Full wwPDB X-ray Structure Validation Report (i)

Jan 23, 2021 – 03:05 PM EST

PDB ID	:	1Q3H
Title	:	mouse CFTR NBD1 with AMP.PNP
Authors	:	Lewis, H.A.; Buchanan, S.G.; Burley, S.K.; Conners, K.; Dickey, M.; Dorwart, M.; Fowler, R.; Gao, X.; Guggino, W.B.; Hendrickson, W.A.
Deposited on	:	2003-07-29
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 (i) symbol.

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

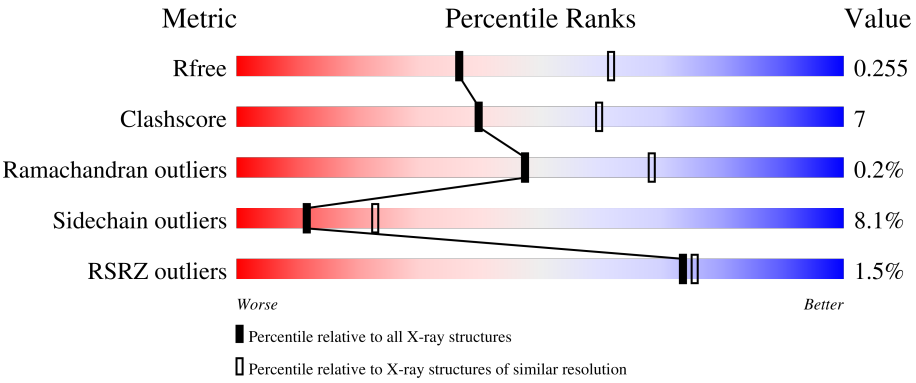
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.16
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.16

1 Overall quality at a glance (i)

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 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 <=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	286	73% 18% • 7%
1	B	286	74% 16% • 7%
1	C	286	75% 15% • 7%
1	D	286	3% 73% 17% • 8%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 8667 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 Cystic fibrosis transmembrane conductance regulator.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	265	Total	C	N	O	S	0	1	0
			2088	1331	345	399	13			
1	B	267	Total	C	N	O	S	0	1	0
			2102	1340	347	402	13			
1	C	266	Total	C	N	O	S	0	1	0
			2095	1335	346	401	13			
1	D	264	Total	C	N	O	S	0	1	0
			2082	1328	344	397	13			

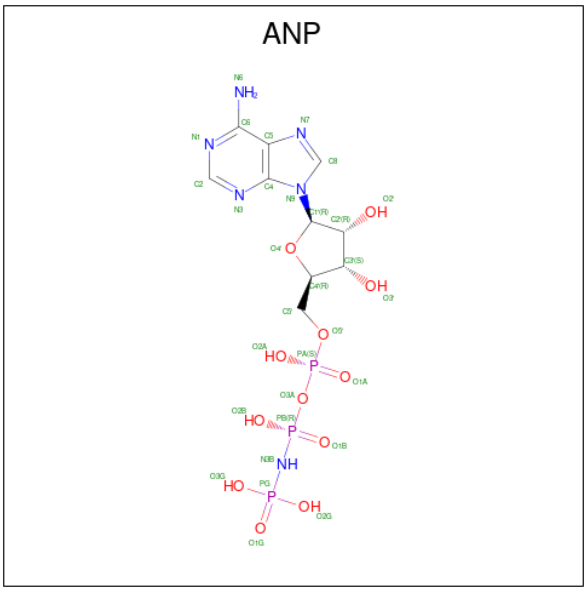
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	388	SER	-	cloning artifact	UNP P26361
B	388	SER	-	cloning artifact	UNP P26361
C	388	SER	-	cloning artifact	UNP P26361
D	388	SER	-	cloning artifact	UNP P26361

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

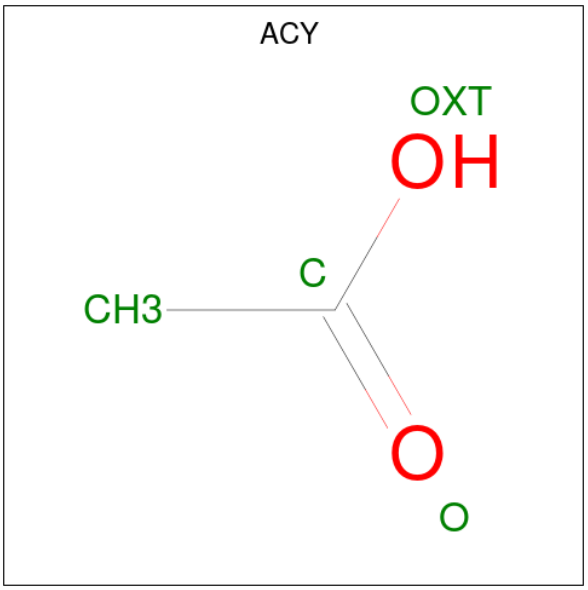
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mg	0	0
			1	1		
2	A	1	Total	Mg	0	0
			1	1		
2	D	1	Total	Mg	0	0
			1	1		
2	C	1	Total	Mg	0	0
			1	1		

- Molecule 3 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).



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

- Molecule 4 is ACETIC ACID (three-letter code: ACY) (formula: $C_2H_4O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0

- Molecule 5 is water.

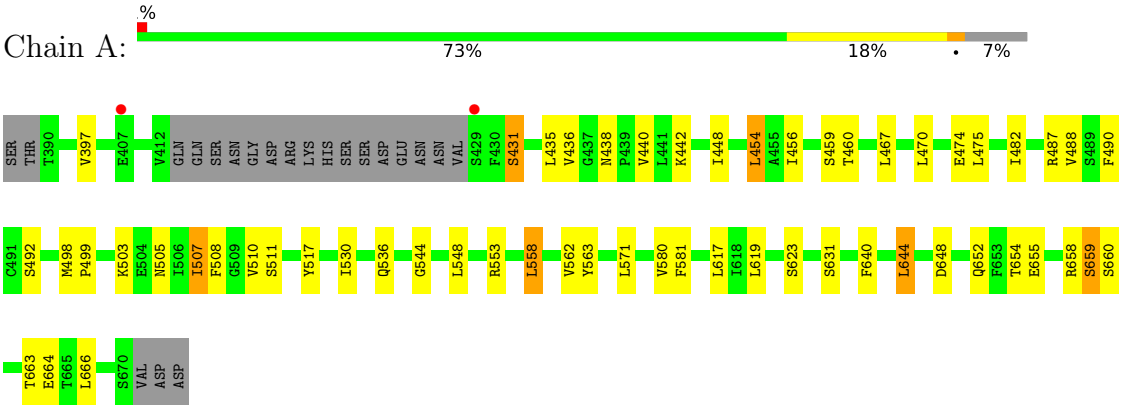
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	39	Total O 39 39	0	0
5	B	42	Total O 42 42	0	0
5	C	43	Total O 43 43	0	0
5	D	32	Total O 32 32	0	0

3 Residue-property plots (i)

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

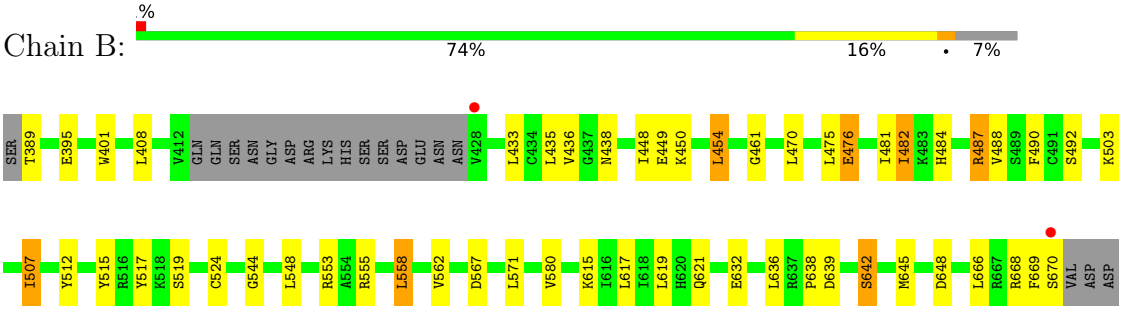
• Molecule 1: Cystic fibrosis transmembrane conductance regulator

Chain A:



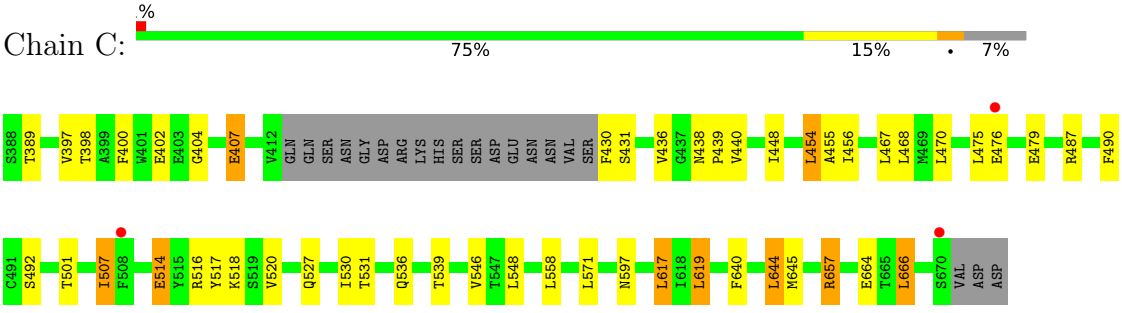
• Molecule 1: Cystic fibrosis transmembrane conductance regulator

Chain B:



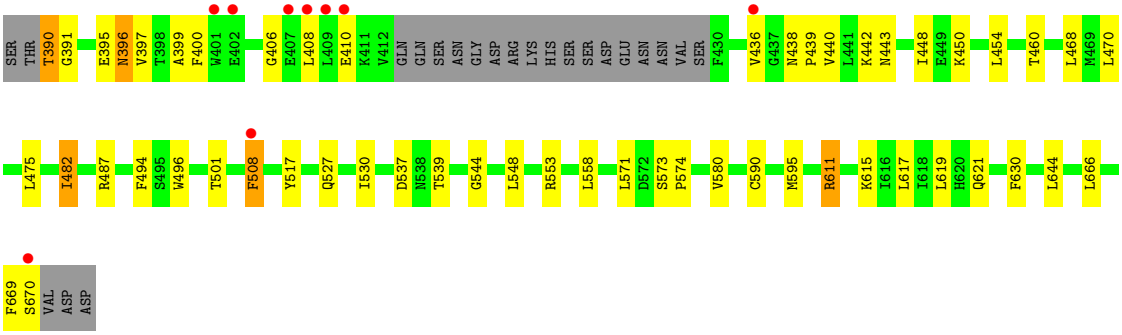
• Molecule 1: Cystic fibrosis transmembrane conductance regulator

Chain C:



• Molecule 1: Cystic fibrosis transmembrane conductance regulator

Chain D:


SER THR T390 G391 E395 N396 V397 T398 A399 F400 W401 E402 G406 E407 L408 L409 E410 K411 V412 GLN GLN SER ASN GLY ASP ARG LYS HIS SER SER ASP GLU ASN ASN VAL SER F430 V436 G437 N438 P439 V440 L441 K442 N443 I448 E449 K450 L454 T460 L468 M469 L470
L475 I482 R487 F494 S495 W496 T501 F508 Y517 Q527 I530 D537 N538 T539 G544 L548 R553 L558 L571 D572 S573 P574 V580 C590 M595 R611 K615 I616 L617 I618 L619 H620 Q621 F630 L644 L666
F669 S670 VAL ASP ASP

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 4 21 2	Depositor
Cell constants a, b, c, α, β, γ	171.68Å 171.68Å 109.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.00 – 2.50 121.40 – 2.18	Depositor EDS
% Data completeness (in resolution range)	(Not available) (33.00-2.50) 99.5 (121.40-2.18)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	1.59 (at 2.18Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.216 , 0.257 0.216 , 0.255	Depositor DCC
R_{free} test set	4278 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	36.9	Xtriage
Anisotropy	0.092	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 31.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	8667	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.84% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: ACY, ANP, MG

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	0.40	0/2128	0.50	0/2862
1	B	0.39	0/2142	0.51	0/2882
1	C	0.39	0/2135	0.50	0/2872
1	D	0.38	0/2122	0.50	0/2854
All	All	0.39	0/8527	0.50	0/11470

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	2088	0	2088	29	0
1	B	2102	0	2104	31	0
1	C	2095	0	2095	31	0
1	D	2082	0	2083	34	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	31	0	13	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	31	0	13	1	0
3	C	31	0	13	0	0
3	D	31	0	13	0	0
4	A	4	0	3	0	0
4	B	4	0	3	0	0
4	C	4	0	3	0	0
4	D	4	0	3	0	0
5	A	39	0	0	1	0
5	B	42	0	0	0	0
5	C	43	0	0	2	0
5	D	32	0	0	2	0
All	All	8667	0	8434	124	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 7.

