wwPDB X-ray Structure Validation Summary Report (i)

Oct 8, 2026 – 07:14 pm BST

PDB ID	:	29ZY / pdb_000029zy
Title	:	Human smooth muscle myosin motor domain co-crystallized with the R(+)2501 inhibitor, MgAMP-PNP form.
Authors	:	Glaser, C.; Kikuti, C.M.; Heidsieck, L.; Houdusse, A.
Deposited on	:	2026-04-16
Resolution	:	2.50 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

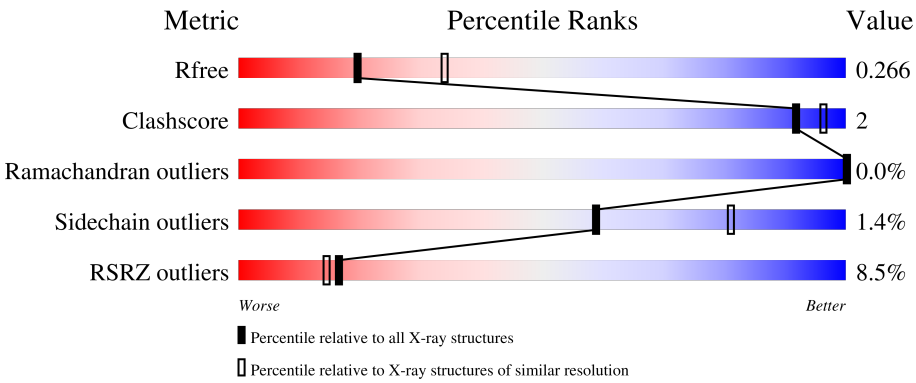
MolProbity	:	4-5-2 with Phenix2.2
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.2
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 2.50 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}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (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	794	6% 84% 5% 11%
1	B	794	9% 85% 6% 9%
1	C	794	9% 86% • 11%
1	D	794	7% 83% 6% 11%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 23405 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 Myosin-11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	707	5685	3623	972	1062	28	0	0	0
1	B	722	5798	3689	992	1087	30	0	0	0
1	C	710	5697	3625	977	1067	28	0	0	0
1	D	706	5682	3617	974	1063	28	0	1	0

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	785	ALA	-	expression tag	UNP P35749
A	786	SER	-	expression tag	UNP P35749
A	787	ASP	-	expression tag	UNP P35749
A	788	TYR	-	expression tag	UNP P35749
A	789	LYS	-	expression tag	UNP P35749
A	790	ASP	-	expression tag	UNP P35749
A	791	ASP	-	expression tag	UNP P35749
A	792	ASP	-	expression tag	UNP P35749
A	793	ASP	-	expression tag	UNP P35749
A	794	LYS	-	expression tag	UNP P35749
B	785	ALA	-	expression tag	UNP P35749
B	786	SER	-	expression tag	UNP P35749
B	787	ASP	-	expression tag	UNP P35749
B	788	TYR	-	expression tag	UNP P35749
B	789	LYS	-	expression tag	UNP P35749
B	790	ASP	-	expression tag	UNP P35749
B	791	ASP	-	expression tag	UNP P35749
B	792	ASP	-	expression tag	UNP P35749
B	793	ASP	-	expression tag	UNP P35749
B	794	LYS	-	expression tag	UNP P35749
C	785	ALA	-	expression tag	UNP P35749

Continued on next page...

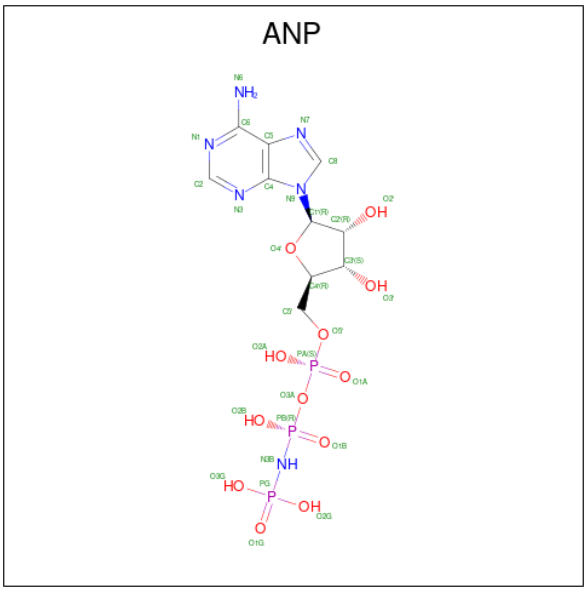
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	786	SER	-	expression tag	UNP P35749
C	787	ASP	-	expression tag	UNP P35749
C	788	TYR	-	expression tag	UNP P35749
C	789	LYS	-	expression tag	UNP P35749
C	790	ASP	-	expression tag	UNP P35749
C	791	ASP	-	expression tag	UNP P35749
C	792	ASP	-	expression tag	UNP P35749
C	793	ASP	-	expression tag	UNP P35749
C	794	LYS	-	expression tag	UNP P35749
D	785	ALA	-	expression tag	UNP P35749
D	786	SER	-	expression tag	UNP P35749
D	787	ASP	-	expression tag	UNP P35749
D	788	TYR	-	expression tag	UNP P35749
D	789	LYS	-	expression tag	UNP P35749
D	790	ASP	-	expression tag	UNP P35749
D	791	ASP	-	expression tag	UNP P35749
D	792	ASP	-	expression tag	UNP P35749
D	793	ASP	-	expression tag	UNP P35749
D	794	LYS	-	expression tag	UNP P35749

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

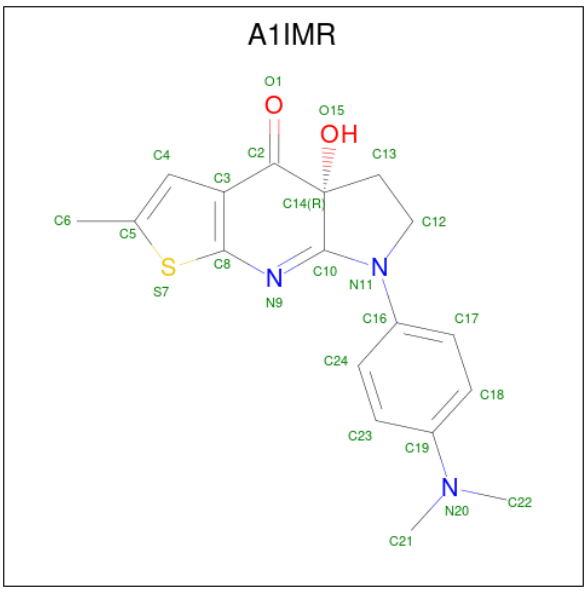
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
2	A	2	2	2	0	0
			Total	Mg		
2	B	2	2	2	0	0
			Total	Mg		
2	C	1	1	1	0	0
			Total	Mg		
2	D	1	1	1	0	0

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



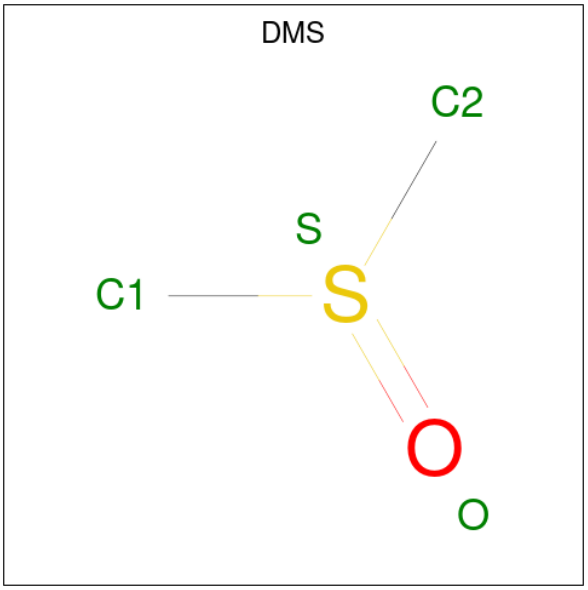
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	A	1	31	10	6	12	3	0	0
			Total	C	N	O	P		
3	B	1	31	10	6	12	3	0	0
			Total	C	N	O	P		
3	C	1	31	10	6	12	3	0	0
			Total	C	N	O	P		
3	D	1	31	10	6	12	3	0	0

- Molecule 4 is (9R)-12-[4-(dimethylamino)phenyl]-5-methyl-9-oxidanyl-4-thia-2,12-diazatricyclo[7.3.0.0^{3,7}]dodeca-1,3(7),5-trien-8-one (CCD ID: A1IMR) (formula: $C_{18}H_{19}N_3O_2S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
4	A	1	24	18	3	2	1	0	0
4	B	1	24	18	3	2	1	0	0
4	C	1	24	18	3	2	1	0	0
4	D	1	24	18	3	2	1	0	0

- Molecule 5 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C_2H_6OS).



