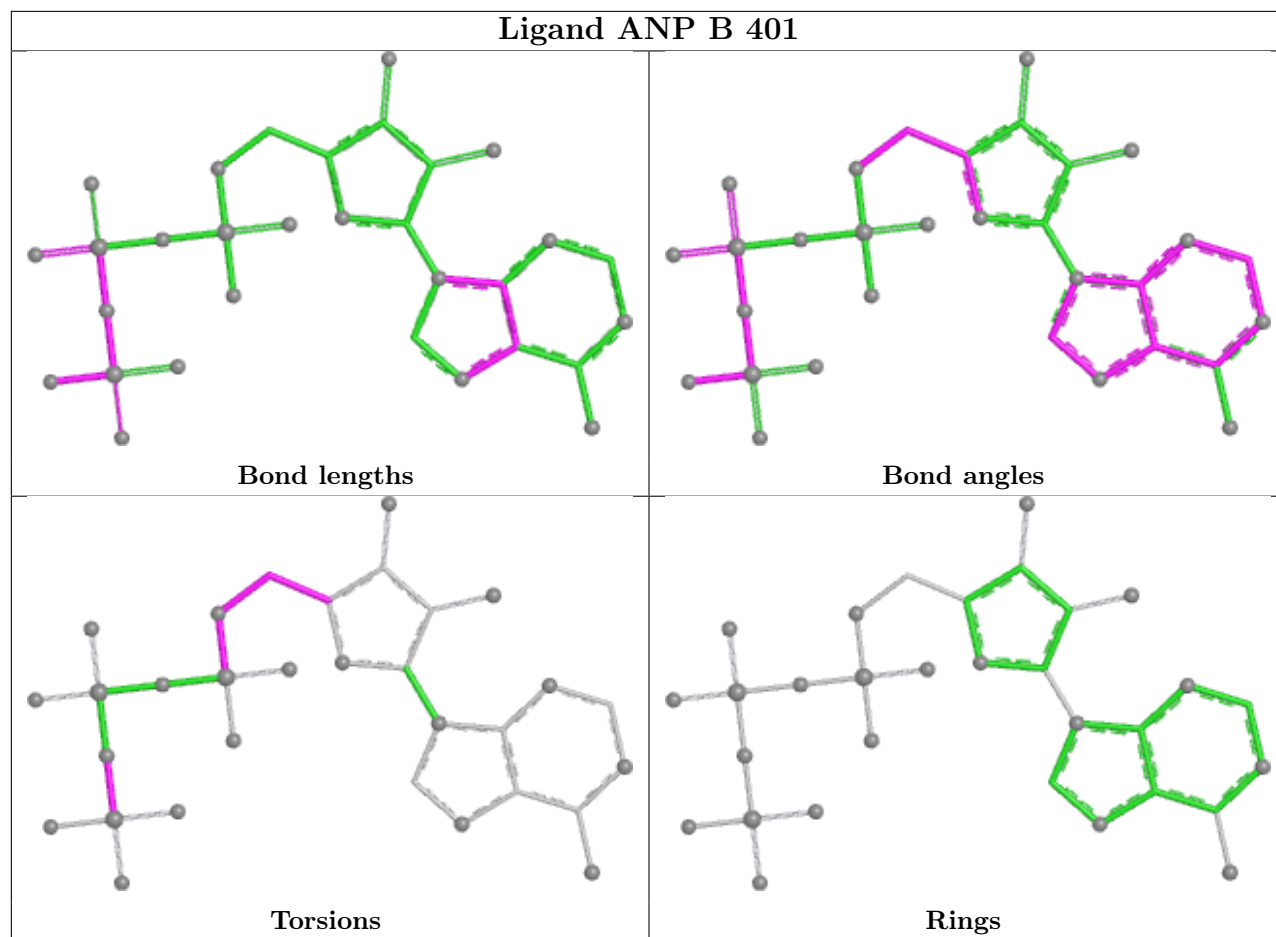
Mol	Chain	Res	Type	Atoms
2	B	401	ANP	C5'-O5'-PA-O3A
2	C	401	ANP	PB-N3B-PG-O1G
2	C	401	ANP	PG-N3B-PB-O1B
2	B	401	ANP	C4'-C5'-O5'-PA
2	B	401	ANP	O4'-C4'-C5'-O5'
2	C	401	ANP	PA-O3A-PB-O1B
2	C	401	ANP	PG-N3B-PB-O3A

