Full wwPDB X-ray Structure Validation Report ⓘ

Nov 11, 2026 – 12:47 pm GMT

PDB ID	:	9QGS / pdb_00009qgs
Title	:	Crystal Structure of human MLH1 N-terminal domain with AMP-PNP
Authors	:	Thomsen, M.; Ganichkin, O.; Thieulin-Pardo, G.; Bandera, A.M.; Finley, M.; Felsenfeld, D.; Haque, T.; Monteagudo, E.; Stamford, A.; Vogt, T.; Prasad, B.C.; Boudet, J.
Deposited on	:	2025-03-14
Resolution	:	1.93 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:

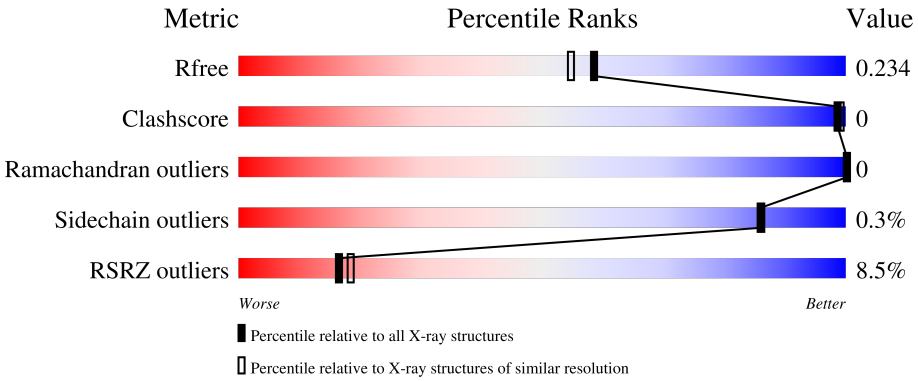
MolProbity	:	4-5-2 with Phenix2.2
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.2
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

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 1.93 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	1452 (1.94-1.94)
Clashscore	190562	1494 (1.94-1.94)
Ramachandran outliers	187476	1479 (1.94-1.94)
Sidechain outliers	187428	1479 (1.94-1.94)
RSRZ outliers	180081	1453 (1.94-1.94)

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	341	6% 96%
1	B	341	9% 96%
1	C	341	6% 97%
1	D	341	12% 96%

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 11762 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.

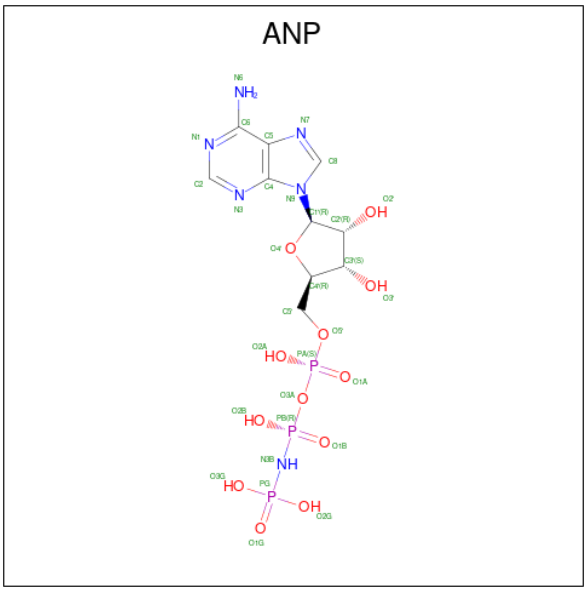
- Molecule 1 is a protein called DNA mismatch repair protein Mlh1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	334	Total	C	N	O	S	26	8	0
			2667	1685	468	506	8			
1	B	333	Total	C	N	O	S	31	6	0
			2647	1672	465	502	8			
1	C	334	Total	C	N	O	S	43	10	0
			2693	1698	476	511	8			
1	D	335	Total	C	N	O	S	41	9	0
			2676	1686	470	510	10			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP P40692
B	0	GLY	-	expression tag	UNP P40692
C	0	GLY	-	expression tag	UNP P40692
D	0	GLY	-	expression tag	UNP P40692

- Molecule 2 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$) (labeled as "Ligand of Interest" by depositor).



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

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

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

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Na 1 1	0	0

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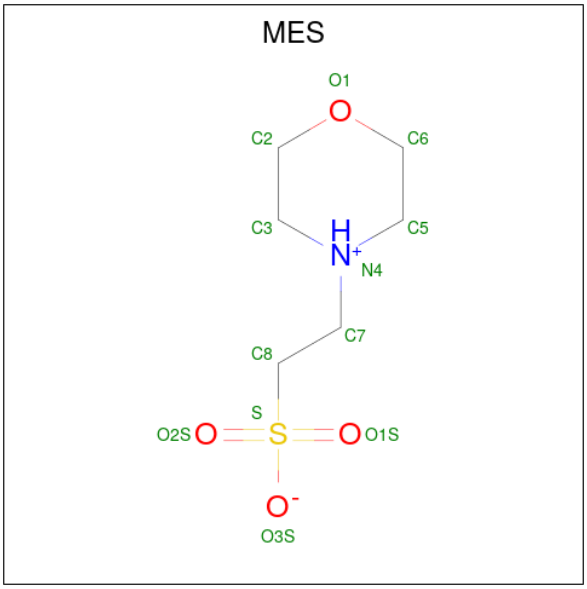
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Na 1 1	0	0
4	C	1	Total Na 1 1	0	0
4	D	1	Total Na 1 1	0	0

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

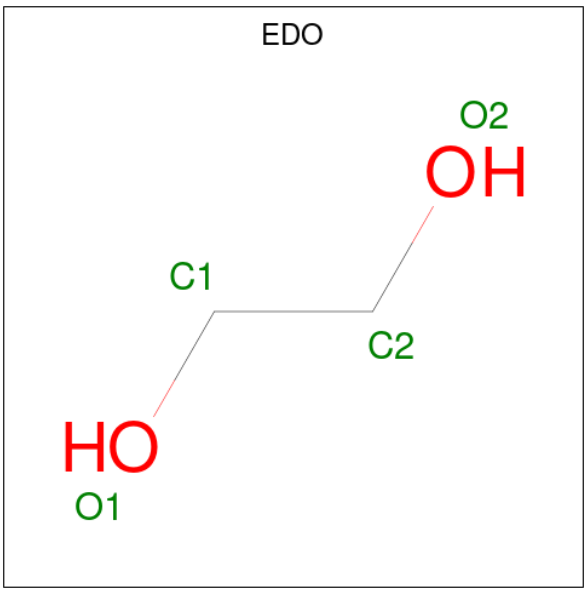
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	2	Total Ca 2 2	0	0
5	B	1	Total Ca 1 1	0	0
5	C	2	Total Ca 2 2	0	0
5	D	1	Total Ca 1 1	0	0

- Molecule 6 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: $C_6H_{13}NO_4S$).



