



Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 08:01 am BST

PDB ID : 5C8Y
Title : Crystal structure of T2R-TTL-Plinabulin complex
Authors : Wang, Y.; Yu, Y.; Chen, Q.; Yang, J.
Deposited on : 2015-06-26
Resolution : 2.59 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

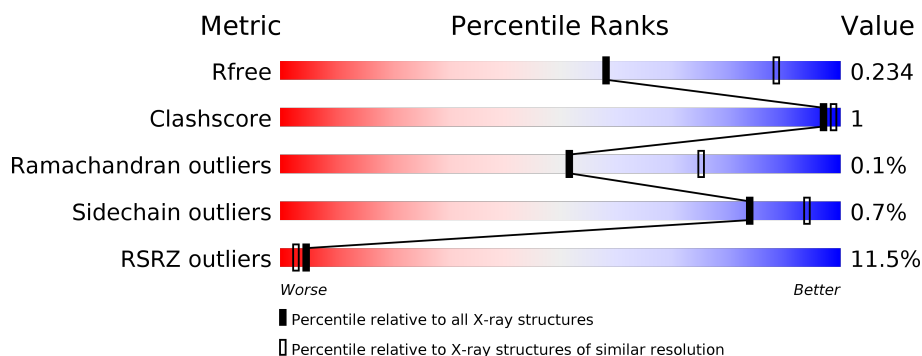
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.59 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	450	<div> <div>6%</div> <div>96%</div> <div>..</div> </div>
1	C	450	<div> <div>2%</div> <div>96%</div> <div>..</div> </div>
2	B	445	<div> <div>7%</div> <div>92%</div> <div>. .</div> </div>
2	D	445	<div> <div>14%</div> <div>92%</div> <div>. 5%</div> </div>
3	E	143	<div> <div>12%</div> <div>84%</div> <div>. 15%</div> </div>
4	F	384	<div> <div>28%</div> <div>83%</div> <div>. 13%</div> </div>

2 Entry composition [i](#)

There are 12 unique types of molecules in this entry. The entry contains 34616 atoms, of which 16867 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 Tubulin alpha.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	437	Total	C	H	N	O	S	0	0	0
			6733	2163	3317	581	650	22			
1	C	440	Total	C	H	N	O	S	0	0	0
			6772	2175	3335	584	656	22			

- Molecule 2 is a protein called Tubulin beta.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	427	Total	C	H	N	O	S	0	0	0
			6589	2110	3228	576	649	26			
2	D	421	Total	C	H	N	O	S	0	0	0
			6488	2080	3179	562	640	27			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	E	121	Total	C	H	N	O	S	0	0	0
			2014	617	1014	181	197	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	3	MET	-	expression tag	UNP P63043
E	4	ALA	-	expression tag	UNP P63043

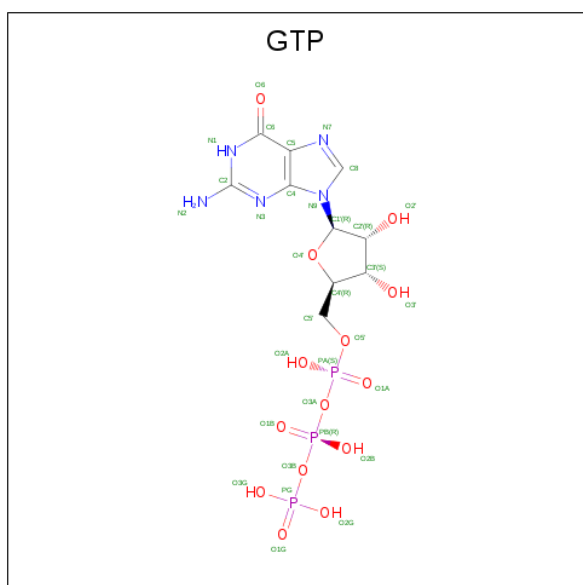
- Molecule 4 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	F	334	Total	C	H	N	O	S	0	0	0
			5442	1761	2698	470	499	14			

There are 6 discrepancies between the modelled and reference sequences:

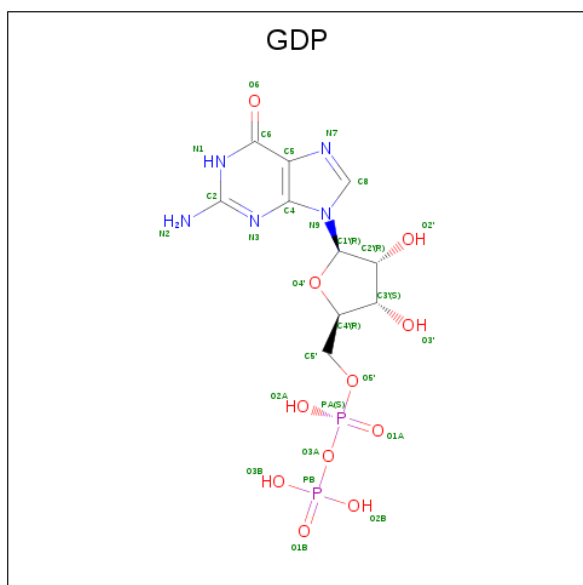
Chain	Residue	Modelled	Actual	Comment	Reference
F	379	HIS	-	expression tag	UNP E1BQ43
F	380	HIS	-	expression tag	UNP E1BQ43
F	381	HIS	-	expression tag	UNP E1BQ43
F	382	HIS	-	expression tag	UNP E1BQ43
F	383	HIS	-	expression tag	UNP E1BQ43
F	384	HIS	-	expression tag	UNP E1BQ43

- Molecule 5 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



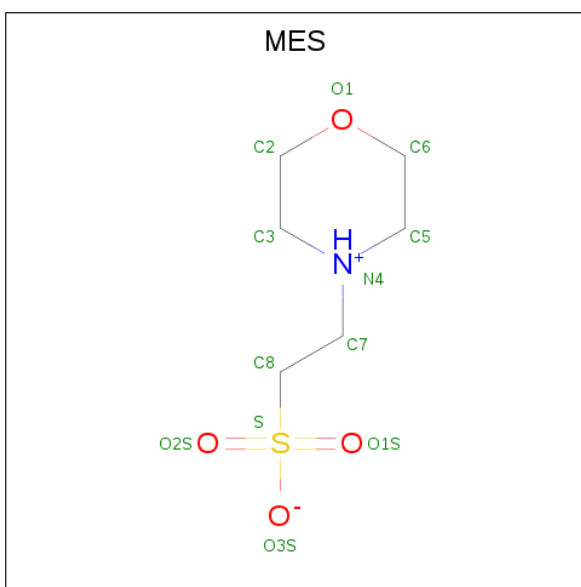
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total Ca 1 1	0	0
7	C	1	Total Ca 1 1	0	0

- Molecule 8 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



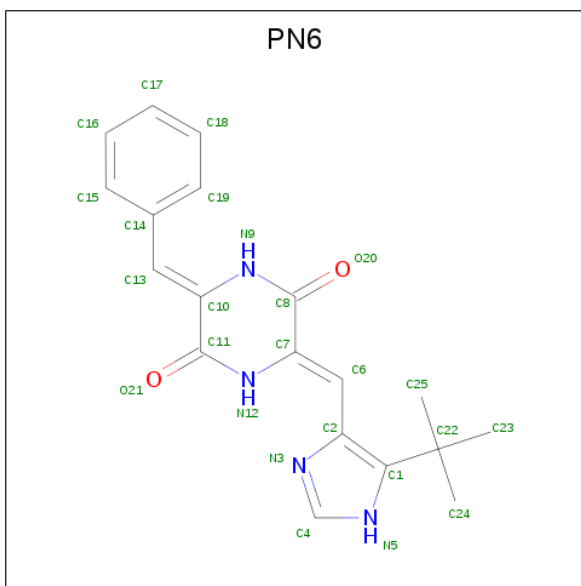
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
8	B	1	Total	C	H	N	O	P	0	0
			38	10	10	5	11	2		
8	D	1	Total	C	H	N	O	P	0	0
			38	10	10	5	11	2		

- Molecule 9 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
9	B	1	Total	C	H	N	O	S	0	0
			24	6	12	1	4	1		

- Molecule 10 is (3Z,6Z)-3-benzylidene-6-[(5-tert-butyl-1H-imidazol-4-yl)methylidene]piperazine-2,5-dione (three-letter code: PN6) (formula: $C_{19}H_{20}N_4O_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	B	1	Total	C	H	N	O	0	0
			45	19	20	4	2		
10	D	1	Total	C	H	N	O	0	0
			45	19	20	4	2		