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	100	100	100	0	0
6	B	90	90	90	0	0
6	C	66	66	66	0	0

Continued on next page...

Continued from previous page...

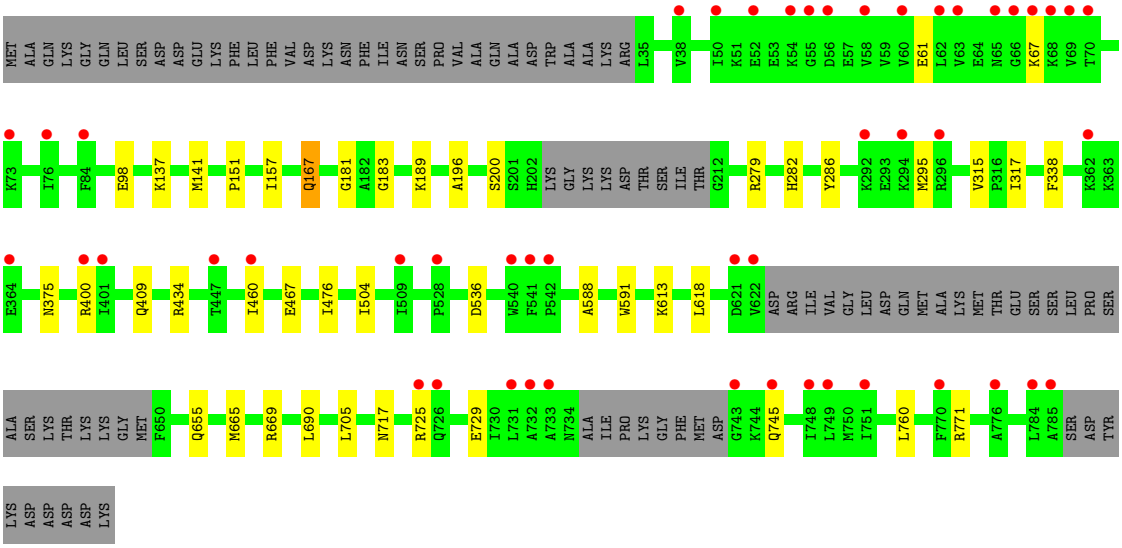
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	D	49	49	49	0	0

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.

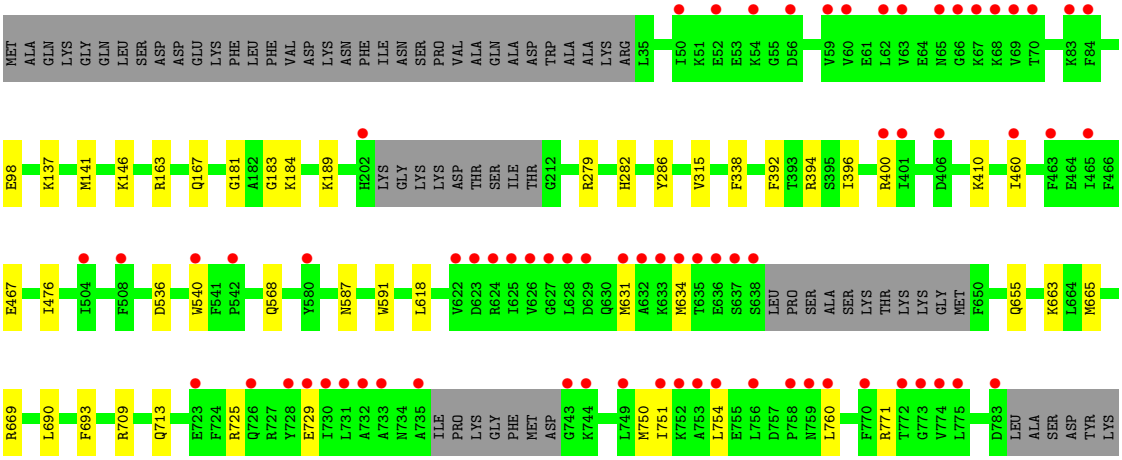
- Molecule 1: Myosin-11

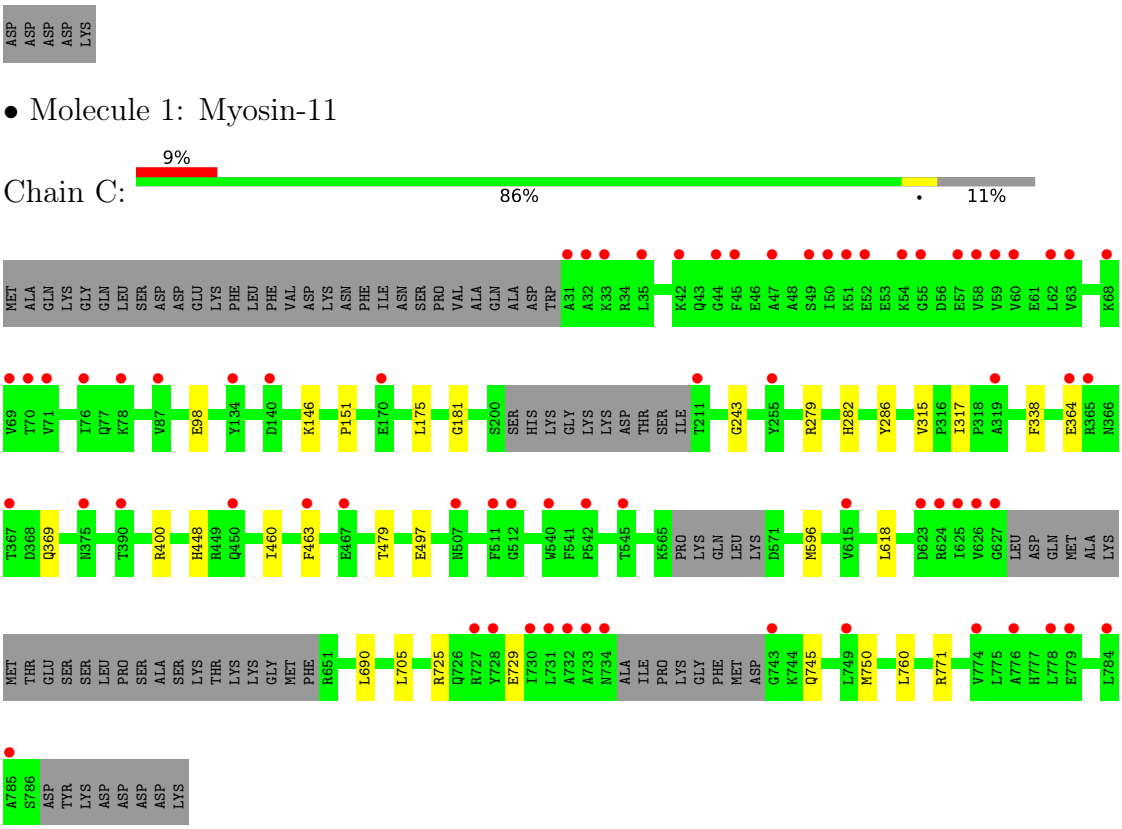
Chain A:

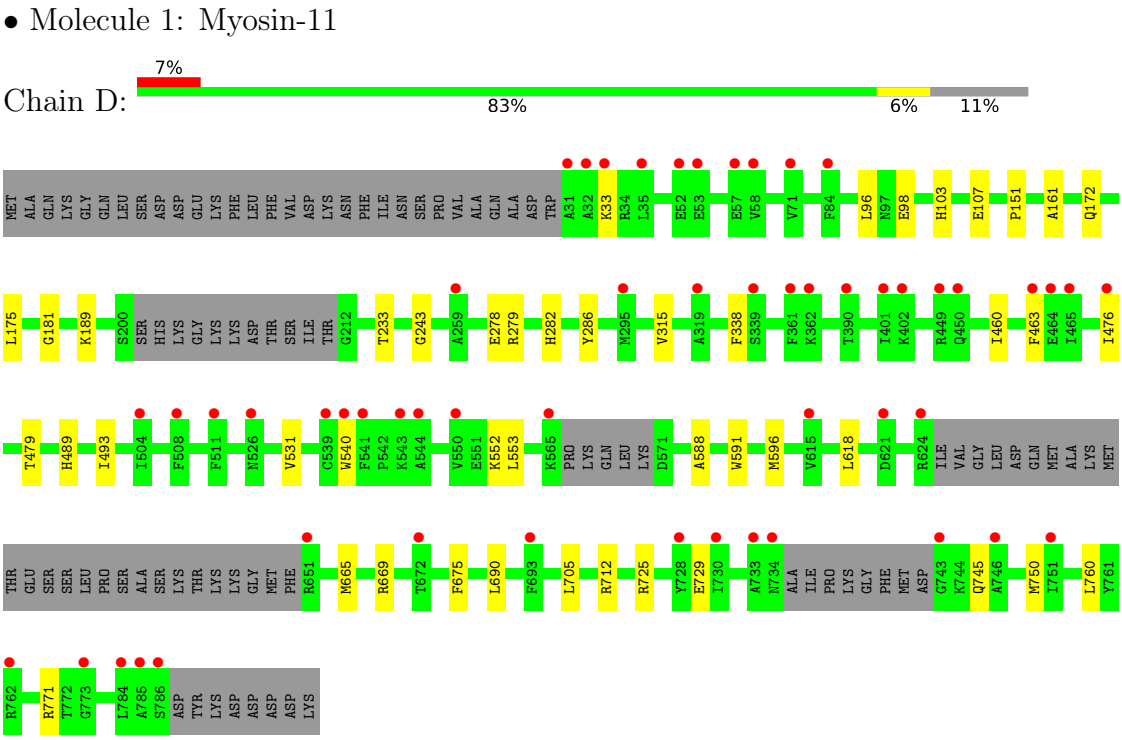


- Molecule 1: Myosin-11

Chain B:




ASP ASP ASP ASP LYS
• Molecule 1: Myosin-11
Chain C:
9%
86%
11%
MET ALA GLN LYS GLY GLN LEU SER ASP ASP GLU LYS PHE LEU PHE VAL ASP LYS ASN PHE ILE ASN SER PRO VAL ALA GLN ALA ASP TRP A31 A32 K33 R34 L35 K42 Q43 G44 F45 E46 A47 A48 S49 I50 K51 E52 E53 K54 G55 D56 E57 V58 V59 V60 E61 L62 V63 K68
V69 T70 V71 I76 Q77 K78 V87 E98 Y134 D140 K146 P151 E170 L175 G181 S200 SER HIS LYS GLY LYS LYS ASP THR SER ILE T211 G243 Y255 R279 H282 Y286 V315 P316 I317 P318 A319 F338 E364 R365 N366
T367 D368 Q369 N375 T390 R400 H448 R449 Q450 I460 F463 E467 T479 E497 N507 F511 G512 W540 F541 P542 T545 K565 PRO LYS GLN LEU LYS D571 M596 V615 L618 D623 R624 I625 V626 G627 LEU ASP GLN MET ALA LYS
MET THR GLU SER SER LEU PRO SER ALA SER LYS THR LYS LYS GLY MET PHE R651 L690 L705 R725 Q726 R727 Y728 E729 I730 L731 A732 A733 N734 ALA ILE PRO LYS GLY PHE MET ASP G743 K744 Q745 L749 M750 L760 R771 V774 L775 A776 H777 L778 E779 L784
A785 S786 ASP TYR LYS ASP ASP ASP ASP LYS


• Molecule 1: Myosin-11
Chain D:
7%
83%
6%
11%
MET ALA GLN LYS GLY GLN LEU SER ASP ASP GLU LYS PHE LEU PHE VAL ASP LYS ASN PHE ILE ASN SER PRO VAL ALA GLN ALA ASP TRP A31 A32 K33 R34 L35 E52 E53 E57 V58 V71 F84 L96 N97 E98 H103 E107 P151 A161 Q172
L175 G181 K189 S200 SER HIS LYS GLY LYS LYS ASP THR SER ILE THR G212 T233 G243 A259 E278 R279 H282 Y286 M295 V315 A319 F338 S339 F361 K362 T390 I401 K402 R449 Q450 I460 F463 E464 I465 I476
T479 H489 I493 I504 F508 F511 N526 V531 C539 W540 F541 P542 K543 A544 V550 E551 K552 L553 K565 PRO LYS GLN LEU LYS D571 A588 W591 M596 V615 L618 D621 R624 ILE VAL GLY GLY LEU ASP GLN MET ALA LYS MET
THR GLU SER SER LEU PRO SER ALA SER LYS THR LYS LYS GLY MET PHE R651 M665 R669 T672 F675 L690 F693 L705 R712 R725 Y728 E729 I730 A733 N734 ALA ILE PRO LYS GLY PHE MET ASP G743 K744 Q745 A746 M750 I751 L760 Y761
R762 R771 T772 G773 L784 A785 S786 ASP TYR LYS ASP ASP ASP ASP LYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	91.18Å 94.94Å 97.72Å 90.12° 94.35° 96.53°	Depositor
Resolution (Å)	94.32 – 2.50 94.32 – 2.50	Depositor EDS
% Data completeness (in resolution range)	66.7 (94.32-2.50) 66.7 (94.32-2.50)	Depositor EDS
R_{merge}	0.33	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.96 (at 2.51Å)	Xtriage
Refinement program	BUSTER 2.10.4	Depositor
R, R_{free}	0.230 , 0.271 0.224 , 0.266	Depositor DCC
R_{free} test set	3961 reflections (3.53%)	wwPDB-VP
Wilson B-factor (Å^2)	34.1	Xtriage
Anisotropy	0.127	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 44.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.007 for -h,-l,-k	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	23405	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.71% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: A1IMR, ANP, MG, DMS, MLY

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	0.71	1/5781 (0.0%)	1.01	5/7795 (0.1%)
1	B	0.69	0/5894	0.99	1/7945 (0.0%)
1	C	0.68	1/5789 (0.0%)	1.00	3/7804 (0.0%)
1	D	0.67	1/5775 (0.0%)	0.97	2/7784 (0.0%)
All	All	0.69	3/23239 (0.0%)	0.99	11/31328 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	151	PRO	CA-C	5.79	1.55	1.51
1	C	151	PRO	CA-C	5.74	1.55	1.51
1	D	151	PRO	CA-C	5.72	1.55	1.51

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	375	ASN	CA-CB-CG	6.91	119.51	112.60
1	A	295	MET	CA-C-N	5.98	128.57	120.38
1	A	295	MET	C-N-CA	5.98	128.57	120.38
1	C	463	PHE	CA-CB-CG	5.94	119.74	113.80
1	D	463	PHE	CA-CB-CG	5.89	119.69	113.80

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	5685	0	5689	19	0
1	B	5798	0	5800	24	0
1	C	5697	0	5703	13	0
1	D	5682	0	5681	20	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	31	0	13	3	0
3	B	31	0	13	5	0
3	C	31	0	13	1	0
3	D	31	0	13	1	0
4	A	24	0	0	0	0
4	B	24	0	0	0	0
4	C	24	0	0	0	0
4	D	24	0	0	0	0
5	A	4	0	6	1	0
5	B	4	0	6	0	0
5	D	4	0	6	0	0
6	A	100	0	0	1	0
6	B	90	0	0	1	0
6	C	66	0	0	0	0
6	D	49	0	0	0	0
All	All	23405	0	22943	73	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 2.

The worst 5 of 73 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:400:ARG:HH21	1:A:409:GLN:NE2	1.90	0.69
1:C:181:GLY:H	3:C:801:ANP:HNB1	1.40	0.68
1:B:663:LYS:NZ	6:B:901:HOH:O	2.22	0.66
1:B:181:GLY:H	3:B:802:ANP:HNB1	1.41	0.66
1:B:392:PHE:O	1:B:396:ILE:HG12	1.96	0.66

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	698/794 (88%)	681 (98%)	16 (2%)	1 (0%)	48	68
1	B	713/794 (90%)	692 (97%)	21 (3%)	0	100	100
1	C	699/794 (88%)	680 (97%)	19 (3%)	0	100	100
1	D	696/794 (88%)	677 (97%)	19 (3%)	0	100	100
All	All	2806/3176 (88%)	2730 (97%)	75 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	67	LYS

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	619/693 (89%)	608 (98%)	11 (2%)	51	77
1	B	632/693 (91%)	621 (98%)	11 (2%)	53	78
1	C	619/693 (89%)	613 (99%)	6 (1%)	68	86
1	D	617/693 (89%)	611 (99%)	6 (1%)	68	86
All	All	2487/2772 (90%)	2453 (99%)	34 (1%)	59	81

5 of 34 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	33	LYS
1	D	476	ILE
1	D	690	LEU
1	B	167	GLN
1	B	98	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 47 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	130	HIS
1	C	683	HIS
1	C	187	ASN
1	C	375	ASN
1	D	65	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)

4 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\#\|Z\| > 2$
1	MLY	D	189	1	9,10,11	0.66	0	6,11,13	1.78	3 (50%)
1	MLY	A	189	1	9,10,11	0.51	0	6,11,13	1.78	2 (33%)
1	MLY	C	189	1	9,10,11	0.72	0	6,11,13	1.25	0
1	MLY	B	189	1	9,10,11	0.96	0	6,11,13	1.64	2 (33%)