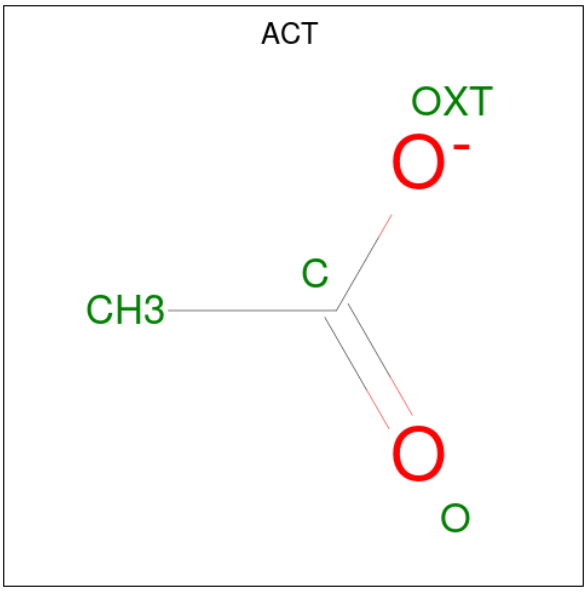
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C N O S 12 6 1 4 1	0	0
6	B	1	Total C N O S 12 6 1 4 1	0	0

- Molecule 7 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



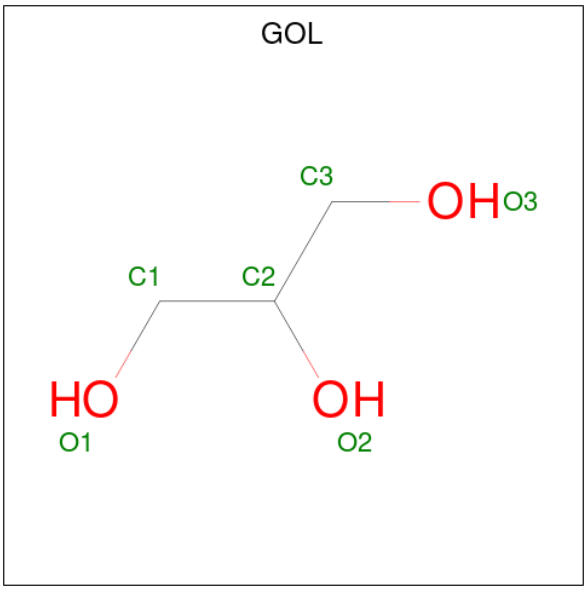
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C O 4 2 2	0	0
7	A	1	Total C O 4 2 2	0	0
7	A	1	Total C O 4 2 2	0	0
7	A	1	Total C O 4 2 2	0	0
7	B	1	Total C O 4 2 2	0	0
7	B	1	Total C O 4 2 2	0	0
7	C	1	Total C O 4 2 2	0	0
7	D	1	Total C O 4 2 2	0	0
7	D	1	Total C O 4 2 2	0	0

- Molecule 8 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



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

- Molecule 9 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total C O 6 3 3	0	0
9	C	1	Total C O 6 3 3	0	0
9	D	1	Total C O 6 3 3	0	0

- Molecule 10 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	B	2	Total Cl 2 2	0	0

- Molecule 11 is water.

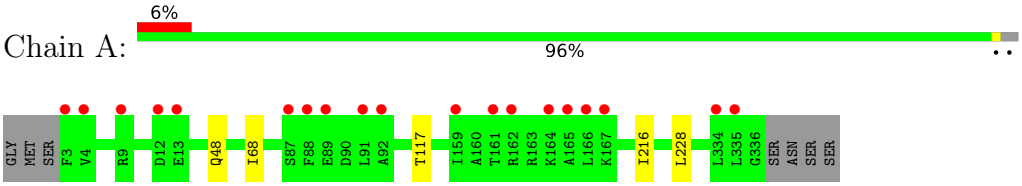
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	274	Total O 274 274	0	0
11	B	195	Total O 196 196	0	1
11	C	194	Total O 194 194	0	0
11	D	180	Total O 181 181	0	1

3 Residue-property plots (i)

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

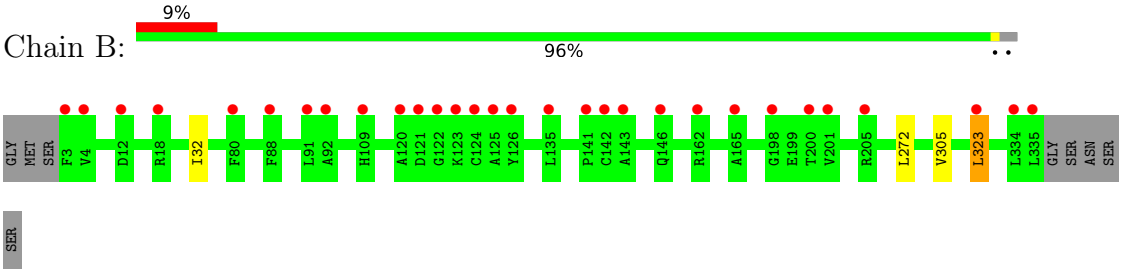
• Molecule 1: DNA mismatch repair protein Mlh1

Chain A:



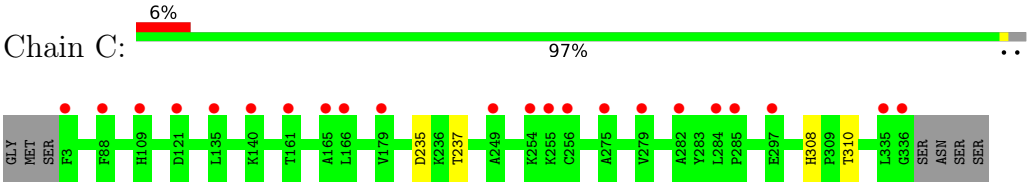
• Molecule 1: DNA mismatch repair protein Mlh1

Chain B:



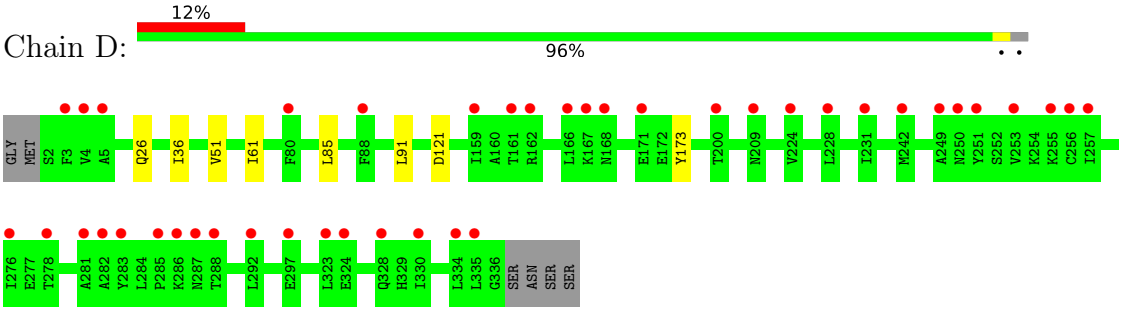
• Molecule 1: DNA mismatch repair protein Mlh1

Chain C:



• Molecule 1: DNA mismatch repair protein Mlh1

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	59.09Å 178.55Å 72.47Å 90.00° 93.92° 90.00°	Depositor
Resolution (Å)	67.10 – 1.93 67.10 – 1.93	Depositor EDS
% Data completeness (in resolution range)	61.7 (67.10-1.93) 62.2 (67.10-1.93)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	1.52 (at 1.92Å)	Xtriage
Refinement program	REFMAC 5.8.0430	Depositor
R, R_{free}	0.199 , 0.228 0.203 , 0.234	Depositor DCC
R_{free} test set	1466 reflections (2.04%)	wwPDB-VP
Wilson B-factor (Å^2)	31.8	Xtriage
Anisotropy	0.065	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 37.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	11762	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.97% 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: ANP, GOL, MG, CA, MES, ACT, CL, EDO, NA

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	0.52	0/2710	0.93	0/3667
1	B	0.52	0/2690	0.93	0/3639
1	C	0.52	0/2737	0.92	0/3701
1	D	0.52	0/2719	0.93	1/3675 (0.0%)
All	All	0.52	0/10856	0.93	1/14682 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	121	ASP	CA-CB-CG	5.07	117.67	112.60

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	2667	0	2711	2	0
1	B	2647	0	2690	2	0
1	C	2693	0	2730	2	0
1	D	2676	0	2708	4	0
2	A	31	0	13	0	0
2	B	31	0	13	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	31	0	13	0	0
2	D	31	0	13	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	2	0	0	0	0
5	B	1	0	0	0	0
5	C	2	0	0	0	0
5	D	1	0	0	0	0
6	A	12	0	13	0	0
6	B	12	0	13	0	0
7	A	16	0	24	0	0
7	B	8	0	12	0	0
7	C	4	0	6	0	0
7	D	8	0	12	0	0
8	A	12	0	9	0	0
8	D	4	0	3	0	0
9	A	6	0	8	0	0
9	C	6	0	8	0	0
9	D	6	0	8	0	0
10	B	2	0	0	0	0
11	A	274	0	0	0	0
11	B	196	0	0	0	0
11	C	194	0	0	0	0
11	D	181	0	0	0	0
All	All	11762	0	11007	10	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 0.

All (10) 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:D:85:LEU:HD21	1:D:91:LEU:HD12	1.95	0.48
1:D:36[B]:ILE:HG22	1:D:61[B]:ILE:HD11	1.94	0.48
1:C:308[B]:HIS:ND1	1:C:310:THR:OG1	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:61[B]:ILE:O	1:D:61[B]:ILE:HG23	2.16	0.46
1:B:305[A]:VAL:HG12	1:B:305[A]:VAL:O	2.16	0.45
1:A:216:ILE:HG21	1:A:228:LEU:HD11	1.99	0.44
1:B:272:LEU:HD13	1:B:323:LEU:HG	2.01	0.42
1:A:68:ILE:HB	1:A:117:THR:HG21	2.03	0.41
1:C:235:ASP:OD1	1:C:237[A]:THR:OG1	2.37	0.41
1:D:51[B]:VAL:HG21	1:D:173:TYR:CD1	2.56	0.41

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	340/341 (100%)	333 (98%)	7 (2%)	0	100	100
1	B	337/341 (99%)	330 (98%)	7 (2%)	0	100	100
1	C	343/341 (101%)	337 (98%)	6 (2%)	0	100	100
1	D	342/341 (100%)	335 (98%)	7 (2%)	0	100	100
All	All	1362/1364 (100%)	1335 (98%)	27 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	296/294 (101%)	295 (100%)	1 (0%)	86 86
1	B	294/294 (100%)	292 (99%)	2 (1%)	76 74
1	C	299/294 (102%)	299 (100%)	0	100 100
1	D	298/294 (101%)	297 (100%)	1 (0%)	86 86
All	All	1187/1176 (101%)	1183 (100%)	4 (0%)	86 86

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	GLN
1	B	32	ILE
1	B	323	LEU
1	D	26	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	ASN
1	A	86	GLN
1	B	112	HIS
1	C	112	HIS
1	D	48	GLN
1	D	306	ASN

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 38 ligands modelled in this entry, 16 are monoatomic - leaving 22 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	$\#\|Z\| > 2$
7	EDO	A	414	-	3,3,3	0.12	0	2,2,2	0.43	0
7	EDO	A	411	-	3,3,3	0.03	0	2,2,2	0.29	0
2	ANP	A	401	3	32,33,33	1.11	4 (12%)	44,52,52	1.01	2 (4%)
9	GOL	C	406	-	5,5,5	0.13	0	5,5,5	0.37	0
7	EDO	B	408	-	3,3,3	0.08	0	2,2,2	0.27	0
9	GOL	D	407	-	5,5,5	0.11	0	5,5,5	0.32	0
6	MES	B	405	-	12,12,12	0.73	0	14,16,16	0.45	0
7	EDO	A	407	-	3,3,3	0.08	0	2,2,2	0.30	0
7	EDO	B	409	-	3,3,3	0.09	0	2,2,2	0.33	0
2	ANP	C	401	3	32,33,33	1.16	5 (15%)	44,52,52	0.98	2 (4%)
8	ACT	A	413	-	3,3,3	0.97	0	3,3,3	0.83	0
7	EDO	D	406	-	3,3,3	0.08	0	2,2,2	0.28	0
7	EDO	C	407	-	3,3,3	0.09	0	2,2,2	0.35	0
8	ACT	D	405	-	3,3,3	1.00	0	3,3,3	0.76	0
2	ANP	B	401	3	32,33,33	1.12	4 (12%)	44,52,52	1.04	3 (6%)
2	ANP	D	401	3	32,33,33	1.24	5 (15%)	44,52,52	1.06	3 (6%)
8	ACT	A	408	-	3,3,3	0.96	0	3,3,3	0.86	0
9	GOL	A	412	-	5,5,5	0.10	0	5,5,5	0.35	0
6	MES	A	406	-	12,12,12	0.75	0	14,16,16	0.42	0
7	EDO	A	409	-	3,3,3	0.08	0	2,2,2	0.35	0
7	EDO	D	408	-	3,3,3	0.08	0	2,2,2	0.29	0
8	ACT	A	410	-	3,3,3	0.99	0	3,3,3	0.76	0

