Full wwPDB X-ray Structure Validation Report ⓘ

Oct 6, 2026 – 07:31 pm BST

PDB ID	:	9QIE / pdb_00009qie
Title	:	Crystal Structure of human MLH1 N-terminal domain I219V with AMP-PNP
Authors	:	Thomsen, M.; Ganichkin, O.; Thieulin-Pardo, G.; Bandera, A.M.; Boudet, J.; Finley, M.; Felsenfeld, D.; Haque, T.; Prasad, B.C.; Monteagudo, E.; Vogt, T.; Stamford, A.
Deposited on	:	2025-03-17
Resolution	:	2.15 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:

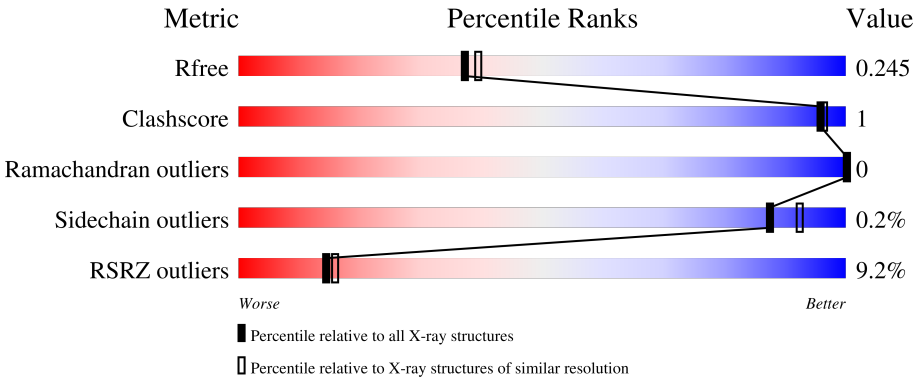
MolProbity	:	4-5-2 with Phenix2.2
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.2
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 2.15 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	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

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	4% 96%
1	B	341	4% 96%
1	C	341	12% 94%
1	D	341	15% 95%

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 11068 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	38	5	0
			2645	1671	465	501	8			
1	B	333	Total	C	N	O	S	48	3	0
			2626	1658	462	498	8			
1	C	334	Total	C	N	O	S	58	4	0
			2643	1666	466	503	8			
1	D	330	Total	C	N	O	S	66	2	0
			2587	1628	456	494	9			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP P40692
A	219	VAL	ILE	variant	UNP P40692
B	0	GLY	-	expression tag	UNP P40692
B	219	VAL	ILE	variant	UNP P40692
C	0	GLY	-	expression tag	UNP P40692
C	219	VAL	ILE	variant	UNP P40692
D	0	GLY	-	expression tag	UNP P40692
D	219	VAL	ILE	variant	UNP P40692

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

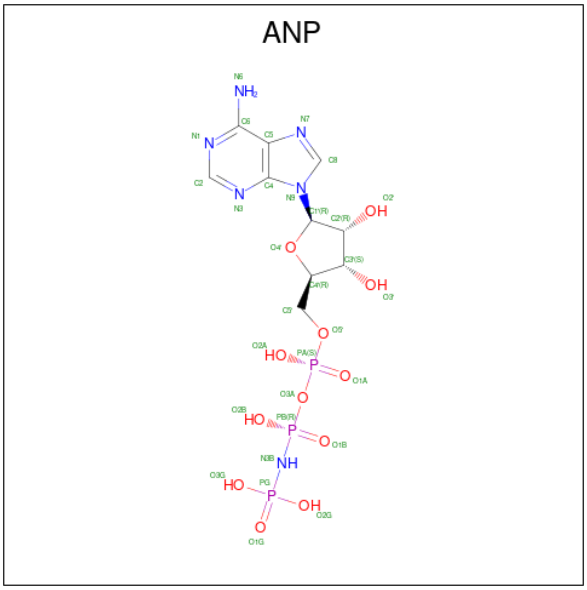
- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

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

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

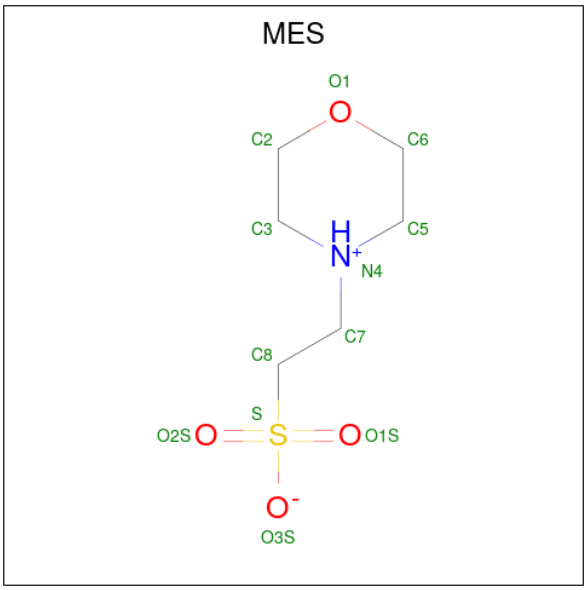
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	2	Total Ca 2 2	0	0
4	B	1	Total Ca 1 1	0	0
4	C	2	Total Ca 2 2	0	0
4	D	1	Total Ca 1 1	0	0

- Molecule 5 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).



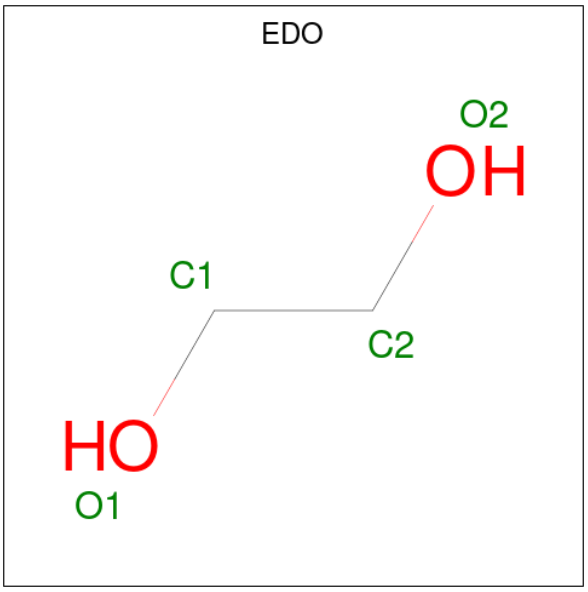
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
5	B	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
5	C	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
5	D	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