-
- The chemical structure of ACP (Adenosine Cyclic Phosphate) is shown. It consists of an adenine base (N1, N3, N7, N9) attached to a ribose sugar (C1', C2', C3', C4', C5') via a glycosidic bond. The ribose sugar is linked to a cyclic phosphate group (P1, P2, P3, P4, P5) through its 5' carbon (C5'). The phosphate group is shown in a cyclic conformation with various oxygen atoms (O1, O2, O3, O4, O5, O6, O7, O8, O9, O10, O11, O12, O13, O14, O15, O16, O17, O18, O19, O20, O21, O22, O23, O24, O25, O26, O27, O28, O29, O30, O31, O32, O33, O34, O35, O36, O37, O38, O39, O40, O41, O42, O43, O44, O45, O46, O47, O48, O49, O50, O51, O52, O53, O54, O55, O56, O57, O58, O59, O60, O61, O62, O63, O64, O65, O66, O67, O68, O69, O70, O71, O72, O73, O74, O75, O76, O77, O78, O79, O80, O81, O82, O83, O84, O85, O86, O87, O88, O89, O90, O91, O92, O93, O94, O95, O96, O97, O98, O99, O100, O101, O102, O103, O104, O105, O106, O107, O108, O109, O110, O111, O112, O113, O114, O115, O116, O117, O118, O119, O120, O121, O122, O123, O124, O125, O126, O127, O128, O129, O130, O131, O132, O133, O134, O135, O136, O137, O138, O139, O140, O141, O142, O143, O144, O145, O146, O147, O148, O149, O150, O151, O152, O153, O154, O155, O156, O157, O158, O159, O160, O161, O162, O163, O164, O165, O166, O167, O168, O169, O170, O171, O172, O173, O174, O175, O176, O177, O178, O179, O180, O181, O182, O183, O184, O185, O186, O187, O188, O189, O190, O191, O192, O193, O194, O195, O196, O197, O198, O199, O200, O201, O202, O203, O204, O205, O206, O207, O208, O209, O210, O211, O212, O213, O214, O215, O216, O217, O218, O219, O220, O221, O222, O223, O224, O225, O226, O227, O228, O229, O230, O231, O232, O233, O234, O235, O236, O237, O238, O239, O240, O241, O242, O243, O244, O245, O246, O247, O248, O249, O250, O251, O252, O253, O254, O255, O256, O257, O258, O259, O260, O261, O262, O263, O264, O265, O266, O267, O268, O269, O270, O271, O272, O273, O274, O275, O276, O277, O278, O279, O280, O281, O282, O283, O284, O285, O286, O287, O288, O289, O290, O291, O292, O293, O294, O295, O296, O297, O298, O299, O300, O301, O302, O303, O304, O305, O306, O307, O308, O309, O310, O311, O312, O313, O314, O315, O316, O317, O318, O319, O320, O321, O322, O323, O324, O325, O326, O327, O328, O329, O330, O331, O332, O333, O334, O335, O336, O337, O338, O339, O340, O341, O342, O343, O344, O345, O346, O347, O348, O349, O350, O351, O352, O353, O354, O355, O356, O357, O358, O359, O360, O361, O362, O363, O364, O365, O366, O367, O368, O369, O370, O371, O372, O373, O374, O375, O376, O377, O378, O379, O380, O381, O382, O383, O384, O385, O386, O387, O388, O389, O390, O391, O392, O393, O394, O395, O396, O397, O398, O399, O400, O401, O402, O403, O404, O405, O406, O407, O408, O409, O410, O411, O412, O413, O414, O415, O416, O417, O418, O419, O420, O421, O422, O423, O424, O425, O426, O427, O428, O429, O430, O431, O432, O433, O434, O435, O436, O437, O438, O439, O440, O441, O442, O443, O444, O445, O446, O447, O448, O449, O450, O451, O452, O453, O454, O455, O456, O457, O458, O459, O460, O461, O462, O463, O464, O465, O466, O467, O468, O469, O470, O471, O472, O473, O474, O475, O476, O477, O478, O479, O480, O481, O482, O483, O484, O485, O486, O487, O488, O489, O490, O491, O492, O493, O494, O495, O496, O497, O498, O499, O500, O501, O502, O503, O504, O505, O506, O507, O508, O509, O510, O511, O512, O513, O514, O515, O516, O517, O518, O519, O520, O521, O522, O523, O524, O525, O526, O527, O528, O529, O530, O531, O532, O533, O534, O535, O536, O537, O538, O539, O540, O541, O542, O543, O544, O545, O546, O547, O548, O549, O550, O551, O552, O553, O554, O555, O556, O557, O558, O559, O560, O561, O562, O563, O564, O565, O566, O567, O568, O569, O570, O571, O572, O573, O574, O575, O576, O577, O578, O579, O580, O581, O582, O583, O584, O585, O586, O587, O588, O589, O590, O591, O592, O593, O594, O595, O596, O597, O598, O599, O600, O601, O602, O603, O604, O605, O606, O607, O608, O609, O610, O611, O612, O613, O614, O615, O616, O617, O618, O619, O620, O621, O622, O623, O624, O625, O626, O627, O628, O629, O630, O631, O632, O633, O634, O635, O636, O637, O638, O639, O640, O641, O642, O643, O644, O645, O646, O647, O648, O649, O650, O651, O652, O653, O654, O655, O656, O657, O658, O659, O660, O661, O662, O663, O664, O665, O666, O667, O668, O669, O670, O671, O672, O673, O674, O675, O676, O677, O678, O679, O680, O681, O682, O683, O684, O685, O686, O687, O688, O689, O690, O691, O692, O693, O694, O695, O696, O697, O698, O699, O700, O701, O702, O703, O704, O705, O706, O707, O708, O709, O710, O711, O712, O713, O714, O715, O716, O717, O718, O719, O720, O721, O722, O723, O724, O725, O726, O727, O728, O729, O730, O731, O732, O733, O734, O735, O736, O737, O738, O739, O740, O741, O742, O743, O744, O745, O746, O747, O748, O749, O750, O751, O752, O753, O754, O755, O756, O757, O758, O759, O760, O761, O762, O763, O764, O765, O766, O767, O768, O769, O770, O771, O772, O773, O774, O775, O776, O777, O778, O779, O780, O781, O782, O783, O784, O785, O786, O787, O788, O789, O790, O791, O792, O793, O794, O795, O796, O797, O798, O799, O800, O801, O802, O803, O804, O805, O806, O807, O808, O809, O810, O8

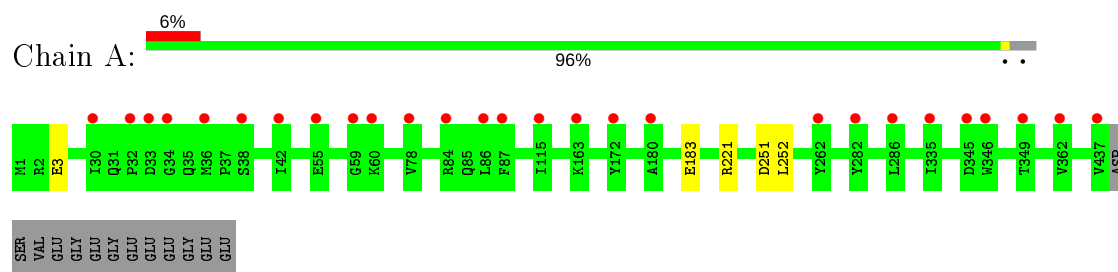
- Molecule 12 is water.



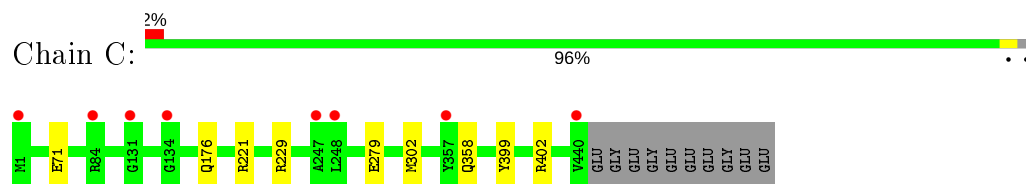
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

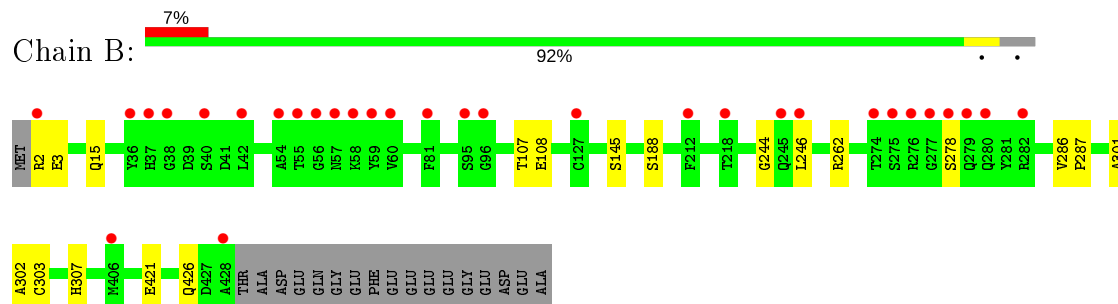
• Molecule 1: Tubulin alpha



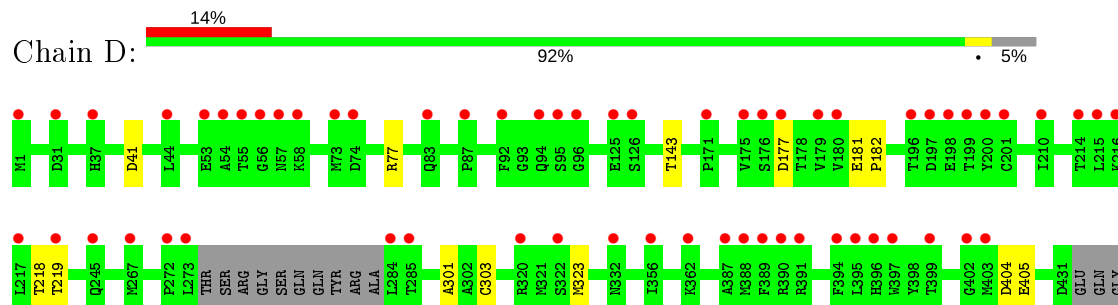
• Molecule 1: Tubulin alpha



• Molecule 2: Tubulin beta

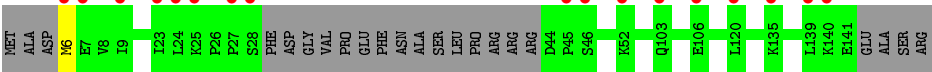
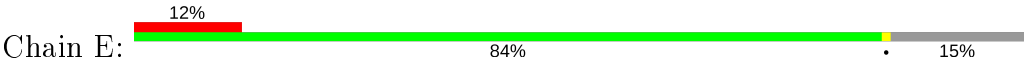