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	3	-	3/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	EDO	A	414	-	-	1/1/1/1	-
2	ANP	C	401	3	-	3/18/38/38	0/3/3/3
2	ANP	D	401	3	-	4/18/38/38	0/3/3/3
7	EDO	A	411	-	-	0/1/1/1	-
2	ANP	A	401	3	-	3/18/38/38	0/3/3/3
7	EDO	B	409	-	-	1/1/1/1	-
7	EDO	C	407	-	-	1/1/1/1	-
7	EDO	B	408	-	-	0/1/1/1	-
6	MES	A	406	-	-	0/6/14/14	0/1/1/1
7	EDO	D	406	-	-	1/1/1/1	-
9	GOL	A	412	-	-	0/4/4/4	-
9	GOL	C	406	-	-	3/4/4/4	-
7	EDO	A	409	-	-	0/1/1/1	-
6	MES	B	405	-	-	0/6/14/14	0/1/1/1
7	EDO	D	408	-	-	0/1/1/1	-
9	GOL	D	407	-	-	2/4/4/4	-
7	EDO	A	407	-	-	1/1/1/1	-

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	401	ANP	PG-O1G	4.22	1.52	1.46
2	C	401	ANP	PG-O1G	3.89	1.52	1.46
2	B	401	ANP	PG-O1G	3.58	1.51	1.46
2	A	401	ANP	PG-O1G	3.54	1.51	1.46
2	D	401	ANP	PB-O1B	3.16	1.51	1.46
2	B	401	ANP	PB-O1B	3.13	1.51	1.46
2	A	401	ANP	PB-O1B	3.12	1.51	1.46
2	C	401	ANP	PB-O1B	3.00	1.50	1.46
2	D	401	ANP	PG-O2G	-2.52	1.50	1.56
2	B	401	ANP	PB-O2B	-2.35	1.50	1.56
2	C	401	ANP	PB-O2B	-2.26	1.50	1.56
2	D	401	ANP	PG-O3G	-2.25	1.50	1.56
2	D	401	ANP	PB-O2B	-2.22	1.50	1.56
2	A	401	ANP	PB-O2B	-2.22	1.50	1.56
2	B	401	ANP	PG-O2G	-2.19	1.50	1.56
2	C	401	ANP	PG-O3G	-2.17	1.50	1.56
2	C	401	ANP	PG-O2G	-2.15	1.51	1.56
2	A	401	ANP	PG-O3G	-2.02	1.51	1.56

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	401	ANP	O2B-PB-O1B	4.57	119.51	109.92
2	D	401	ANP	O2B-PB-O1B	4.23	118.78	109.92
2	C	401	ANP	O2B-PB-O1B	4.13	118.58	109.92
2	B	401	ANP	O2B-PB-O1B	4.11	118.54	109.92
2	B	401	ANP	O1G-PG-N3B	-3.81	106.16	111.77
2	D	401	ANP	O1G-PG-N3B	-3.32	106.89	111.77
2	A	401	ANP	O1G-PG-N3B	-3.24	107.00	111.77
2	C	401	ANP	O1G-PG-N3B	-2.89	107.51	111.77
2	D	401	ANP	O1B-PB-N3B	-2.82	107.62	111.77
2	B	401	ANP	O3G-PG-O1G	-2.15	108.05	113.45

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	ANP	PG-N3B-PB-O1B
2	A	401	ANP	PA-O3A-PB-O1B
2	A	401	ANP	PA-O3A-PB-O2B
2	B	401	ANP	PG-N3B-PB-O1B
2	B	401	ANP	PA-O3A-PB-O1B
2	B	401	ANP	PA-O3A-PB-O2B
2	C	401	ANP	PG-N3B-PB-O1B
2	C	401	ANP	PA-O3A-PB-O1B
2	C	401	ANP	PA-O3A-PB-O2B
2	D	401	ANP	PB-N3B-PG-O1G
2	D	401	ANP	PG-N3B-PB-O1B
2	D	401	ANP	PA-O3A-PB-O1B
2	D	401	ANP	PA-O3A-PB-O2B
9	C	406	GOL	C1-C2-C3-O3
9	C	406	GOL	O2-C2-C3-O3
9	D	407	GOL	C1-C2-C3-O3
9	D	407	GOL	O2-C2-C3-O3
7	B	409	EDO	O1-C1-C2-O2
7	C	407	EDO	O1-C1-C2-O2
9	C	406	GOL	O1-C1-C2-C3
7	A	407	EDO	O1-C1-C2-O2
7	A	414	EDO	O1-C1-C2-O2
7	D	406	EDO	O1-C1-C2-O2

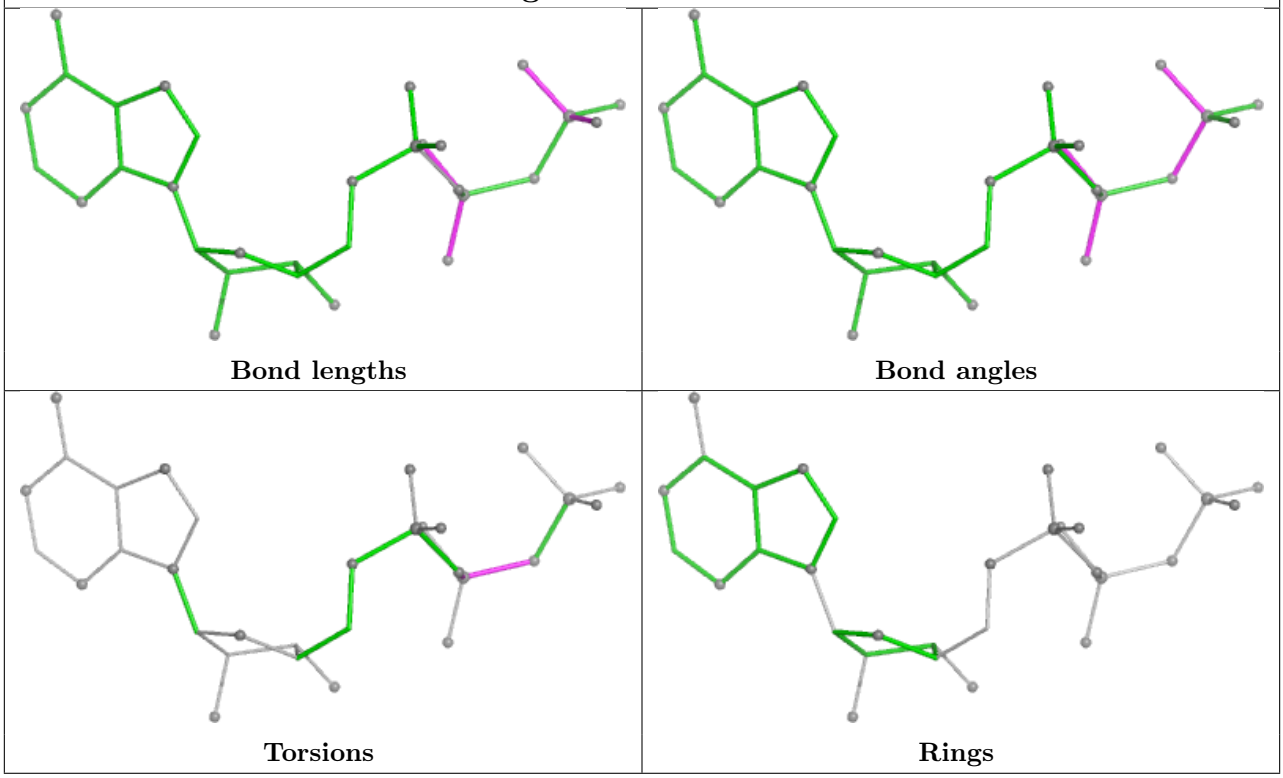
There are no ring outliers.

