



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 10:45 PM UTC

PDB ID : 7CE6 / pdb_00007ce6
Title : Crystal structure of T2R-TTL-Compound9 complex
Authors : Chen, L.J.; Chen, Q.; Yu, Y.; Yang, J.H.
Deposited on : 2020-06-22
Resolution : 2.69 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

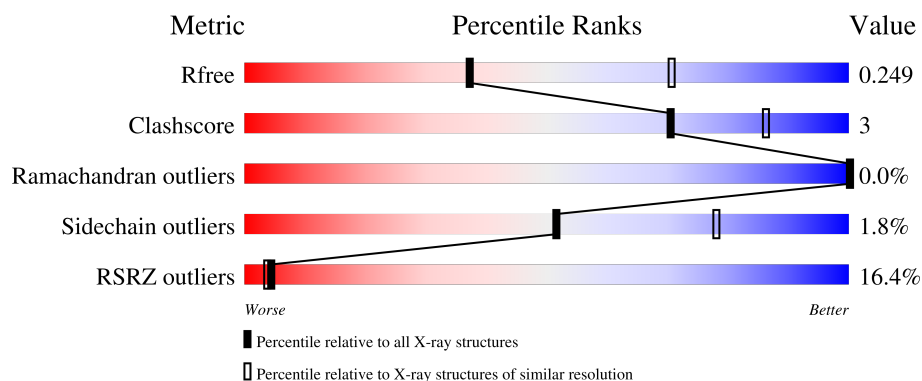
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.69 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	2% 93% 5% •
1	C	450	4% 93% 5% •
2	B	445	12% 87% 9% •
2	D	445	31% 84% 10% 5% •
3	E	143	17% 78% 6% 15%

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Mol	Chain	Length	Quality of chain
4	F	384	31% 77% 10% 13%

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 34712 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-1B chain.

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	1	0
			6783	2178	3340	585	657	23			

- Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	427	Total	C	H	N	O	S	0	0	0
			6586	2110	3225	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

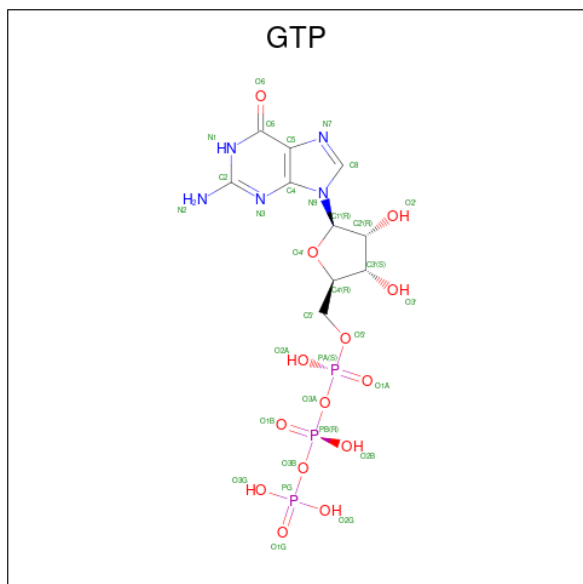
- Molecule 4 is a protein called Tubulin tyrosine ligase.

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 (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	A	1	Total 42	C 10	H 10	N 5	O 14	P 3	0	0
5	C	1	Total 42	C 10	H 10	N 5	O 14	P 3	0	0
5	D	1	Total 42	C 10	H 10	N 5	O 14	P 3	0	0

- 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		

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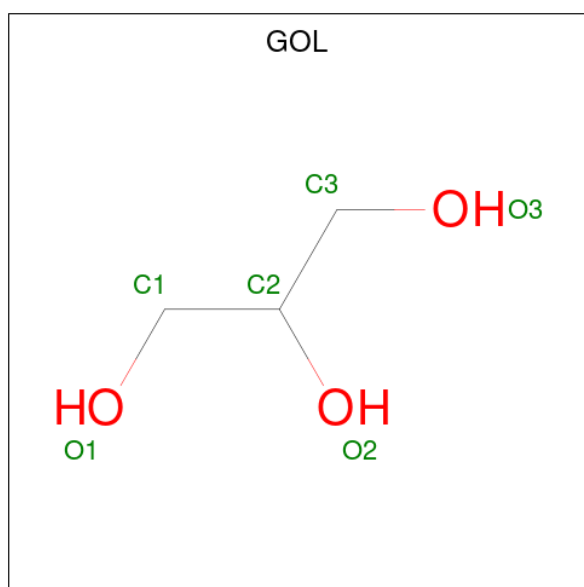
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	1	Total	Mg	0	0
			1	1		