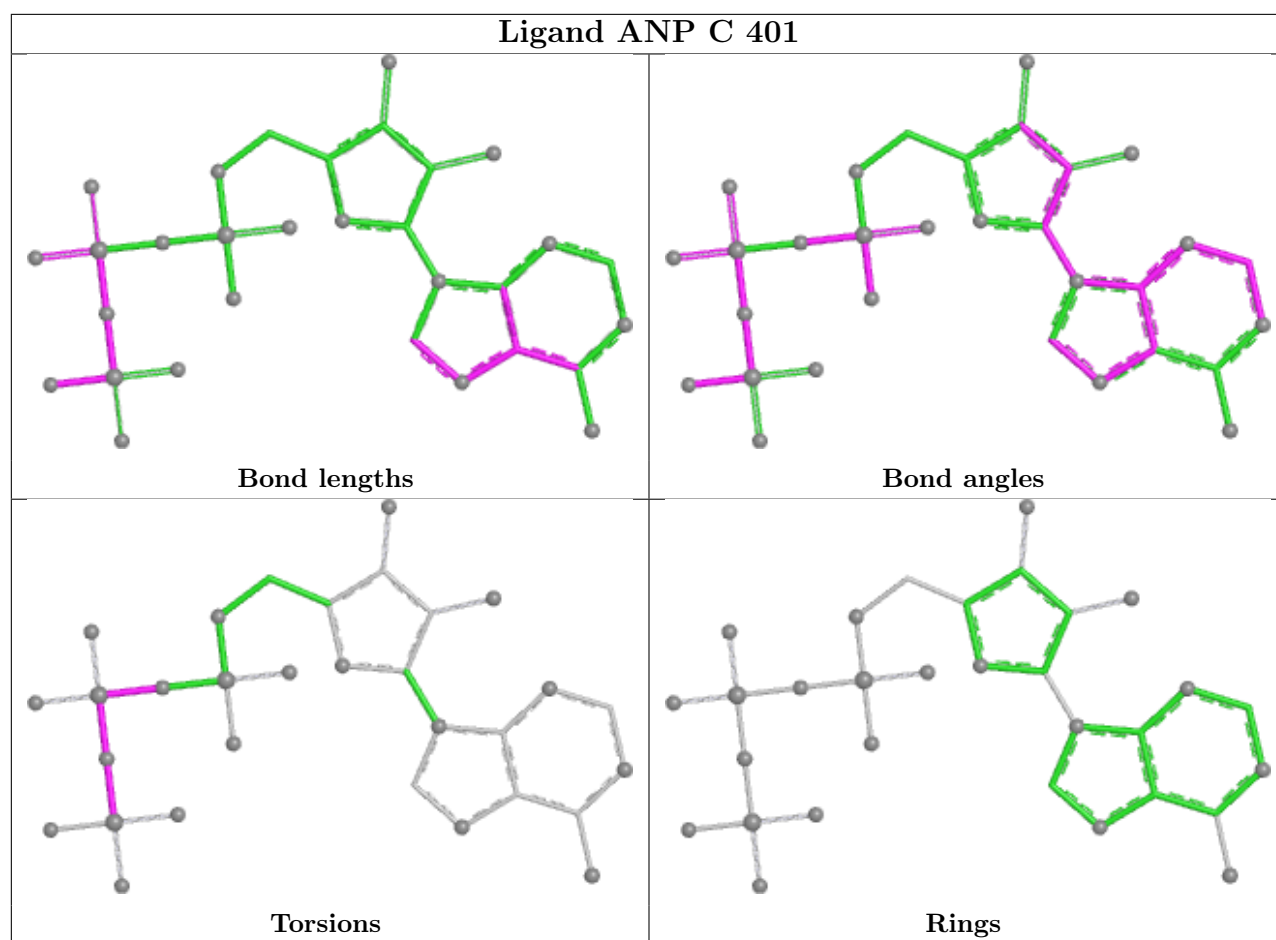
There are no ring outliers.

