



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 06:38 AM UTC

PDB ID : 5XI5 / pdb_00005xi5
Title : Crystal structure of T2R-TTL-PO5 complex
Authors : Chu, Y.; Wang, Y.; Yang, J.; Li, W.
Deposited on : 2017-04-26
Resolution : 2.81 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 Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
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 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

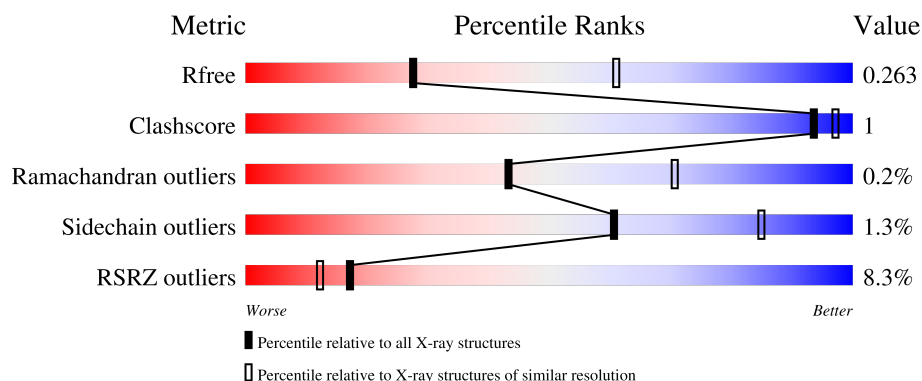
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.81 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	4591 (2.84-2.80)
Clashscore	190562	5010 (2.84-2.80)
Ramachandran outliers	187476	4916 (2.84-2.80)
Sidechain outliers	187428	4918 (2.84-2.80)
RSRZ outliers	180081	4594 (2.84-2.80)

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 $\leq 5\%$. 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	3% 93% • •
1	C	450	2% 95% • •
2	B	445	4% 91% • 5%
2	D	445	15% 90% • 5%
3	E	184	8% 65% • 35%

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Mol	Chain	Length	Quality of chain
4	F	384	14% 78% • 20%

2 Entry composition [i](#)

There are 12 unique types of molecules in this entry. The entry contains 17473 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 Tubulin alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	437	Total	C	N	O	S	0	4	0
			3441	2179	586	652	24			
1	C	440	Total	C	N	O	S	0	9	0
			3482	2200	589	668	25			

- Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	424	Total	C	N	O	S	0	2	0
			3353	2107	574	645	27			
2	D	421	Total	C	N	O	S	0	1	0
			3306	2079	562	638	27			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	120	Total	C	N	O	S	0	2	0
			1004	621	181	196	6			

- Molecule 4 is a protein called Tubulin tyrosine ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	309	Total	C	N	O	S	0	3	0
			2553	1645	438	455	15			

There are 6 discrepancies between the modelled and reference sequences:

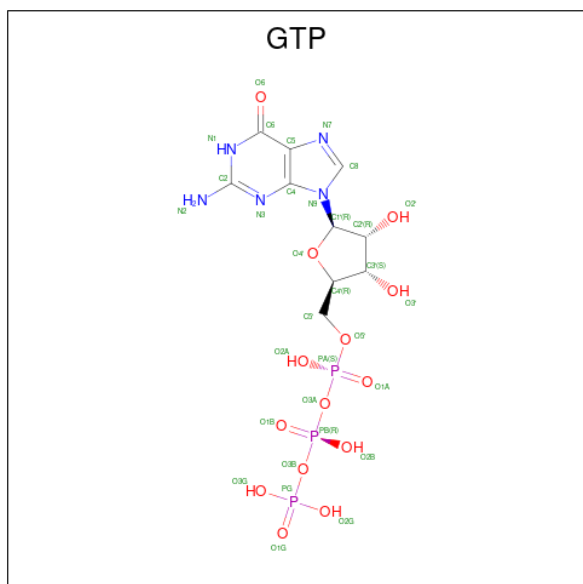
Chain	Residue	Modelled	Actual	Comment	Reference
F	379	HIS	-	expression tag	UNP E1BQ43
F	380	HIS	-	expression tag	UNP E1BQ43
F	381	HIS	-	expression tag	UNP E1BQ43
F	382	HIS	-	expression tag	UNP E1BQ43

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Chain	Residue	Modelled	Actual	Comment	Reference
F	383	HIS	-	expression tag	UNP E1BQ43
F	384	HIS	-	expression tag	UNP E1BQ43

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
5	C	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
5	D	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

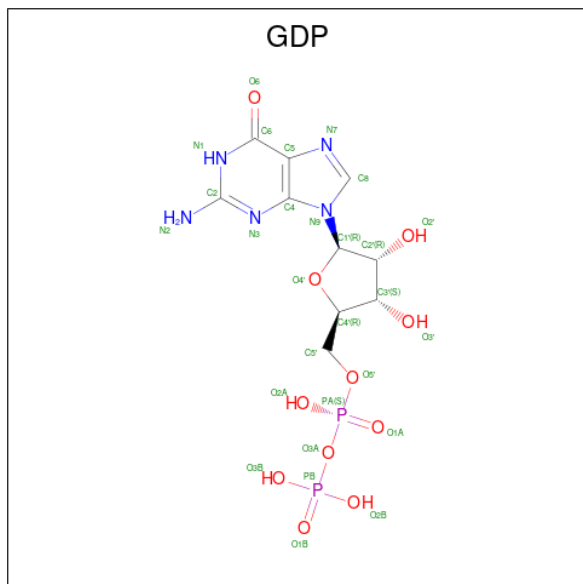
- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 7 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

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



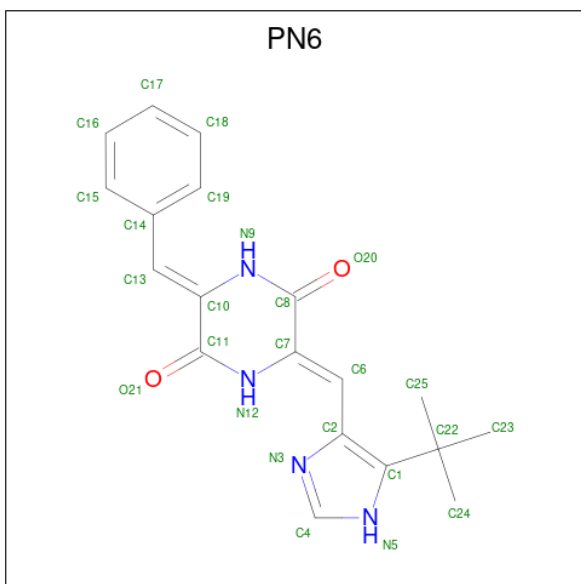
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	B	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

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



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

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



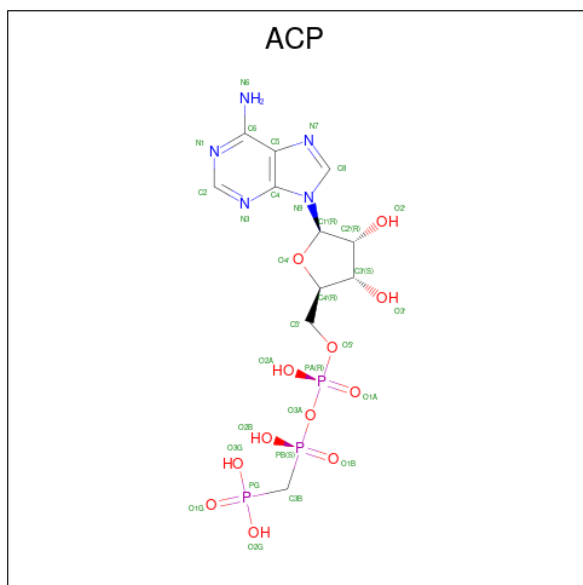
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	B	1	Total	C	N	O	0	0
			25	19	4	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	D	1	Total	C	N	O	0	0
			25	19	4	2		

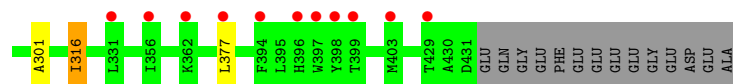
- Molecule 11 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (CCD ID: ACP) (formula: $C_{11}H_{18}N_5O_{12}P_3$).



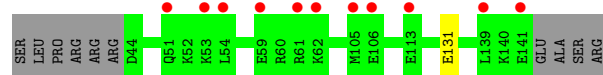
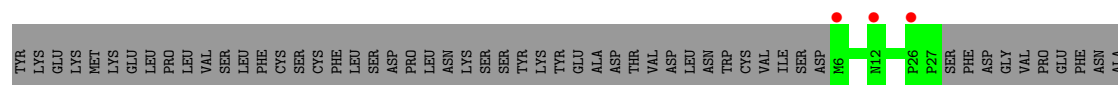
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	F	1	Total	C	N	O	P	0	0
			31	11	5	12	3		

- Molecule 12 is water.