• Molecule 2: Tubulin beta

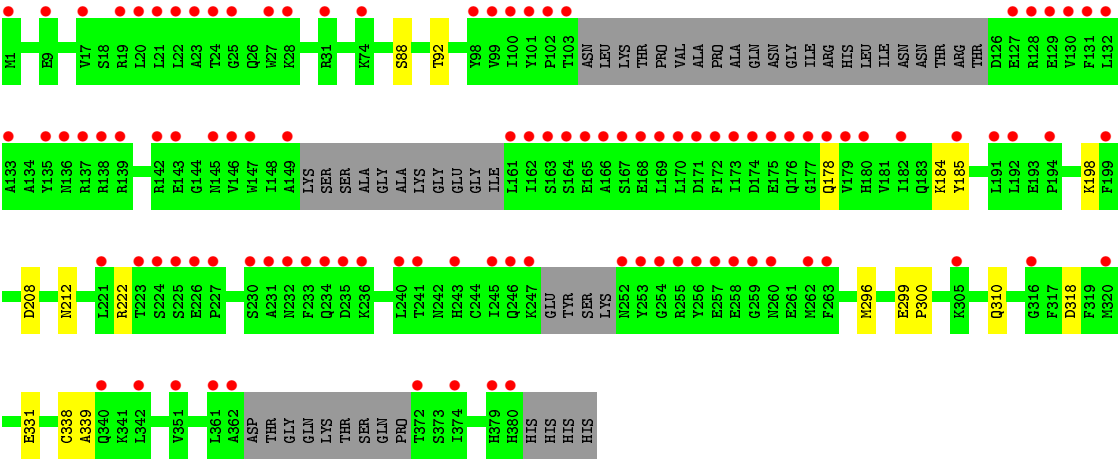
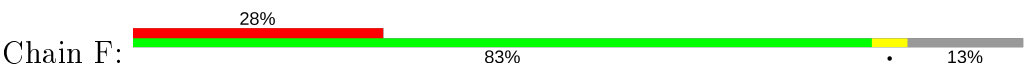


GLU
PHE
GLU
GLU
GLU
GLY
GLU
ASP
GLU
ALA

● Molecule 3: Stathmin-4



● Molecule 4: Uncharacterized protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	105.06Å 158.44Å 181.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.70 – 2.59 45.48 – 2.59	Depositor EDS
% Data completeness (in resolution range)	98.8 (39.70-2.59) 98.8 (45.48-2.59)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.89 (at 2.58Å)	Xtriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, R_{free}	0.222 , 0.271 0.227 , 0.234	Depositor DCC
R_{free} test set	4633 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	44.9	Xtriage
Anisotropy	0.236	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 59.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	34616	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.75% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GDP, MG, CA, PN6, GTP, ACP, MES

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	0.22	0/3494	0.37	0/4743
1	C	0.22	0/3515	0.37	0/4772
2	B	0.22	0/3436	0.38	0/4654
2	D	0.22	0/3382	0.37	0/4581
3	E	0.21	0/1008	0.32	0/1337
4	F	0.22	0/2806	0.36	0/3791
All	All	0.22	0/17641	0.37	0/23878

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [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	3416	3317	3330	3	0
1	C	3437	3335	3348	5	0
2	B	3361	3228	3238	8	0
2	D	3309	3179	3189	6	0
3	E	1000	1014	1018	1	0
4	F	2744	2698	2709	7	0
5	A	32	10	12	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	32	10	12	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
7	A	1	0	0	0	0
7	C	1	0	0	0	0
8	B	28	10	12	0	0
8	D	28	10	12	1	0
9	B	12	12	12	0	0
10	B	25	20	20	0	0
10	D	25	20	20	1	0
11	F	31	4	14	0	0
12	A	68	0	0	0	0
12	B	49	0	0	1	0
12	C	89	0	0	3	0
12	D	20	0	0	1	0
12	E	13	0	0	1	0
12	F	25	0	0	0	0
All	All	17749	16867	16946	31	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 (31) 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)
2:B:2:ARG:NH1	12:B:603:HOH:O	2.27	0.67
2:D:77:ARG:NH2	12:D:1201:HOH:O	2.30	0.64
4:F:222:ARG:NH1	4:F:318:ASP:OD1	2.33	0.62
2:B:301:ALA:O	2:B:303:CYS:N	2.32	0.61
2:D:404:ASP:OD1	2:D:405:GLU:N	2.35	0.59
1:C:176:GLN:NE2	12:C:604:HOH:O	2.35	0.58
1:A:251:ASP:OD1	1:A:252:LEU:N	2.37	0.58
2:B:145:SER:HG	2:B:188:SER:HG	1.53	0.56
1:C:229:ARG:NH2	12:C:606:HOH:O	2.38	0.56
4:F:185:TYR:OH	4:F:198:LYS:NZ	2.39	0.56
2:D:143:THR:N	8:D:501:GDP:O2B	2.43	0.51
10:D:502:PN6:N12	10:D:502:PN6:N3	2.49	0.51
2:B:262:ARG:NE	2:B:421:GLU:OE2	2.45	0.49
4:F:178:GLN:OE1	4:F:178:GLN:N	2.45	0.49
1:C:399:TYR:O	1:C:402:ARG:NH2	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:279:GLU:OE1	1:C:279:GLU:N	2.46	0.46
1:C:71:GLU:O	12:C:601:HOH:O	2.20	0.46
2:D:301:ALA:O	2:D:303:CYS:N	2.48	0.45
2:D:181:GLU:N	2:D:182:PRO:HD2	2.31	0.45
4:F:208:ASP:OD1	4:F:212:ASN:N	2.47	0.44
2:B:307:HIS:O	2:B:426:GLN:NE2	2.51	0.43
1:A:183:GLU:OE2	5:A:501:GTP:O3'	2.20	0.43
3:E:6:MET:N	12:E:204:HOH:O	2.51	0.43
4:F:338:CYS:SG	4:F:339:ALA:N	2.92	0.42
4:F:184:LYS:NZ	4:F:185:TYR:O	2.51	0.42
2:B:107:THR:OG1	2:B:108:GLU:N	2.53	0.41
2:B:3:GLU:OE2	2:B:3:GLU:N	2.53	0.41
2:D:218:THR:O	2:D:219:THR:OG1	2.37	0.41
1:A:3:GLU:N	1:A:3:GLU:OE1	2.54	0.40
2:B:286:VAL:HB	2:B:287:PRO:HD3	2.03	0.40
4:F:299:GLU:N	4:F:300:PRO:HD2	2.36	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	435/450 (97%)	414 (95%)	21 (5%)	0	100	100
1	C	438/450 (97%)	427 (98%)	11 (2%)	0	100	100
2	B	425/445 (96%)	408 (96%)	14 (3%)	3 (1%)	22	43
2	D	417/445 (94%)	401 (96%)	16 (4%)	0	100	100
3	E	117/143 (82%)	115 (98%)	2 (2%)	0	100	100
4	F	324/384 (84%)	312 (96%)	12 (4%)	0	100	100
All	All	2156/2317 (93%)	2077 (96%)	76 (4%)	3 (0%)	51	75

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	244	GLY
2	B	302	ALA
2	B	278	SER

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	368/378 (97%)	367 (100%)	1 (0%)	92	98
1	C	371/378 (98%)	368 (99%)	3 (1%)	81	92
2	B	369/383 (96%)	367 (100%)	2 (0%)	88	96
2	D	364/383 (95%)	361 (99%)	3 (1%)	81	92
3	E	109/127 (86%)	109 (100%)	0	100	100
4	F	301/342 (88%)	296 (98%)	5 (2%)	60	81
All	All	1882/1991 (94%)	1868 (99%)	14 (1%)	84	94

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	221	ARG
2	B	15	GLN
2	B	246	LEU
1	C	221	ARG
1	C	302	MET
1	C	358	GLN
2	D	41	ASP
2	D	177	ASP
2	D	323	MET
4	F	88	SER
4	F	92	THR
4	F	296	MET
4	F	310	GLN
4	F	331	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 5 are monoatomic - leaving 8 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	GTP	C	501	6	26,34,34	0.97	1 (3%)	33,54,54	1.80	7 (21%)
5	GTP	A	501	6	26,34,34	0.97	1 (3%)	33,54,54	1.79	7 (21%)
8	GDP	D	501	-	24,30,30	1.16	2 (8%)	31,47,47	1.93	9 (29%)
10	PN6	B	504	-	19,27,27	2.11	6 (31%)	20,39,39	2.27	4 (20%)
9	MES	B	503	-	12,12,12	2.28	1 (8%)	14,16,16	1.96	4 (28%)
10	PN6	D	502	-	19,27,27	2.21	6 (31%)	20,39,39	2.21	4 (20%)
11	ACP	F	401	-	27,33,33	1.96	6 (22%)	32,52,52	1.79	7 (21%)
8	GDP	B	501	6	24,30,30	1.15	2 (8%)	31,47,47	1.92	8 (25%)

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
5	GTP	C	501	6	-	9/18/38/38	0/3/3/3
5	GTP	A	501	6	-	8/18/38/38	0/3/3/3
8	GDP	D	501	-	-	2/12/32/32	0/3/3/3
10	PN6	B	504	-	-	2/10/14/14	0/3/3/3
9	MES	B	503	-	-	5/6/14/14	0/1/1/1
10	PN6	D	502	-	-	2/10/14/14	0/3/3/3
11	ACP	F	401	-	-	5/15/38/38	0/3/3/3
8	GDP	B	501	6	-	5/12/32/32	0/3/3/3

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	503	MES	C8-S	-7.64	1.66	1.77
10	D	502	PN6	C8-N9	5.42	1.42	1.33
11	F	401	ACP	PG-O1G	5.40	1.61	1.50
10	B	504	PN6	C8-N9	4.87	1.41	1.33
8	B	501	GDP	C6-C5	4.08	1.48	1.41
8	D	501	GDP	C6-C5	4.05	1.48	1.41
11	F	401	ACP	PB-O2B	-4.02	1.46	1.56
10	B	504	PN6	C11-N12	3.90	1.39	1.33
10	D	502	PN6	C10-N9	3.87	1.41	1.35
10	D	502	PN6	C11-N12	3.83	1.39	1.33
11	F	401	ACP	PB-O1B	3.60	1.60	1.51
10	B	504	PN6	C14-C13	-3.57	1.39	1.47
10	D	502	PN6	C14-C13	-3.54	1.39	1.47
11	F	401	ACP	PG-O2G	-3.52	1.46	1.54
10	B	504	PN6	C10-N9	3.29	1.40	1.35
5	A	501	GTP	C6-N1	3.09	1.38	1.33
11	F	401	ACP	C2'-C1'	-3.07	1.49	1.53
5	C	501	GTP	C6-N1	3.06	1.38	1.33
10	B	504	PN6	C7-N12	2.93	1.40	1.35
10	D	502	PN6	C7-N12	2.71	1.39	1.35
10	B	504	PN6	C22-C1	2.47	1.57	1.54
11	F	401	ACP	PG-O3G	2.38	1.60	1.54
10	D	502	PN6	C22-C1	2.38	1.57	1.54
8	D	501	GDP	C5-C4	2.37	1.47	1.40
8	B	501	GDP	C5-C4	2.32	1.47	1.40