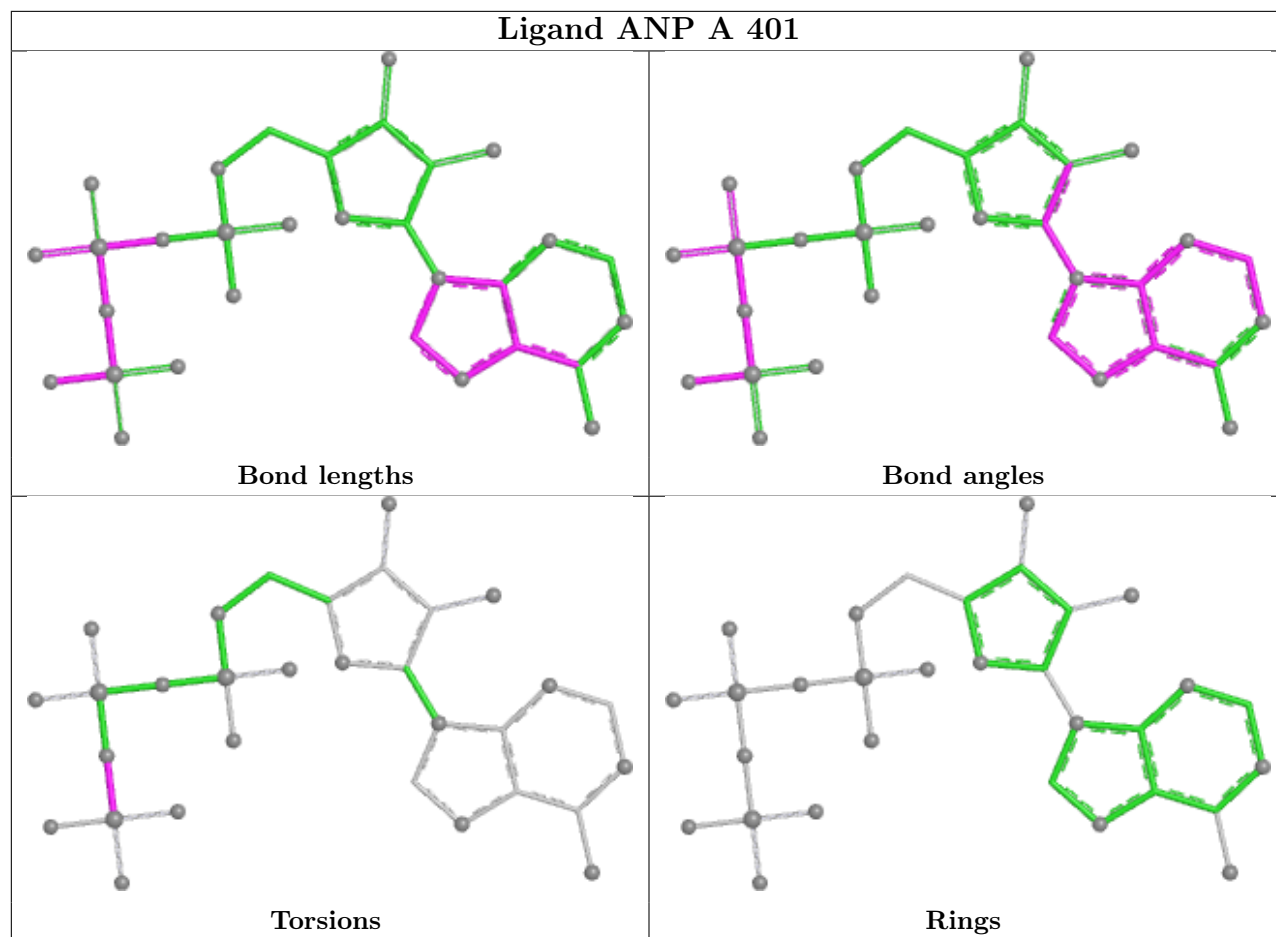
2 monomers are involved in 4 short contacts:

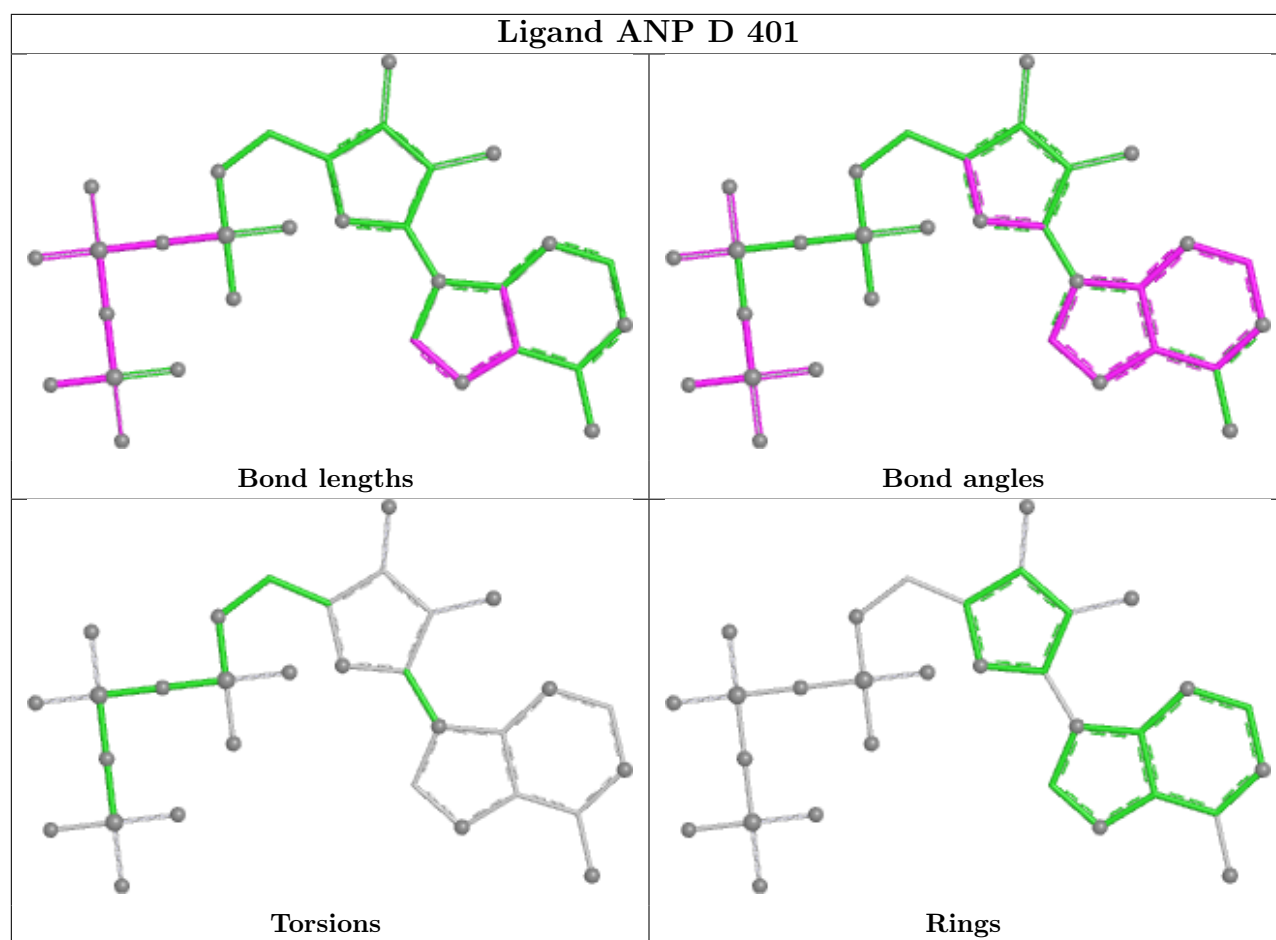
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	401	ANP	1	0
2	D	401	ANP	3	0

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









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	297/350 (84%)	-0.56	2 (0%) 84 79	29, 64, 115, 140	0
1	B	311/350 (88%)	-0.55	0 100 100	30, 61, 112, 139	0
1	C	288/350 (82%)	-0.29	3 (1%) 79 73	29, 64, 118, 151	0
1	D	309/350 (88%)	-0.59	0 100 100	30, 58, 112, 152	0
All	All	1205/1400 (86%)	-0.50	5 (0%) 88 85	29, 61, 114, 152	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	382	ASN	5.7
1	C	277	CYS	3.9
1	A	382	ASN	3.2
1	C	108	ARG	2.1
1	A	182	GLU	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.