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
1	MLY	D	189	1	-	1/8/9/11	-
1	MLY	A	189	1	-	1/8/9/11	-
1	MLY	C	189	1	-	0/8/9/11	-
1	MLY	B	189	1	-	3/8/9/11	-

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	189	MLY	CH1-NZ-CE	-2.87	99.38	110.74
1	A	189	MLY	CH2-NZ-CH1	-2.80	102.49	109.73
1	D	189	MLY	CH2-NZ-CH1	-2.60	103.02	109.73
1	B	189	MLY	CH2-NZ-CE	2.35	120.06	110.74
1	D	189	MLY	CH2-NZ-CE	-2.28	101.71	110.74

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	D	189	MLY	CG-CD-CE-NZ
1	A	189	MLY	CG-CD-CE-NZ
1	B	189	MLY	CG-CD-CE-NZ
1	B	189	MLY	CD-CE-NZ-CH2
1	B	189	MLY	CE-CD-CG-CB

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 17 ligands modelled in this entry, 6 are monoatomic - leaving 11 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	A1IMR	C	802	-	23,27,27	0.24	0	28,42,42	0.41	0
3	ANP	D	801	2	32,33,33	1.11	4 (12%)	44,52,52	0.65	2 (4%)
5	DMS	D	803	-	3,3,3	0.76	0	3,3,3	0.50	0
3	ANP	A	802	2	32,33,33	1.03	4 (12%)	44,52,52	0.67	1 (2%)
4	A1IMR	D	802	-	23,27,27	0.24	0	28,42,42	0.37	0
5	DMS	B	804	-	3,3,3	0.76	0	3,3,3	0.09	0
4	A1IMR	A	803	-	23,27,27	0.28	0	28,42,42	0.40	0
3	ANP	C	801	2	32,33,33	1.11	4 (12%)	44,52,52	0.69	2 (4%)
3	ANP	B	802	2	32,33,33	1.04	4 (12%)	44,52,52	0.60	1 (2%)
5	DMS	A	804	-	3,3,3	0.78	0	3,3,3	0.19	0
4	A1IMR	B	803	-	23,27,27	0.31	0	28,42,42	0.42	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
4	A1IMR	C	802	-	-	1/8/38/38	0/4/4/4
3	ANP	D	801	2	-	3/18/38/38	0/3/3/3
3	ANP	A	802	2	-	3/18/38/38	0/3/3/3
4	A1IMR	D	802	-	-	0/8/38/38	0/4/4/4
4	A1IMR	A	803	-	-	0/8/38/38	0/4/4/4
3	ANP	C	801	2	-	3/18/38/38	0/3/3/3
3	ANP	B	802	2	-	3/18/38/38	0/3/3/3
4	A1IMR	B	803	-	-	1/8/38/38	0/4/4/4

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	801	ANP	PG-O2G	-3.11	1.48	1.56
3	C	801	ANP	PG-O2G	-3.08	1.48	1.56
3	C	801	ANP	PB-O2B	-3.01	1.48	1.56
3	A	802	ANP	PG-O2G	-2.96	1.48	1.56
3	D	801	ANP	PG-O3G	-2.93	1.48	1.56

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	802	ANP	O2B-PB-O1B	3.13	116.48	109.92
3	C	801	ANP	O2B-PB-O1B	2.38	114.92	109.92
3	D	801	ANP	O2B-PB-O1B	2.38	114.90	109.92
3	C	801	ANP	O3G-PG-O1G	-2.33	107.59	113.45
3	D	801	ANP	O2G-PG-O3G	2.05	113.10	107.64

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	802	ANP	PG-N3B-PB-O1B
3	A	802	ANP	PA-O3A-PB-O1B
3	A	802	ANP	PA-O3A-PB-O2B
3	B	802	ANP	PG-N3B-PB-O1B
3	B	802	ANP	PA-O3A-PB-O1B

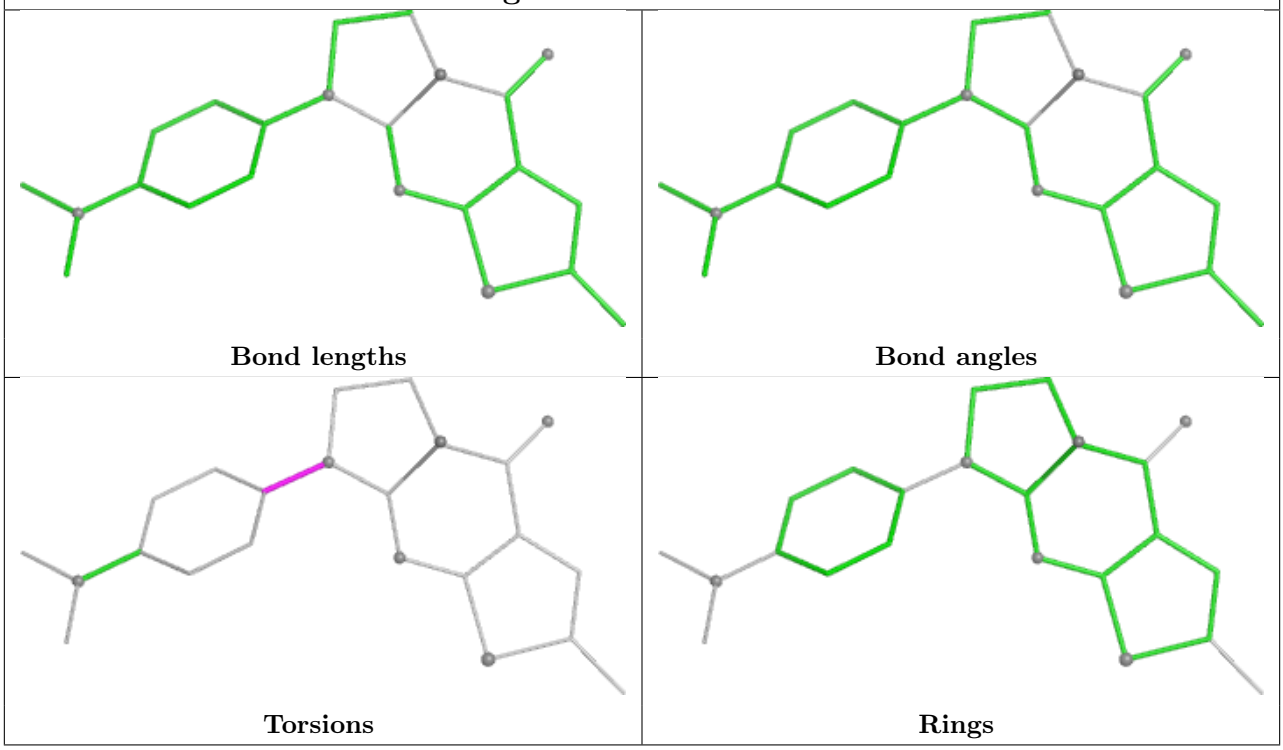
There are no ring outliers.

5 monomers are involved in 11 short contacts:

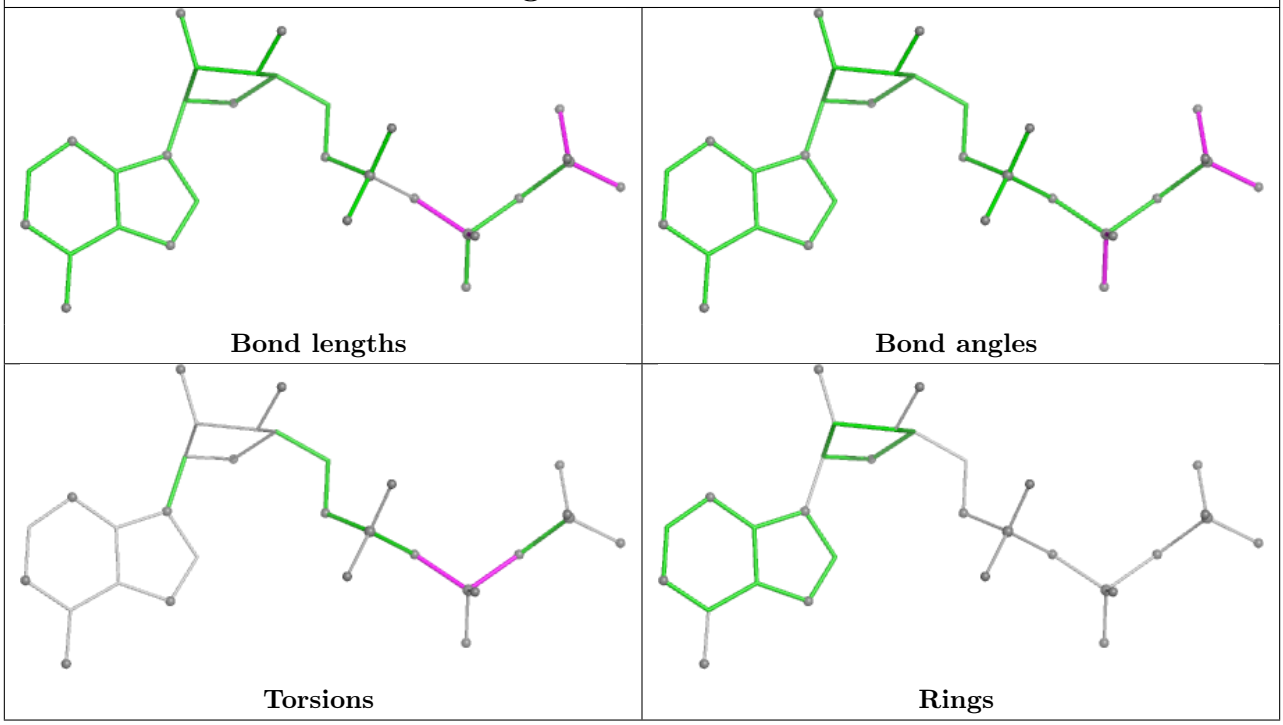
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	801	ANP	1	0
3	A	802	ANP	3	0
3	C	801	ANP	1	0
3	B	802	ANP	5	0
5	A	804	DMS	1	0