No monomer is involved in short contacts.

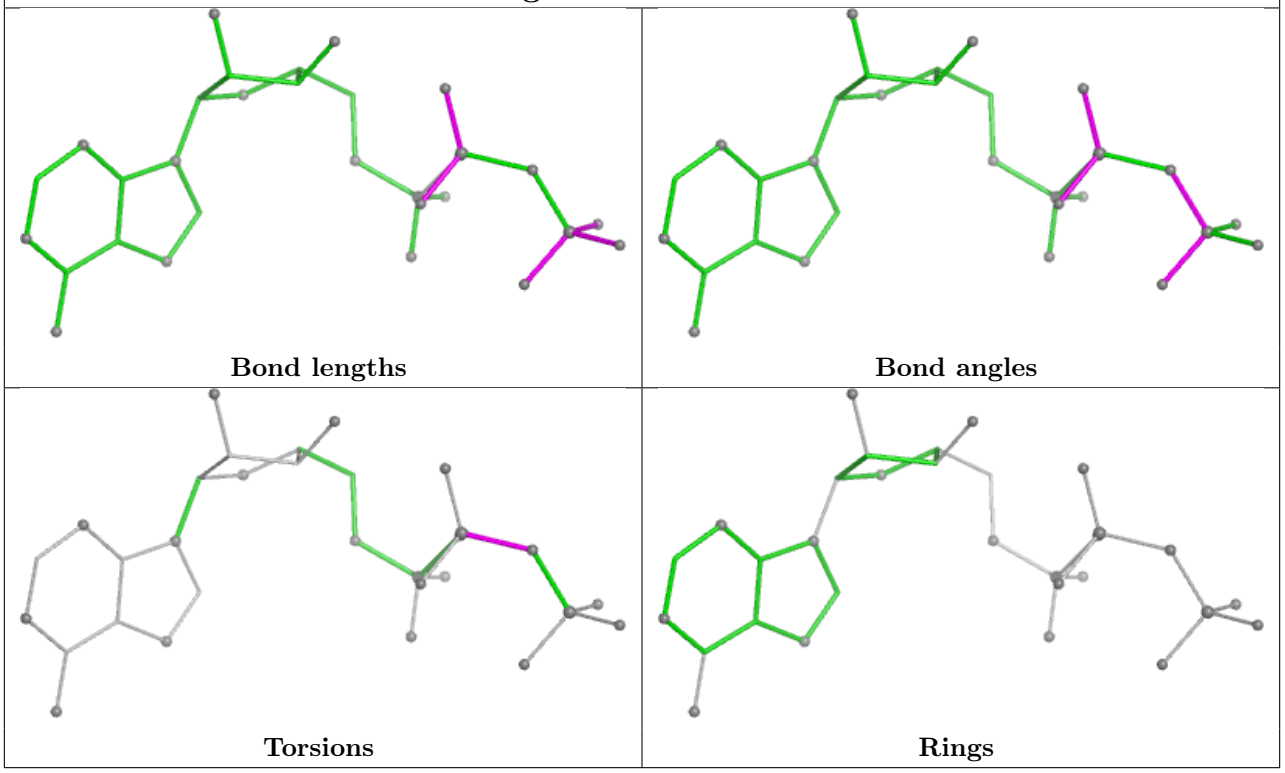
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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.