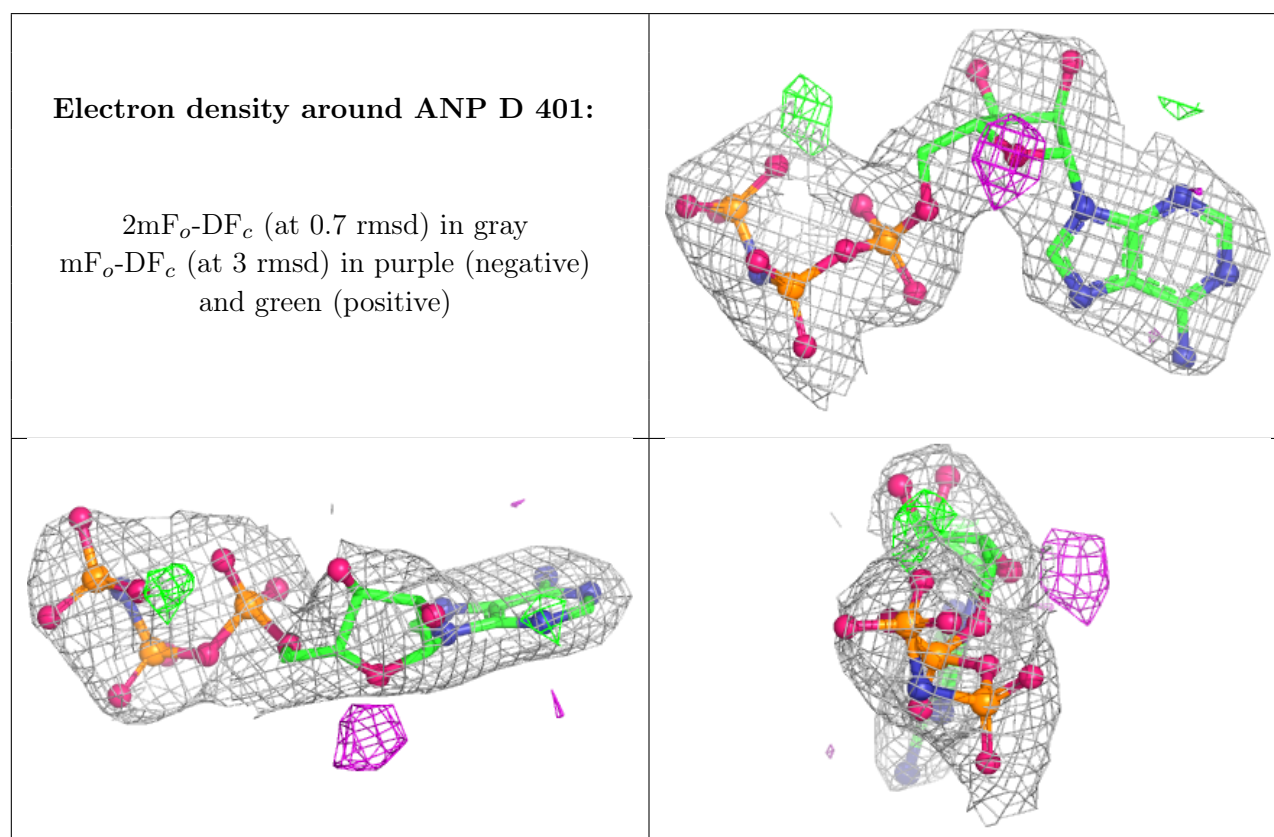
6.4 Ligands [i](#)

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.

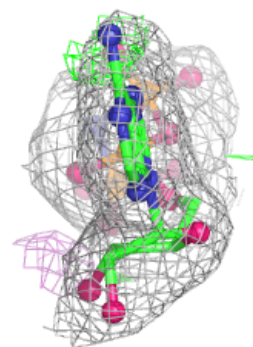
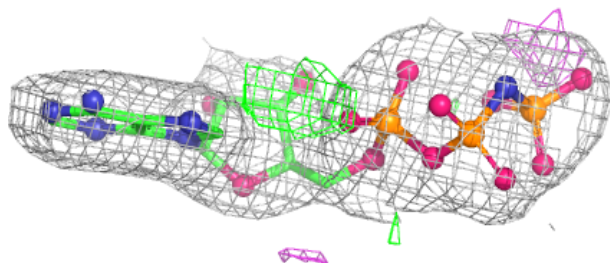
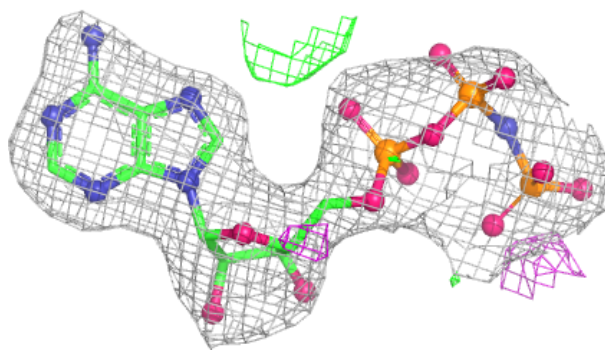
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	ANP	D	401	31/31	0.92	0.08	34,46,88,90	0
2	ANP	B	401	31/31	0.94	0.08	36,45,104,128	0
2	ANP	C	401	31/31	0.97	0.07	35,49,63,75	0
3	MG	C	402	1/1	0.97	0.05	60,60,60,60	0
3	MG	A	402	1/1	0.98	0.09	50,50,50,50	0
2	ANP	A	401	31/31	0.98	0.05	39,45,52,57	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.