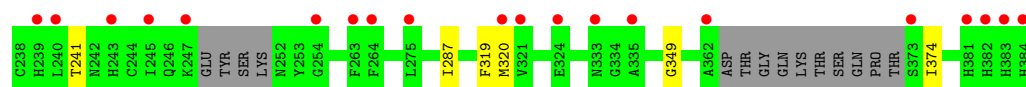
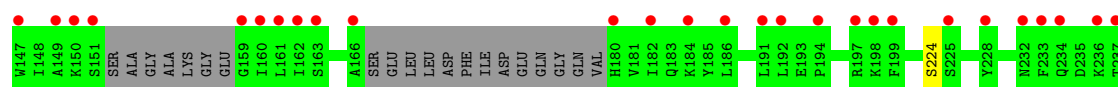
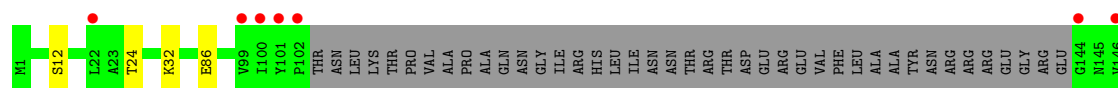
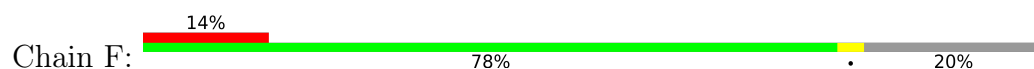
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	19	Total	O	0	0
			19	19		
12	B	24	Total	O	0	0
			24	24		
12	C	50	Total	O	0	0
			50	50		
12	E	2	Total	O	0	0
			2	2		
12	F	3	Total	O	0	0
			3	3		



● Molecule 3: Stathmin-4



● Molecule 4: Tubulin tyrosine ligase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	105.25Å 157.38Å 182.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	119.17 – 2.81 119.17 – 2.81	Depositor EDS
% Data completeness (in resolution range)	96.5 (119.17-2.81) 96.7 (119.17-2.81)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.09 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.8.0135, PHENIX	Depositor
R, R_{free}	0.227 , 0.265 0.226 , 0.263	Depositor DCC
R_{free} test set	3562 reflections (4.77%)	wwPDB-VP
Wilson B-factor (Å ²)	45.7	Xtriage
Anisotropy	0.053	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 24.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	17473	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.72% 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: PN6, MG, MES, GDP, GTP, ACP, CA

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	0.57	0/3525	0.80	0/4784
1	C	0.54	0/3572	0.81	0/4850
2	B	0.56	0/3427	0.80	1/4640 (0.0%)
2	D	0.58	0/3379	0.82	2/4577 (0.0%)
3	E	0.57	0/1018	0.80	0/1350
4	F	0.55	0/2618	0.73	0/3537
All	All	0.56	0/17539	0.80	3/23738 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	243	PRO	CB-CA-C	5.83	121.18	111.56
2	B	316	ILE	CB-CA-C	5.53	118.18	110.99
2	D	316	ILE	CB-CA-C	5.25	116.40	110.41

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	3441	0	3363	13	0
1	C	3482	0	3384	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	3353	0	3228	13	0
2	D	3306	0	3181	13	0
3	E	1004	0	1028	0	0
4	F	2553	0	2519	4	0
5	A	32	0	12	0	0
5	C	32	0	12	0	0
5	D	32	0	12	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
8	B	28	0	12	0	0
9	B	24	0	26	2	0
10	B	25	0	20	3	0
10	D	25	0	20	2	0
11	F	31	0	14	1	0
12	A	19	0	0	0	0
12	B	24	0	0	0	0
12	C	50	0	0	0	0
12	E	2	0	0	0	0
12	F	3	0	0	0	0
All	All	17473	0	16831	49	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 (49) 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:229[A]:ARG:HG2	1:A:229[A]:ARG:HH11	1.08	1.08
1:A:229[A]:ARG:HH11	1:A:229[A]:ARG:CG	1.73	1.01
1:A:229[A]:ARG:HG2	1:A:229[A]:ARG:NH1	1.87	0.81
1:C:178:SER:HB2	1:C:183:GLU:OE2	1.86	0.76
2:B:243:PRO:CB	2:B:244:GLY:HA2	2.20	0.71
1:A:229[A]:ARG:CG	1:A:229[A]:ARG:NH1	2.45	0.71
2:B:243:PRO:HB2	2:B:244:GLY:HA2	1.74	0.68
2:B:295:ASP:HA	9:B:505:MES:O2S	1.99	0.62
2:D:243:PRO:HB2	2:D:244:GLY:HA2	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:SER:HB3	1:A:391:LEU:HD21	1.84	0.58
1:A:368[B]:LEU:HD12	1:A:368[B]:LEU:N	2.18	0.58
1:A:101:ASN:HD22	2:B:256:ASN:HD21	1.50	0.58
1:A:346:TRP:CD1	1:A:347:CYS:HG	2.22	0.57
2:B:316:ILE:O	2:B:316:ILE:HD13	2.05	0.56
1:A:368[B]:LEU:HD12	1:A:368[B]:LEU:H	1.70	0.54
1:A:187:SER:CB	1:A:391:LEU:HD21	2.38	0.54
1:A:68:VAL:HG11	1:A:149:PHE:CE2	2.45	0.52
1:C:187:SER:HB3	1:C:391:LEU:HD21	1.92	0.51
2:D:243:PRO:HB2	2:D:244:GLY:CA	2.42	0.49
1:C:180:ALA:HB3	1:C:183:GLU:HG3	1.94	0.49
2:D:4:ILE:HD11	2:D:240:LEU:HD13	1.95	0.48
1:A:265:ILE:HG23	1:A:432:TYR:CZ	2.49	0.48
1:C:230:LEU:O	1:C:234:ILE:HD12	2.15	0.47
4:F:224:SER:HB2	4:F:241:THR:HG22	1.97	0.46
2:B:251:ARG:NH1	9:B:503:MES:O2S	2.47	0.46
2:B:179:VAL:HG12	1:C:348:PRO:HG2	1.97	0.45
2:D:165:ASN:ND2	2:D:198:GLU:HG3	2.32	0.45
1:A:270:ALA:HB3	1:A:302:MET:CG	2.46	0.45
2:B:240:LEU:HD12	10:B:506:PN6:H18	1.97	0.45
2:B:251:ARG:O	2:B:255:VAL:HG23	2.17	0.45
4:F:349:GLY:HA3	4:F:374:ILE:HD11	1.97	0.45
2:B:4:ILE:HD11	2:B:240:LEU:HD13	2.00	0.44
2:D:170:MET:HE2	2:D:377:LEU:HD21	1.98	0.44
4:F:287:ILE:HG23	4:F:319:PHE:CE2	2.53	0.44
2:D:139:LEU:HD12	2:D:170:MET:SD	2.58	0.43
2:B:7:ILE:HB	2:B:135:LEU:HD12	2.00	0.43
2:D:243:PRO:CB	2:D:244:GLY:HA2	2.48	0.43
2:D:267:MET:HG3	2:D:301:ALA:HB3	2.01	0.43
4:F:320:MET:HE2	11:F:401:ACP:C2	2.49	0.43
2:D:139:LEU:HD11	2:D:168:SER:HB3	2.00	0.42
2:D:237:THR:HG22	10:D:503:PN6:C18	2.48	0.42
2:B:198:GLU:OE2	10:B:506:PN6:H15	2.20	0.41
10:B:506:PN6:N3	10:B:506:PN6:N12	2.54	0.41
2:D:136:THR:CG2	2:D:233:MET:HE1	2.51	0.41
2:D:139:LEU:HD22	2:D:188:SER:HB3	2.03	0.40
10:D:503:PN6:H7	10:D:503:PN6:H1	2.04	0.40
2:B:170:MET:HG3	2:B:377:LEU:HD11	2.03	0.40
1:C:4[A]:CYS:SG	1:C:136:LEU:HG	2.61	0.40
2:D:4:ILE:HD12	2:D:49:VAL:CG1	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	439/450 (98%)	426 (97%)	13 (3%)	0	100	100
1	C	446/450 (99%)	439 (98%)	7 (2%)	0	100	100
2	B	422/445 (95%)	408 (97%)	12 (3%)	2 (0%)	24	53
2	D	417/445 (94%)	401 (96%)	13 (3%)	3 (1%)	18	45
3	E	118/184 (64%)	116 (98%)	2 (2%)	0	100	100
4	F	300/384 (78%)	287 (96%)	13 (4%)	0	100	100
All	All	2142/2358 (91%)	2077 (97%)	60 (3%)	5 (0%)	43	71

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	243	PRO
2	B	71	GLY
2	D	243	PRO
2	D	39	ASP
2	D	244	GLY

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	372/378 (98%)	364 (98%)	8 (2%)	45	77
1	C	379/378 (100%)	375 (99%)	4 (1%)	65	86
2	B	367/383 (96%)	360 (98%)	7 (2%)	50	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	362/383 (94%)	359 (99%)	3 (1%)	73	90
3	E	110/168 (66%)	109 (99%)	1 (1%)	70	89
4	F	281/342 (82%)	277 (99%)	4 (1%)	59	84
All	All	1871/2032 (92%)	1844 (99%)	27 (1%)	61	84