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.

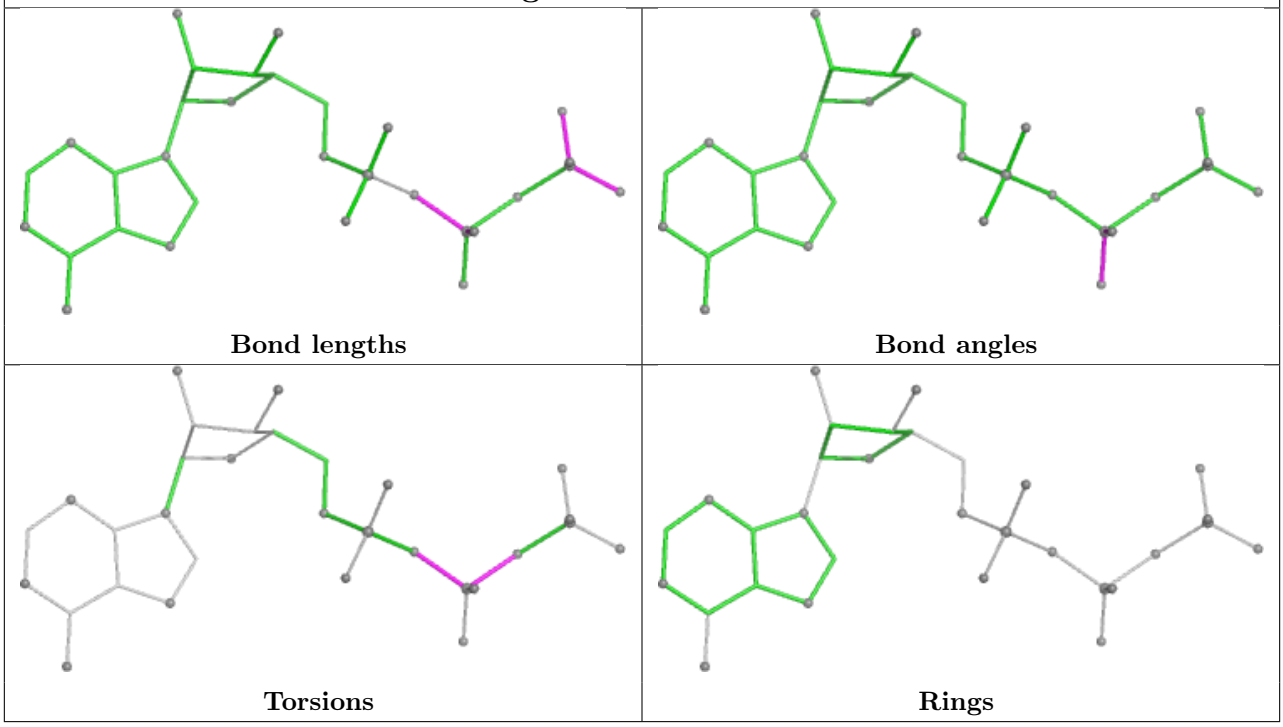
Ligand A1IMR C 802



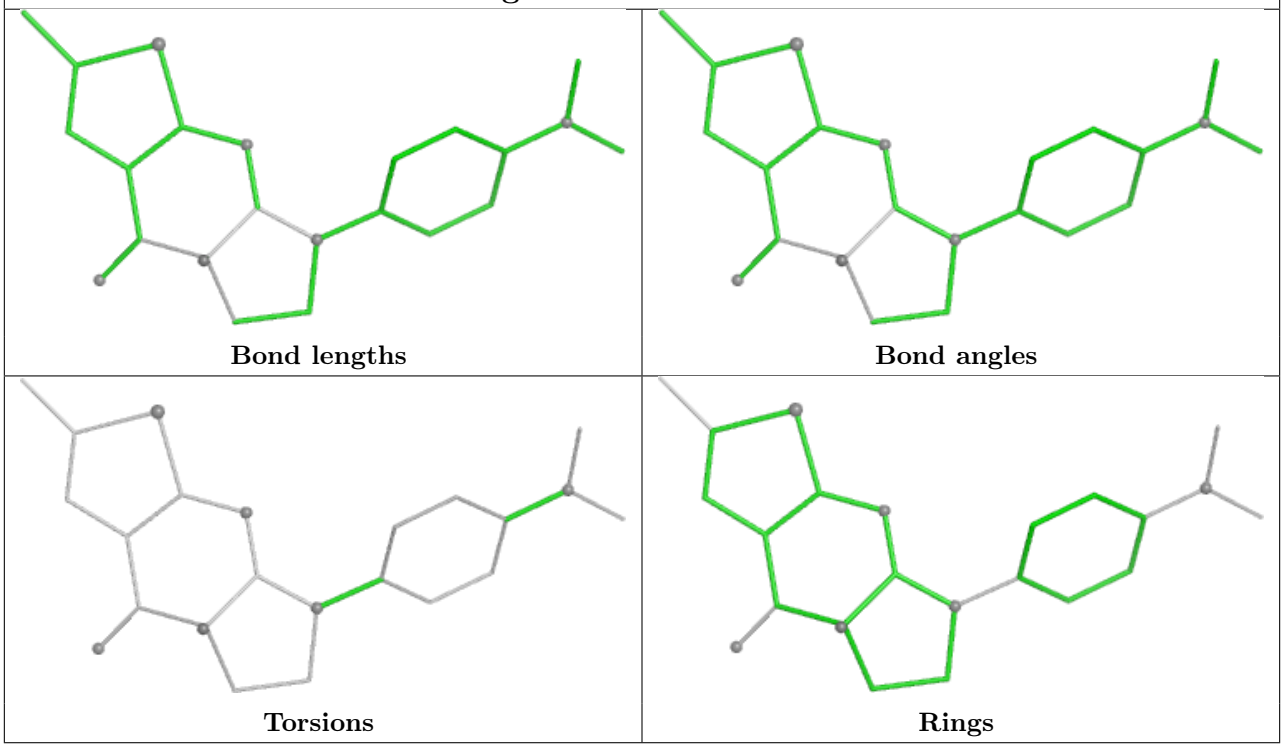
Ligand ANP D 801



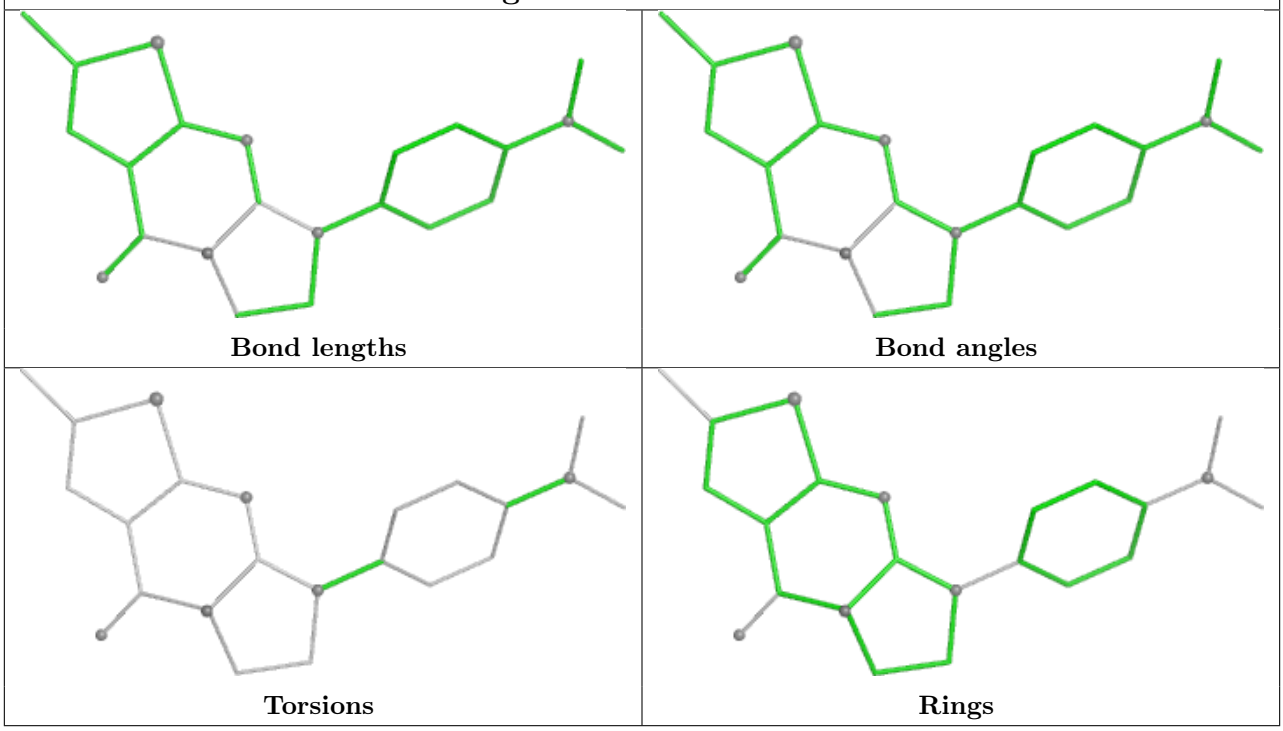
Ligand ANP A 802



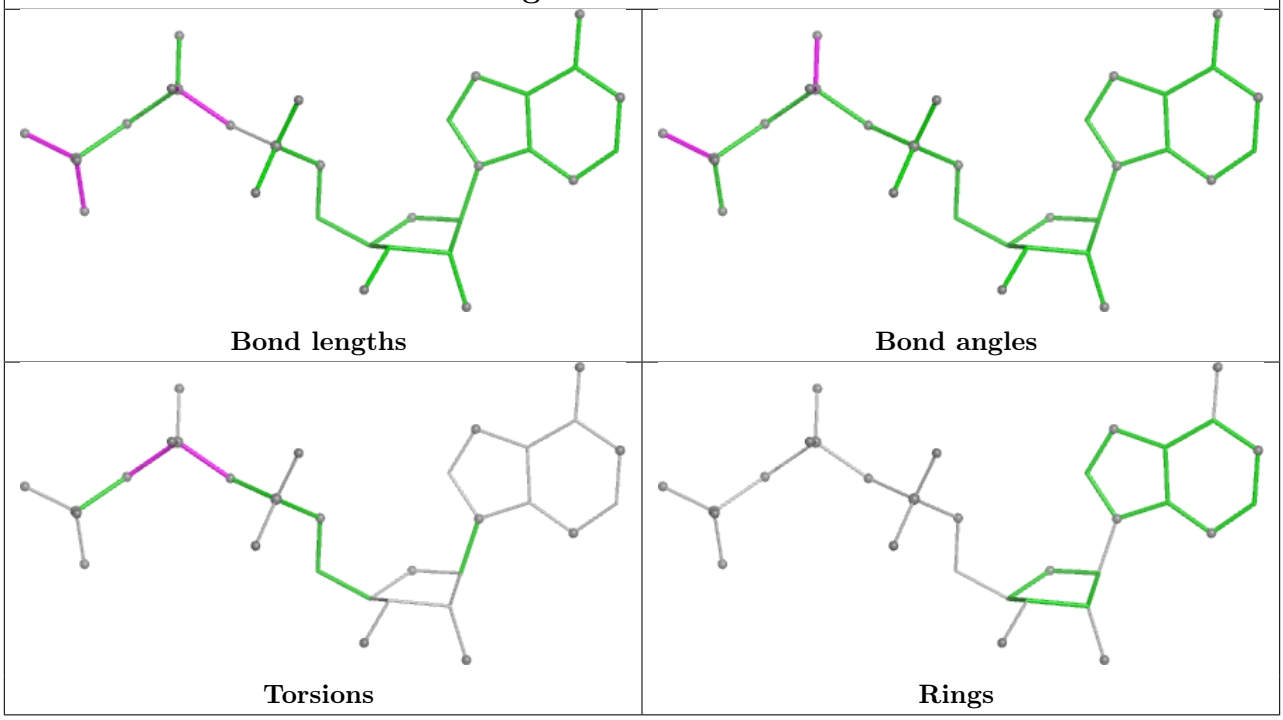
Ligand A1IMR D 802



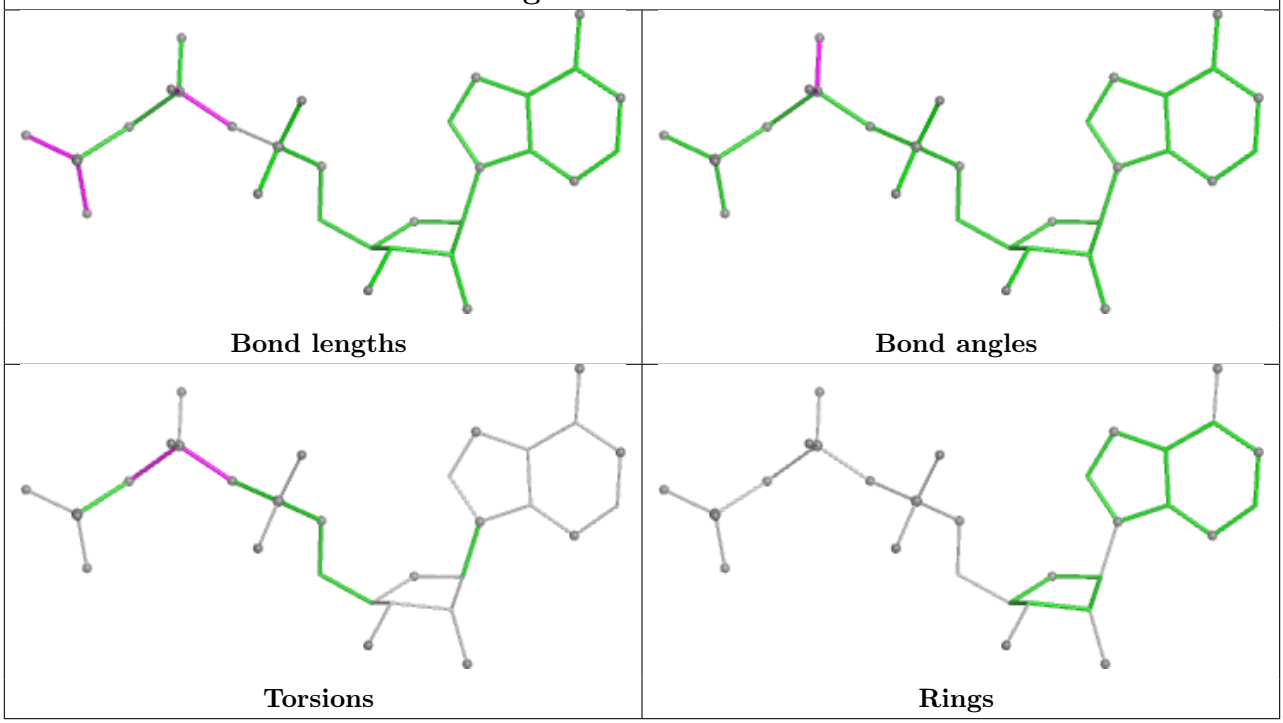
Ligand A1IMR A 803



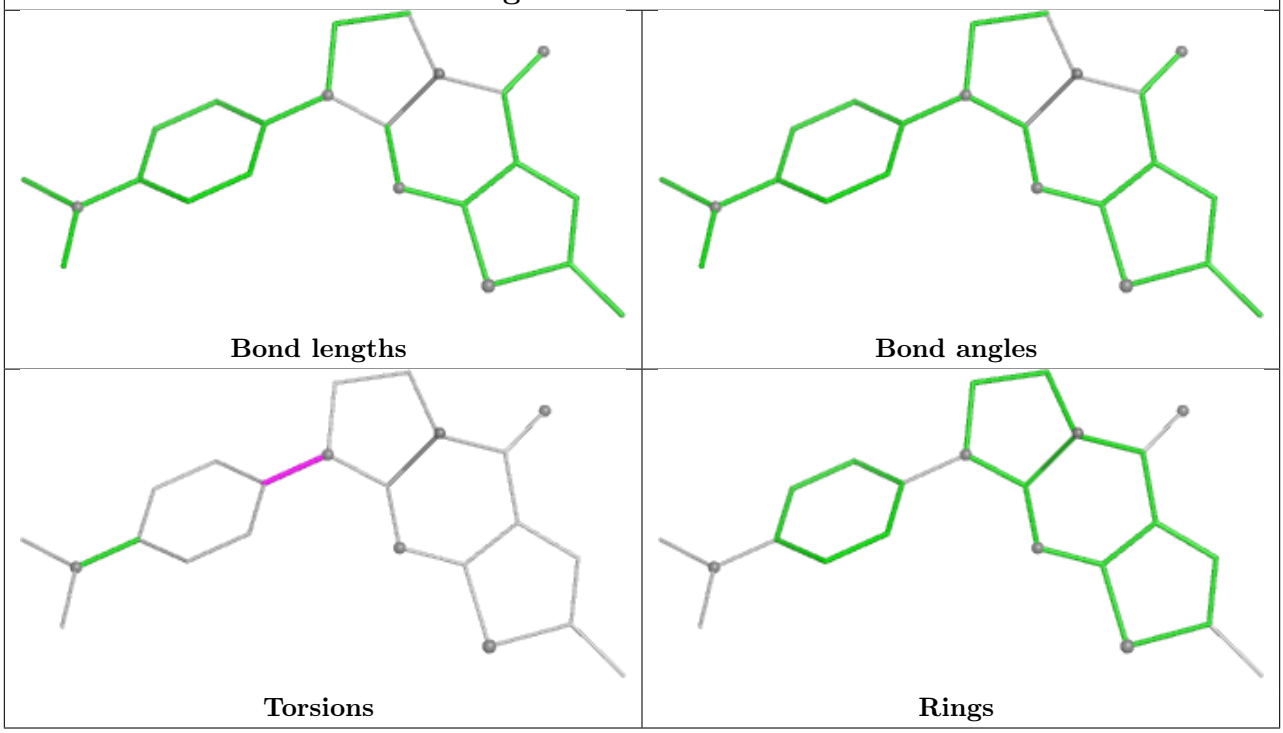
Ligand ANP C 801



Ligand ANP B 802



Ligand A1IMR B 803



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	706/794 (88%)	0.50	49 (6%)	23	20	16, 39, 77, 109	0
1	B	721/794 (90%)	0.63	70 (9%)	13	11	17, 38, 87, 100	0
1	C	709/794 (89%)	0.72	68 (9%)	13	11	16, 45, 85, 112	0
1	D	705/794 (88%)	0.76	54 (7%)	19	17	21, 48, 78, 91	1 (0%)
All	All	2841/3176 (89%)	0.65	241 (8%)	16	14	16, 42, 81, 112	1 (0%)

The worst 5 of 241 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	733	ALA	5.4
1	D	733	ALA	5.0