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



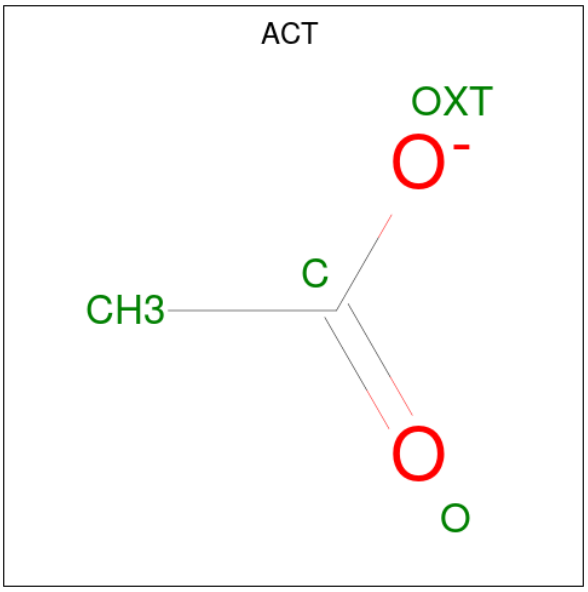
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
6	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

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



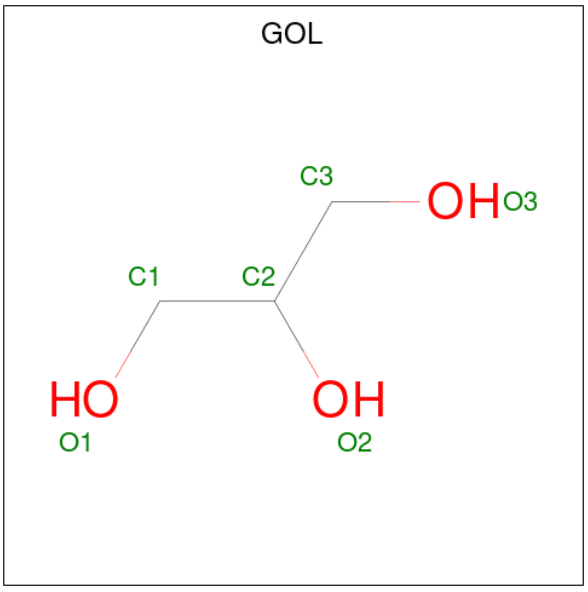
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C O 4 2 2	0	0
7	A	1	Total C O 4 2 2	0	0
7	A	1	Total C O 4 2 2	0	0
7	B	1	Total C O 4 2 2	0	0
7	B	1	Total C O 4 2 2	0	0
7	C	1	Total C O 4 2 2	0	0
7	D	1	Total C O 4 2 2	0	0
7	D	1	Total C O 4 2 2	0	0

- 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

- 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.

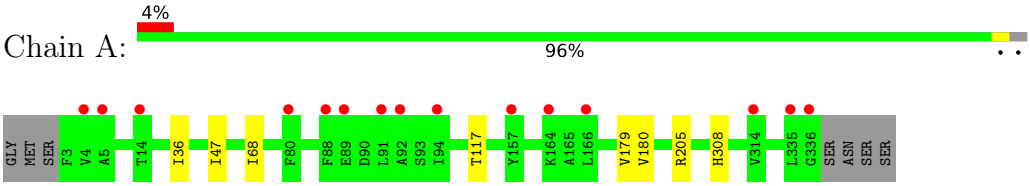
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	130	Total O 130 130	0	0
11	B	84	Total O 84 84	0	0
11	C	61	Total O 61 61	0	0
11	D	68	Total O 68 68	0	0

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.

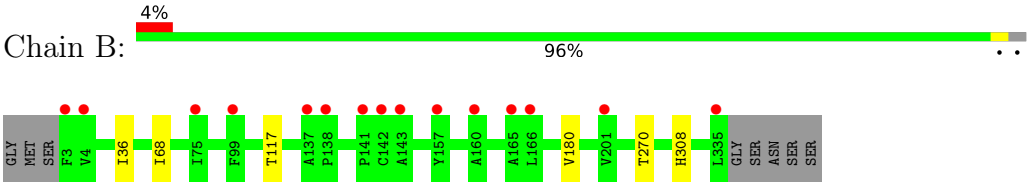
• Molecule 1: DNA mismatch repair protein Mlh1

Chain A:



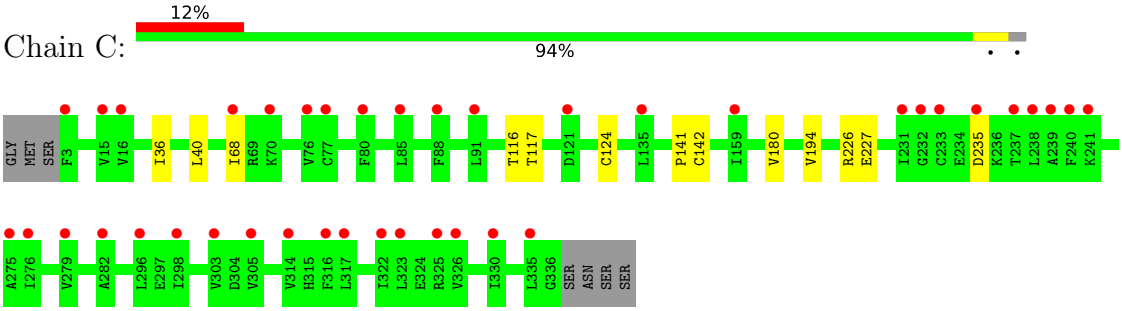
• Molecule 1: DNA mismatch repair protein Mlh1

Chain B:



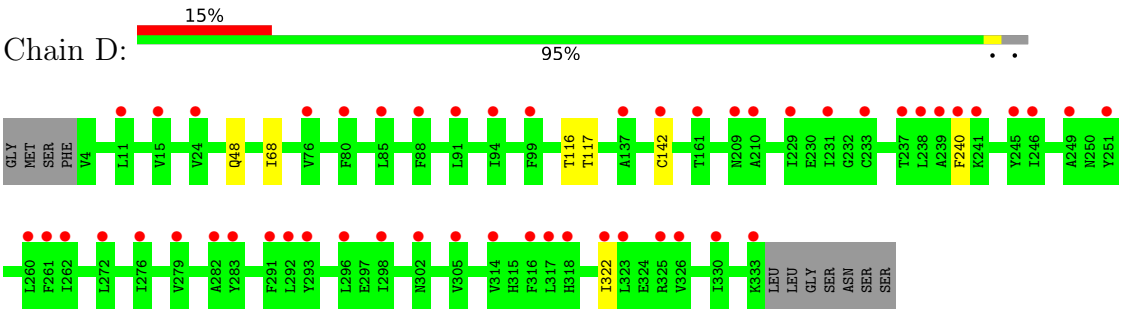
• Molecule 1: DNA mismatch repair protein Mlh1