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	THR
1	A	188	ILE
1	A	229[A]	ARG
1	A	229[B]	ARG
1	A	237	SER
1	A	320	ARG
1	A	326	LYS
1	A	402	ARG
2	B	2	ARG
2	B	15	GLN
2	B	48	ASN
2	B	83	GLN
2	B	135	LEU
2	B	214	THR
2	B	316	ILE
1	C	179	THR
1	C	251[A]	ASP
1	C	251[B]	ASP
1	C	368	LEU
2	D	245	GLN
2	D	247	ASN
2	D	316	ILE
3	E	131	GLU
4	F	12	SER
4	F	24	THR
4	F	32	LYS
4	F	86	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	309	HIS

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Mol	Chain	Res	Type
1	A	393	HIS
2	B	8	GLN
2	B	11	GLN
2	B	14	ASN
2	B	83	GLN
2	B	94	GLN
2	B	134	GLN
2	B	165	ASN
2	B	247	ASN
2	B	256	ASN
2	B	292	GLN
2	B	375	GLN
2	B	426	GLN
1	C	11	GLN
1	C	15	GLN
1	C	128	GLN
1	C	249	ASN
1	C	283	HIS
1	C	356	ASN
1	C	372	GLN
1	C	393	HIS
2	D	15	GLN
2	D	37	HIS
2	D	329	GLN
2	D	396	HIS
2	D	426	GLN
3	E	18	GLN
3	E	90	ASN
3	E	124	GLN
4	F	333	ASN
4	F	384	HIS

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 7 are monoatomic - leaving 9 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	A	501	6	33,34,34	1.34	7 (21%)	50,54,54	1.62	8 (16%)
8	GDP	B	501	6	29,30,30	1.26	4 (13%)	45,47,47	1.65	6 (13%)
10	PN6	D	503	-	26,27,27	1.91	8 (30%)	34,39,39	1.96	11 (32%)
5	GTP	C	501	6	33,34,34	1.24	6 (18%)	50,54,54	1.60	7 (14%)
10	PN6	B	506	-	26,27,27	1.83	8 (30%)	34,39,39	2.00	11 (32%)
9	MES	B	503	-	12,12,12	2.05	1 (8%)	15,16,16	6.17	10 (66%)
9	MES	B	505	-	12,12,12	2.07	2 (16%)	15,16,16	5.48	6 (40%)
11	ACP	F	401	-	31,33,33	2.19	11 (35%)	47,52,52	1.83	11 (23%)
5	GTP	D	501	6	33,34,34	1.17	2 (6%)	50,54,54	1.65	6 (12%)

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	A	501	6	-	4/22/38/38	0/3/3/3
8	GDP	B	501	6	-	3/16/32/32	0/3/3/3
10	PN6	D	503	-	-	2/14/14/14	0/3/3/3
5	GTP	C	501	6	-	8/22/38/38	0/3/3/3
10	PN6	B	506	-	-	2/14/14/14	0/3/3/3
9	MES	B	503	-	-	3/6/14/14	0/1/1/1
9	MES	B	505	-	-	2/6/14/14	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	ACP	F	401	-	-	5/19/38/38	0/3/3/3
5	GTP	D	501	6	-	5/22/38/38	0/3/3/3

All (49) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	503	MES	C8-S	-6.48	1.68	1.77
9	B	505	MES	C8-S	-6.40	1.68	1.77
11	F	401	ACP	PG-O1G	5.60	1.61	1.50
11	F	401	ACP	C5-C4	4.88	1.47	1.39
10	D	503	PN6	C22-C1	4.16	1.57	1.52
11	F	401	ACP	PB-O1B	4.10	1.61	1.51
10	B	506	PN6	C10-C11	-4.02	1.40	1.48
10	D	503	PN6	C10-C11	-3.97	1.40	1.48
10	B	506	PN6	C14-C13	-3.87	1.39	1.46
10	B	506	PN6	C7-C8	-3.66	1.41	1.48
10	D	503	PN6	C7-C8	-3.58	1.41	1.48
11	F	401	ACP	PB-O3A	3.46	1.62	1.58
5	D	501	GTP	C5-C4	3.39	1.48	1.38
10	D	503	PN6	C13-C10	3.26	1.41	1.34
5	C	501	GTP	C5-C4	3.21	1.47	1.38
5	A	501	GTP	C5-C4	3.20	1.47	1.38
11	F	401	ACP	PB-O2B	-3.14	1.48	1.56
5	A	501	GTP	PB-O3B	3.08	1.62	1.59
8	B	501	GDP	C5-C4	3.05	1.47	1.38
10	D	503	PN6	C14-C13	-2.99	1.41	1.46
11	F	401	ACP	PG-O2G	2.95	1.61	1.55
10	B	506	PN6	C22-C1	2.90	1.55	1.52
11	F	401	ACP	C5-C6	2.88	1.49	1.41
11	F	401	ACP	PG-O3G	-2.87	1.48	1.55
10	B	506	PN6	C13-C10	2.66	1.39	1.34
8	B	501	GDP	PA-O3A	2.62	1.62	1.59
11	F	401	ACP	PA-O3A	2.47	1.62	1.59
11	F	401	ACP	C8-N7	2.43	1.36	1.31
5	A	501	GTP	PA-O3A	2.41	1.62	1.59
5	C	501	GTP	PA-O3A	2.37	1.62	1.59
8	B	501	GDP	C5-N7	-2.34	1.34	1.39
10	B	506	PN6	C6-C2	-2.32	1.35	1.40
10	B	506	PN6	C2-N3	-2.31	1.33	1.39
8	B	501	GDP	C6-N1	-2.31	1.34	1.38
11	F	401	ACP	C5-N7	-2.29	1.34	1.39
10	D	503	PN6	C2-N3	-2.23	1.33	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	505	MES	O2S-S	2.21	1.51	1.45
5	D	501	GTP	C5-N7	-2.19	1.34	1.39
10	D	503	PN6	C1-N5	-2.19	1.34	1.37
5	A	501	GTP	C4-N9	-2.18	1.32	1.38
5	A	501	GTP	PB-O3A	2.14	1.61	1.59
5	C	501	GTP	C5-N7	-2.13	1.34	1.39
5	C	501	GTP	C6-N1	-2.13	1.34	1.38
5	A	501	GTP	C6-N1	-2.11	1.34	1.38
5	C	501	GTP	PB-O3B	2.10	1.61	1.59
10	D	503	PN6	C6-C2	-2.08	1.35	1.40
10	B	506	PN6	C1-N5	-2.07	1.34	1.37
5	C	501	GTP	PB-O3A	2.05	1.61	1.59
5	A	501	GTP	C5-N7	-2.04	1.35	1.39