All (124) 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:436:VAL:HB	1:C:438:ASN:HD21	1.32	0.92
1:D:669:PHE:O	1:D:670:SER:HB3	1.83	0.78
1:C:440:VAL:HG11	1:C:475:LEU:HD21	1.68	0.76
1:D:436:VAL:HB	1:D:438:ASN:HD21	1.51	0.76
1:C:657:ARG:HD3	5:C:73:HOH:O	1.88	0.72
1:C:389:THR:HG21	1:C:597:ASN:O	1.90	0.71
1:D:487:ARG:HH21	1:D:487:ARG:HG3	1.60	0.65
1:C:398:THR:HB	1:C:479:GLU:HB2	1.78	0.65
1:C:397:VAL:HG11	1:C:470:LEU:HD21	1.79	0.65
1:D:448:ILE:HD13	1:D:615:LYS:HD3	1.80	0.63
1:C:456:ILE:HD13	1:C:467:LEU:HD23	1.81	0.63
1:A:490:PHE:CE2	1:A:492:SER:HB3	2.33	0.63
1:B:515:TYR:O	1:B:519:SER:HB2	2.00	0.62
1:A:440:VAL:HG11	1:A:475:LEU:HD21	1.81	0.61
1:C:402:GLU:HG3	1:C:476:GLU:CD	2.21	0.61
1:B:482:ILE:HD11	1:B:484:HIS:CD2	2.36	0.61
1:C:436:VAL:CB	1:C:438:ASN:HD21	2.11	0.61
1:C:404:GLY:O	1:C:407:GLU:HG2	2.00	0.60
1:A:474:GLU:HG3	1:B:435:LEU:HD11	1.84	0.60
1:A:436:VAL:HB	1:A:438:ASN:OD1	2.01	0.59
1:C:490:PHE:CE2	1:C:492:SER:HB3	2.37	0.59
1:D:440:VAL:HG11	1:D:475:LEU:HD21	1.84	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:104:HOH:O	1:B:621:GLN:HG2	2.04	0.57
1:A:456:ILE:HD13	1:A:467:LEU:HD23	1.87	0.56
1:C:436:VAL:HB	1:C:438:ASN:ND2	2.13	0.56
1:D:390:THR:CG2	1:D:391:GLY:N	2.68	0.56
1:D:390:THR:HG22	1:D:391:GLY:N	2.23	0.54
1:D:580:VAL:HG22	5:D:56:HOH:O	2.09	0.53
1:A:558:LEU:HD22	1:A:562:VAL:HG23	1.91	0.53
1:A:498[B]:MET:HE1	1:A:499:PRO:O	2.09	0.53
1:B:401:TRP:CE2	1:B:433:LEU:HD13	2.45	0.52
1:D:669:PHE:O	1:D:670:SER:CB	2.57	0.52
1:A:640:PHE:CZ	1:A:644:LEU:HD13	2.45	0.51
1:B:490:PHE:CE2	1:B:492:SER:HB3	2.45	0.51
1:A:581:PHE:HE2	1:A:652:GLN:HE22	1.58	0.51
1:D:482:ILE:C	1:D:482:ILE:HD13	2.30	0.51
1:A:654:THR:O	1:A:658:ARG:HG3	2.11	0.51
1:C:617:LEU:HD13	1:C:619:LEU:HD13	1.92	0.51
1:B:638:PRO:O	1:B:642:SER:HB3	2.10	0.51
1:D:436:VAL:HB	1:D:438:ASN:ND2	2.23	0.51
1:B:448:ILE:HD11	1:B:454:LEU:HG	1.92	0.50
1:B:461:GLY:O	3:B:202:ANP:O3'	2.29	0.50
1:A:448:ILE:HD11	1:A:454:LEU:HG	1.94	0.50
1:A:498[B]:MET:HG2	1:A:508:PHE:CD1	2.46	0.50
1:A:397:VAL:HG11	1:A:470:LEU:HD21	1.93	0.50
1:C:440:VAL:CG1	1:C:475:LEU:HD21	2.40	0.49
1:D:442:LYS:HG2	1:D:443:ASN:ND2	2.26	0.49
1:B:395:GLU:HB2	1:B:481:ILE:CG2	2.43	0.49
1:B:476:GLU:H	1:B:476:GLU:CD	2.15	0.49
1:B:507:ILE:HD13	1:B:512:TYR:HD1	1.78	0.49
1:B:487:ARG:CZ	1:B:487:ARG:HB2	2.43	0.49
1:D:487:ARG:HG3	1:D:487:ARG:NH2	2.28	0.48
1:A:544:GLY:O	1:A:553:ARG:HD3	2.14	0.48
1:C:507:ILE:HD13	1:C:517:TYR:CD1	2.49	0.48
1:A:660:SER:O	1:A:664:GLU:HG3	2.14	0.48
1:C:527:GLN:O	1:C:531:THR:HG22	2.15	0.47
1:D:496:TRP:HH2	1:D:508:PHE:CE2	2.32	0.47
1:A:436:VAL:O	1:A:436:VAL:HG12	2.14	0.47
1:D:527:GLN:HE22	1:D:530:ILE:HD11	1.80	0.47
1:B:470:LEU:HD12	1:B:475:LEU:O	2.14	0.47
1:B:436:VAL:HB	1:B:438:ASN:HD21	1.80	0.46
1:A:459:SER:HB3	1:A:663:THR:HA	1.98	0.46
1:B:507:ILE:CG2	1:B:507:ILE:O	2.63	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:530:ILE:O	1:A:536:GLN:HA	2.16	0.46
1:D:390:THR:HG22	1:D:391:GLY:H	1.80	0.46
1:C:507:ILE:O	1:C:507:ILE:HG23	2.16	0.46
1:D:448:ILE:CD1	1:D:615:LYS:HD3	2.46	0.46
1:B:544:GLY:O	1:B:553:ARG:HD3	2.16	0.46
1:B:481:ILE:HD12	1:B:482:ILE:H	1.80	0.45
1:A:507:ILE:HG23	1:A:507:ILE:O	2.16	0.45
1:D:611:ARG:HA	1:D:630:PHE:CD1	2.51	0.45
1:A:498[B]:MET:SD	1:A:499:PRO:O	2.75	0.45
1:C:514:GLU:HG3	1:C:518:LYS:HD2	1.99	0.45
1:D:391:GLY:HA3	1:D:448:ILE:O	2.17	0.45
1:C:640:PHE:CZ	1:C:644:LEU:HD13	2.51	0.45
1:C:516:ARG:O	1:C:520:VAL:HG23	2.17	0.45
1:D:399:ALA:O	1:D:440:VAL:HG12	2.17	0.44
1:A:507:ILE:HD13	1:A:517:TYR:CD1	2.52	0.44
1:A:498[B]:MET:HE2	1:A:508:PHE:HE1	1.82	0.44
1:B:435:LEU:HA	1:B:435:LEU:HD12	1.90	0.44
1:B:476:GLU:N	1:B:476:GLU:CD	2.71	0.44
1:A:498[B]:MET:CE	1:A:508:PHE:HE1	2.31	0.44
1:D:527:GLN:NE2	1:D:530:ILE:HD11	2.32	0.44
1:A:431:SER:O	1:A:435:LEU:HD13	2.18	0.44
1:C:448:ILE:HD11	1:C:454:LEU:HG	1.99	0.43
1:D:390:THR:HG23	1:D:450:LYS:HB2	2.00	0.43
1:D:494:PHE:CE2	1:D:496:TRP:HB3	2.53	0.43
1:C:666:LEU:HD12	1:C:666:LEU:HA	1.86	0.43
1:C:617:LEU:CD1	1:C:619:LEU:HD13	2.48	0.43
1:A:507:ILE:HD11	1:A:563:TYR:CZ	2.53	0.43
1:A:655:GLU:O	1:A:659:SER:HB2	2.19	0.43
1:B:487:ARG:NH2	1:B:567:ASP:OD2	2.51	0.43
1:B:454:LEU:HD23	1:B:615:LYS:O	2.19	0.43
1:B:524:CYS:O	1:B:555:ARG:HD2	2.18	0.43
1:D:406:GLY:O	1:D:410:GLU:HB2	2.19	0.43
1:D:395:GLU:O	1:D:396:ASN:C	2.57	0.42
1:D:397:VAL:HG11	1:D:470:LEU:HD21	2.01	0.42
1:C:404:GLY:C	1:C:407:GLU:HG2	2.39	0.42
1:C:430:PHE:N	5:C:79:HOH:O	2.52	0.42
1:B:507:ILE:CD1	1:B:512:TYR:HD1	2.33	0.42
1:D:517:TYR:HE2	1:D:537:ASP:OD2	2.02	0.42
1:D:544:GLY:O	1:D:553:ARG:HD3	2.20	0.42
1:C:530:ILE:O	1:C:536:GLN:HA	2.19	0.42
1:C:501:THR:HA	1:C:539:THR:O	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:402:GLU:HG3	1:C:476:GLU:OE1	2.19	0.42
1:D:470:LEU:HD12	1:D:475:LEU:O	2.20	0.42
1:C:400:PHE:HA	1:C:439:PRO:HA	2.02	0.42
1:B:558:LEU:HD22	1:B:562:VAL:HG23	2.03	0.41
1:D:400:PHE:HA	1:D:439:PRO:HA	2.01	0.41
1:B:639:ASP:HB3	1:B:669:PHE:CZ	2.55	0.41
1:B:507:ILE:HD13	1:B:512:TYR:CD1	2.56	0.41
1:C:454:LEU:HD22	1:C:455:ALA:N	2.36	0.41
1:D:501:THR:HA	1:D:539:THR:O	2.21	0.41
1:B:507:ILE:HG23	1:B:507:ILE:O	2.21	0.41
1:D:573:SER:N	1:D:574:PRO:CD	2.83	0.41
1:C:507:ILE:CD1	1:C:517:TYR:CD1	3.04	0.41
1:B:632:GLU:O	1:B:636:LEU:HB2	2.21	0.41
1:D:580:VAL:CG2	5:D:56:HOH:O	2.69	0.41
1:B:389:THR:N	1:B:567:ASP:OD1	2.54	0.41
1:A:510:VAL:HG12	1:A:511:SER:N	2.35	0.40
1:B:503:LYS:HE3	1:B:517:TYR:CE2	2.56	0.40
1:D:590:CYS:O	1:D:595:MET:HG3	2.22	0.40
1:A:498[B]:MET:HE2	1:A:498[B]:MET:HB2	1.85	0.40
1:A:498[B]:MET:HG3	1:A:505:ASN:OD1	2.21	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	262/286 (92%)	255 (97%)	7 (3%)	0	100	100
1	B	264/286 (92%)	256 (97%)	8 (3%)	0	100	100
1	C	263/286 (92%)	256 (97%)	7 (3%)	0	100	100
1	D	261/286 (91%)	251 (96%)	8 (3%)	2 (1%)	19	35
All	All	1050/1144 (92%)	1018 (97%)	30 (3%)	2 (0%)	47	68

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	396	ASN
1	D	508	PHE

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	232/252 (92%)	211 (91%)	21 (9%)	9 18
1	B	234/252 (93%)	213 (91%)	21 (9%)	9 19
1	C	233/252 (92%)	215 (92%)	18 (8%)	13 25
1	D	231/252 (92%)	216 (94%)	15 (6%)	17 33
All	All	930/1008 (92%)	855 (92%)	75 (8%)	11 23