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	D	502	PN6	C7-C6-C2	-6.31	119.95	128.66
10	B	504	PN6	C10-C13-C14	-6.16	122.05	130.01
10	B	504	PN6	C7-C6-C2	-5.96	120.43	128.66
5	A	501	GTP	N3-C2-N1	-5.30	120.15	127.22
10	D	502	PN6	C10-C13-C14	-5.30	123.16	130.01
5	C	501	GTP	N3-C2-N1	-5.27	120.19	127.22
11	F	401	ACP	PA-O3A-PB	-5.15	116.24	132.56
8	D	501	GDP	C2-N3-C4	4.78	120.81	115.36
9	B	503	MES	C5-N4-C3	4.69	119.38	108.83
8	B	501	GDP	C2-N3-C4	4.61	120.62	115.36
5	A	501	GTP	C2-N3-C4	4.30	120.27	115.36
5	C	501	GTP	C2-N3-C4	4.19	120.14	115.36
8	B	501	GDP	C6-N1-C2	4.04	122.36	115.93
8	B	501	GDP	C5-C6-N1	-3.97	118.00	123.43
8	B	501	GDP	C6-C5-C4	-3.93	117.04	120.80
8	D	501	GDP	C6-N1-C2	3.91	122.14	115.93
8	D	501	GDP	C5-C6-N1	-3.87	118.14	123.43
10	B	504	PN6	C22-C1-N5	3.80	125.24	120.50
11	F	401	ACP	C3'-C2'-C1'	3.77	106.65	100.98
10	D	502	PN6	C22-C1-N5	3.76	125.19	120.50
8	D	501	GDP	C6-C5-C4	-3.70	117.27	120.80
5	A	501	GTP	PB-O3B-PG	-3.51	120.79	132.83
5	C	501	GTP	PB-O3B-PG	-3.44	121.01	132.83
11	F	401	ACP	N3-C2-N1	-3.29	123.54	128.68
5	A	501	GTP	PA-O3A-PB	-3.27	121.61	132.83
8	B	501	GDP	N3-C2-N1	-3.24	122.91	127.22
8	D	501	GDP	N3-C2-N1	-3.23	122.92	127.22
5	C	501	GTP	PA-O3A-PB	-3.21	121.80	132.83
11	F	401	ACP	C4-C5-N7	-3.18	106.08	109.40
8	D	501	GDP	PA-O3A-PB	-3.14	122.06	132.83
5	C	501	GTP	C3'-C2'-C1'	2.87	105.29	100.98
8	D	501	GDP	C3'-C2'-C1'	2.86	105.29	100.98
9	B	503	MES	O1S-S-C8	2.83	110.33	106.92
8	B	501	GDP	PA-O3A-PB	-2.81	123.19	132.83
5	C	501	GTP	C5-C6-N1	-2.73	119.70	123.43
5	A	501	GTP	C5-C6-N1	-2.73	119.70	123.43
8	B	501	GDP	C3'-C2'-C1'	2.66	104.99	100.98
9	B	503	MES	C7-N4-C5	2.62	117.94	111.23
8	B	501	GDP	C4-C5-N7	-2.58	106.71	109.40
8	D	501	GDP	C4-C5-N7	-2.50	106.80	109.40
5	A	501	GTP	C6-N1-C2	2.47	119.85	115.93
5	C	501	GTP	C6-N1-C2	2.46	119.84	115.93
11	F	401	ACP	O2'-C2'-C3'	-2.39	104.09	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	503	MES	O3S-S-C8	2.37	109.60	105.77
10	D	502	PN6	C11-N12-C7	2.33	121.58	116.41
10	B	504	PN6	C11-N12-C7	2.17	121.22	116.41
11	F	401	ACP	C2-N1-C6	2.08	122.32	118.75
11	F	401	ACP	O1B-PB-C3B	2.05	114.50	109.07
5	A	501	GTP	C3'-C2'-C1'	2.04	104.05	100.98
8	D	501	GDP	C2'-C3'-C4'	2.03	106.58	102.64

There are no chirality outliers.

All (38) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O2A
5	A	501	GTP	C5'-O5'-PA-O1A
5	A	501	GTP	C5'-O5'-PA-O2A
8	D	501	GDP	C5'-O5'-PA-O3A
10	B	504	PN6	C1-C2-C6-C7
10	B	504	PN6	N3-C2-C6-C7
10	D	502	PN6	C1-C2-C6-C7
10	D	502	PN6	N3-C2-C6-C7
9	B	503	MES	C8-C7-N4-C5
9	B	503	MES	C7-C8-S-O2S
9	B	503	MES	C7-C8-S-O3S
11	F	401	ACP	PG-C3B-PB-O1B
11	F	401	ACP	PG-C3B-PB-O3A
11	F	401	ACP	O4'-C4'-C5'-O5'
8	B	501	GDP	PA-O3A-PB-O3B
8	B	501	GDP	C5'-O5'-PA-O3A
8	B	501	GDP	C5'-O5'-PA-O1A
8	B	501	GDP	C5'-O5'-PA-O2A
11	F	401	ACP	C3'-C4'-C5'-O5'
9	B	503	MES	C8-C7-N4-C3
5	C	501	GTP	C4'-C5'-O5'-PA
5	C	501	GTP	PB-O3B-PG-O2G
5	C	501	GTP	PB-O3A-PA-O2A
8	D	501	GDP	C5'-O5'-PA-O2A
9	B	503	MES	C7-C8-S-O1S
11	F	401	ACP	PG-C3B-PB-O2B
5	A	501	GTP	C4'-C5'-O5'-PA
5	C	501	GTP	C3'-C4'-C5'-O5'
5	A	501	GTP	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
5	A	501	GTP	PB-O3A-PA-O2A
5	C	501	GTP	O4'-C4'-C5'-O5'
5	A	501	GTP	O4'-C4'-C5'-O5'
5	C	501	GTP	C5'-O5'-PA-O3A
5	A	501	GTP	C5'-O5'-PA-O3A
5	C	501	GTP	PB-O3A-PA-O1A
5	A	501	GTP	PB-O3A-PA-O1A
8	B	501	GDP	PA-O3A-PB-O1B

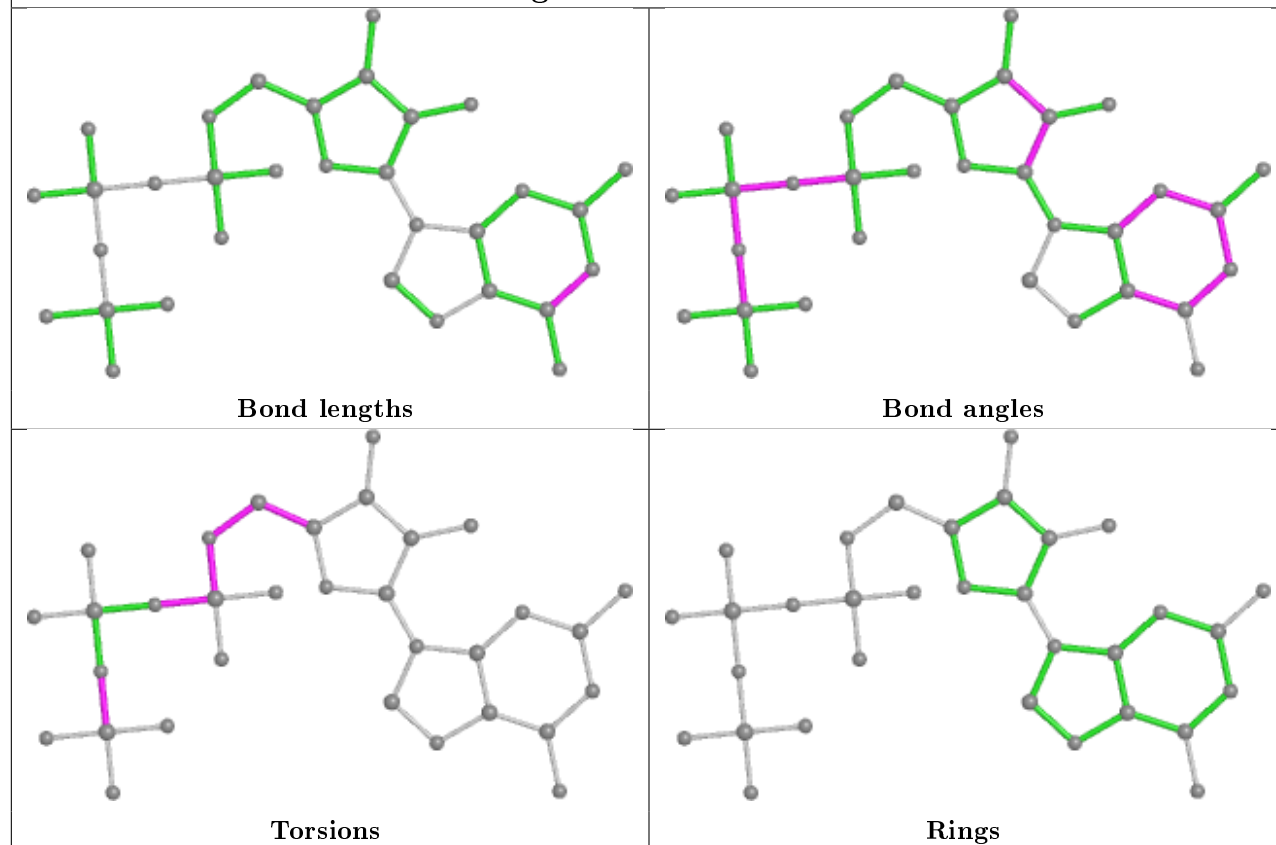
There are no ring outliers.