All (76) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	503	MES	O1S-S-C8	-14.23	85.23	106.73
9	B	505	MES	O3S-S-O1S	-13.15	78.49	111.40
9	B	503	MES	O3S-S-O1S	-10.58	84.92	111.40
9	B	503	MES	O2S-S-O1S	-9.69	82.31	113.82
9	B	505	MES	O2S-S-O1S	-9.43	83.14	113.82
9	B	503	MES	O2S-S-C8	9.03	120.38	106.73
9	B	505	MES	O3S-S-C8	8.40	122.43	106.00
9	B	505	MES	O1S-S-C8	-7.68	95.12	106.73
9	B	503	MES	O3S-S-C8	6.07	117.88	106.00
9	B	505	MES	O3S-S-O2S	5.98	126.37	111.40
5	D	501	GTP	C5-C4-N3	-5.66	119.39	128.39
8	B	501	GDP	C5-C4-N3	-5.52	119.61	128.39
11	F	401	ACP	C5-C4-N3	-5.52	119.12	126.72
5	C	501	GTP	C5-C4-N3	-5.30	119.95	128.39
5	A	501	GTP	C5-C4-N3	-5.09	120.29	128.39
8	B	501	GDP	C2-N3-C4	4.73	120.45	112.30
5	D	501	GTP	C2-N3-C4	4.54	120.11	112.30
5	C	501	GTP	C2-N3-C4	4.52	120.08	112.30
5	D	501	GTP	N9-C4-N3	4.49	134.93	125.95
8	B	501	GDP	N9-C4-N3	4.40	134.75	125.95
11	F	401	ACP	N3-C4-N9	4.37	134.59	127.17
5	A	501	GTP	C2-N3-C4	4.27	119.65	112.30
10	B	506	PN6	C7-C8-N9	4.24	120.19	116.02
10	D	503	PN6	C7-C8-N9	4.19	120.14	116.02
10	B	506	PN6	N5-C4-N3	-4.16	108.16	112.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	501	GTP	N9-C4-N3	4.13	134.21	125.95
10	D	503	PN6	N5-C4-N3	-4.07	108.26	112.98
9	B	503	MES	C2-C3-N4	4.07	116.30	110.12
5	A	501	GTP	N9-C4-N3	4.05	134.06	125.95
10	D	503	PN6	C10-C11-N12	3.97	119.93	116.02
10	B	506	PN6	C10-C11-N12	3.87	119.82	116.02
11	F	401	ACP	C2-N3-C4	3.82	121.17	111.83
11	F	401	ACP	N3-C2-N1	-3.79	122.84	128.58
10	B	506	PN6	C10-N9-C8	-3.74	121.27	125.51
10	D	503	PN6	C10-N9-C8	-3.59	121.44	125.51
11	F	401	ACP	C4-C5-N7	-3.57	106.50	110.58
10	B	506	PN6	C22-C1-C2	-3.41	127.83	135.52
5	A	501	GTP	C6-C5-N7	3.39	136.47	130.29
8	B	501	GDP	C6-C5-N7	3.33	136.35	130.29
10	D	503	PN6	C22-C1-C2	-3.26	128.17	135.52
5	D	501	GTP	C6-C5-N7	3.16	136.05	130.29
5	C	501	GTP	C6-C5-N7	3.02	135.79	130.29
10	B	506	PN6	C7-C6-C2	-2.93	120.86	128.06
10	B	506	PN6	C7-N12-C11	-2.92	122.20	125.51
9	B	503	MES	O3S-S-O2S	2.90	118.67	111.40
11	F	401	ACP	C4-N9-C8	2.87	108.75	105.74
11	F	401	ACP	C5-N7-C8	2.70	107.69	103.45
10	D	503	PN6	C7-N12-C11	-2.61	122.55	125.51
9	B	503	MES	C6-C5-N4	2.60	114.08	110.12
9	B	503	MES	C5-N4-C3	2.52	114.26	108.84
10	D	503	PN6	C7-C6-C2	-2.50	121.92	128.06
10	B	506	PN6	C6-C7-N12	-2.46	119.31	122.75
5	A	501	GTP	O6-C6-C5	-2.44	120.10	126.53
5	C	501	GTP	O6-C6-C5	-2.43	120.12	126.53
5	D	501	GTP	C4-C5-N7	-2.42	106.83	110.67
5	A	501	GTP	C4-C5-N7	-2.38	106.90	110.67
10	B	506	PN6	C14-C13-C10	-2.36	125.90	130.66
10	D	503	PN6	C22-C1-N5	2.36	124.40	119.48
5	D	501	GTP	O6-C6-C5	-2.36	120.31	126.53
5	C	501	GTP	O2B-PB-O3B	2.35	113.63	107.27
10	B	506	PN6	C11-C10-N9	2.34	118.75	116.65
10	B	506	PN6	C22-C1-N5	2.31	124.30	119.48
11	F	401	ACP	C6-C5-N7	2.31	136.54	132.09
10	D	503	PN6	C16-C15-C14	2.27	123.30	120.64
9	B	505	MES	C6-C5-N4	2.27	113.56	110.12
10	D	503	PN6	C14-C13-C10	-2.24	126.14	130.66
8	B	501	GDP	C4-C5-N7	-2.24	107.12	110.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	F	401	ACP	N9-C8-N7	-2.23	110.78	113.94
9	B	503	MES	O1-C6-C5	-2.17	107.11	111.77
5	C	501	GTP	C4-C5-N7	-2.15	107.25	110.67
10	D	503	PN6	C6-C7-N12	-2.14	119.76	122.75
11	F	401	ACP	C2-N1-C6	2.12	122.22	118.73
8	B	501	GDP	O6-C6-C5	-2.12	120.94	126.53
11	F	401	ACP	C3'-C2'-C1'	2.11	105.46	101.46
5	A	501	GTP	O3B-PB-O1B	-2.11	104.36	110.70
5	A	501	GTP	O2B-PB-O3B	2.02	112.75	107.27

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	501	GTP	C5'-O5'-PA-O3A
5	A	501	GTP	C5'-O5'-PA-O1A
5	A	501	GTP	C5'-O5'-PA-O2A
5	C	501	GTP	PB-O3B-PG-O3G
5	C	501	GTP	C5'-O5'-PA-O3A
5	C	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O2A
5	D	501	GTP	C5'-O5'-PA-O3A
5	D	501	GTP	C5'-O5'-PA-O1A
5	D	501	GTP	C5'-O5'-PA-O2A
8	B	501	GDP	C5'-O5'-PA-O3A
8	B	501	GDP	C5'-O5'-PA-O1A
8	B	501	GDP	C5'-O5'-PA-O2A
9	B	503	MES	N4-C7-C8-S
10	B	506	PN6	N9-C10-C13-C14
10	D	503	PN6	N9-C10-C13-C14
10	D	503	PN6	C11-C10-C13-C14
11	F	401	ACP	PB-C3B-PG-O1G
9	B	503	MES	C7-C8-S-O3S
9	B	505	MES	C7-C8-S-O3S
9	B	503	MES	C7-C8-S-O2S
9	B	505	MES	C7-C8-S-O1S
11	F	401	ACP	O4'-C4'-C5'-O5'
11	F	401	ACP	PB-C3B-PG-O2G
11	F	401	ACP	PB-C3B-PG-O3G
5	C	501	GTP	C4'-C5'-O5'-PA
10	B	506	PN6	C11-C10-C13-C14
5	D	501	GTP	C4'-C5'-O5'-PA

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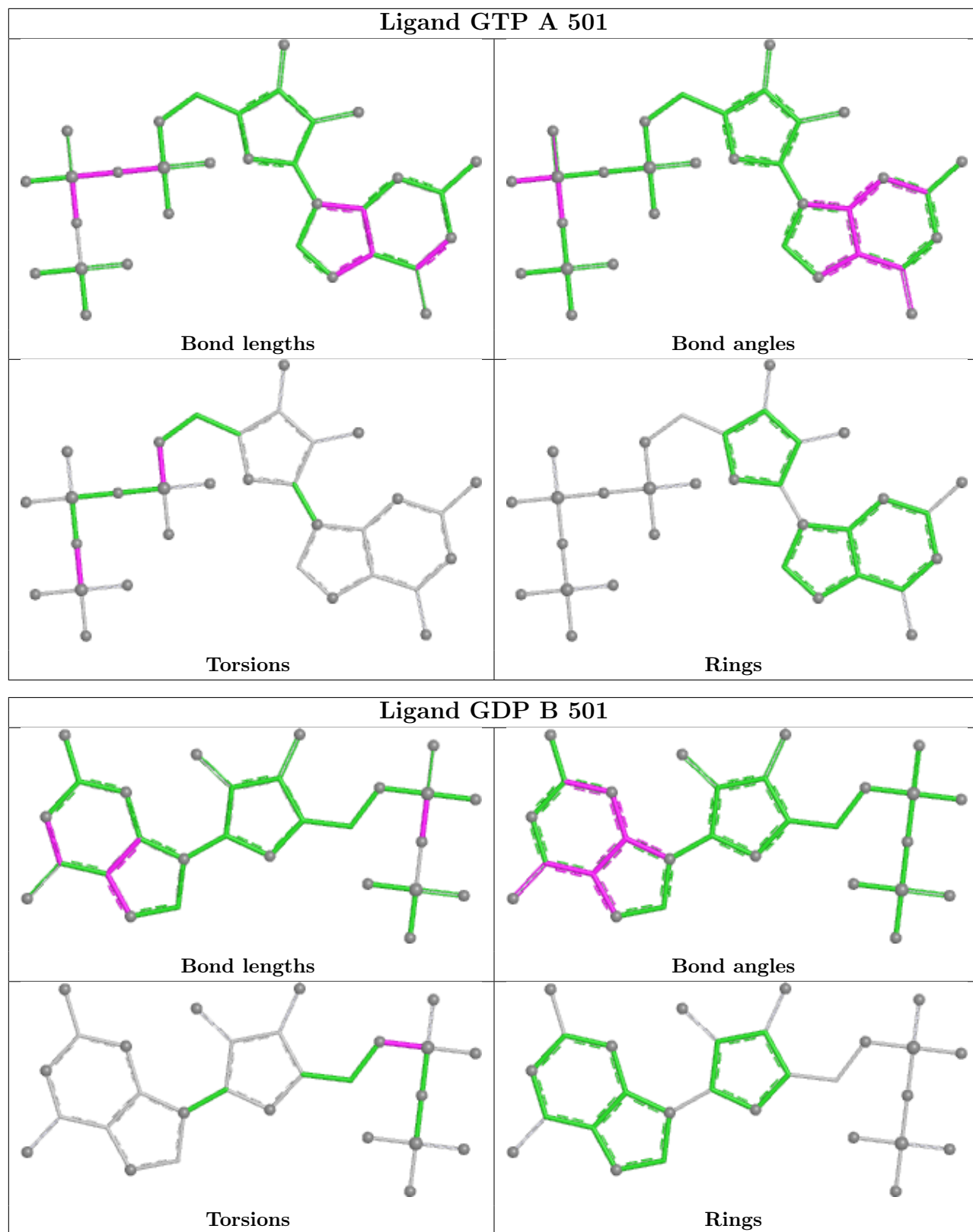
Mol	Chain	Res	Type	Atoms
5	A	501	GTP	PB-O3B-PG-O1G
5	C	501	GTP	PB-O3B-PG-O1G
5	C	501	GTP	PB-O3B-PG-O2G
11	F	401	ACP	C3'-C4'-C5'-O5'
5	C	501	GTP	PB-O3A-PA-O2A
5	D	501	GTP	PB-O3A-PA-O2A

There are no ring outliers.