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	58.88Å 180.01Å 72.61Å 90.00° 93.66° 90.00°	Depositor
Resolution (Å)	72.56 – 2.15 72.56 – 2.15	Depositor EDS
% Data completeness (in resolution range)	51.9 (72.56-2.15) 51.9 (72.56-2.15)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	2.19 (at 2.14Å)	Xtriage
Refinement program	REFMAC 5.8.0430	Depositor
R, R_{free}	0.217 , 0.241 0.220 , 0.245	Depositor DCC
R_{free} test set	1958 reflections (2.40%)	wwPDB-VP
Wilson B-factor (Å^2)	53.1	Xtriage
Anisotropy	0.064	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 38.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	11068	wwPDB-VP
Average B, all atoms (Å^2)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.60% 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: EDO, MG, GOL, MES, CA, ACT, ANP, NA, CL

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	0.53	1/2688 (0.0%)	0.95	0/3637
1	B	0.52	0/2669	0.96	1/3610 (0.0%)
1	C	0.52	0/2685	0.97	1/3629 (0.0%)
1	D	0.53	0/2628	0.96	0/3553
All	All	0.53	1/10670 (0.0%)	0.96	2/14429 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	205	ARG	NE-CZ	5.23	1.38	1.33

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	270	THR	CA-CB-OG1	-5.20	101.80	109.60
1	C	235	ASP	CA-CB-CG	5.04	117.64	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	2645	0	2689	10	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2626	0	2667	9	0
1	C	2643	0	2684	7	0
1	D	2587	0	2623	3	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	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	2	0	0	0	0
4	B	1	0	0	0	0
4	C	2	0	0	0	0
4	D	1	0	0	0	0
5	A	31	0	13	0	0
5	B	31	0	13	0	0
5	C	31	0	13	0	0
5	D	31	0	13	0	0
6	A	12	0	13	0	0
6	B	12	0	13	0	0
7	A	12	0	18	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
10	B	2	0	0	0	0
11	A	130	0	0	0	0
11	B	84	0	0	0	0
11	C	61	0	0	0	0
11	D	68	0	0	0	0
All	All	11068	0	10817	22	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 1.

All (22) 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:308[A]:HIS:CD2	1:B:308[A]:HIS:CD2	1.88	1.58
1:A:308[A]:HIS:HD2	1:B:308[A]:HIS:NE2	1.07	1.47
1:A:308[A]:HIS:NE2	1:B:308[A]:HIS:HD2	0.95	1.45
1:A:308[A]:HIS:NE2	1:B:308[A]:HIS:CD2	1.78	1.43
1:A:308[A]:HIS:CD2	1:B:308[A]:HIS:NE2	1.84	1.39
1:A:308[A]:HIS:HE2	1:B:308[A]:HIS:CD2	1.47	1.23
1:A:308[A]:HIS:HE2	1:B:308[A]:HIS:HD2	0.61	0.60
1:D:116:THR:HG23	1:D:142:CYS:SG	2.46	0.55
1:C:68:ILE:HB	1:C:117:THR:HG21	1.95	0.49
1:A:36[A]:ILE:HD11	1:A:180:VAL:HG22	1.95	0.48
1:C:226:ARG:HG3	1:C:227:GLU:HG2	1.96	0.47
1:D:68:ILE:HB	1:D:117:THR:HG21	1.99	0.44
1:D:240:PHE:CD2	1:D:322:ILE:HG12	2.52	0.44
1:C:36[A]:ILE:HD11	1:C:180:VAL:HG22	2.01	0.43
1:A:68:ILE:HB	1:A:117:THR:HG21	2.01	0.43
1:C:124:CYS:SG	1:C:141:PRO:HB3	2.59	0.43
1:B:36[A]:ILE:HD11	1:B:180:VAL:HG22	2.00	0.42
1:C:116:THR:HG23	1:C:142:CYS:SG	2.60	0.42
1:C:40[B]:LEU:HD12	1:C:40[B]:LEU:HA	1.84	0.41
1:C:180:VAL:HG11	1:C:194:VAL:CG2	2.51	0.41
1:B:68:ILE:HB	1:B:117:THR:HG21	2.03	0.41
1:A:36[B]:ILE:CD1	1:A:47:ILE:HG21	2.52	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	337/341 (99%)	330 (98%)	7 (2%)	0	100	100
1	B	334/341 (98%)	327 (98%)	7 (2%)	0	100	100
1	C	337/341 (99%)	329 (98%)	8 (2%)	0	100	100
1	D	330/341 (97%)	324 (98%)	6 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1338/1364 (98%)	1310 (98%)	28 (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	293/294 (100%)	291 (99%)	2 (1%)	76 82
1	B	291/294 (99%)	291 (100%)	0	100 100
1	C	293/294 (100%)	293 (100%)	0	100 100
1	D	287/294 (98%)	286 (100%)	1 (0%)	86 91
All	All	1164/1176 (99%)	1161 (100%)	3 (0%)	87 91

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	179[A]	VAL
1	A	179[B]	VAL
1	D	48	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	112	HIS
1	A	306	ASN
1	B	60	GLN
1	B	112	HIS
1	B	209	ASN
1	C	60	GLN
1	C	149	GLN
1	C	209	ASN
1	D	60	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	209	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 36 ligands modelled in this entry, 16 are monoatomic - leaving 20 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	$\#\|Z\| > 2$
5	ANP	C	405	2	32,33,33	1.07	4 (12%)	44,52,52	1.10	3 (6%)
6	MES	A	406	-	12,12,12	0.73	0	14,16,16	0.51	0
9	GOL	A	412	-	5,5,5	0.17	0	5,5,5	0.52	0
9	GOL	C	406	-	5,5,5	0.12	0	5,5,5	0.46	0
7	EDO	B	408	-	3,3,3	0.08	0	2,2,2	0.24	0
5	ANP	A	405	2	32,33,33	1.11	4 (12%)	44,52,52	1.14	3 (6%)
7	EDO	B	409	-	3,3,3	0.11	0	2,2,2	0.32	0
5	ANP	B	404	2	32,33,33	1.17	4 (12%)	44,52,52	1.10	2 (4%)
7	EDO	D	406	-	3,3,3	0.12	0	2,2,2	0.29	0
7	EDO	A	409	-	3,3,3	0.10	0	2,2,2	0.43	0
7	EDO	C	407	-	3,3,3	0.14	0	2,2,2	0.45	0
6	MES	B	405	-	12,12,12	0.73	0	14,16,16	0.47	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
8	ACT	A	408	-	3,3,3	1.01	0	3,3,3	0.79	0
5	ANP	D	404	2	32,33,33	1.14	5 (15%)	44,52,52	1.05	2 (4%)
8	ACT	A	413	-	3,3,3	1.02	0	3,3,3	0.71	0
8	ACT	D	405	-	3,3,3	1.01	0	3,3,3	0.75	0
7	EDO	D	407	-	3,3,3	0.13	0	2,2,2	0.25	0
7	EDO	A	407	-	3,3,3	0.13	0	2,2,2	0.35	0
7	EDO	A	411	-	3,3,3	0.10	0	2,2,2	0.35	0
8	ACT	A	410	-	3,3,3	0.99	0	3,3,3	0.79	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
7	EDO	B	409	-	-	1/1/1/1	-
7	EDO	A	407	-	-	1/1/1/1	-
5	ANP	C	405	2	-	3/18/38/38	0/3/3/3
6	MES	A	406	-	-	0/6/14/14	0/1/1/1
7	EDO	A	409	-	-	1/1/1/1	-
5	ANP	D	404	2	-	6/18/38/38	0/3/3/3
6	MES	B	405	-	-	0/6/14/14	0/1/1/1
9	GOL	A	412	-	-	2/4/4/4	-
9	GOL	C	406	-	-	1/4/4/4	-
7	EDO	D	406	-	-	0/1/1/1	-
7	EDO	B	408	-	-	0/1/1/1	-
7	EDO	C	407	-	-	1/1/1/1	-
5	ANP	A	405	2	-	4/18/38/38	0/3/3/3
7	EDO	D	407	-	-	1/1/1/1	-
5	ANP	B	404	2	-	5/18/38/38	0/3/3/3
7	EDO	A	411	-	-	0/1/1/1	-