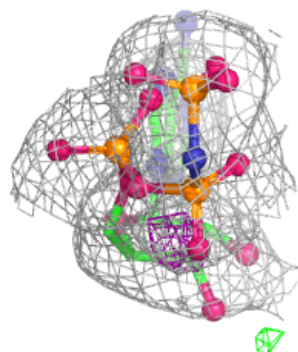
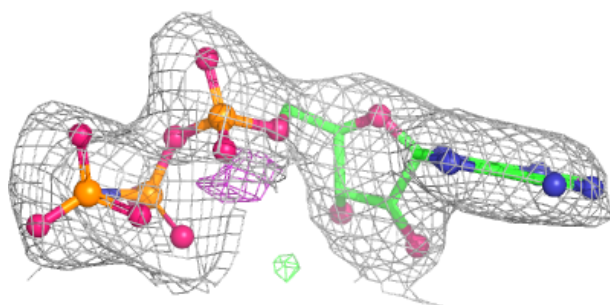
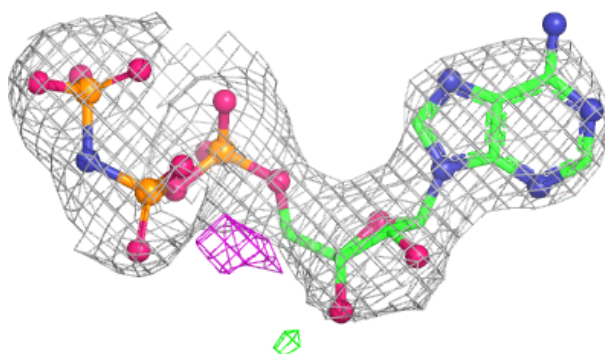


Electron density around ANP B 401:

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

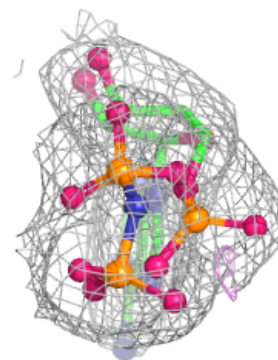
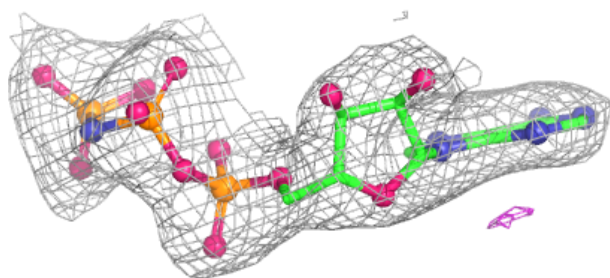
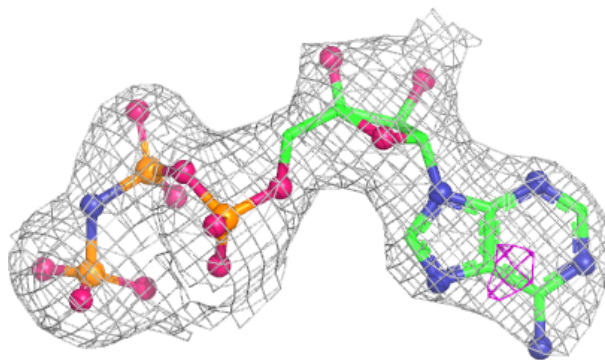
**Electron density around ANP C 401:**

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



Electron density around ANP A 401:

$2mF_o - DF_c$ (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.