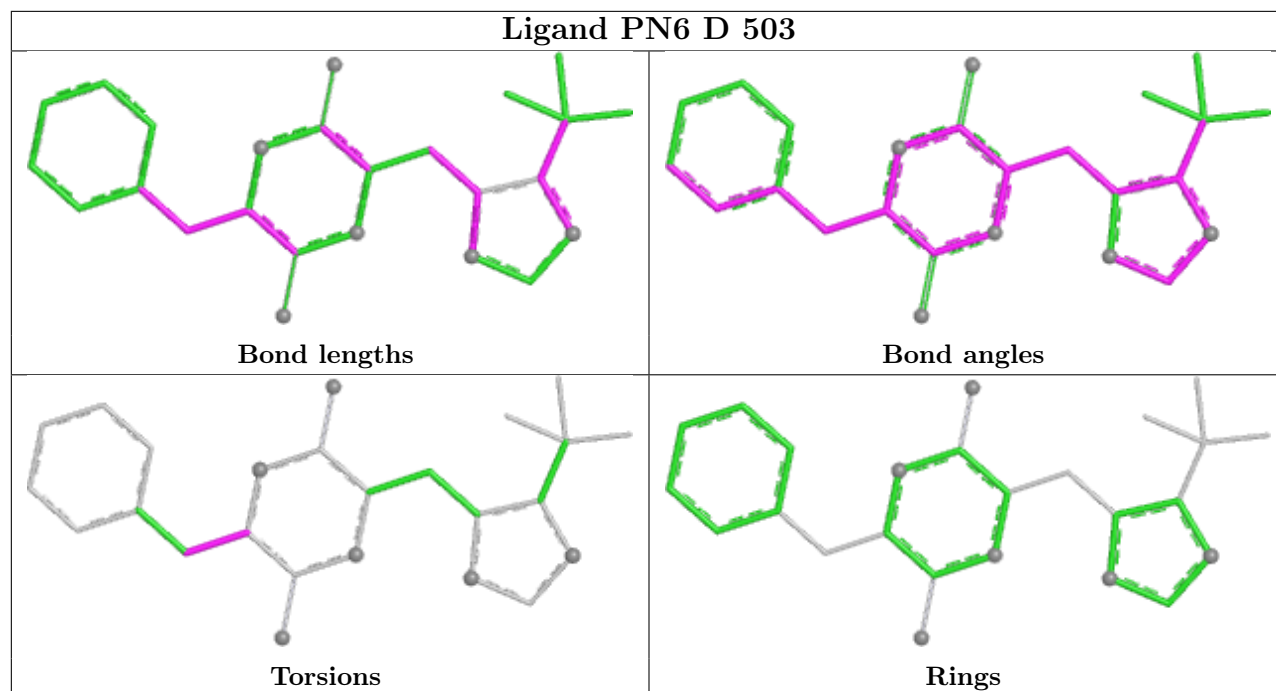
5 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	D	503	PN6	2	0
10	B	506	PN6	3	0
9	B	503	MES	1	0
9	B	505	MES	1	0
11	F	401	ACP	1	0

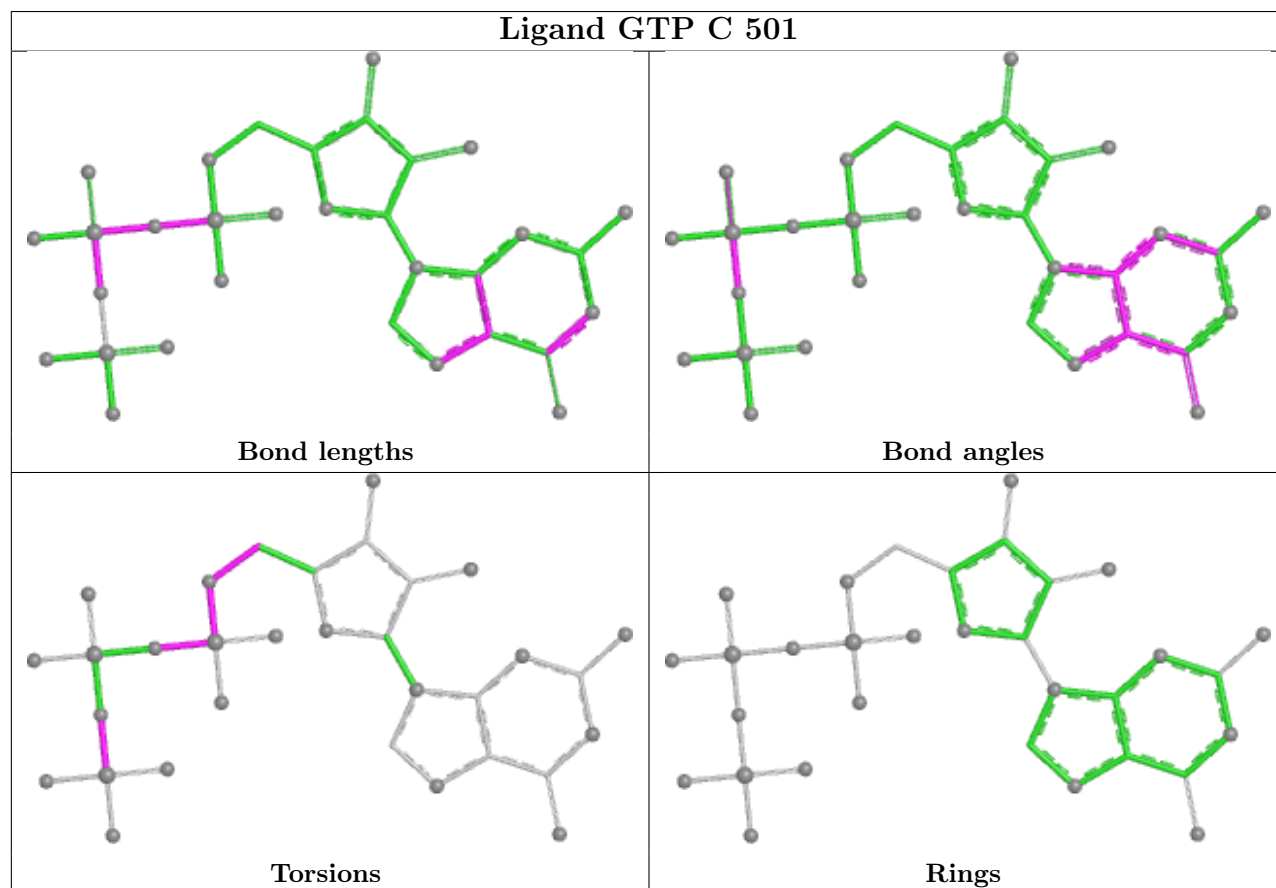
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