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	404	ANP	PG-O1G	4.03	1.52	1.46
5	D	404	ANP	PG-O1G	3.94	1.52	1.46
5	A	405	ANP	PG-O1G	3.61	1.51	1.46
5	C	405	ANP	PG-O1G	3.20	1.51	1.46
5	B	404	ANP	PB-O1B	3.10	1.51	1.46
5	A	405	ANP	PB-O1B	2.95	1.50	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	404	ANP	PB-O1B	2.76	1.50	1.46
5	C	405	ANP	PB-O1B	2.71	1.50	1.46
5	A	405	ANP	PB-O2B	-2.42	1.50	1.56
5	D	404	ANP	PB-O2B	-2.36	1.50	1.56
5	C	405	ANP	PB-O2B	-2.30	1.50	1.56
5	B	404	ANP	PB-O2B	-2.29	1.50	1.56
5	C	405	ANP	PG-O2G	-2.24	1.50	1.56
5	D	404	ANP	PG-O2G	-2.24	1.50	1.56
5	D	404	ANP	PG-O3G	-2.12	1.51	1.56
5	B	404	ANP	PG-O2G	-2.06	1.51	1.56
5	A	405	ANP	PG-O2G	-2.05	1.51	1.56

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	C	405	ANP	O1G-PG-N3B	-4.43	105.25	111.77
5	B	404	ANP	O1G-PG-N3B	-4.26	105.50	111.77
5	D	404	ANP	O2B-PB-O1B	4.20	118.73	109.92
5	A	405	ANP	O1G-PG-N3B	-4.16	105.64	111.77
5	C	405	ANP	O2B-PB-O1B	3.91	118.12	109.92
5	A	405	ANP	O2B-PB-O1B	3.89	118.08	109.92
5	B	404	ANP	O2B-PB-O1B	3.88	118.06	109.92
5	D	404	ANP	O1G-PG-N3B	-3.79	106.19	111.77
5	A	405	ANP	O3A-PB-N3B	-2.66	99.22	106.59
5	C	405	ANP	O3A-PB-N3B	-2.47	99.74	106.59

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	405	ANP	PG-N3B-PB-O1B
5	A	405	ANP	PA-O3A-PB-O1B
5	A	405	ANP	PA-O3A-PB-O2B
5	B	404	ANP	PG-N3B-PB-O1B
5	B	404	ANP	PA-O3A-PB-O1B
5	B	404	ANP	PA-O3A-PB-O2B
5	C	405	ANP	PG-N3B-PB-O1B
5	C	405	ANP	PA-O3A-PB-O1B
5	C	405	ANP	PA-O3A-PB-O2B
5	D	404	ANP	PB-N3B-PG-O1G
5	D	404	ANP	PG-N3B-PB-O1B
5	D	404	ANP	PA-O3A-PB-O1B

Continued on next page...

Continued from previous page...

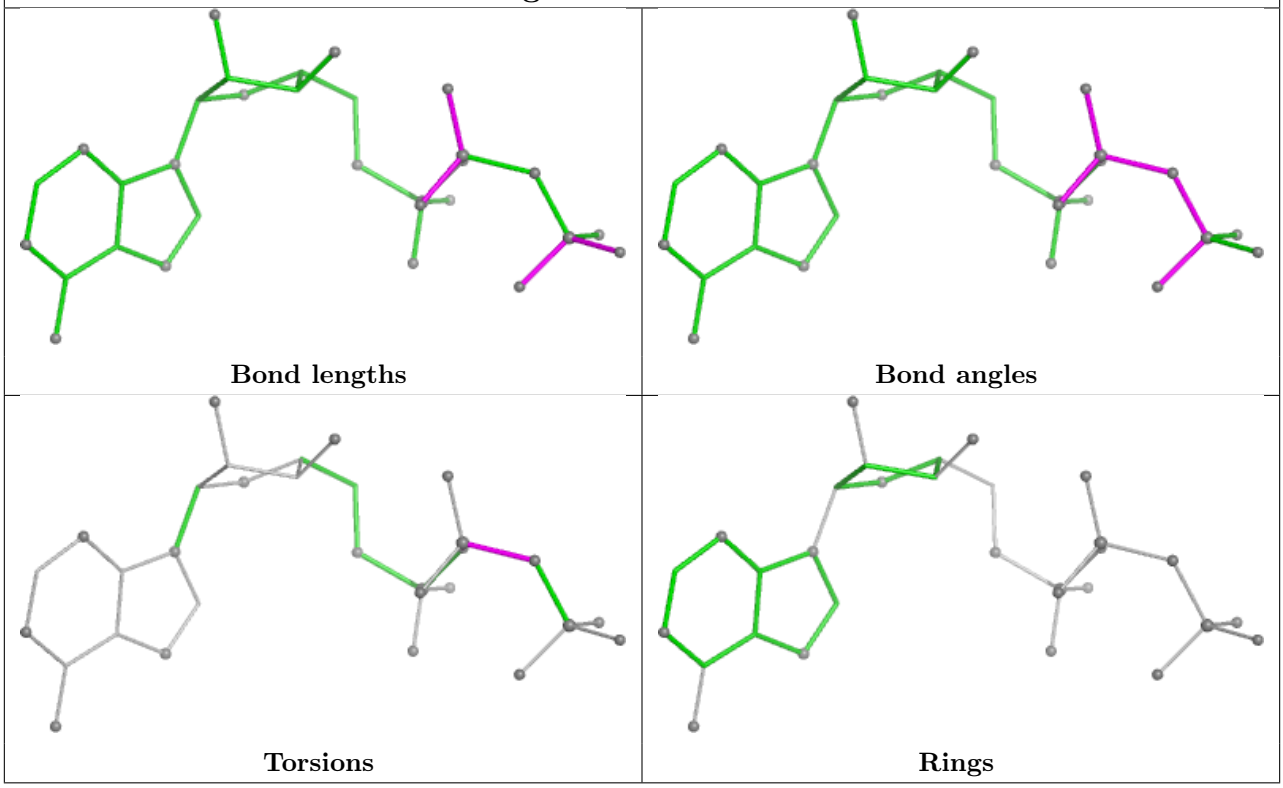
Mol	Chain	Res	Type	Atoms
5	D	404	ANP	PA-O3A-PB-O2B
9	A	412	GOL	C1-C2-C3-O3
9	A	412	GOL	O2-C2-C3-O3
9	C	406	GOL	C1-C2-C3-O3
7	C	407	EDO	O1-C1-C2-O2
7	D	407	EDO	O1-C1-C2-O2
7	A	409	EDO	O1-C1-C2-O2
5	B	404	ANP	C5'-O5'-PA-O3A
5	D	404	ANP	C5'-O5'-PA-O3A
7	A	407	EDO	O1-C1-C2-O2
5	B	404	ANP	C5'-O5'-PA-O1A
5	D	404	ANP	C5'-O5'-PA-O1A
7	B	409	EDO	O1-C1-C2-O2
5	A	405	ANP	PB-N3B-PG-O1G