3 monomers are involved in 3 short contacts:

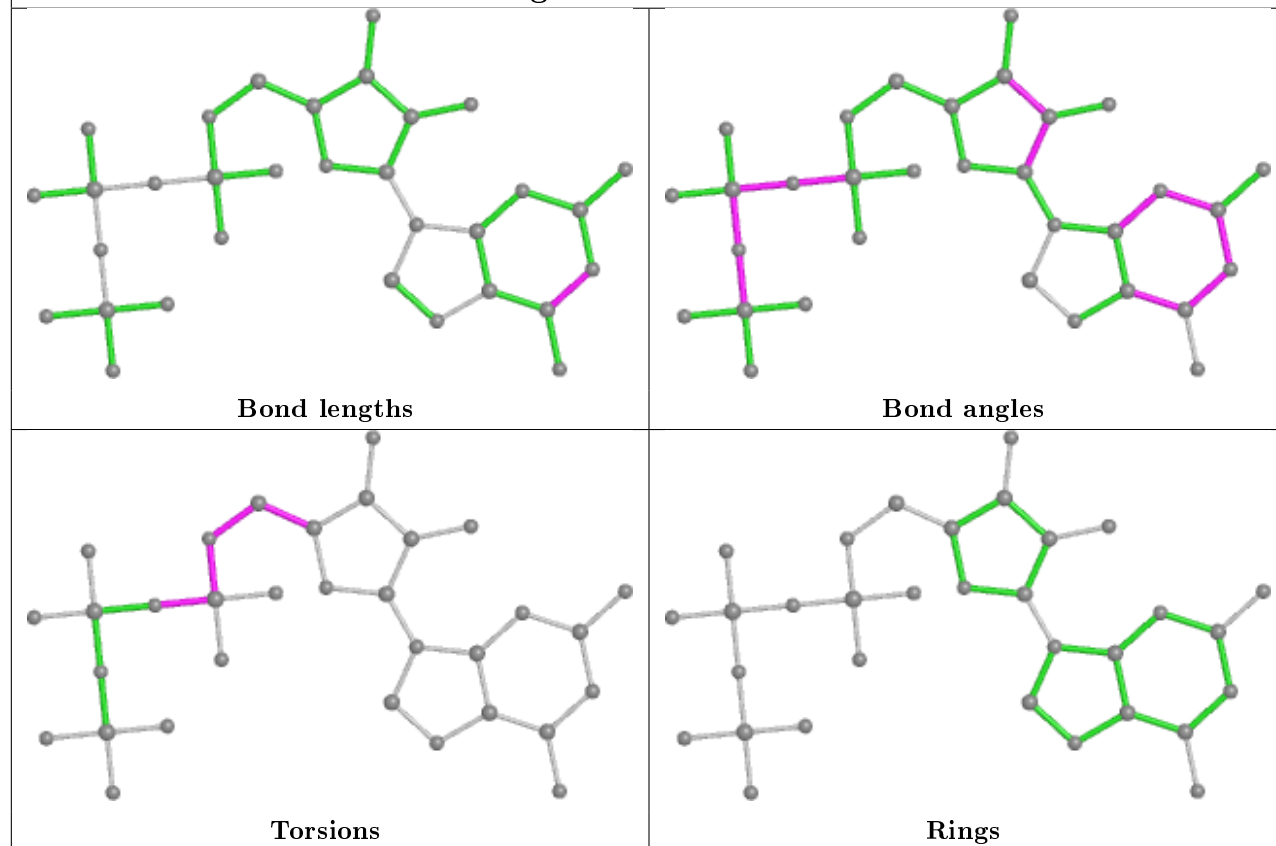
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	501	GTP	1	0
8	D	501	GDP	1	0
10	D	502	PN6	1	0

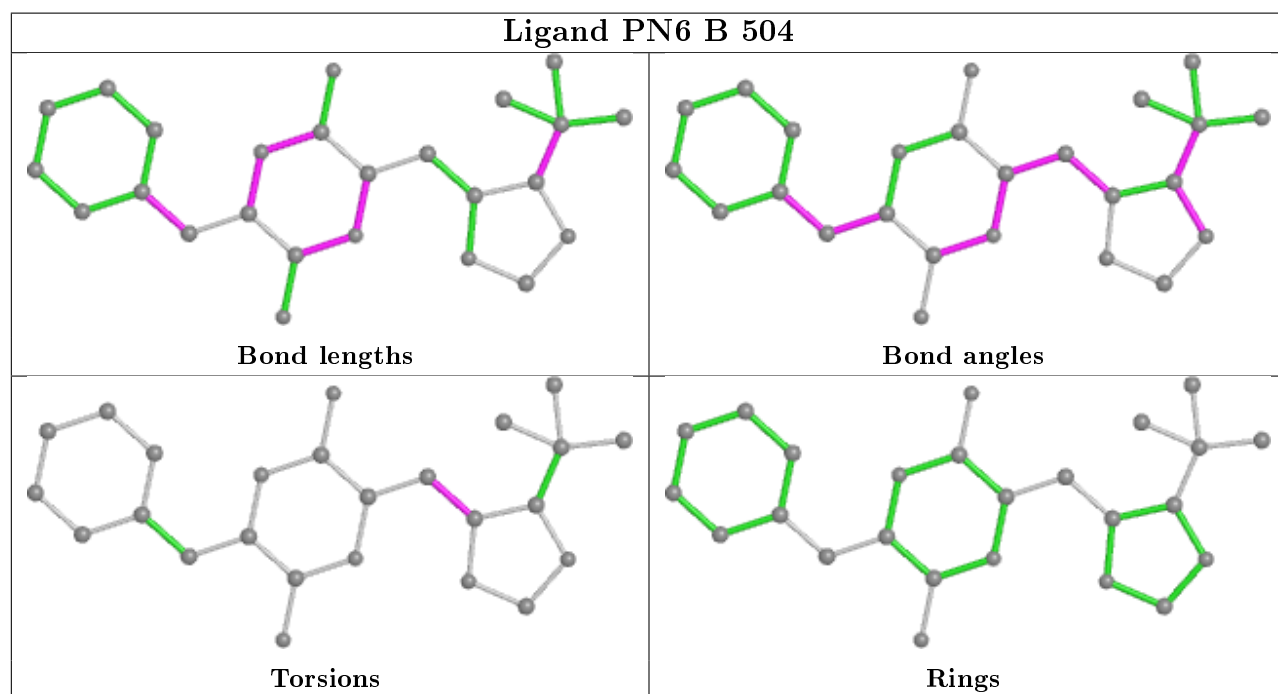
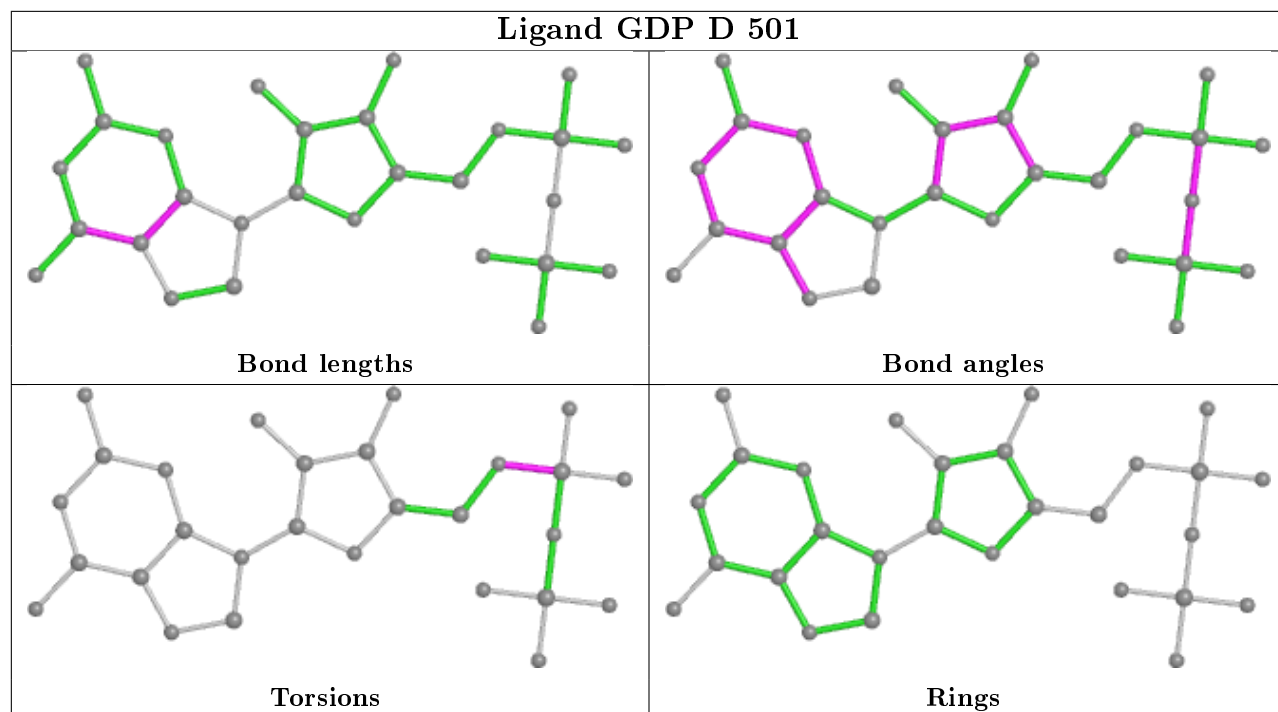
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