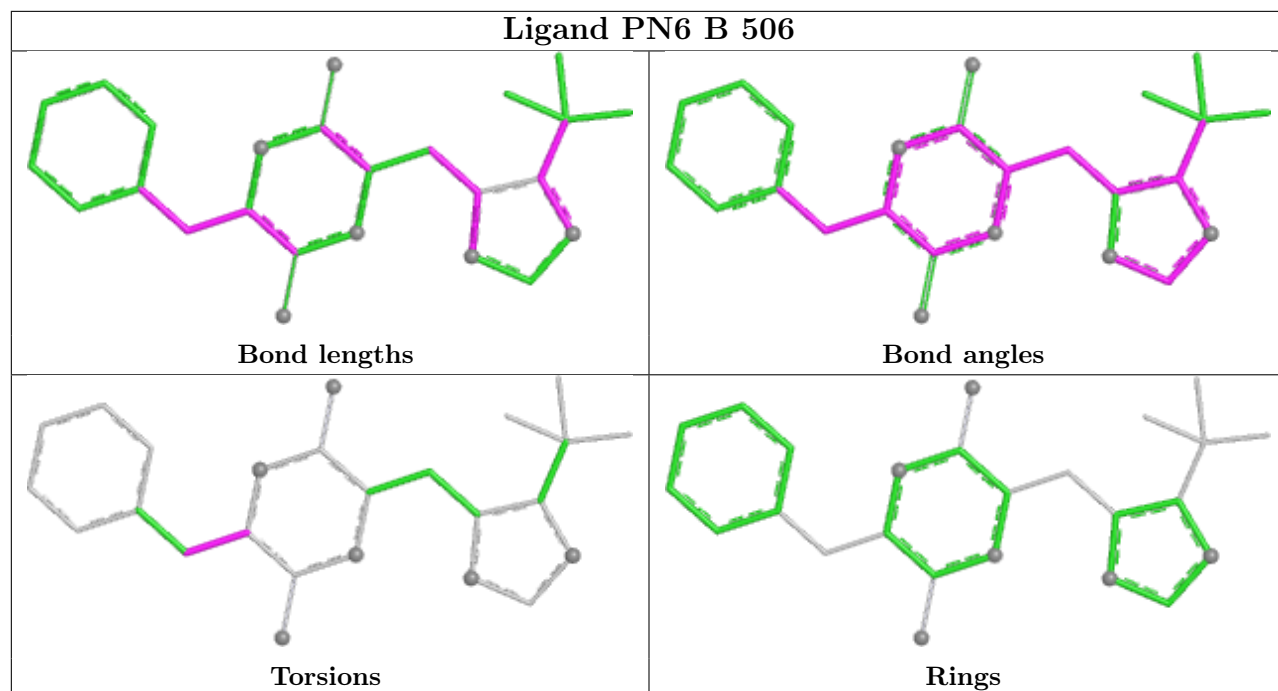
Ligand PN6 D 503



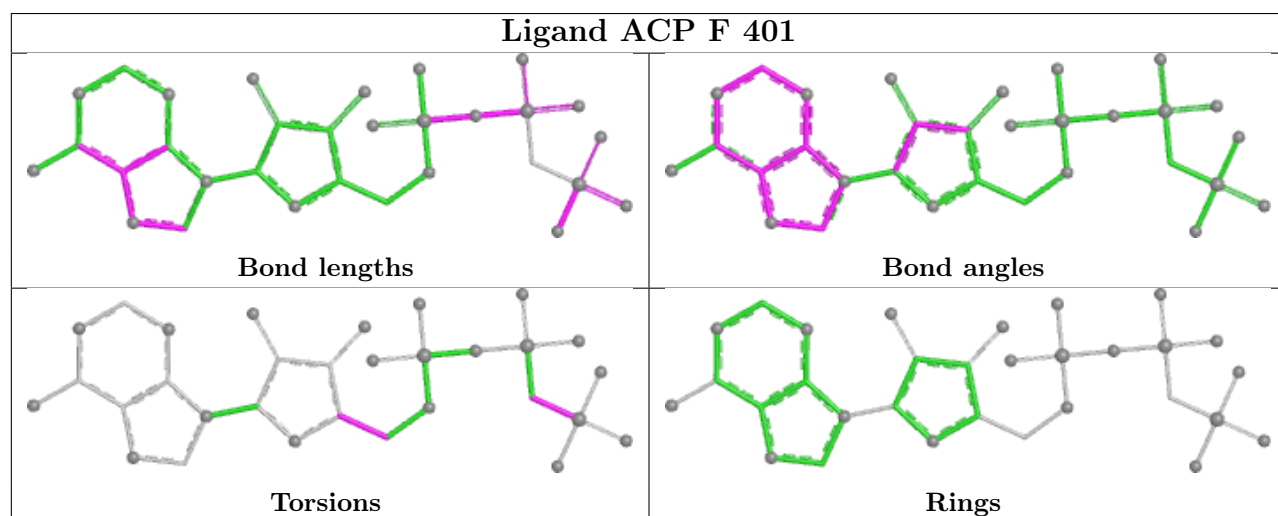
Ligand GTP C 501

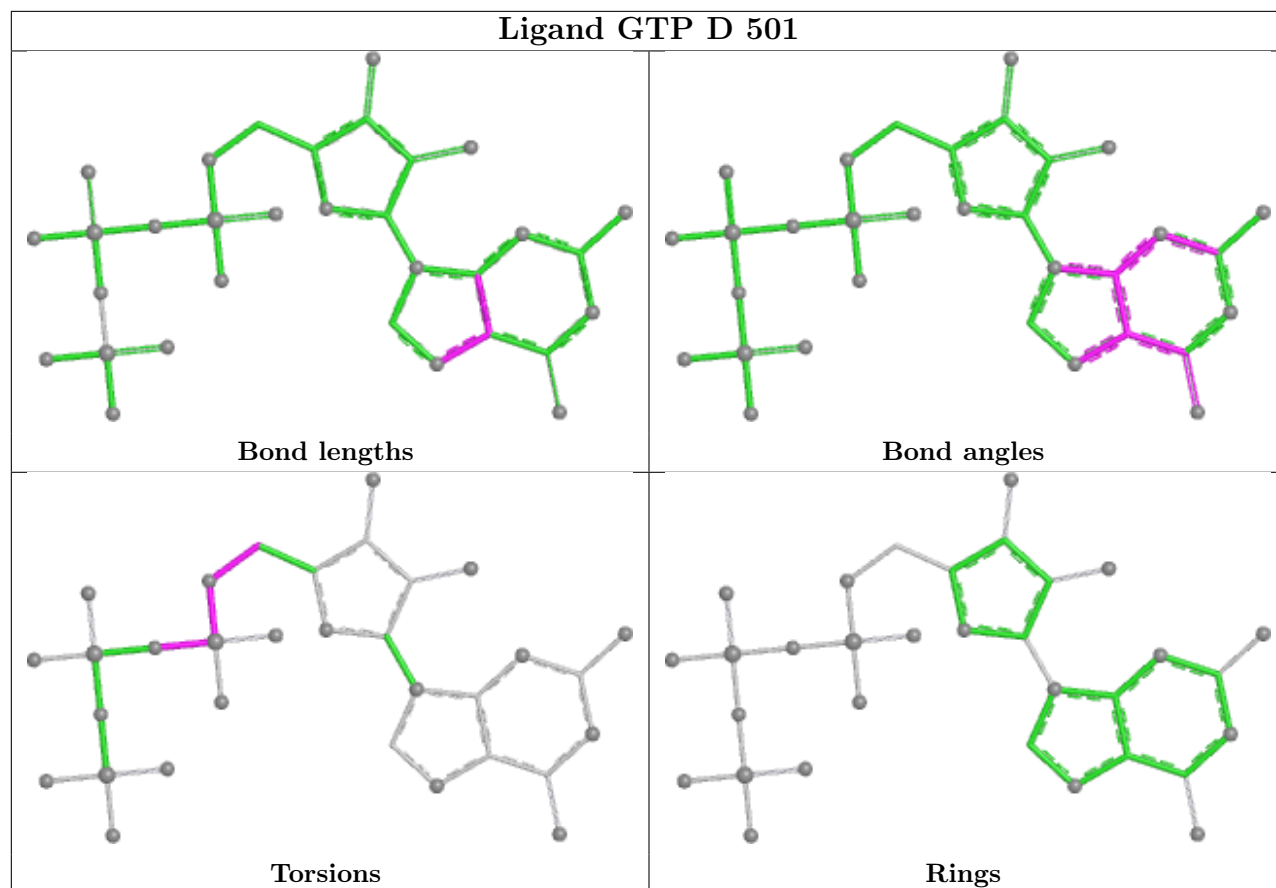


Ligand PN6 B 506



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%)	0.22	12 (2%)	56	46	19, 43, 69, 86	4 (0%)
1	C	440/450 (97%)	-0.06	10 (2%)	61	51	14, 34, 58, 73	9 (2%)
2	B	424/445 (95%)	0.29	20 (4%)	36	28	17, 42, 72, 102	3 (0%)
2	D	421/445 (94%)	1.10	68 (16%)	4	3	32, 65, 101, 131	4 (0%)
3	E	120/184 (65%)	0.95	14 (11%)	9	7	31, 64, 93, 102	2 (1%)
4	F	309/384 (80%)	1.11	54 (17%)	4	3	18, 68, 111, 130	3 (0%)
All	All	2151/2358 (91%)	0.52	178 (8%)	17	12	14, 49, 92, 131	25 (1%)

All (178) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	166	ALA	7.7
4	F	100	ILE	6.2
4	F	161	LEU	5.6
2	D	245	GLN	5.3
4	F	102	PRO	5.0
4	F	182	ILE	4.9
1	C	245	ASP	4.9
1	C	211[A]	ASP	4.6
4	F	233	PHE	4.6
3	E	12[A]	ASN	4.5
1	A	262	TYR	4.3
4	F	237	THR	4.2
2	D	73	MET	4.0
4	F	159	GLY	3.9
2	B	246	LEU	3.8
2	B	243	PRO	3.8
2	B	55	THR	3.8
4	F	382	HIS	3.6
2	D	243	PRO	3.6