There are no ring outliers.

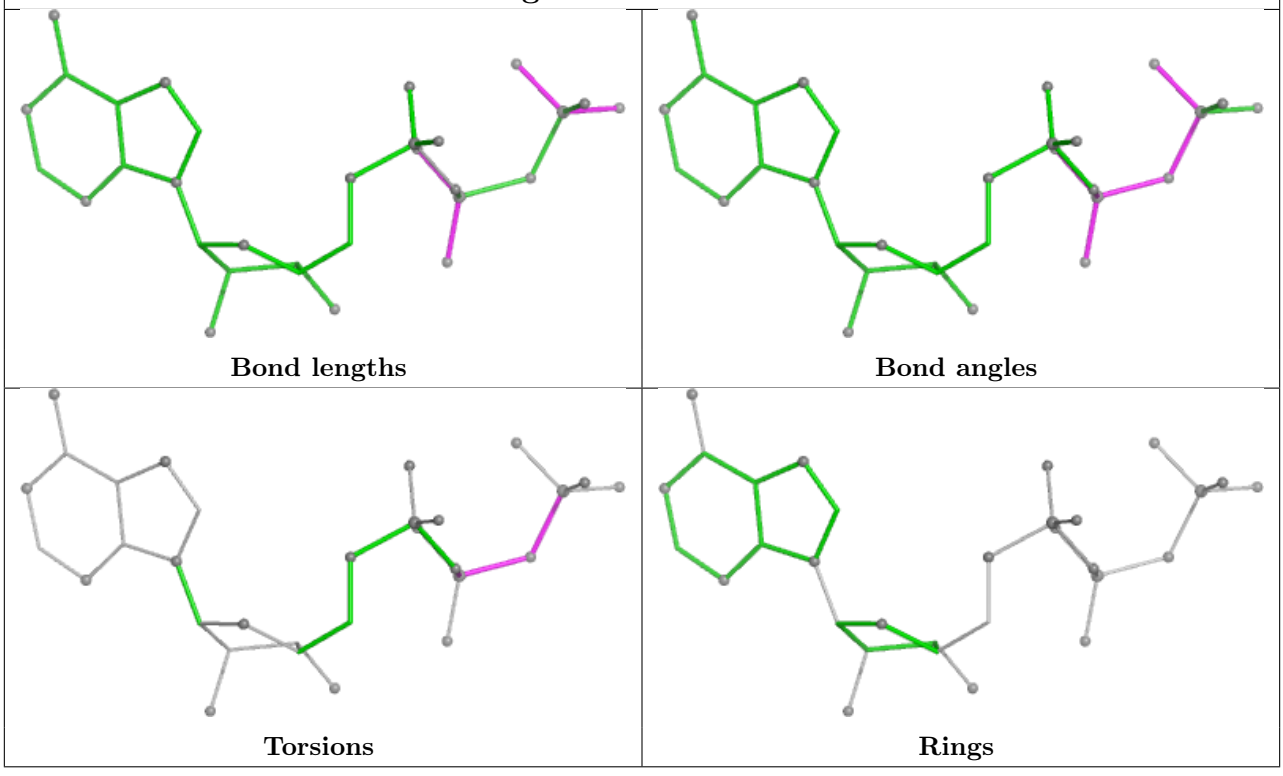
No monomer is involved in short contacts.

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.