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	431	SER
1	A	442	LYS
1	A	454	LEU
1	A	460	THR
1	A	482	ILE
1	A	487	ARG
1	A	488	VAL
1	A	503	LYS
1	A	507	ILE
1	A	548	LEU
1	A	558	LEU
1	A	571	LEU
1	A	580	VAL
1	A	617	LEU
1	A	619	LEU
1	A	623	SER
1	A	631	SER
1	A	644	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	648	ASP
1	A	659	SER
1	A	666	LEU
1	B	408	LEU
1	B	449	GLU
1	B	450	LYS
1	B	454	LEU
1	B	476	GLU
1	B	482	ILE
1	B	487	ARG
1	B	488	VAL
1	B	507	ILE
1	B	548	LEU
1	B	558	LEU
1	B	571	LEU
1	B	580	VAL
1	B	617	LEU
1	B	619	LEU
1	B	642	SER
1	B	645	MET
1	B	648	ASP
1	B	666	LEU
1	B	668	ARG
1	B	670	SER
1	C	407	GLU
1	C	431	SER
1	C	454	LEU
1	C	468	LEU
1	C	487	ARG
1	C	507	ILE
1	C	514	GLU
1	C	546	VAL
1	C	548	LEU
1	C	558	LEU
1	C	571	LEU
1	C	617	LEU
1	C	619	LEU
1	C	644	LEU
1	C	645	MET
1	C	657	ARG
1	C	664	GLU
1	C	666	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	390	THR
1	D	408	LEU
1	D	454	LEU
1	D	460	THR
1	D	468	LEU
1	D	482	ILE
1	D	548	LEU
1	D	558	LEU
1	D	571	LEU
1	D	611	ARG
1	D	617	LEU
1	D	619	LEU
1	D	621	GLN
1	D	644	LEU
1	D	666	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	443	ASN
1	A	538	ASN
1	A	652	GLN
1	B	396	ASN
1	B	438	ASN
1	B	443	ASN
1	B	621	GLN
1	C	438	ASN
1	D	438	ASN
1	D	443	ASN
1	D	527	GLN
1	D	634	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 12 ligands modelled in this entry, 4 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	ACY	A	301	-	1,3,3	2.70	1 (100%)	0,3,3	0.00	-
3	ANP	A	201	2	29,33,33	3.28	12 (41%)	31,52,52	2.07	12 (38%)
4	ACY	B	302	-	1,3,3	3.01	1 (100%)	0,3,3	0.00	-
3	ANP	B	202	2	29,33,33	3.31	12 (41%)	31,52,52	2.13	11 (35%)
4	ACY	C	303	-	1,3,3	2.33	1 (100%)	0,3,3	0.00	-
3	ANP	C	203	2	29,33,33	3.38	12 (41%)	31,52,52	2.15	12 (38%)
4	ACY	D	304	-	1,3,3	2.73	1 (100%)	0,3,3	0.00	-
3	ANP	D	204	2	29,33,33	3.37	12 (41%)	31,52,52	2.04	10 (32%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ANP	C	203	2	-	4/14/38/38	0/3/3/3
3	ANP	B	202	2	-	4/14/38/38	0/3/3/3
3	ANP	D	204	2	-	3/14/38/38	0/3/3/3
3	ANP	A	201	2	-	4/14/38/38	0/3/3/3

All (52) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	203	ANP	PG-O1G	8.71	1.60	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	204	ANP	PG-O1G	8.62	1.59	1.46
3	A	201	ANP	PB-O1B	8.14	1.59	1.46
3	A	201	ANP	PG-O1G	8.07	1.59	1.46
3	D	204	ANP	PB-O1B	7.87	1.58	1.46
3	B	202	ANP	PB-O1B	7.86	1.58	1.46
3	B	202	ANP	PG-O1G	7.74	1.58	1.46
3	C	203	ANP	PB-O1B	6.91	1.57	1.46
3	C	203	ANP	C4-N3	6.76	1.45	1.35
3	B	202	ANP	C4-N3	6.59	1.44	1.35
3	C	203	ANP	O2'-C2'	6.22	1.57	1.43
3	D	204	ANP	O2'-C2'	6.16	1.57	1.43
3	D	204	ANP	C4-N3	6.06	1.44	1.35
3	A	201	ANP	O2'-C2'	5.77	1.56	1.43
3	B	202	ANP	O2'-C2'	5.71	1.56	1.43
3	A	201	ANP	C5'-C4'	-5.65	1.34	1.51
3	A	201	ANP	C4-N3	5.54	1.43	1.35
3	D	204	ANP	C5'-C4'	-5.41	1.34	1.51
3	C	203	ANP	C5'-C4'	-5.41	1.34	1.51
3	B	202	ANP	C5'-C4'	-4.99	1.36	1.51
3	D	204	ANP	C2-N1	4.55	1.42	1.33
3	C	203	ANP	C2-N1	4.55	1.42	1.33
3	A	201	ANP	C2-N1	4.48	1.42	1.33
3	B	202	ANP	C2-N1	4.45	1.42	1.33
3	B	202	ANP	PB-N3B	4.43	1.74	1.63
3	C	203	ANP	PB-N3B	4.30	1.74	1.63
3	D	204	ANP	PB-N3B	3.93	1.73	1.63
3	A	201	ANP	PB-N3B	3.93	1.73	1.63
3	C	203	ANP	PG-N3B	3.78	1.73	1.63
3	D	204	ANP	PG-N3B	3.65	1.72	1.63
3	A	201	ANP	PG-N3B	3.57	1.72	1.63
3	B	202	ANP	PG-N3B	3.41	1.72	1.63
3	B	202	ANP	O5'-C5'	3.03	1.56	1.44
4	B	302	ACY	CH3-C	3.01	1.52	1.48
3	C	203	ANP	C2-N3	2.96	1.36	1.32
3	B	202	ANP	C2-N3	2.80	1.36	1.32
4	D	304	ACY	CH3-C	2.73	1.52	1.48
3	D	204	ANP	C3'-C4'	2.72	1.60	1.53
4	A	301	ACY	CH3-C	2.70	1.52	1.48
3	D	204	ANP	C2-N3	2.57	1.36	1.32
3	A	201	ANP	C2-N3	2.49	1.36	1.32
3	A	201	ANP	C3'-C4'	2.43	1.59	1.53
3	D	204	ANP	O3'-C3'	-2.35	1.37	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	303	ACY	CH3-C	2.33	1.51	1.48
3	C	203	ANP	O3'-C3'	-2.24	1.37	1.43
3	D	204	ANP	PA-O1A	2.17	1.58	1.50
3	A	201	ANP	O3'-C3'	-2.13	1.38	1.43
3	B	202	ANP	C8-N7	-2.11	1.30	1.34
3	A	201	ANP	PA-O1A	2.10	1.58	1.50
3	B	202	ANP	O3'-C3'	-2.05	1.38	1.43
3	C	203	ANP	C3'-C4'	2.04	1.58	1.53
3	C	203	ANP	C8-N7	-2.03	1.31	1.34

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	202	ANP	O3'-C3'-C4'	5.74	127.64	111.05
3	D	204	ANP	O3'-C3'-C4'	5.46	126.83	111.05
3	C	203	ANP	O3'-C3'-C4'	5.42	126.72	111.05
3	A	201	ANP	O3'-C3'-C4'	4.57	124.26	111.05
3	B	202	ANP	O4'-C4'-C5'	-4.13	95.79	109.37
3	A	201	ANP	C3'-C2'-C1'	3.99	106.99	100.98
3	C	203	ANP	O4'-C4'-C5'	-3.98	96.28	109.37
3	B	202	ANP	C3'-C2'-C1'	3.85	106.78	100.98
3	C	203	ANP	C4-C5-N7	3.80	113.36	109.40
3	D	204	ANP	C3'-C2'-C1'	3.79	106.68	100.98
3	A	201	ANP	O4'-C4'-C5'	-3.77	96.97	109.37
3	D	204	ANP	O4'-C4'-C5'	-3.72	97.14	109.37
3	C	203	ANP	C3'-C2'-C1'	3.70	106.55	100.98
3	A	201	ANP	C4-C5-N7	3.60	113.15	109.40
3	D	204	ANP	C4-C5-N7	3.57	113.12	109.40
3	B	202	ANP	C4-C5-N7	3.49	113.03	109.40
3	C	203	ANP	O4'-C4'-C3'	-3.48	98.23	105.11
3	A	201	ANP	O4'-C4'-C3'	-3.46	98.27	105.11
3	D	204	ANP	O4'-C4'-C3'	-3.42	98.35	105.11
3	B	202	ANP	O4'-C4'-C3'	-2.93	99.31	105.11
3	D	204	ANP	PA-O3A-PB	-2.92	122.34	132.62
3	B	202	ANP	O2B-PB-O3A	2.87	114.22	104.64
3	A	201	ANP	O2'-C2'-C3'	-2.75	102.92	111.82
3	C	203	ANP	O2'-C2'-C3'	-2.73	102.99	111.82
3	B	202	ANP	O2'-C2'-C3'	-2.61	103.37	111.82
3	A	201	ANP	C2'-C3'-C4'	-2.53	97.72	102.64
3	A	201	ANP	O4'-C1'-C2'	-2.48	103.31	106.93
3	B	202	ANP	C1'-N9-C4	2.47	130.98	126.64
3	A	201	ANP	O3'-C3'-C2'	2.46	119.78	111.82