Ligand GTP C 501

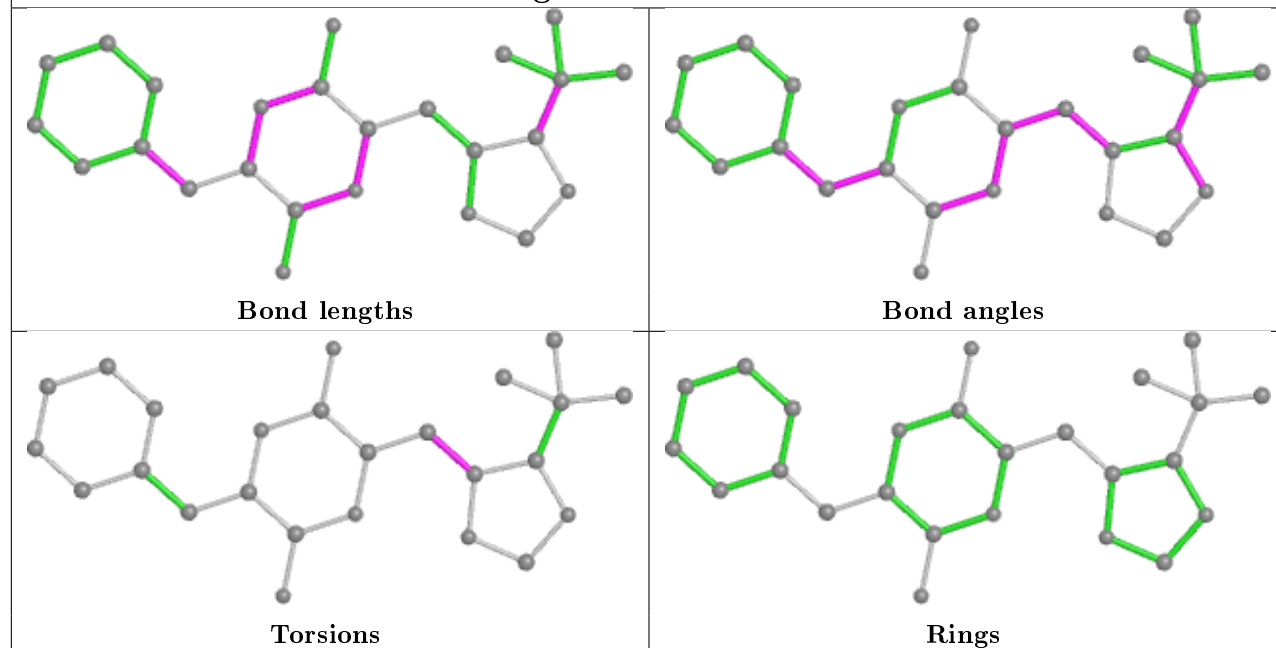


Ligand GTP A 501

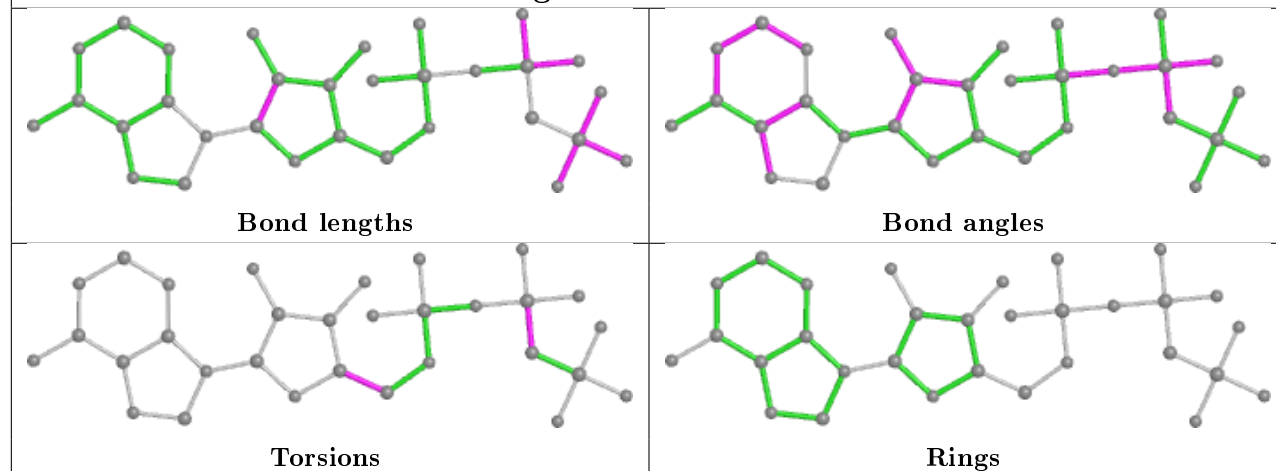


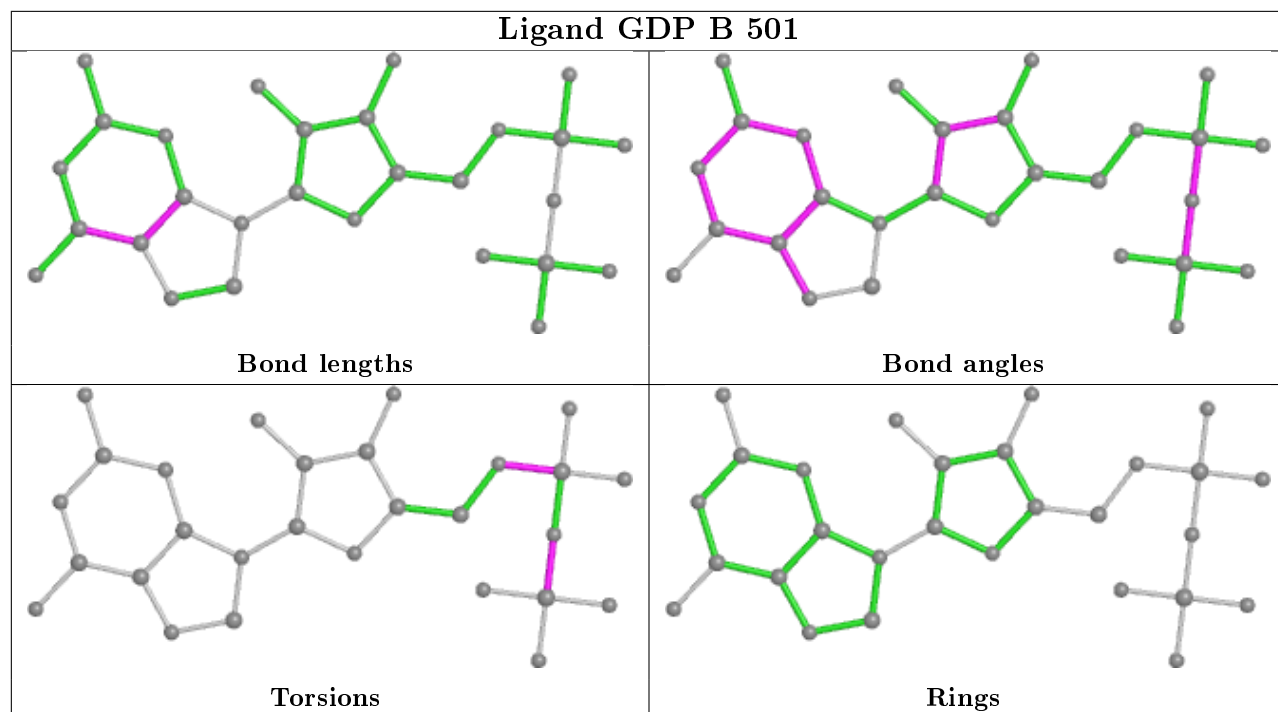


Ligand PN6 D 502



Ligand ACP F 401





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, 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	437/450 (97%)	0.80	27 (6%)	20 15	27, 49, 78, 145	0
1	C	440/450 (97%)	0.26	8 (1%)	68 64	21, 37, 66, 90	0
2	B	427/445 (95%)	0.66	31 (7%)	15 11	23, 47, 88, 121	0
2	D	421/445 (94%)	1.01	61 (14%)	2 1	33, 65, 102, 124	0
3	E	121/143 (84%)	1.04	17 (14%)	2 1	30, 67, 100, 127	0
4	F	334/384 (86%)	1.62	106 (31%)	0 0	38, 76, 126, 153	0
All	All	2180/2317 (94%)	0.84	250 (11%)	4 3	21, 54, 102, 153	0

All (250) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	282	TYR	8.6
4	F	233	PHE	8.1
4	F	234	GLN	7.9
4	F	161	LEU	7.6
2	D	394	PHE	7.3
4	F	169	LEU	7.1
4	F	132	LEU	6.8
4	F	173	ILE	6.3
2	D	1	MET	6.3
4	F	142	ARG	6.3
2	D	55	THR	6.2
4	F	100	ILE	5.9
4	F	103	THR	5.8
4	F	167	SER	5.8
4	F	245	ILE	5.6
4	F	135	TYR	5.6
4	F	253	TYR	5.6
4	F	232	ASN	5.6
4	F	170	LEU	5.3

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Mol	Chain	Res	Type	RSRZ
4	F	225	SER	5.0
2	D	94	GLN	5.0
2	D	390	ARG	4.9
4	F	372	THR	4.9
2	B	279	GLN	4.9
4	F	172	PHE	4.9
4	F	194	PRO	4.8
4	F	178	GLN	4.7
4	F	162	ILE	4.7
4	F	256	TYR	4.6
2	D	92	PHE	4.6
4	F	180	HIS	4.5
2	D	397	TRP	4.5
4	F	168	GLU	4.4
4	F	31	ARG	4.4
2	D	216	LYS	4.4
4	F	130	VAL	4.4
2	B	280	GLN	4.3
2	D	37	HIS	4.3
4	F	101	TYR	4.3
4	F	182	ILE	4.2
4	F	227	PRO	4.2
4	F	240	LEU	4.2
2	D	391	ARG	4.2
4	F	139	ARG	4.2
4	F	361	LEU	4.2
2	B	37	HIS	4.1
2	B	245	GLN	4.0
2	D	389	PHE	4.0
4	F	255	ARG	3.9
2	D	180	VAL	3.9
1	A	86	LEU	3.9
3	E	139	LEU	3.9
4	F	98	TYR	3.9
2	D	54	ALA	3.9
2	D	356	ILE	3.8
4	F	252	ASN	3.8
2	D	396	HIS	3.7
4	F	246	GLN	3.7
3	E	27	PRO	3.7
4	F	25	GLY	3.7
3	E	24	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
4	F	243	HIS	3.6
2	D	56	GLY	3.6
2	B	282	ARG	3.6
2	D	285	THR	3.6
2	D	177	ASP	3.6
4	F	223	THR	3.5
4	F	231	ALA	3.5
4	F	236	LYS	3.5
4	F	128	ARG	3.5
4	F	27	TRP	3.5
4	F	137	ARG	3.5
4	F	235	ASP	3.5
4	F	199	PHE	3.4
4	F	254	GLY	3.4
1	A	34	GLY	3.4
2	B	55	THR	3.4
2	B	276	ARG	3.4
2	B	95	SER	3.4
4	F	133	ALA	3.4
2	D	53	GLU	3.4
2	B	277	GLY	3.3
4	F	136	ASN	3.3
4	F	175	GLU	3.3
4	F	258	GLU	3.3
4	F	176	GLN	3.3
2	D	214	THR	3.3
2	D	245	GLN	3.3
2	D	362	LYS	3.3
2	D	322	SER	3.3
2	D	219	THR	3.3
2	D	320	ARG	3.3
2	D	217	LEU	3.2
2	D	96	GLY	3.2
3	E	6	MET	3.2
1	A	42	ILE	3.2
4	F	145	ASN	3.1
1	A	437	VAL	3.1
4	F	179	VAL	3.1
1	C	247	ALA	3.1
2	D	395	LEU	3.1
2	D	87	PRO	3.1
4	F	171	ASP	3.1