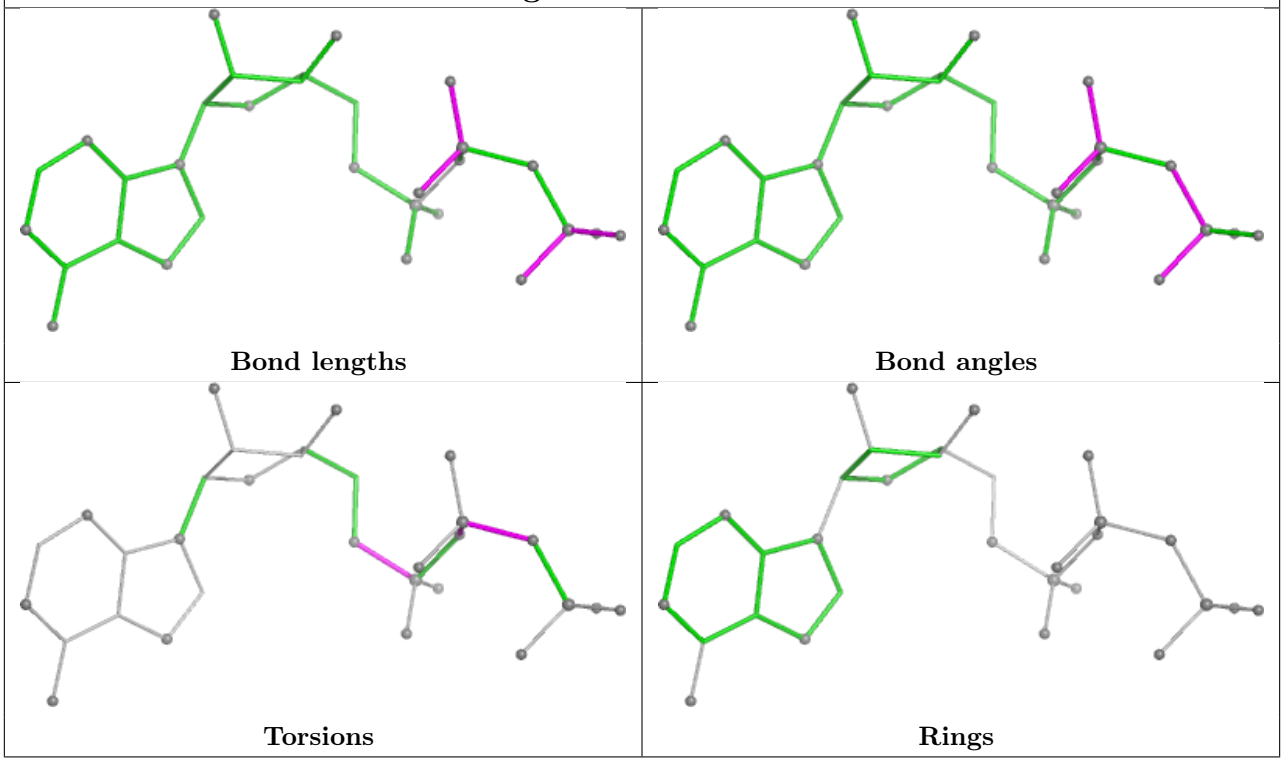
Ligand ANP C 405



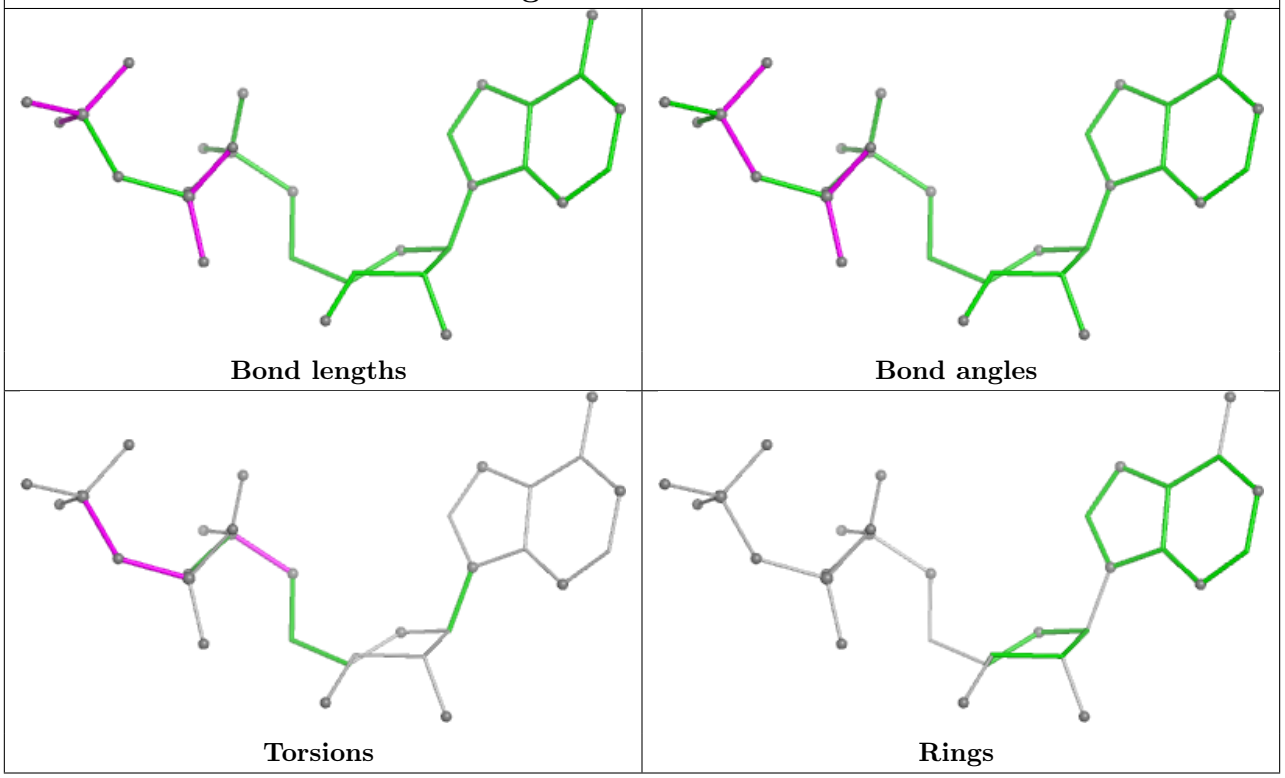
Ligand ANP A 405



Ligand ANP B 404



Ligand ANP D 404



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	334/341 (97%)	0.41	15 (4%)	38	43	17, 46, 77, 117	21 (6%)
1	B	333/341 (97%)	0.61	15 (4%)	38	43	17, 51, 82, 99	26 (7%)
1	C	334/341 (97%)	1.02	40 (11%)	9	9	20, 64, 95, 109	32 (9%)
1	D	330/341 (96%)	1.21	52 (15%)	5	5	26, 66, 100, 124	37 (11%)
All	All	1331/1364 (97%)	0.81	122 (9%)	14	16	17, 57, 93, 124	116 (8%)