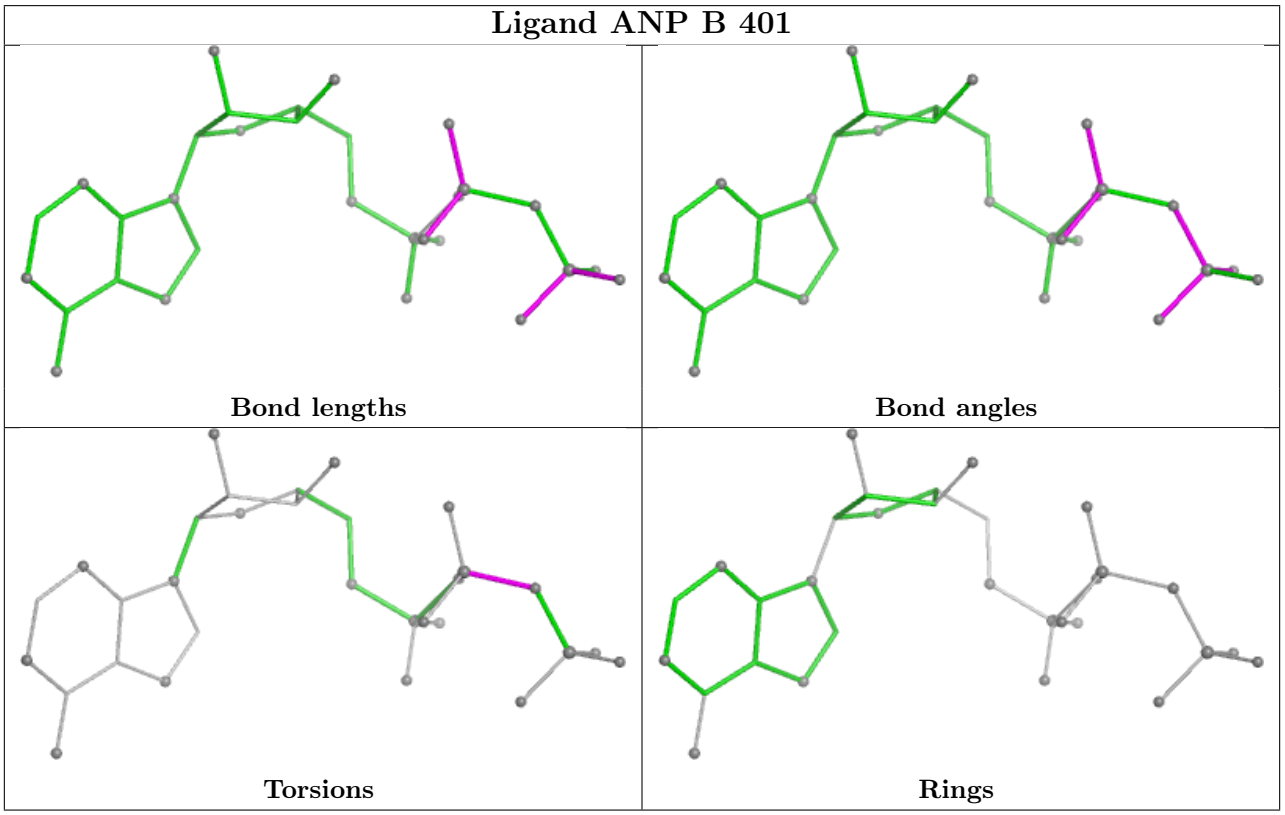
Ligand ANP A 401



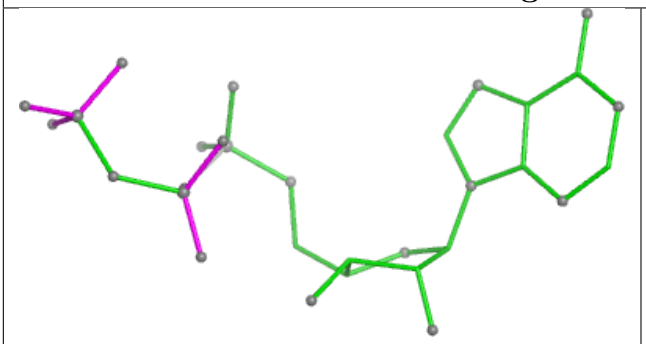
Ligand ANP C 401



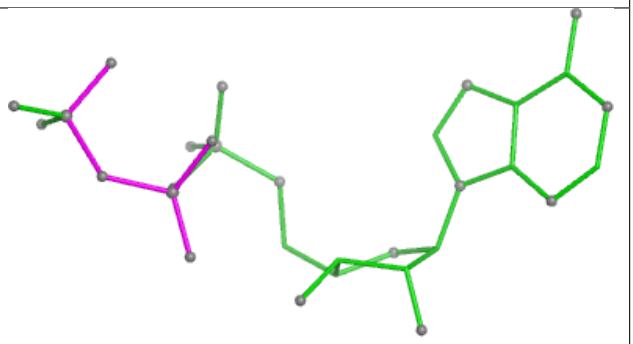
Ligand ANP B 401



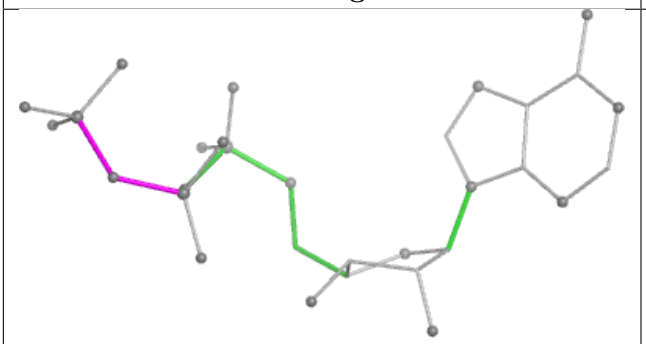
Ligand ANP D 401



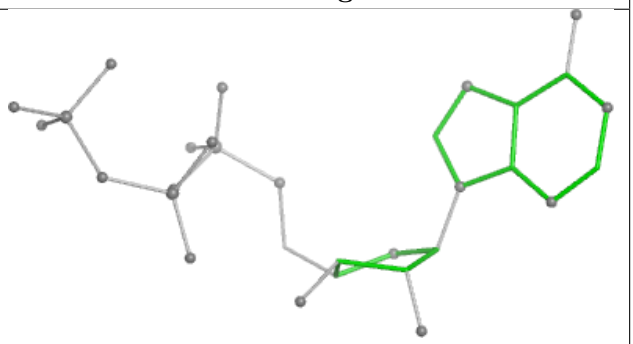
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	334/341 (97%)	0.36	19 (5%) 29 32	11, 29, 53, 80	21 (6%)
1	B	333/341 (97%)	0.71	30 (9%) 15 17	12, 35, 61, 74	21 (6%)
1	C	334/341 (97%)	0.69	22 (6%) 24 27	12, 37, 61, 76	29 (8%)
1	D	335/341 (98%)	0.88	42 (12%) 8 9	12, 39, 68, 90	27 (8%)
All	All	1336/1364 (97%)	0.66	113 (8%) 16 18	11, 35, 62, 90	98 (7%)