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	201	ANP	O5'-C5'-C4'	-2.46	100.54	108.99
3	C	203	ANP	O1G-PG-N3B	-2.41	108.22	111.77
3	D	204	ANP	O3G-PG-O1G	-2.37	107.49	113.45
3	C	203	ANP	C1'-N9-C4	2.36	130.80	126.64
3	C	203	ANP	PA-O3A-PB	-2.36	124.30	132.62
3	C	203	ANP	C2'-C3'-C4'	-2.33	98.11	102.64
3	B	202	ANP	O2G-PG-O1G	-2.32	107.63	113.45
3	C	203	ANP	O4'-C1'-C2'	-2.28	103.59	106.93
3	C	203	ANP	O1B-PB-N3B	-2.27	108.43	111.77
3	D	204	ANP	O2'-C2'-C3'	-2.25	104.55	111.82
3	D	204	ANP	C2'-C3'-C4'	-2.21	98.36	102.64
3	B	202	ANP	PA-O3A-PB	-2.12	125.13	132.62
3	A	201	ANP	PA-O3A-PB	-2.10	125.21	132.62
3	A	201	ANP	O3G-PG-O1G	-2.08	108.22	113.45
3	D	204	ANP	O3'-C3'-C2'	2.07	118.50	111.82
3	B	202	ANP	C2'-C3'-C4'	-2.03	98.71	102.64

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	201	ANP	PB-N3B-PG-O1G
3	A	201	ANP	PG-N3B-PB-O1B
3	A	201	ANP	PG-N3B-PB-O3A
3	B	202	ANP	PB-N3B-PG-O1G
3	B	202	ANP	PG-N3B-PB-O1B
3	B	202	ANP	PG-N3B-PB-O3A
3	C	203	ANP	PB-N3B-PG-O1G
3	C	203	ANP	PG-N3B-PB-O1B
3	C	203	ANP	PG-N3B-PB-O3A
3	D	204	ANP	PB-N3B-PG-O1G
3	D	204	ANP	PG-N3B-PB-O1B
3	D	204	ANP	PG-N3B-PB-O3A
3	A	201	ANP	O4'-C4'-C5'-O5'
3	C	203	ANP	O4'-C4'-C5'-O5'
3	B	202	ANP	C5'-O5'-PA-O1A

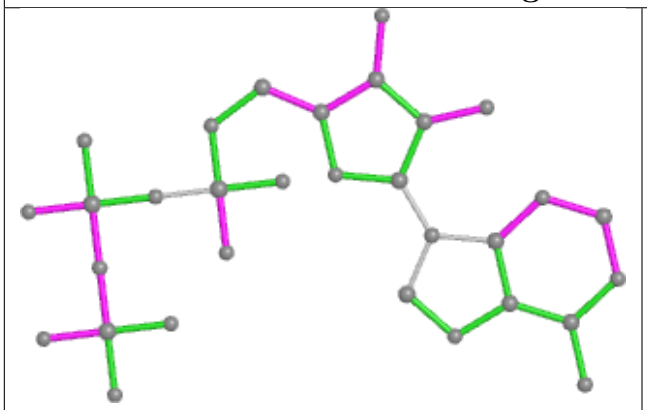
There are no ring outliers.

1 monomer is involved in 1 short contact:

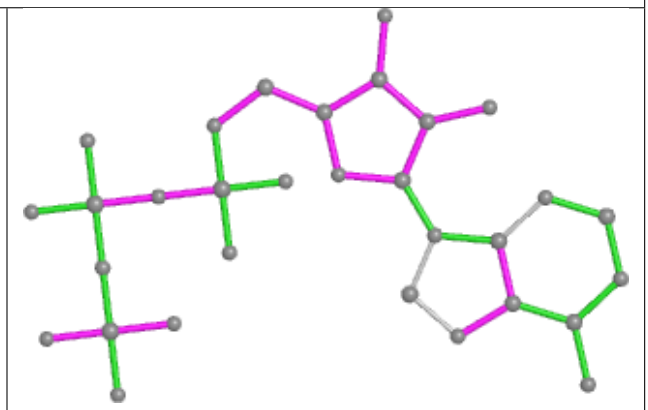
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	202	ANP	1	0

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 then 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.