1	B	625	ILE	4.7
1	C	730	ILE	4.6
1	D	31	ALA	4.5

6.2 Non-standard residues in protein, DNA, RNA chains (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
1	MLY	D	189	11/12	0.90	0.14	26,27,40,40	0
1	MLY	C	189	11/12	0.92	0.12	27,29,42,42	0
1	MLY	B	189	11/12	0.92	0.10	18,21,36,36	0
1	MLY	A	189	11/12	0.93	0.08	21,24,38,38	0

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

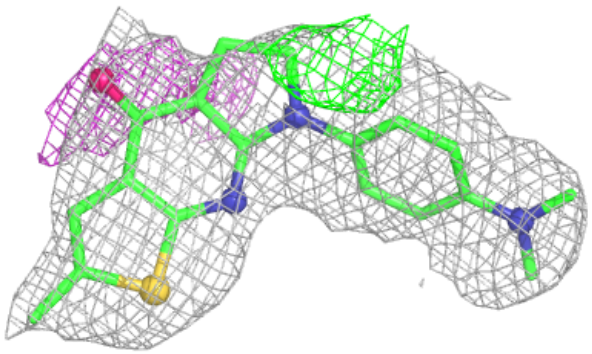
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

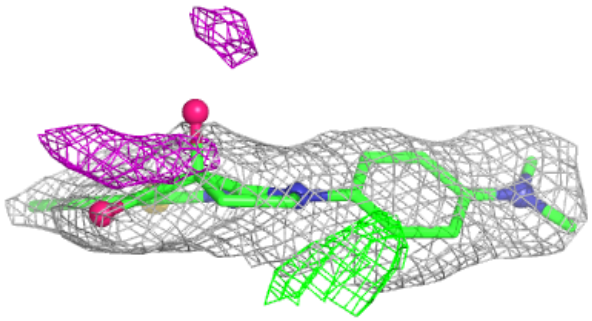
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	DMS	D	803	4/4	0.75	0.24	82,82,82,82	0
5	DMS	A	804	4/4	0.81	0.26	65,66,66,66	0
4	A1IMR	D	802	24/24	0.81	0.17	56,56,57,57	0
5	DMS	B	804	4/4	0.83	0.23	72,72,72,72	0
4	A1IMR	C	802	24/24	0.85	0.17	64,65,66,67	0
4	A1IMR	B	803	24/24	0.90	0.13	52,53,54,54	0
2	MG	A	805	1/1	0.91	0.13	3,3,3,3	0
4	A1IMR	A	803	24/24	0.91	0.12	42,45,45,45	0