All (122) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	233	CYS	6.3
1	D	326	VAL	5.3
1	D	330	ILE	5.2
1	D	240	PHE	4.6
1	D	316	PHE	4.6
1	D	239	ALA	4.4
1	D	262	ILE	4.2
1	C	326	VAL	4.2
1	C	233	CYS	4.2
1	D	317	LEU	4.1
1	D	80	PHE	4.1
1	A	88	PHE	4.1
1	D	238	LEU	4.1
1	C	316	PHE	4.0
1	D	276	ILE	3.9
1	C	240	PHE	3.9
1	C	239	ALA	3.8
1	C	238	LEU	3.7
1	D	296	LEU	3.7
1	D	291	PHE	3.7
1	A	336	GLY	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	335	LEU	3.5
1	C	322	ILE	3.4
1	D	323	LEU	3.4
1	C	77	CYS	3.4
1	A	91	LEU	3.4
1	D	251	TYR	3.4
1	A	335	LEU	3.3
1	C	237	THR	3.3
1	C	314	VAL	3.3
1	D	283	TYR	3.3
1	D	229	ILE	3.3
1	D	298	ILE	3.3
1	D	88	PHE	3.3
1	C	323	LEU	3.2
1	C	88	PHE	3.2
1	D	209	ASN	3.1
1	C	91	LEU	3.1
1	D	231	ILE	3.1
1	D	322	ILE	3.1
1	B	3	PHE	3.0
1	A	14	THR	3.0
1	D	260	LEU	2.9
1	C	330	ILE	2.9
1	C	80	PHE	2.9
1	D	99	PHE	2.8
1	C	121	ASP	2.8
1	A	92	ALA	2.8
1	C	85	LEU	2.8
1	D	325	ARG	2.8
1	D	245	TYR	2.8
1	A	80	PHE	2.7
1	B	143	ALA	2.7
1	C	3	PHE	2.7
1	D	237	THR	2.7
1	C	232	GLY	2.7
1	D	272	LEU	2.6
1	D	333	LYS	2.6
1	C	296	LEU	2.6
1	C	335	LEU	2.6
1	A	314	VAL	2.6
1	C	317	LEU	2.6
1	D	282	ALA	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	15	VAL	2.5
1	A	166	LEU	2.5
1	C	298	ILE	2.5
1	B	99	PHE	2.5
1	B	201	VAL	2.5
1	C	231	ILE	2.5
1	C	241	LYS	2.5
1	C	276	ILE	2.5
1	D	314	VAL	2.4
1	A	5	ALA	2.4
1	B	142	CYS	2.4
1	D	11	LEU	2.4
1	D	302	ASN	2.4
1	C	76	VAL	2.4
1	D	142	CYS	2.4
1	D	261	PHE	2.4
1	A	4	VAL	2.4
1	C	279	VAL	2.4
1	D	292	LEU	2.3
1	B	75	ILE	2.3
1	D	246	ILE	2.3
1	B	4	VAL	2.3
1	A	89	GLU	2.3
1	D	249	ALA	2.3
1	C	135	LEU	2.3
1	C	275	ALA	2.3
1	D	137	ALA	2.3
1	D	91	LEU	2.3
1	D	305	VAL	2.3
1	D	293	TYR	2.3
1	C	68	ILE	2.2
1	A	157	TYR	2.2
1	B	141	PRO	2.2
1	C	15	VAL	2.2
1	C	303	VAL	2.2
1	B	160	ALA	2.2
1	C	282	ALA	2.2
1	D	210	ALA	2.2
1	D	318	HIS	2.2
1	D	161	THR	2.2
1	C	70	LYS	2.1
1	B	157	TYR	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	235	ASP	2.1
1	B	165	ALA	2.1
1	A	164	LYS	2.1
1	C	305	VAL	2.1
1	D	241	LYS	2.1
1	B	166	LEU	2.1
1	D	85	LEU	2.1
1	B	138	PRO	2.1
1	A	94	ILE	2.1
1	C	159	ILE	2.1
1	D	94	ILE	2.1
1	C	16	VAL	2.1
1	D	24	VAL	2.0
1	D	76	VAL	2.0
1	D	279	VAL	2.0
1	B	137	ALA	2.0
1	C	325	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, 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
9	GOL	A	412	6/6	0.66	0.18	61,64,66,72	0
8	ACT	A	413	4/4	0.74	0.20	66,68,72,73	0
10	CL	B	406	1/1	0.75	0.18	104,104,104,104	0
7	EDO	A	409	4/4	0.76	0.20	76,77,78,79	0
8	ACT	A	408	4/4	0.78	0.22	93,97,97,98	0
9	GOL	C	406	6/6	0.80	0.17	91,93,93,94	0

Continued on next page...

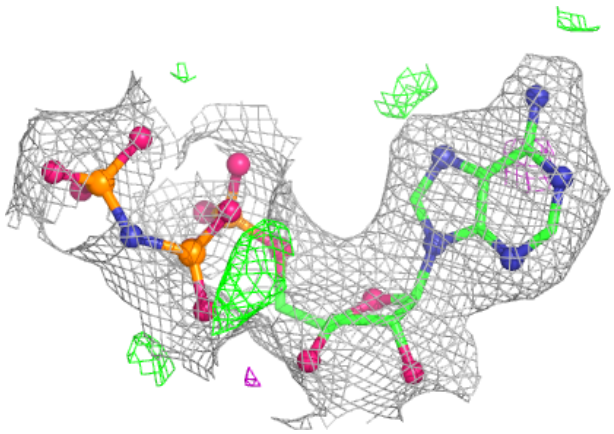
Continued from previous page...

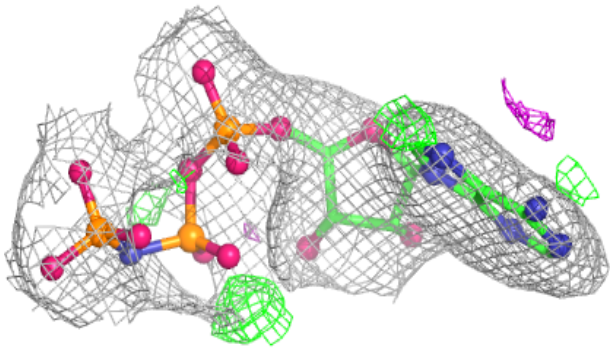
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	EDO	D	407	4/4	0.84	0.12	58,59,61,62	0
7	EDO	A	407	4/4	0.84	0.12	48,49,49,49	0
3	NA	B	402	1/1	0.85	0.18	51,51,51,51	0
7	EDO	A	411	4/4	0.86	0.17	67,70,72,72	0
4	CA	C	403	1/1	0.87	0.08	86,86,86,86	0
7	EDO	C	407	4/4	0.88	0.14	70,74,75,77	0
8	ACT	A	410	4/4	0.89	0.13	77,78,79,81	0
7	EDO	B	408	4/4	0.90	0.13	66,70,73,75	0
8	ACT	D	405	4/4	0.91	0.12	76,77,78,79	0
7	EDO	B	409	4/4	0.91	0.15	46,48,48,50	0
10	CL	B	407	1/1	0.91	0.11	78,78,78,78	0
4	CA	A	404	1/1	0.92	0.08	72,72,72,72	0
4	CA	C	404	1/1	0.92	0.06	85,85,85,85	0
6	MES	B	405	12/12	0.92	0.12	48,63,69,70	0
3	NA	D	402	1/1	0.93	0.07	57,57,57,57	0
5	ANP	D	404	31/31	0.93	0.08	43,49,62,64	0
7	EDO	D	406	4/4	0.94	0.11	62,66,67,71	0
5	ANP	C	405	31/31	0.94	0.08	42,48,55,57	0
3	NA	A	402	1/1	0.95	0.16	47,47,47,47	0
3	NA	C	402	1/1	0.96	0.06	61,61,61,61	0
5	ANP	A	405	31/31	0.96	0.06	31,36,41,42	0
6	MES	A	406	12/12	0.96	0.08	37,49,53,54	0
5	ANP	B	404	31/31	0.96	0.06	36,39,42,44	0
4	CA	D	403	1/1	0.97	0.06	79,79,79,79	0
4	CA	A	403	1/1	0.98	0.03	47,47,47,47	0
2	MG	B	401	1/1	0.98	0.03	38,38,38,38	0
2	MG	D	401	1/1	0.98	0.03	56,56,56,56	0
2	MG	A	401	1/1	0.99	0.05	38,38,38,38	0
4	CA	B	403	1/1	0.99	0.04	56,56,56,56	0
2	MG	C	401	1/1	0.99	0.04	51,51,51,51	0