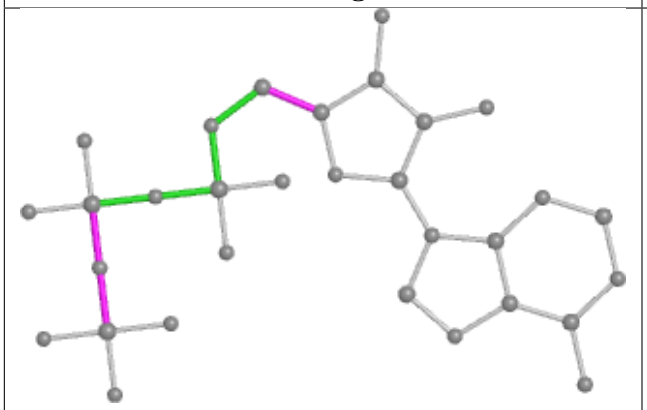
Ligand ANP A 201



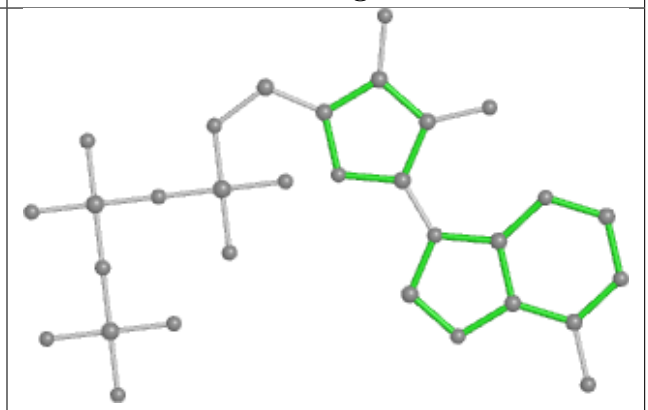
Bond lengths



Bond angles

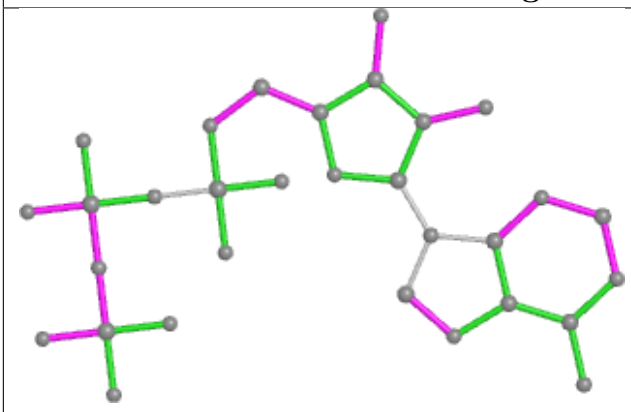


Torsions

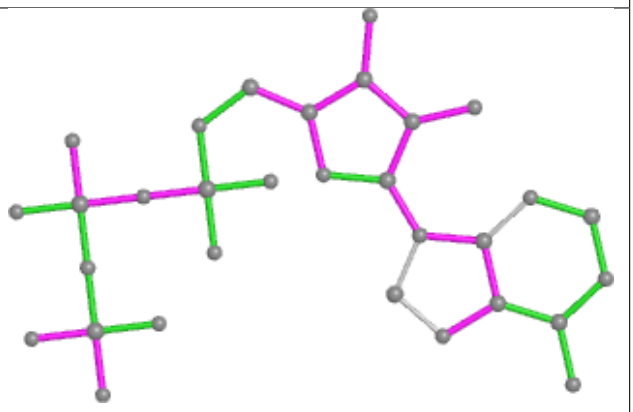


Rings

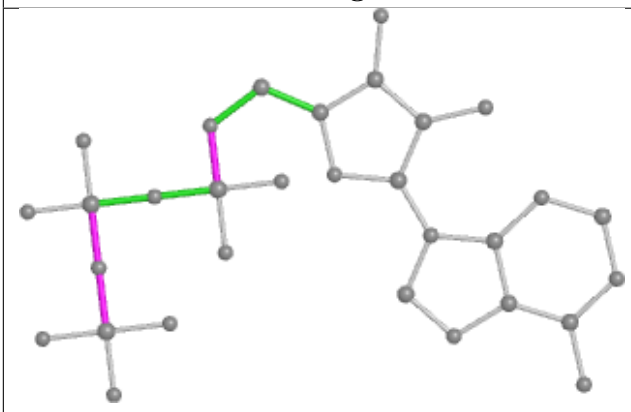
Ligand ANP B 202



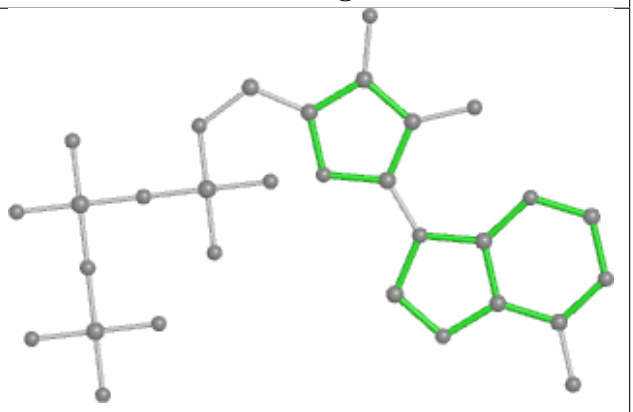
Bond lengths



Bond angles

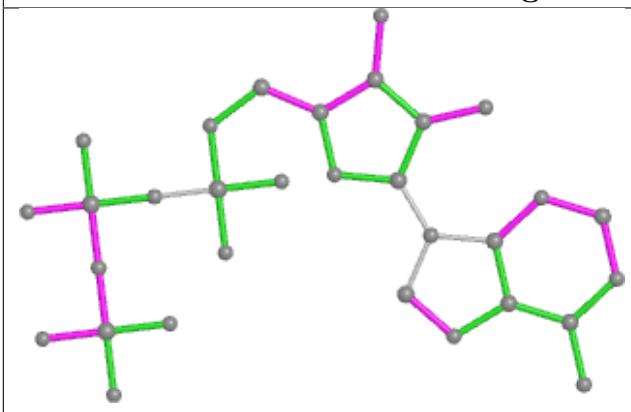


Torsions

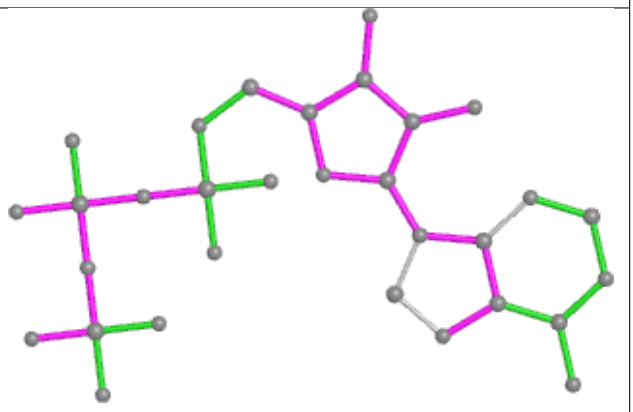


Rings

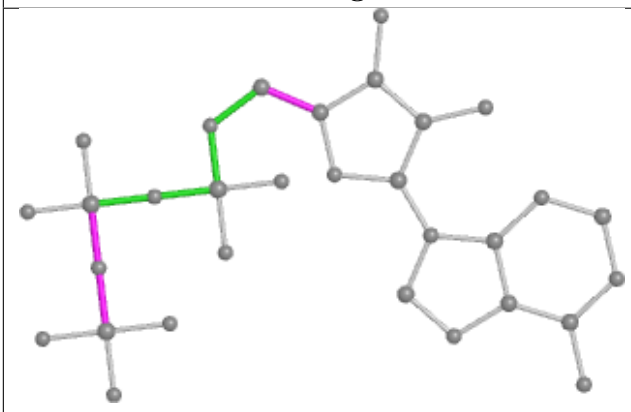
Ligand ANP C 203



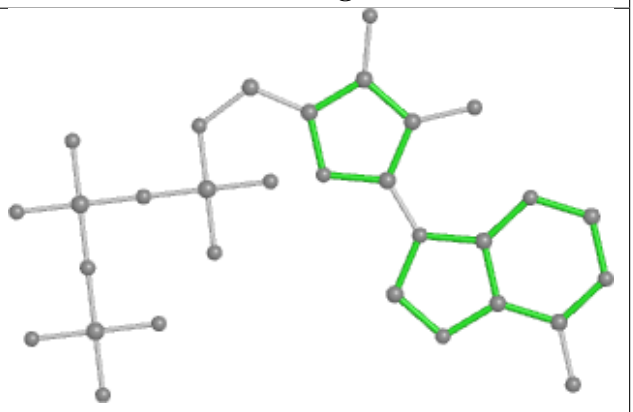
Bond lengths



Bond angles

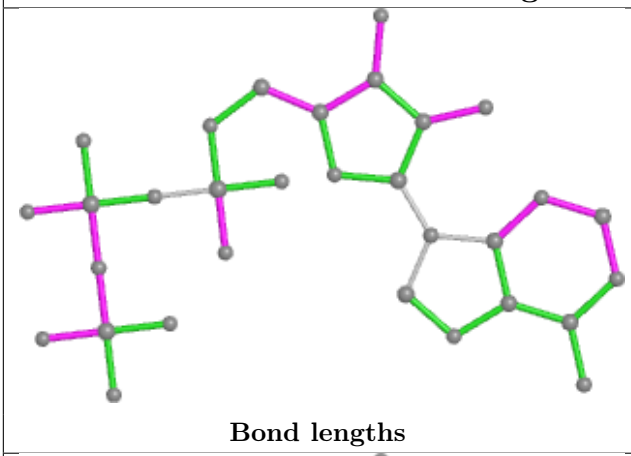


Torsions

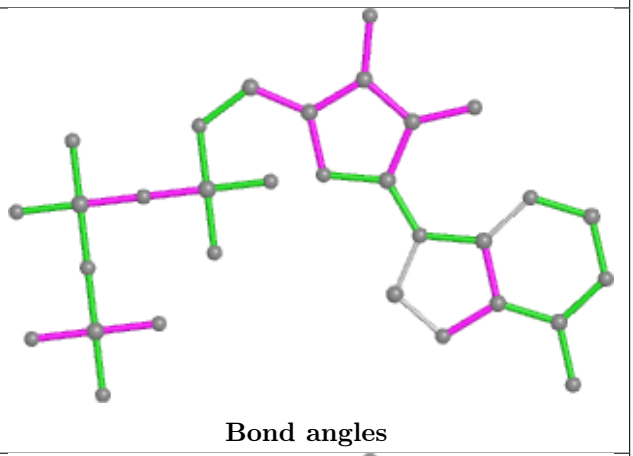


Rings

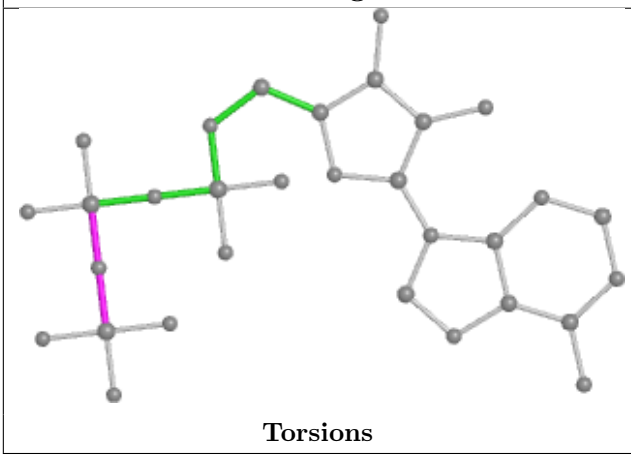
Ligand ANP D 204



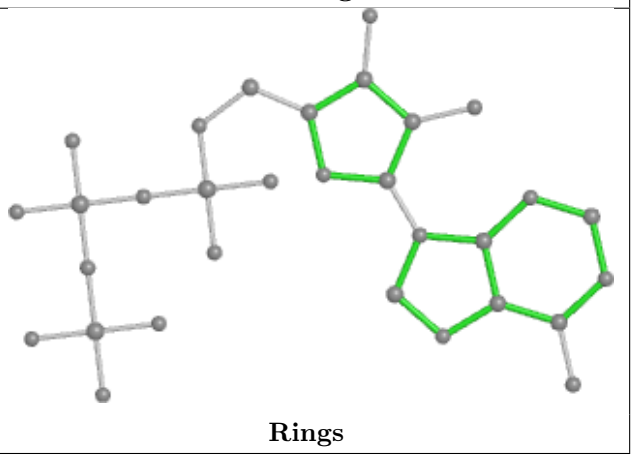
Bond lengths



Bond angles



Torsions



Rings

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, 95^{th} 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	265/286 (92%)	-0.29	2 (0%)	86	87	16, 33, 56, 71	0
1	B	267/286 (93%)	-0.27	2 (0%)	87	89	17, 33, 55, 66	0
1	C	266/286 (93%)	-0.25	3 (1%)	80	82	17, 31, 54, 68	0
1	D	264/286 (92%)	-0.22	9 (3%)	45	48	17, 36, 64, 78	0