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

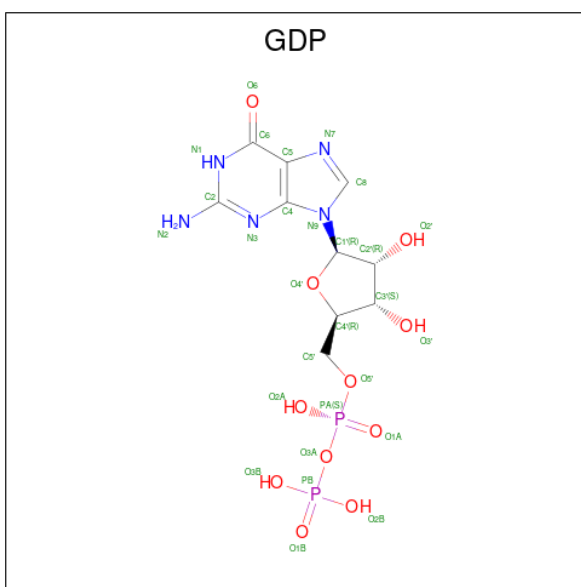
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Ca	0	0
			1	1		
7	C	1	Total	Ca	0	0
			1	1		

- Molecule 8 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



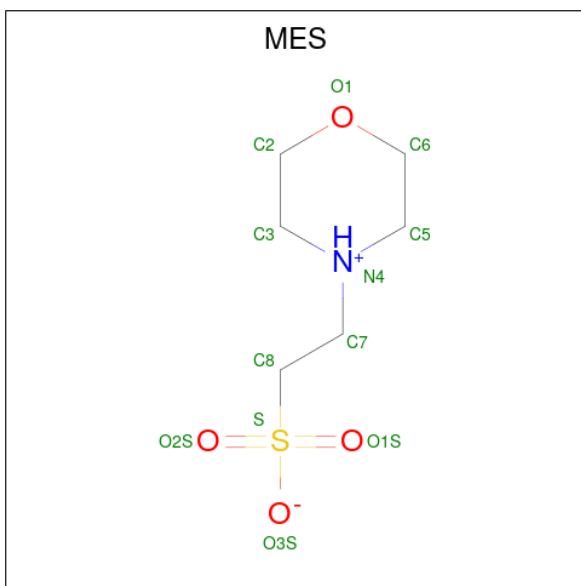
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 9 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



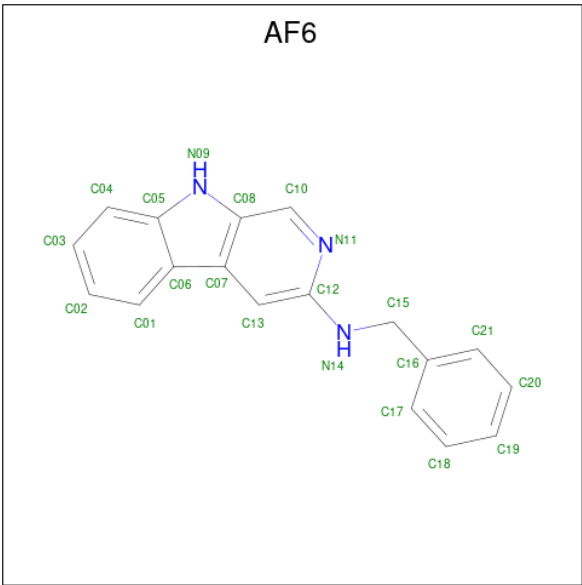
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
9	B	1	Total	C	H	N	O	P	0	0
			38	10	10	5	11	2		

- Molecule 10 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: $\text{C}_6\text{H}_{13}\text{NO}_4\text{S}$).