All (113) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	88	PHE	6.5
1	B	3	PHE	5.8
1	D	323	LEU	5.3
1	A	3	PHE	5.1
1	C	3	PHE	4.8
1	B	88	PHE	4.4
1	B	335	LEU	4.1
1	D	166	LEU	4.1
1	C	166	LEU	4.1
1	C	249	ALA	4.0
1	D	282	ALA	4.0
1	D	256	CYS	4.0
1	B	143	ALA	3.7
1	B	122	GLY	3.6
1	D	287	ASN	3.6
1	A	91	LEU	3.6
1	B	91	LEU	3.5
1	A	4	VAL	3.4
1	D	276	ILE	3.4
1	D	335	LEU	3.4
1	B	124	CYS	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	135	LEU	3.2
1	D	324	GLU	3.2
1	D	167	LYS	3.2
1	D	3	PHE	3.2
1	C	254	LYS	3.1
1	D	4	VAL	3.1
1	D	249	ALA	3.1
1	D	334	LEU	3.1
1	C	88	PHE	3.1
1	B	80	PHE	3.0
1	B	201	VAL	3.0
1	C	336	GLY	3.0
1	C	121	ASP	2.9
1	D	5	ALA	2.9
1	D	200	THR	2.9
1	C	109[A]	HIS	2.9
1	C	282	ALA	2.9
1	D	330	ILE	2.9
1	B	198	GLY	2.9
1	A	89	GLU	2.8
1	B	135	LEU	2.8
1	B	162	ARG	2.8
1	D	253	VAL	2.8
1	B	165	ALA	2.8
1	B	323	LEU	2.8
1	D	285	PRO	2.8
1	C	275	ALA	2.7
1	A	167	LYS	2.7
1	B	109	HIS	2.7
1	B	121	ASP	2.6
1	B	142	CYS	2.6
1	D	251	TYR	2.6
1	A	87	SER	2.6
1	A	335	LEU	2.6
1	B	92	ALA	2.6
1	B	200	THR	2.6
1	D	88	PHE	2.6
1	D	257	ILE	2.6
1	B	123	LYS	2.6
1	D	80	PHE	2.5
1	D	278	THR	2.5
1	B	146	GLN	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	242[A]	MET	2.5
1	C	256	CYS	2.5
1	D	286	LYS	2.5
1	C	279	VAL	2.5
1	C	165	ALA	2.5
1	B	18	ARG	2.4
1	B	4	VAL	2.4
1	C	140	LYS	2.4
1	D	281	ALA	2.4
1	A	162	ARG	2.4
1	D	288	THR	2.3
1	D	283	TYR	2.3
1	D	159	ILE	2.3
1	B	12	ASP	2.3
1	A	161	THR	2.3
1	B	141	PRO	2.3
1	C	335	LEU	2.3
1	A	9	ARG	2.2
1	A	166	LEU	2.2
1	D	231	ILE	2.2
1	D	168	ASN	2.2
1	D	162	ARG	2.2
1	C	297	GLU	2.2
1	D	224	VAL	2.2
1	A	334	LEU	2.2
1	C	285	PRO	2.2
1	B	120	ALA	2.2
1	D	255	LYS	2.2
1	C	284	LEU	2.1
1	D	171	GLU	2.1
1	A	92	ALA	2.1
1	D	328	GLN	2.1
1	A	12	ASP	2.1
1	D	297	GLU	2.1
1	A	13	GLU	2.1
1	A	164	LYS	2.1
1	D	161	THR	2.1
1	D	209	ASN	2.1
1	D	250	ASN	2.1
1	B	125	ALA	2.1
1	C	179	VAL	2.0
1	B	334	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	228	LEU	2.0
1	D	292	LEU	2.0
1	A	165	ALA	2.0
1	C	255	LYS	2.0
1	A	159	ILE	2.0
1	C	161	THR	2.0
1	B	126	TYR	2.0
1	B	205	ARG	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
8	ACT	A	413	4/4	0.55	0.27	63,65,65,66	0
8	ACT	A	408	4/4	0.70	0.27	72,73,73,73	0
9	GOL	A	412	6/6	0.71	0.19	52,56,56,60	0
7	EDO	A	409	4/4	0.73	0.21	62,62,62,62	0
9	GOL	C	406	6/6	0.73	0.26	79,80,81,82	0
8	ACT	A	410	4/4	0.81	0.20	49,51,52,52	0
7	EDO	B	408	4/4	0.81	0.15	51,51,51,51	0
9	GOL	D	407	6/6	0.83	0.20	87,87,88,88	0
8	ACT	D	405	4/4	0.84	0.14	59,61,61,63	0
4	NA	C	403	1/1	0.84	0.10	34,34,34,34	0
10	CL	B	407	1/1	0.85	0.16	74,74,74,74	0
7	EDO	D	406	4/4	0.86	0.13	41,42,43,44	0
7	EDO	A	414	4/4	0.86	0.14	45,46,46,46	0
4	NA	A	403	1/1	0.86	0.08	25,25,25,25	0
7	EDO	A	411	4/4	0.87	0.18	49,49,52,54	0

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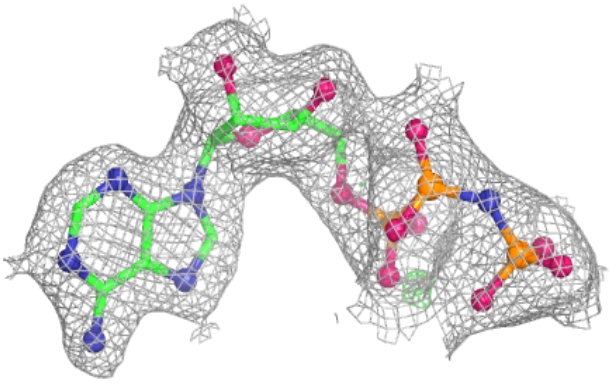
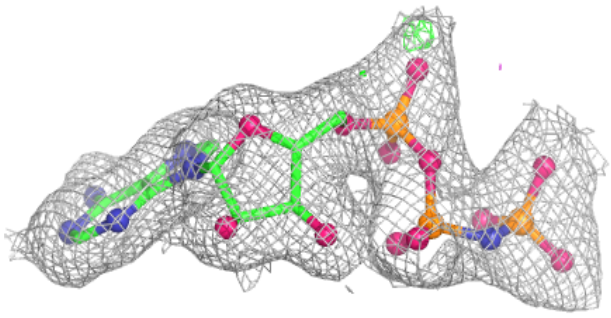
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	CA	C	405	1/1	0.89	0.12	65,65,65,65	0
4	NA	B	403	1/1	0.89	0.14	28,28,28,28	0
4	NA	D	403	1/1	0.90	0.08	28,28,28,28	0
10	CL	B	406	1/1	0.91	0.24	63,63,63,63	0
7	EDO	D	408	4/4	0.93	0.07	37,37,37,38	0
7	EDO	B	409	4/4	0.93	0.10	35,37,38,39	0
5	CA	D	404	1/1	0.94	0.08	47,47,47,47	0
7	EDO	C	407	4/4	0.95	0.07	34,34,35,35	0
7	EDO	A	407	4/4	0.95	0.08	33,33,33,34	0
3	MG	B	402	1/1	0.95	0.05	20,20,20,20	0
5	CA	C	404	1/1	0.95	0.06	53,53,53,53	0
6	MES	B	405	12/12	0.96	0.08	33,39,41,41	0
2	ANP	C	401	31/31	0.97	0.06	24,26,26,27	0
5	CA	B	404	1/1	0.97	0.04	30,30,30,30	0
3	MG	C	402	1/1	0.98	0.04	23,23,23,23	0
2	ANP	A	401	31/31	0.98	0.04	17,18,19,20	0
2	ANP	D	401	31/31	0.98	0.04	20,23,24,24	0
3	MG	A	402	1/1	0.98	0.03	17,17,17,17	0
6	MES	A	406	12/12	0.98	0.06	27,29,30,30	0
2	ANP	B	401	31/31	0.98	0.05	20,22,24,24	0
3	MG	D	402	1/1	0.99	0.02	22,22,22,22	0
5	CA	A	404	1/1	0.99	0.02	24,24,24,24	0
5	CA	A	405	1/1	0.99	0.08	35,35,35,35	0