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Mol	Chain	Res	Type	RSRZ
3	E	135	LYS	3.1
4	F	129	GLU	3.1
2	D	200	TYR	3.1
2	B	278	SER	3.1
1	C	440	VAL	3.0
2	D	74	ASP	3.0
4	F	247	LYS	3.0
2	D	215	LEU	3.0
4	F	165	GLU	3.0
4	F	380	HIS	3.0
2	D	388	MET	2.9
4	F	17	VAL	2.9
2	B	96	GLY	2.9
4	F	22	LEU	2.9
1	A	163	LYS	2.9
2	D	73	MET	2.9
1	A	59	GLY	2.9
4	F	20	LEU	2.9
1	A	180	ALA	2.8
4	F	191	LEU	2.8
2	D	176	SER	2.8
3	E	7	GLU	2.8
2	B	218	THR	2.8
2	B	127	CYS	2.8
4	F	163	SER	2.8
1	C	357	TYR	2.8
1	A	345	ASP	2.8
4	F	138	ARG	2.8
2	D	95	SER	2.8
4	F	1	MET	2.8
4	F	147	TRP	2.8
2	B	81	PHE	2.8
4	F	149	ALA	2.8
3	E	46	SER	2.8
1	A	262	TYR	2.7
4	F	226	GLU	2.7
2	B	56	GLY	2.7
4	F	362	ALA	2.7
4	F	305	LYS	2.7
2	B	275	SER	2.7
4	F	21	LEU	2.7
3	E	106	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
2	D	175	VAL	2.7
2	B	54	ALA	2.7
2	B	246	LEU	2.7
2	D	171	PRO	2.7
4	F	260	ASN	2.7
1	A	60	LYS	2.6
4	F	379	HIS	2.6
4	F	19	ARG	2.6
3	E	9	ILE	2.6
4	F	24	THR	2.6
4	F	146	VAL	2.6
2	B	38	GLY	2.6
4	F	221	LEU	2.6
3	E	25	LYS	2.6
2	D	387	ALA	2.6
4	F	131	PHE	2.6
3	E	103	GLN	2.6
2	D	197	ASP	2.6
2	D	179	VAL	2.5
2	D	199	THR	2.5
2	B	57	ASN	2.5
4	F	166	ALA	2.5
4	F	340	GLN	2.5
4	F	320	MET	2.5
4	F	23	ALA	2.5
4	F	102	PRO	2.5
4	F	192	LEU	2.5
2	B	2	ARG	2.5
4	F	143	GLU	2.5
2	D	58	LYS	2.5
1	C	248	LEU	2.5
4	F	263	PHE	2.5
2	B	428	ALA	2.5
1	A	78	VAL	2.5
1	A	335	ILE	2.5
2	B	406	MET	2.5
2	D	57	ASN	2.5
2	D	201	CYS	2.4
2	D	126	SER	2.4
4	F	177	GLY	2.4
4	F	185	TYR	2.4
3	E	23	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	1	MET	2.4
4	F	316	GLY	2.4
1	A	349	THR	2.4
1	A	38	SER	2.4
2	D	284	LEU	2.4
2	D	399	THR	2.4
1	A	362	VAL	2.4
2	B	58	LYS	2.4
4	F	241	THR	2.4
2	D	267	MET	2.4
4	F	74	LYS	2.3
2	D	198	GLU	2.3
2	D	210	ILE	2.3
2	B	59	TYR	2.3
1	C	84	ARG	2.3
3	E	140	LYS	2.3
4	F	164	SER	2.3
2	B	36	TYR	2.3
2	B	212	PHE	2.3
2	D	332	ASN	2.2
4	F	174	ASP	2.2
1	A	115	ILE	2.2
4	F	28	LYS	2.2
1	C	134	GLY	2.2
4	F	257	GLU	2.2
2	D	196	THR	2.2
4	F	262	MET	2.2
1	A	30	ILE	2.2
2	D	273	LEU	2.2
4	F	127	GLU	2.2
2	B	40	SER	2.2
4	F	351	VAL	2.2
2	D	125	GLU	2.2
1	C	131	GLY	2.2
1	A	346	TRP	2.2
1	A	32	PRO	2.2
4	F	259	GLY	2.2
1	A	55	GLU	2.2
4	F	374	ILE	2.2
1	A	36	MET	2.1
2	D	403	MET	2.1
2	D	402	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	87	PHE	2.1
2	B	42	LEU	2.1
2	D	31	ASP	2.1
1	A	84	ARG	2.1
1	A	172	TYR	2.1
4	F	99	VAL	2.1
4	F	342	LEU	2.1
4	F	224	SER	2.1
2	B	274	THR	2.1
1	A	286	LEU	2.1
2	D	83	GLN	2.1
1	A	33	ASP	2.1
3	E	120	LEU	2.1
2	D	272	PRO	2.0
4	F	230	SER	2.0
2	D	44	LEU	2.0
3	E	45	PRO	2.0
2	B	60	VAL	2.0
3	E	28	SER	2.0
4	F	9	GLU	2.0
3	E	52	LYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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(\AA^2)	Q<0.9
7	CA	A	503	1/1	0.82	0.10	76,76,76,76	0
10	PN6	D	502	25/25	0.87	0.32	41,77,120,145	0

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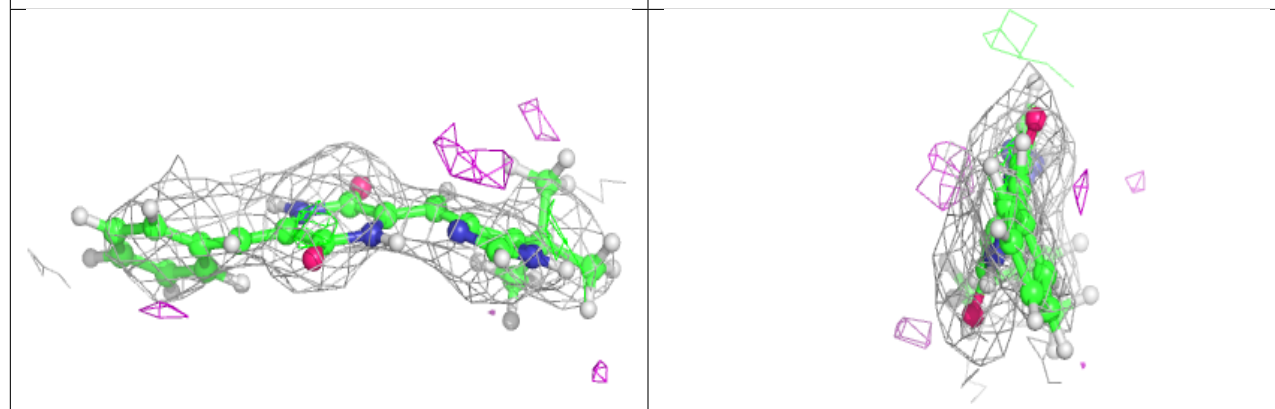
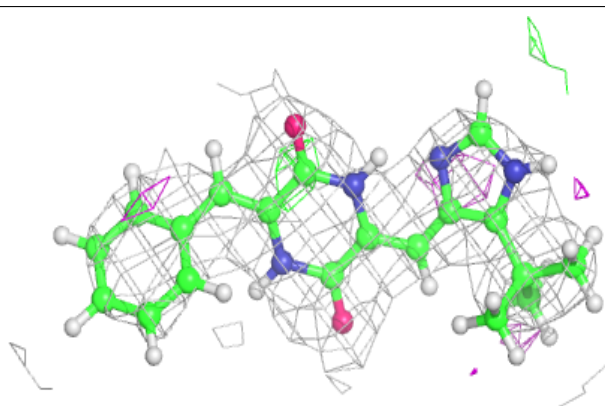
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
11	ACP	F	401	31/31	0.88	0.20	72,107,155,168	0
8	GDP	D	501	28/28	0.90	0.19	35,64,100,112	0
9	MES	B	503	12/12	0.91	0.19	38,57,82,89	0
8	GDP	B	501	28/28	0.94	0.24	18,38,62,71	0
10	PN6	B	504	25/25	0.95	0.25	30,51,79,97	0
6	MG	B	502	1/1	0.95	0.33	40,40,40,40	0
6	MG	A	502	1/1	0.95	0.23	26,26,26,26	0
5	GTP	A	501	32/32	0.96	0.24	13,35,46,79	0
6	MG	C	502	1/1	0.96	0.33	39,39,39,39	0
5	GTP	C	501	32/32	0.97	0.21	16,32,53,91	0
7	CA	C	503	1/1	0.98	0.11	55,55,55,55	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.