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Mol	Chain	Res	Type	RSRZ
2	D	99	ASN	3.6
2	D	94	GLN	3.5
2	D	175	VAL	3.5
1	A	346	TRP	3.5
2	B	360	GLY	3.4
2	D	239	CYS	3.4
1	C	251[A]	ASP	3.3
2	D	92	PHE	3.3
2	D	55	THR	3.3
2	D	72	THR	3.3
4	F	99	VAL	3.3
2	D	377	LEU	3.3
4	F	144	GLY	3.2
2	D	170	MET	3.2
2	D	81	PHE	3.2
2	B	281	TYR	3.2
3	E	139	LEU	3.1
2	D	214	THR	3.1
4	F	162	ILE	3.1
1	A	436	GLY	3.1
2	D	98	GLY	3.1
2	D	1	MET	3.1
2	D	284	LEU	3.1
4	F	163	SER	3.0
2	B	280	GLN	3.0
4	F	320	MET	3.0
4	F	245	ILE	3.0
2	D	215	LEU	3.0
4	F	234	GLN	3.0
2	D	115	SER	3.0
3	E	51	GLN	2.9
2	D	39	ASP	2.9
2	B	282	ARG	2.9
2	D	176	SER	2.9
1	A	94	THR	2.9
2	D	399	THR	2.9
4	F	275	LEU	2.9
4	F	247	LYS	2.9
4	F	186	LEU	2.9
2	D	396	HIS	2.9
4	F	383	HIS	2.9
1	A	437	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
2	D	218	THR	2.8
2	B	2	ARG	2.8
3	E	61	ARG	2.8
4	F	160	ILE	2.8
3	E	59	GLU	2.8
4	F	101	TYR	2.8
2	D	217	LEU	2.8
4	F	180	HIS	2.8
4	F	225	SER	2.8
2	D	93	GLY	2.8
2	D	140	GLY	2.8
4	F	243	HIS	2.7
4	F	381	HIS	2.7
2	D	244	GLY	2.7
2	D	172	SER	2.7
2	D	246	LEU	2.7
2	D	248	ALA	2.7
2	D	28	HIS	2.7
2	D	76	VAL	2.7
1	A	282	TYR	2.7
1	C	357	TYR	2.7
2	D	178	THR	2.7
2	D	80	PRO	2.6
1	C	285	GLN	2.6
2	D	228	LEU	2.6
1	C	340	SER	2.6
2	D	54	ALA	2.6
4	F	228	TYR	2.6
2	D	42	LEU	2.6
3	E	54	LEU	2.6
2	D	356	ILE	2.6
2	B	245	GLN	2.6
3	E	6	MET	2.6
4	F	151	SER	2.6
1	A	89	PRO	2.5
2	D	181	GLU	2.5
2	B	48	ASN	2.5
2	D	403	MET	2.5
4	F	199	PHE	2.5
2	D	293	MET	2.5
4	F	191	LEU	2.5
2	D	296	SER	2.5

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Mol	Chain	Res	Type	RSRZ
2	D	397	TRP	2.5
2	D	362	LYS	2.4
4	F	149	ALA	2.4
2	D	30	ILE	2.4
2	D	229	VAL	2.4
4	F	263	PHE	2.4
2	D	394	PHE	2.4
2	D	185	ALA	2.4
4	F	232	ASN	2.4
1	A	91	GLN	2.4
4	F	373	SER	2.4
2	D	219	THR	2.4
2	D	37	HIS	2.4
1	C	120[A]	ASP	2.3
4	F	184	LYS	2.3
2	B	214	THR	2.3
4	F	150	LYS	2.3
2	B	244	GLY	2.3
4	F	198	LYS	2.3
4	F	254	GLY	2.3
2	D	294	PHE	2.3
4	F	335	ALA	2.3
4	F	236	LYS	2.3
2	D	75	SER	2.3
2	D	96	GLY	2.3
4	F	197	ARG	2.2
4	F	194	PRO	2.2
4	F	264	PHE	2.2
3	E	106	GLU	2.2
3	E	113	GLU	2.2
2	B	128	ASP	2.2
2	D	74	ASP	2.2
4	F	147	TRP	2.2
2	D	86	ARG	2.2
4	F	384	HIS	2.2
3	E	53	LYS	2.2
2	D	82	GLY	2.2
1	A	350	GLY	2.1
2	D	331	LEU	2.1
1	C	358	GLN	2.1
2	B	414	ASN	2.1
1	A	56	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	179	THR	2.1
2	D	429	THR	2.1
2	B	42	LEU	2.1
2	D	207	LEU	2.1
4	F	22	LEU	2.1
2	D	97	ALA	2.1
2	D	110	ALA	2.1
2	D	398	TYR	2.1
4	F	362	ALA	2.1
2	D	145[A]	SER	2.1
4	F	239	HIS	2.1
2	B	323	MET	2.1
2	B	336	LYS	2.1
3	E	62	LYS	2.1
4	F	192	LEU	2.1
2	B	170	MET	2.1
1	C	440	VAL	2.1
2	D	116	VAL	2.1
2	D	171	PRO	2.1
3	E	26	PRO	2.1
1	A	58	ALA	2.1
3	E	141	GLU	2.1
4	F	324[A]	GLU	2.1
2	B	1	MET	2.0
3	E	105[A]	MET	2.0
4	F	240	LEU	2.0
4	F	333	ASN	2.0
2	B	428	ALA	2.0
2	D	180	VAL	2.0
2	D	71	GLY	2.0
1	A	335	ILE	2.0
4	F	146	VAL	2.0
4	F	321	VAL	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

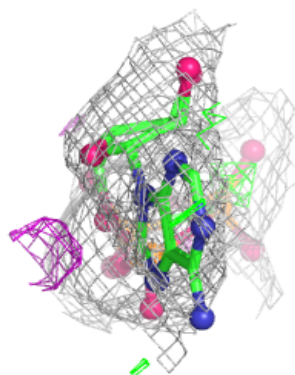
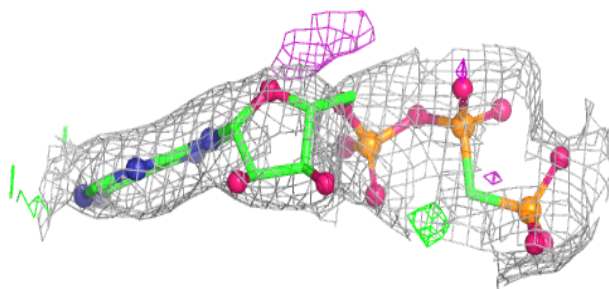
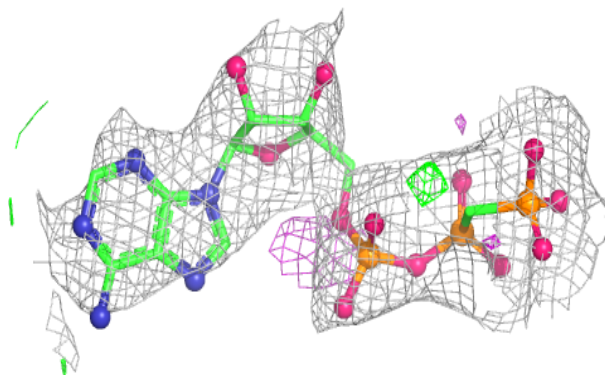
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
11	ACP	F	401	31/31	0.76	0.14	86,94,112,113	0
10	PN6	D	503	25/25	0.83	0.17	52,57,63,63	0
9	MES	B	505	12/12	0.84	0.20	91,93,98,100	0
6	MG	D	502	1/1	0.85	0.24	67,67,67,67	0
9	MES	B	503	12/12	0.86	0.19	62,66,71,71	0
5	GTP	D	501	32/32	0.87	0.12	50,53,69,72	0
7	CA	B	504	1/1	0.90	0.08	67,67,67,67	0
7	CA	C	503	1/1	0.92	0.07	58,58,58,58	0
10	PN6	B	506	25/25	0.94	0.09	28,30,37,37	0
7	CA	A	503	1/1	0.95	0.07	63,63,63,63	0
6	MG	B	502	1/1	0.95	0.05	27,27,27,27	0
5	GTP	C	501	32/32	0.97	0.07	22,24,24,24	0
5	GTP	A	501	32/32	0.97	0.07	24,26,27,27	0
8	GDP	B	501	28/28	0.98	0.06	22,26,27,28	0
6	MG	A	502	1/1	0.98	0.06	17,17,17,17	0
6	MG	C	502	1/1	0.99	0.02	26,26,26,26	0

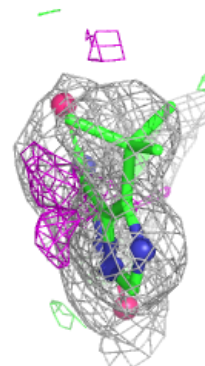
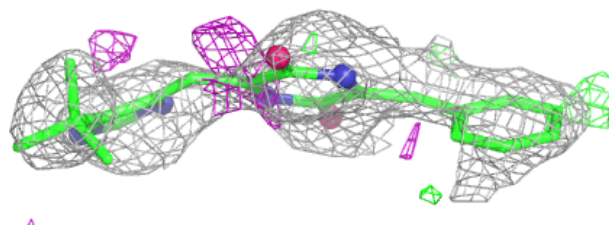
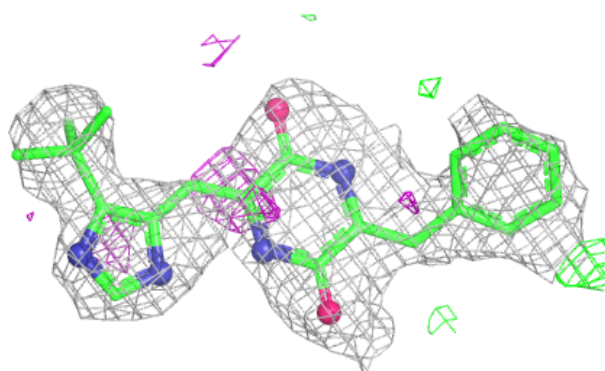
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 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)