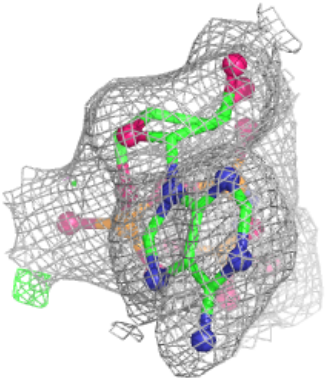
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

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)

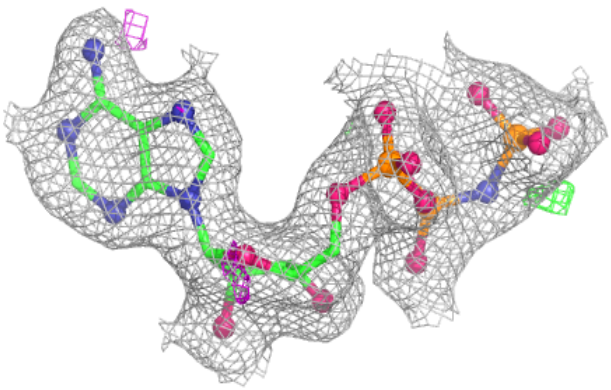


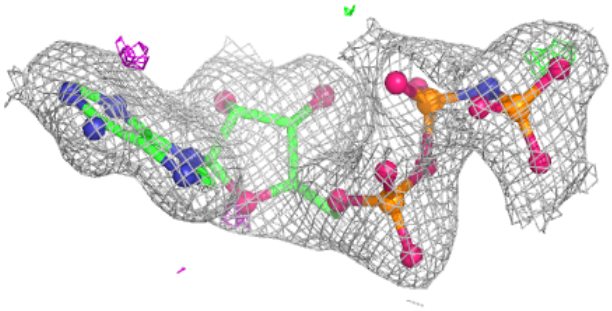


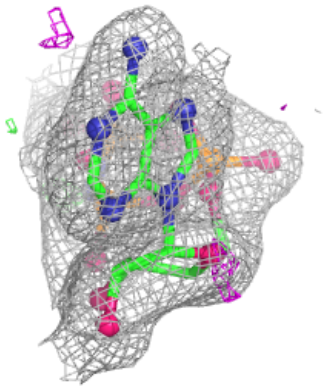


Electron density around ANP A 401:

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

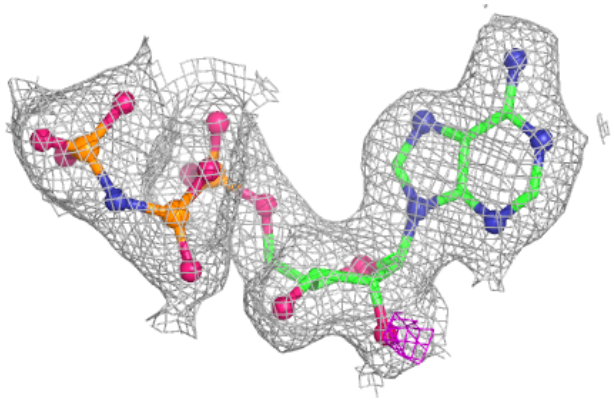


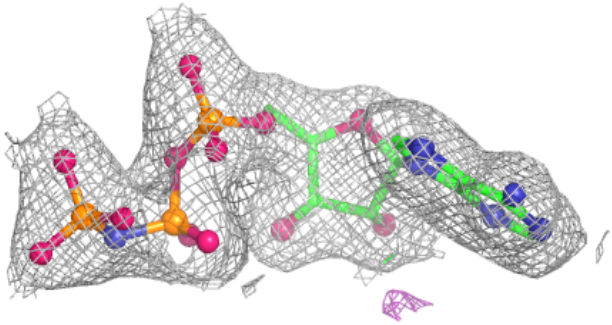


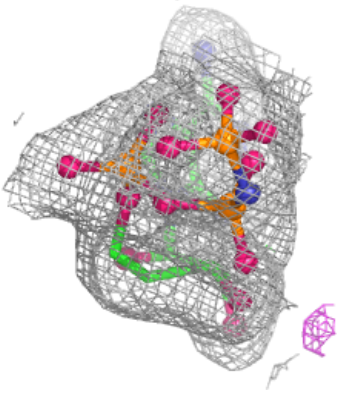


Electron density around ANP D 401:

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

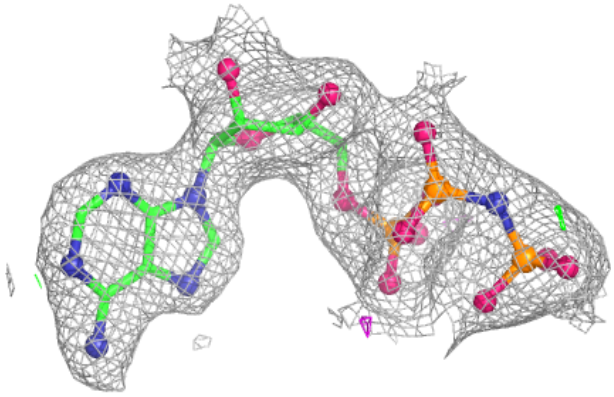


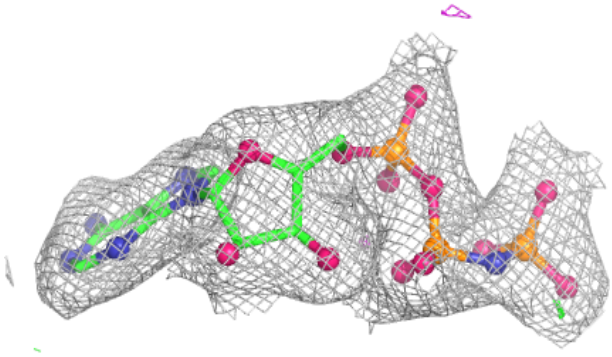


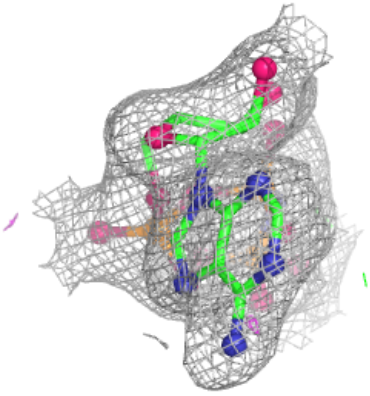


Electron density around ANP B 401:

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







6.5 Other polymers (i)

There are no such residues in this entry.