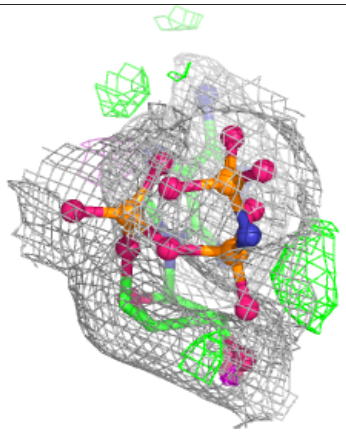
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ANP D 404:

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

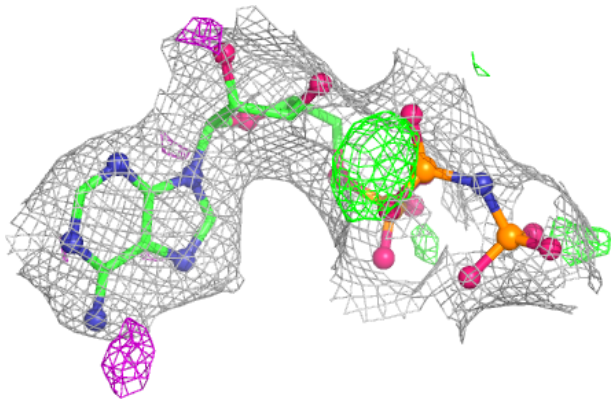


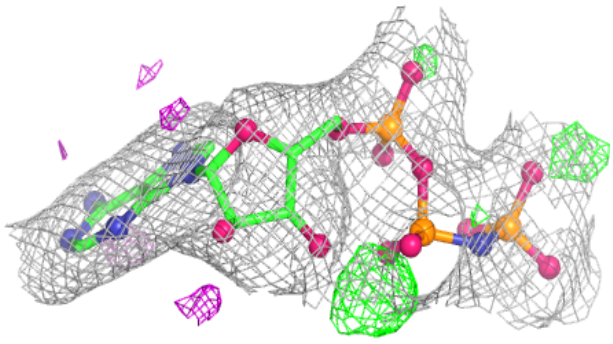


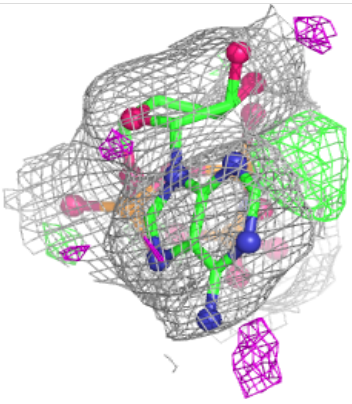


Electron density around ANP C 405:

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

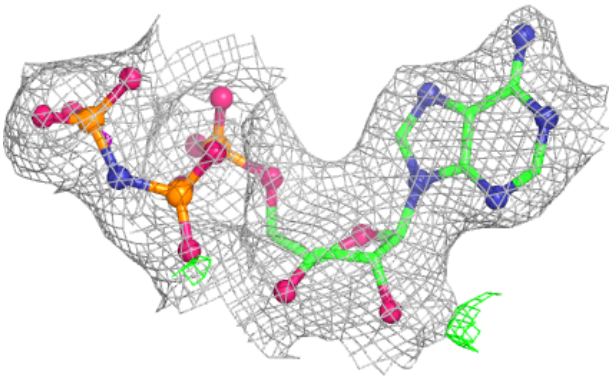


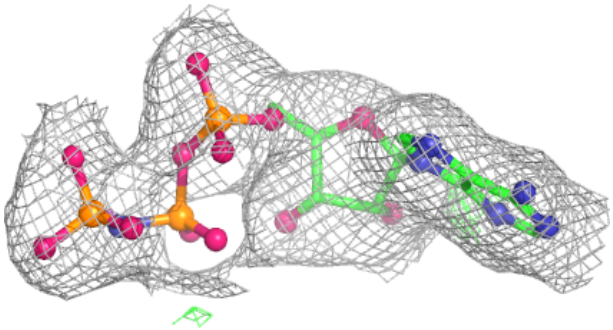


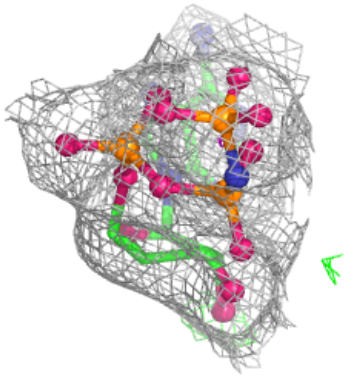


Electron density around ANP A 405:

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

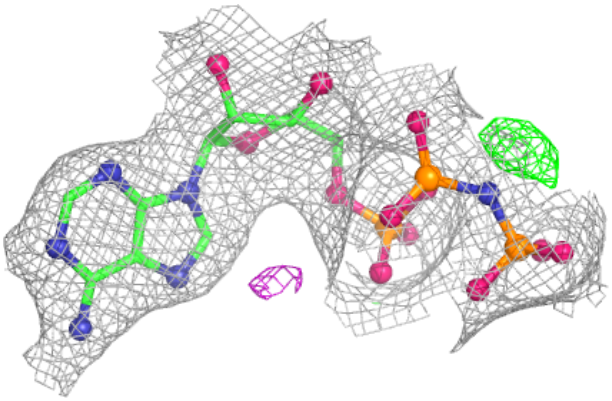


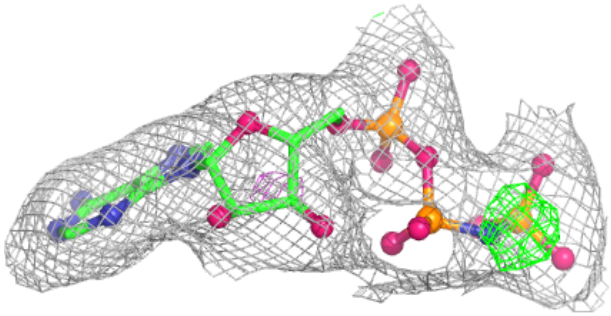


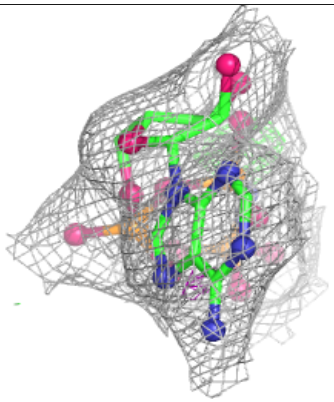


Electron density around ANP B 404:

$2mF_o$-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.