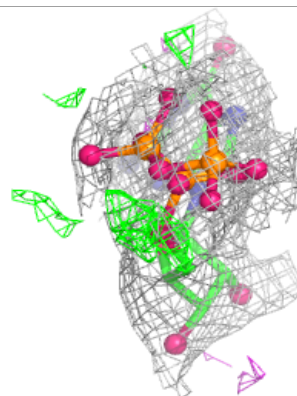
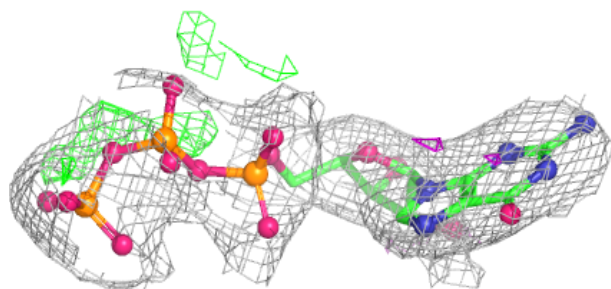
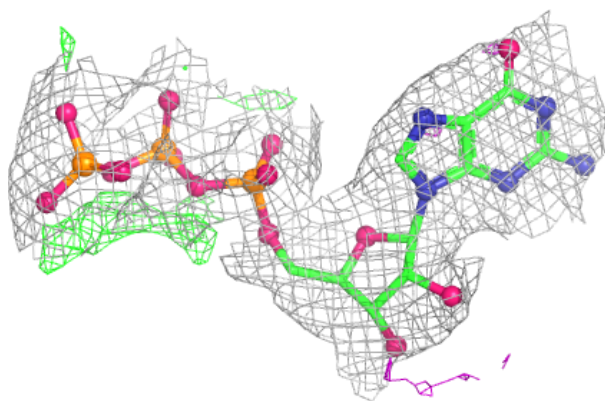
**Electron density around PN6 D 503:**

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

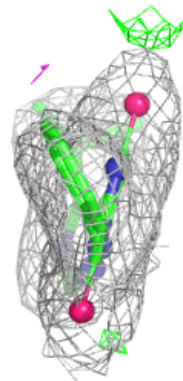
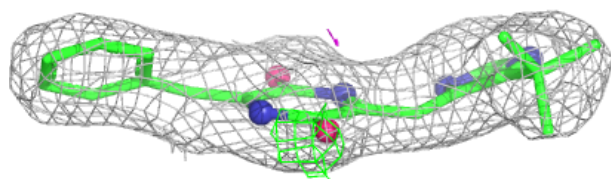
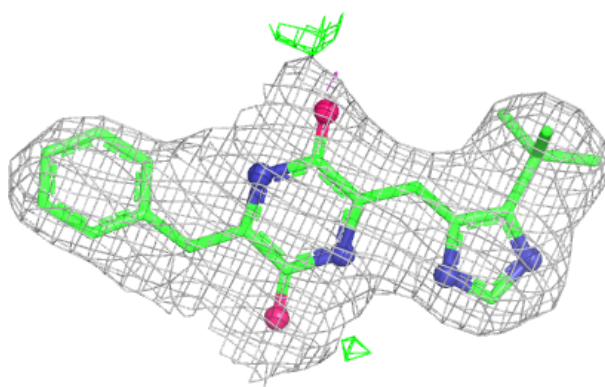


Electron density around GTP D 501:

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

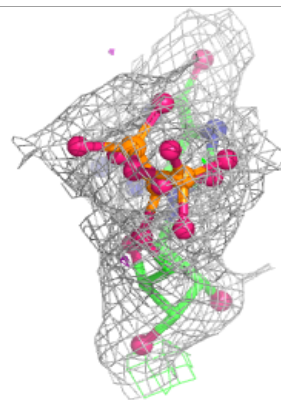
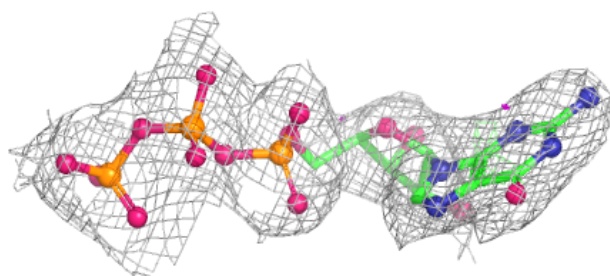
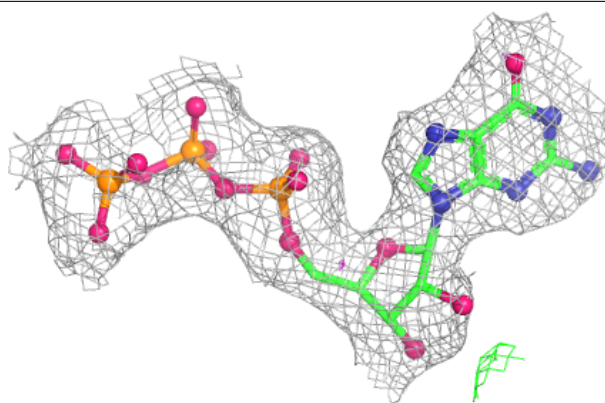
**Electron density around PN6 B 506:**

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

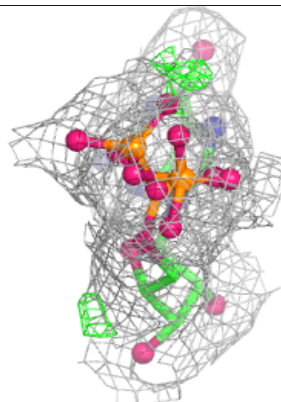
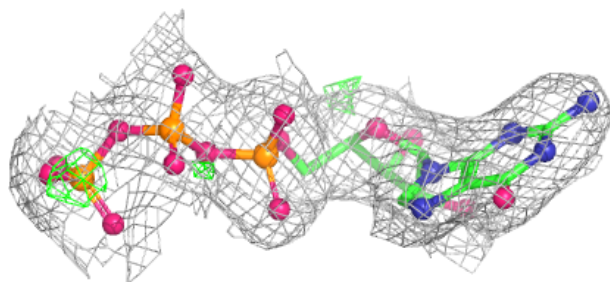
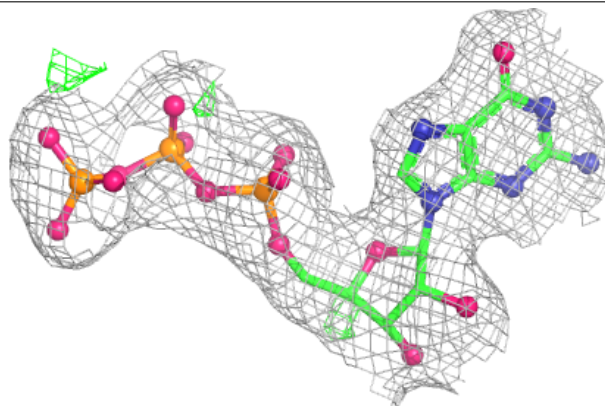


Electron density around GTP C 501:

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

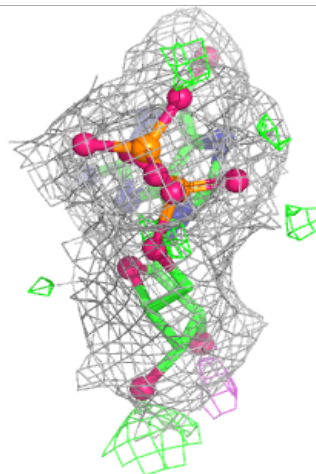
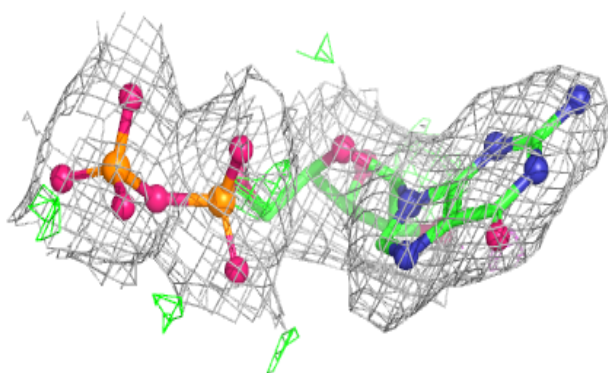
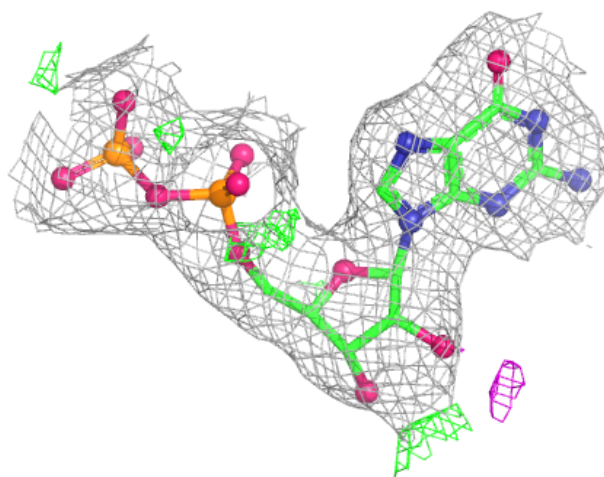
**Electron density around GTP A 501:**

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



Electron density around 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.