3	ANP	D	801	31/31	0.95	0.08	29,33,35,35	0
2	MG	B	805	1/1	0.95	0.10	3,3,3,3	0
3	ANP	B	802	31/31	0.96	0.08	21,26,28,28	0
3	ANP	A	802	31/31	0.97	0.07	28,29,29,32	0
3	ANP	C	801	31/31	0.97	0.07	26,33,34,34	0
2	MG	D	800	1/1	0.98	0.10	26,26,26,26	0
2	MG	B	801	1/1	0.99	0.06	19,19,19,19	0
2	MG	A	801	1/1	0.99	0.04	10,10,10,10	0
2	MG	C	800	1/1	0.99	0.04	21,21,21,21	0

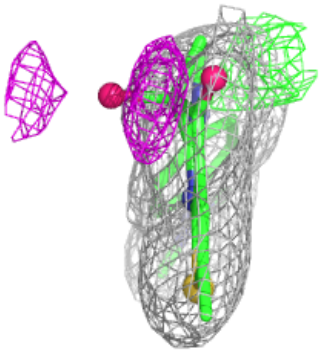
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around A1IMR D 802:

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

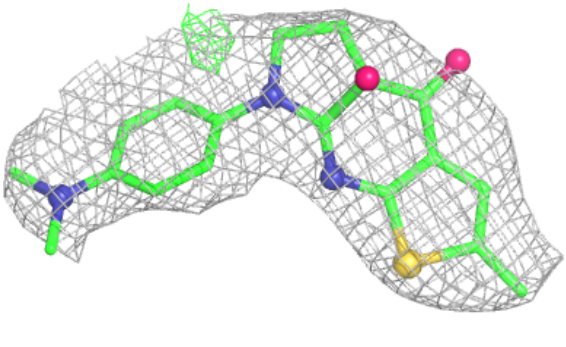


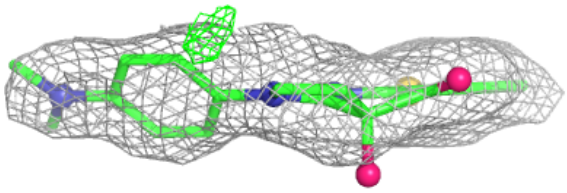


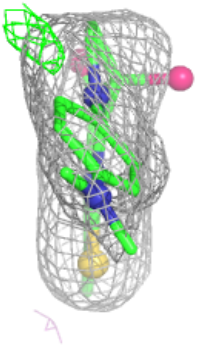


Electron density around A1IMR C 802:

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

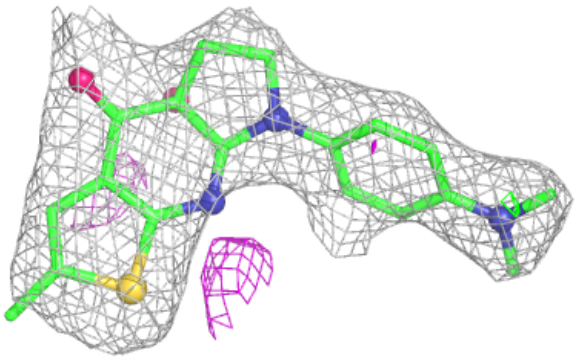


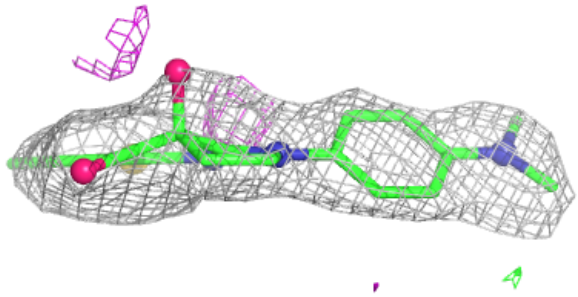


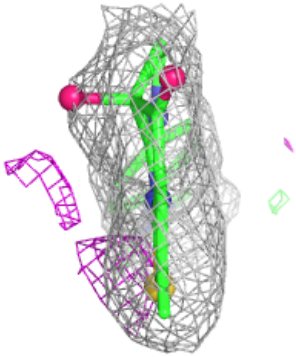


Electron density around A1IMR B 803:

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

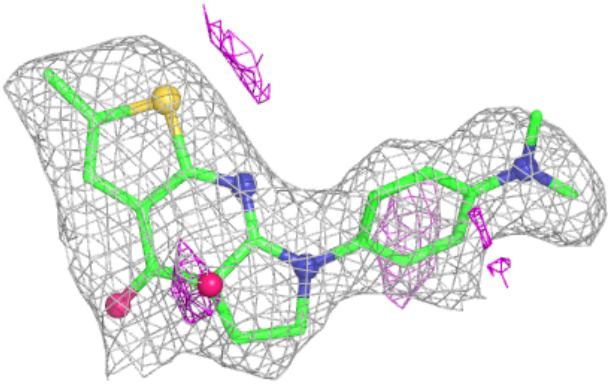


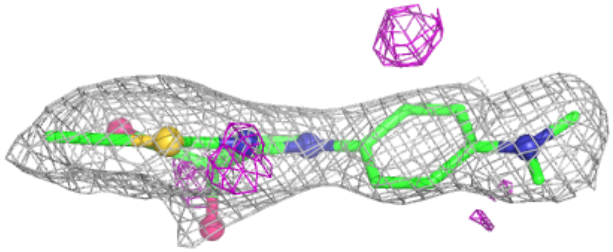


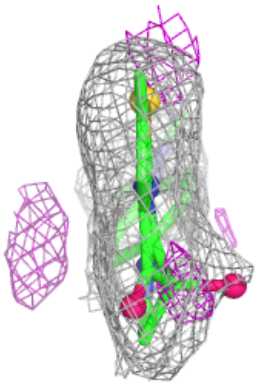


Electron density around A1IMR A 803:

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

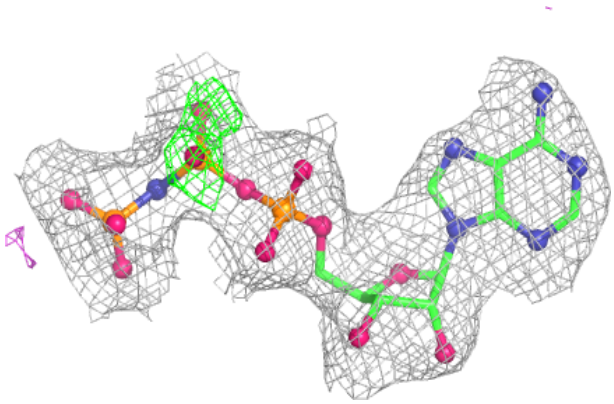


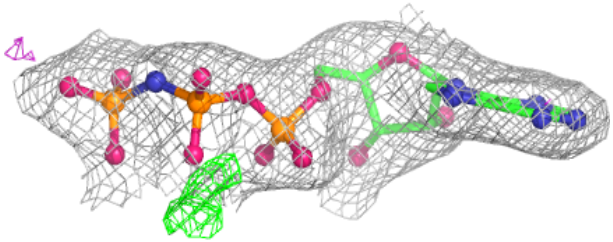


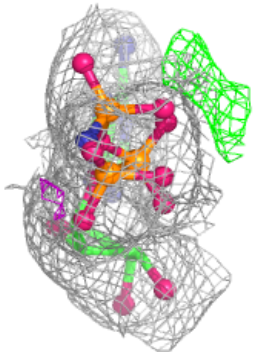


Electron density around ANP D 801:

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

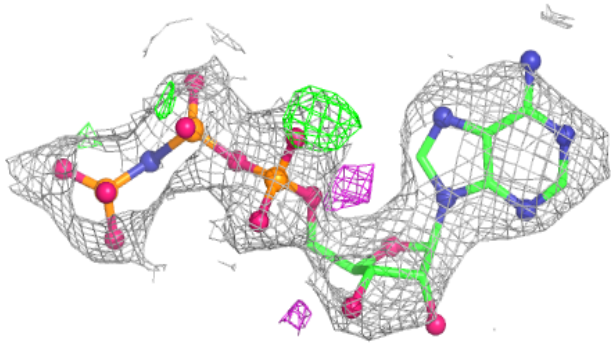


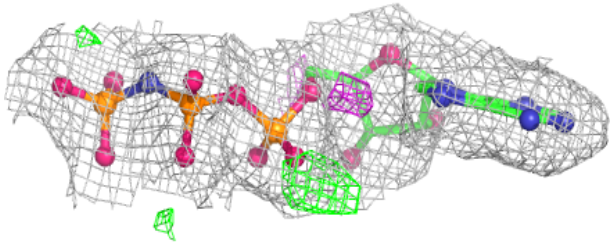


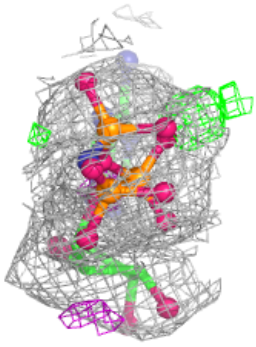


Electron density around ANP B 802:

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

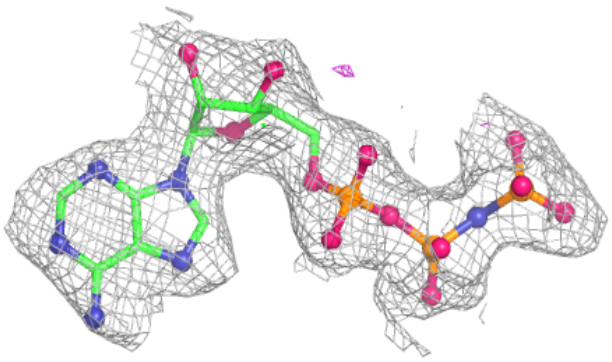


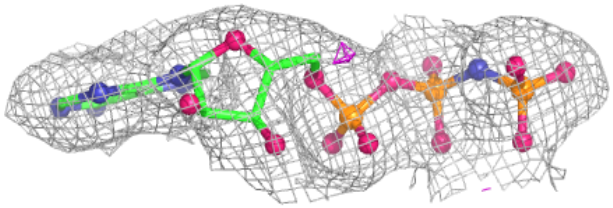


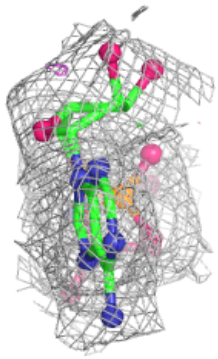


Electron density around ANP A 802:

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

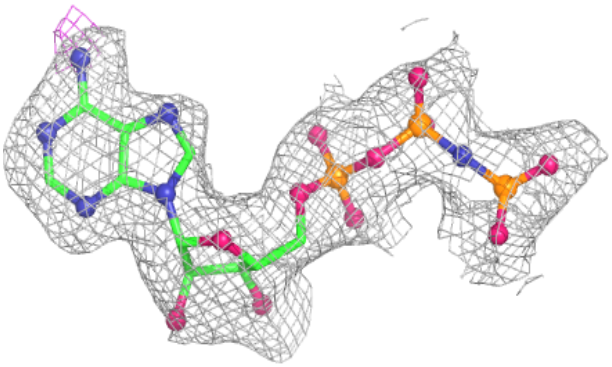


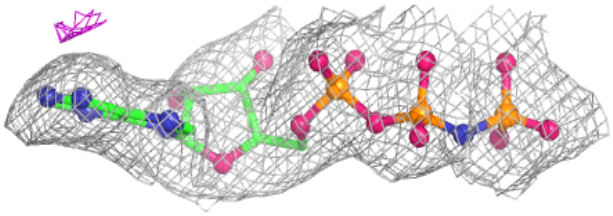


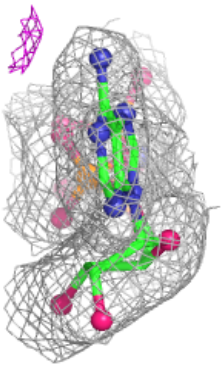


Electron density around ANP C 801:

$2mF_o$-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.