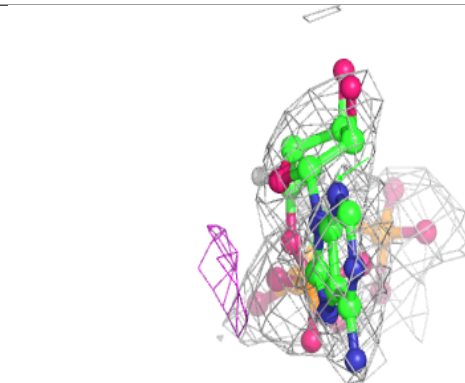
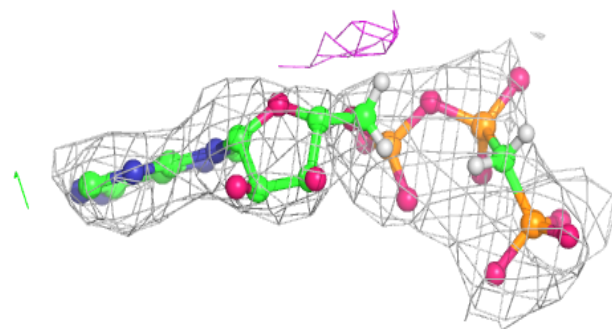
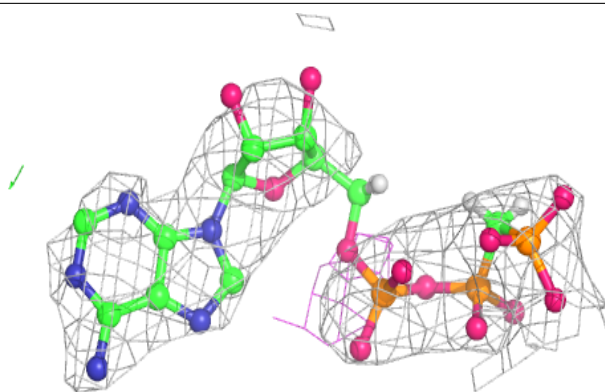
Electron density around PN6 D 502:

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

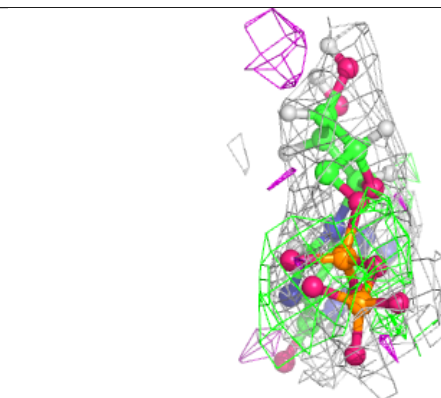
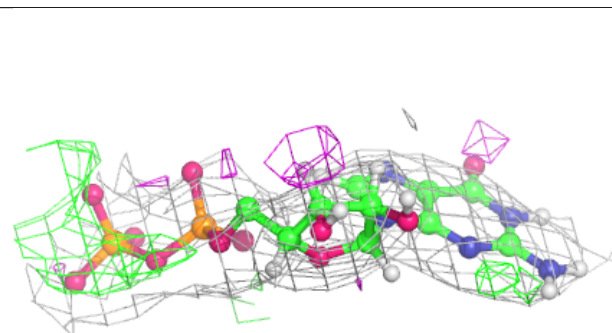
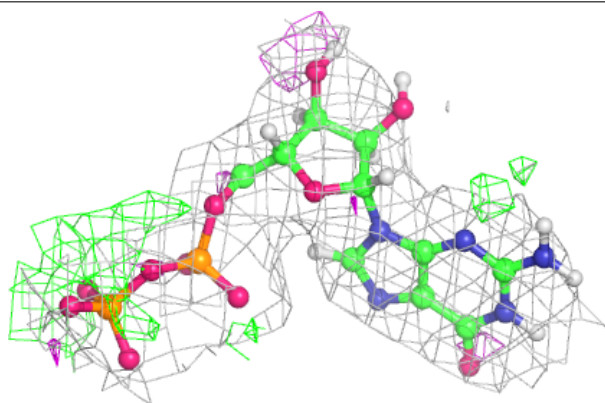


Electron density around ACP F 401:

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

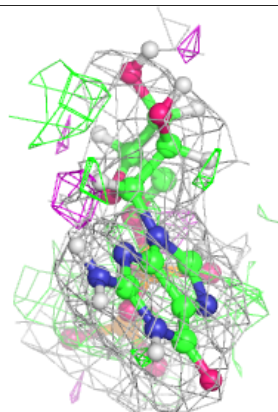
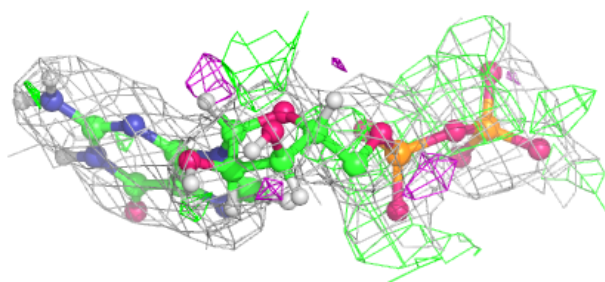
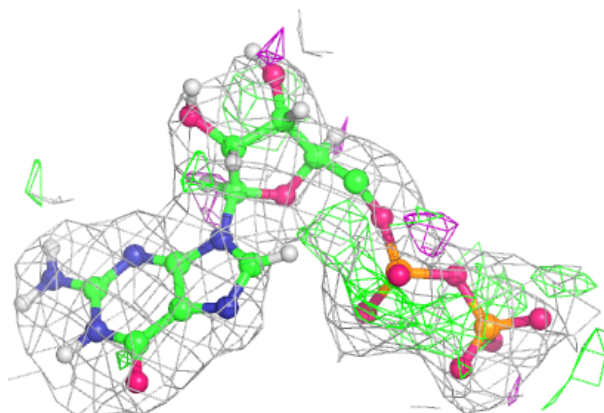
**Electron density around GDP D 501:**

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

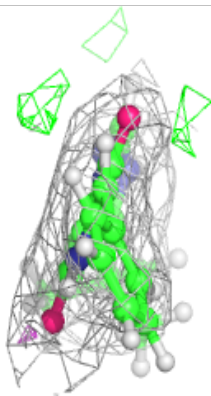
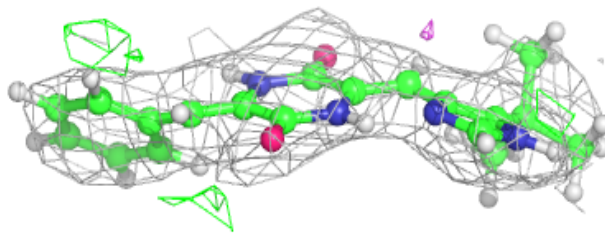
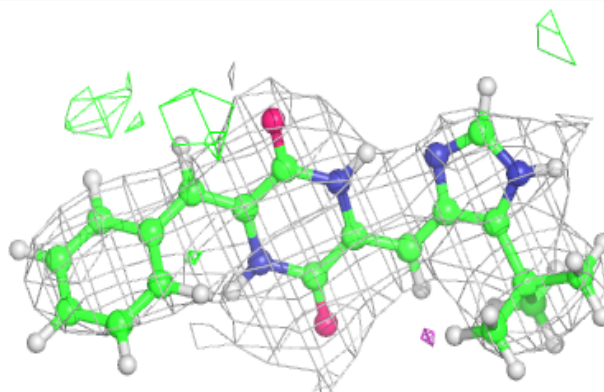


Electron density around GDP B 501:

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

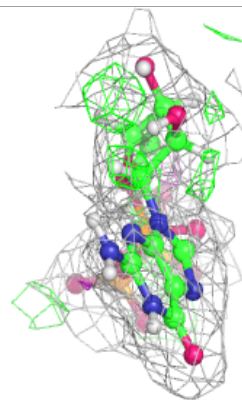
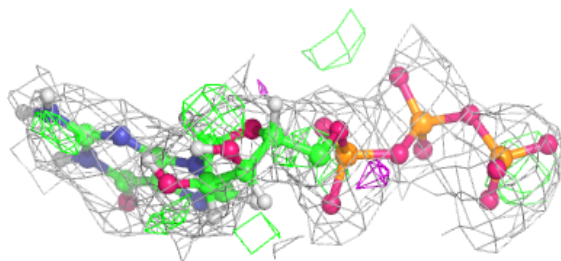
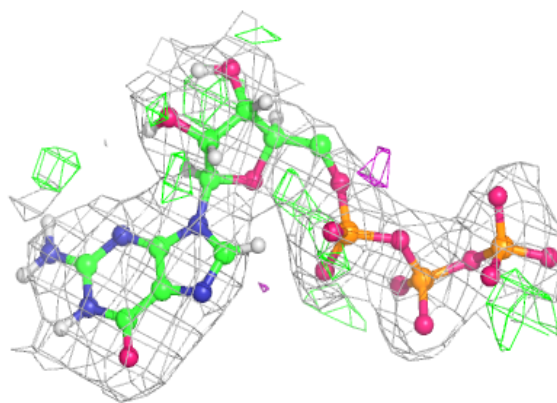
**Electron density around PN6 B 504:**

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

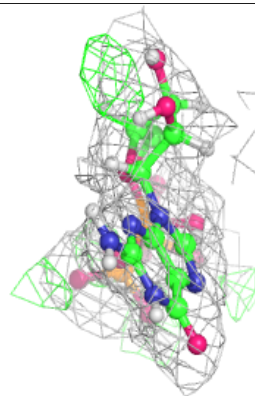
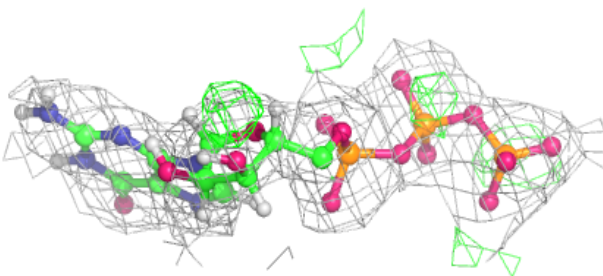
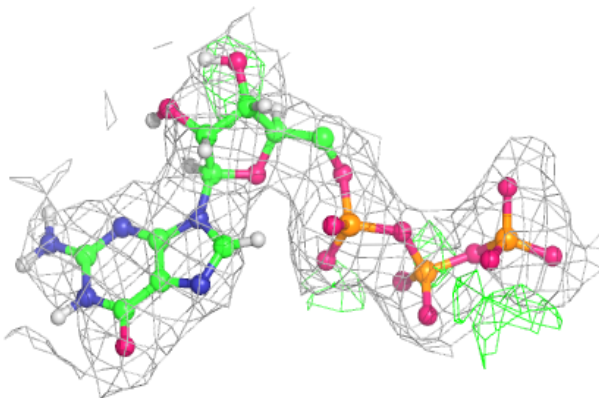


Electron density around GTP A 501:

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

**Electron density around GTP C 501:**

$2mF_o-DF_c$ (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.