All	All	1062/1144 (92%)	-0.26	16 (1%)	73	75	16, 33, 58, 78	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	670	SER	4.4
1	C	670	SER	4.3
1	B	670	SER	3.8
1	D	410	GLU	2.8
1	A	429	SER	2.8
1	D	508	PHE	2.8
1	D	408	LEU	2.6
1	C	476	GLU	2.6
1	D	401	TRP	2.4
1	D	407	GLU	2.4
1	D	409	LEU	2.3
1	B	428	VAL	2.1
1	C	508	PHE	2.1
1	A	407	GLU	2.0
1	D	402	GLU	2.0
1	D	436	VAL	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 (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

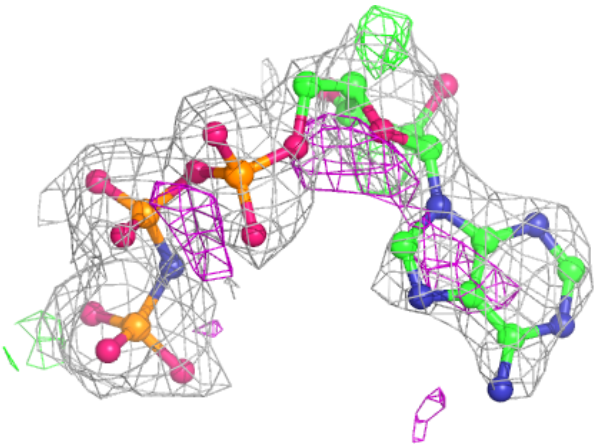
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

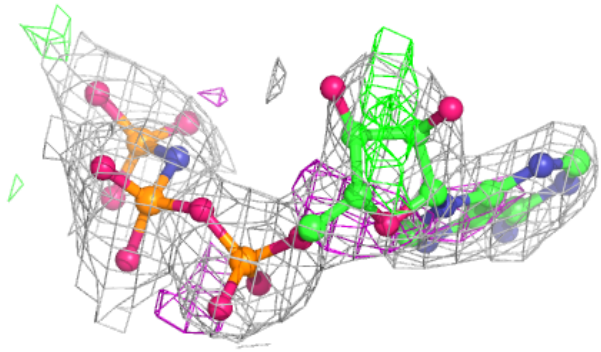
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	MG	B	674	1/1	0.87	0.15	31,31,31,31	0
2	MG	A	674	1/1	0.89	0.12	37,37,37,37	0
2	MG	C	674	1/1	0.89	0.05	31,31,31,31	0
2	MG	D	674	1/1	0.91	0.10	43,43,43,43	0
3	ANP	C	203	31/31	0.93	0.21	36,52,63,64	0
3	ANP	D	204	31/31	0.93	0.23	39,66,81,81	0
3	ANP	A	201	31/31	0.94	0.23	38,58,70,70	0
4	ACY	A	301	4/4	0.95	0.17	30,31,32,33	0
4	ACY	B	302	4/4	0.95	0.15	35,37,37,38	0
3	ANP	B	202	31/31	0.96	0.20	28,50,61,62	0
4	ACY	D	304	4/4	0.97	0.14	36,36,37,38	0
4	ACY	C	303	4/4	0.97	0.17	29,31,31,35	0

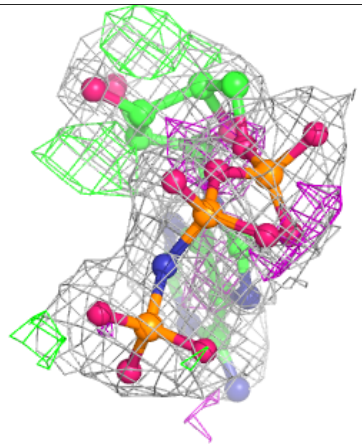
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ANP C 203:

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

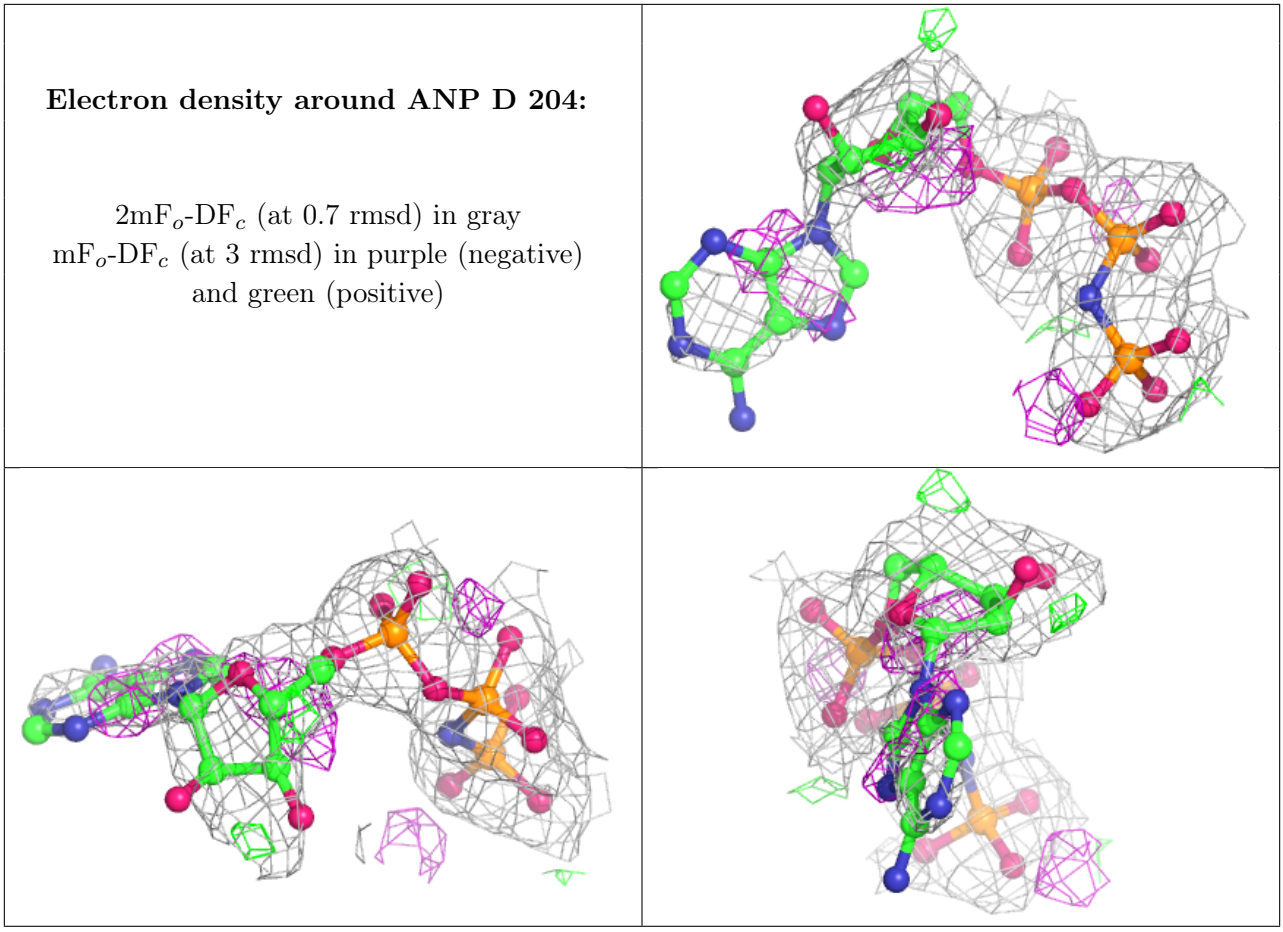






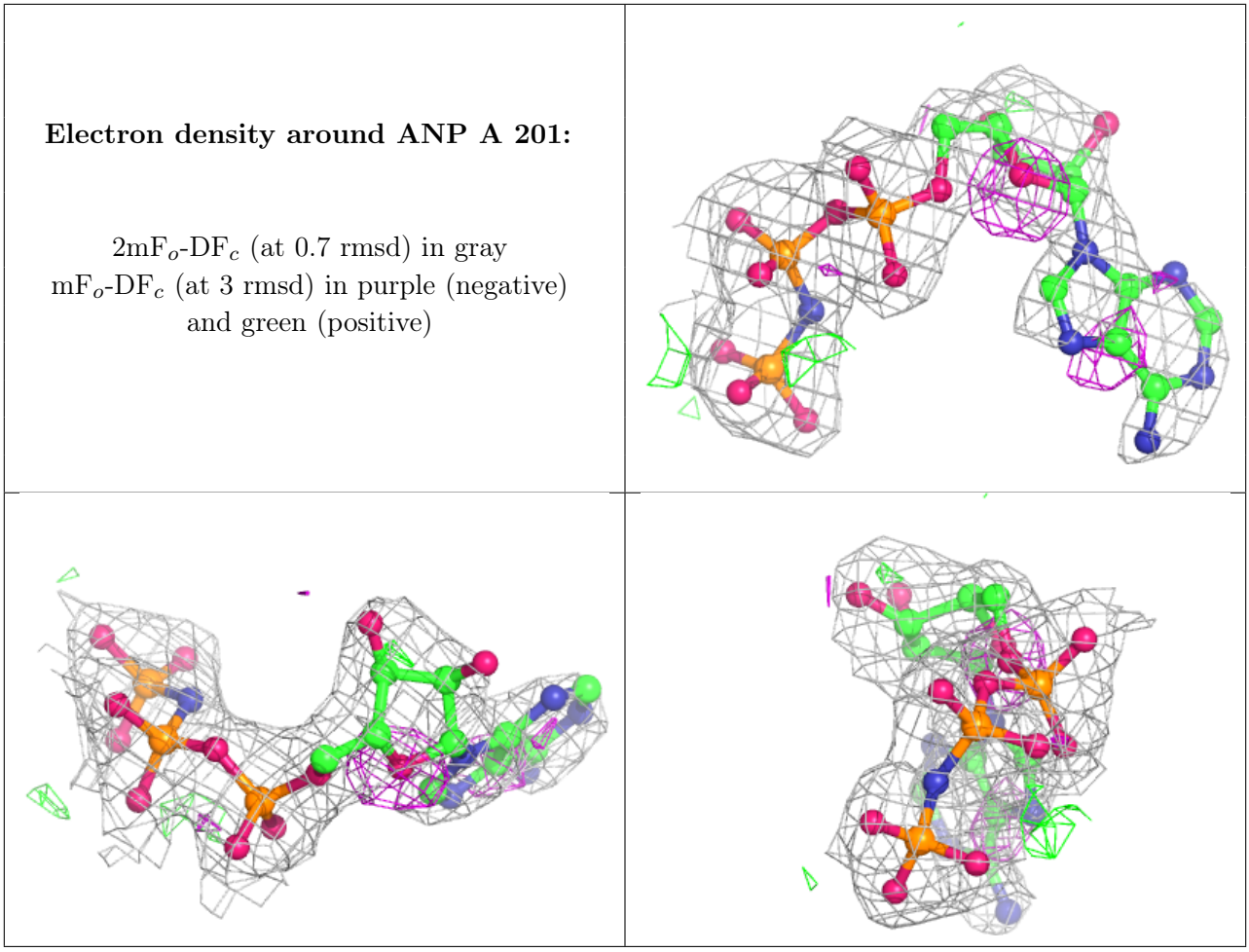
Electron density around ANP D 204:

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



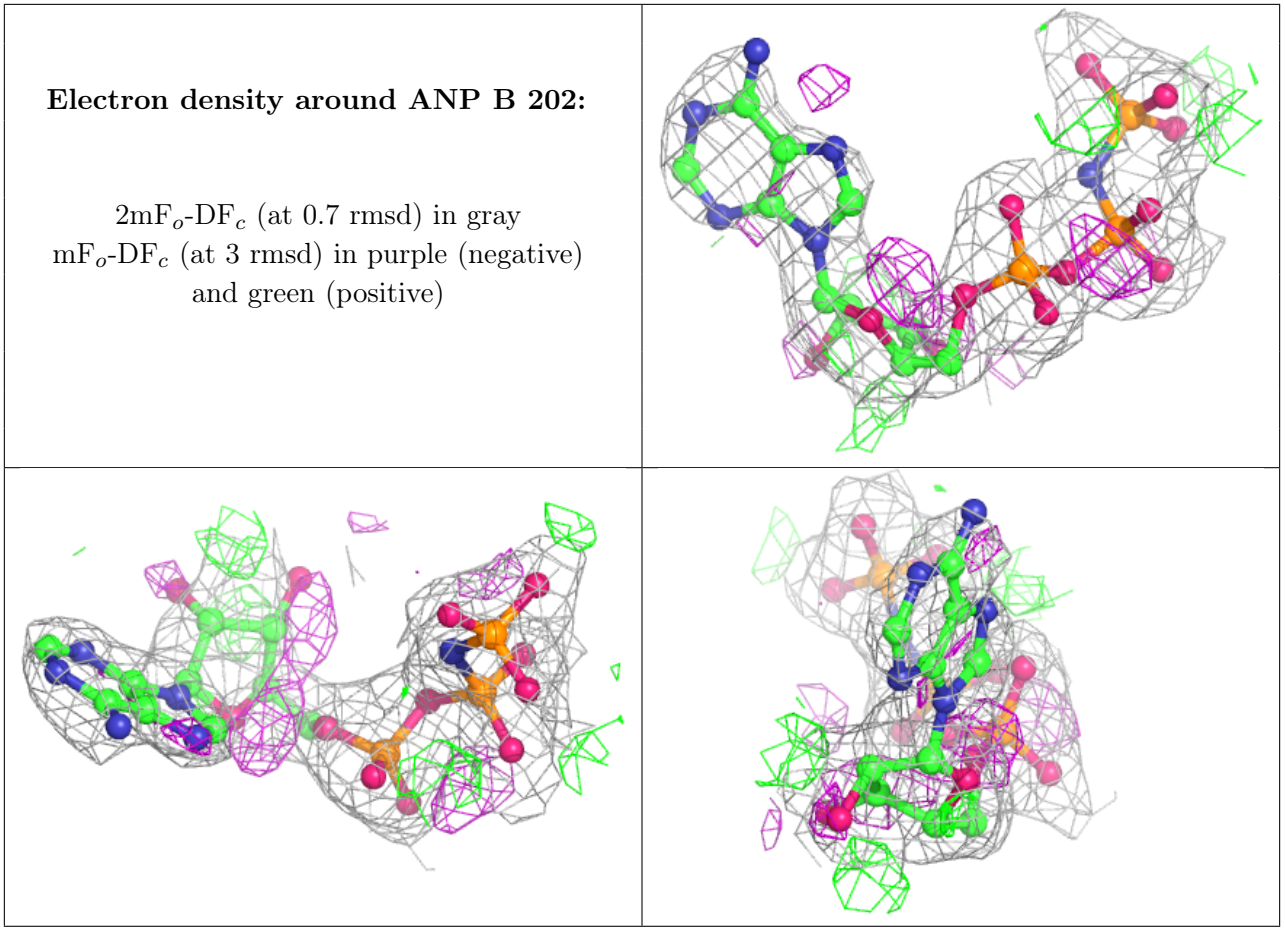
Electron density around ANP A 201:

$2mF_o$-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 202:

$2mF_o$-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.