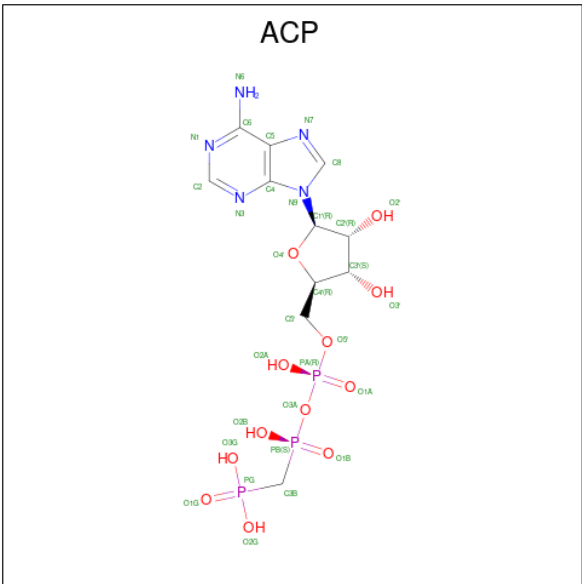
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
10	B	1	Total	C	H	N	O	S	0	0
			24	6	12	1	4	1		

- Molecule 11 is N-benzyl-9H-beta-carboline-3-amine (CCD ID: AF6) (formula: $C_{18}H_{15}N_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	B	1	Total	C	H	N	0	0
			36	18	15	3		
11	D	1	Total	C	H	N	0	0
			36	18	15	3		

- Molecule 12 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (CCD ID: ACP) (formula: C₁₁H₁₈N₅O₁₂P₃).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
12	F	1	Total	C	H	N	O	P	0	0
			35	11	4	5	12	3		

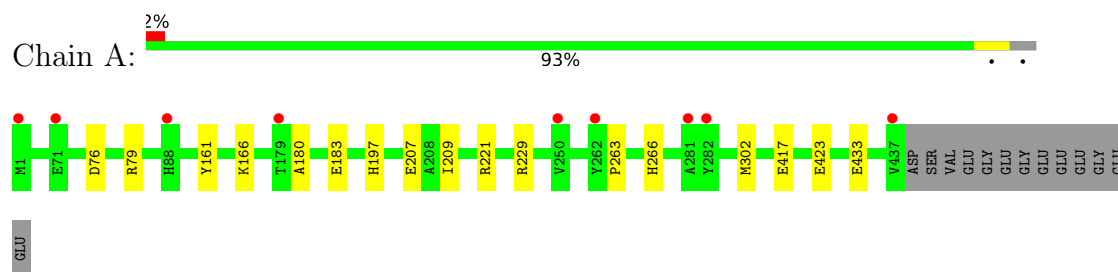
- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	68	Total 68	O 68	0	0
13	B	76	Total 76	O 76	0	0
13	C	130	Total 130	O 130	0	0
13	D	20	Total 20	O 20	0	0
13	E	20	Total 20	O 20	0	0
13	F	37	Total 37	O 37	0	0

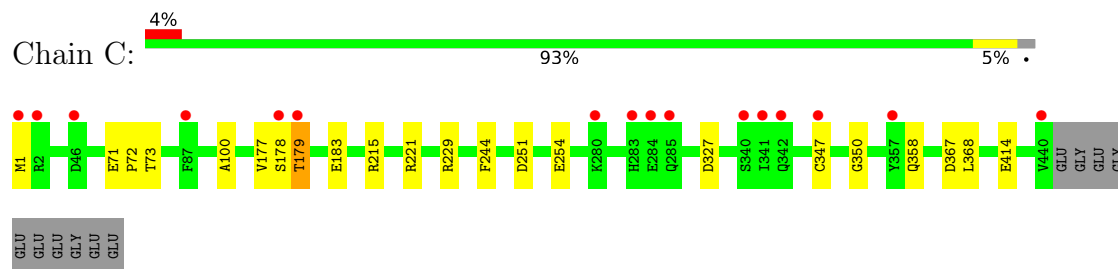
3 Residue-property plots

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.

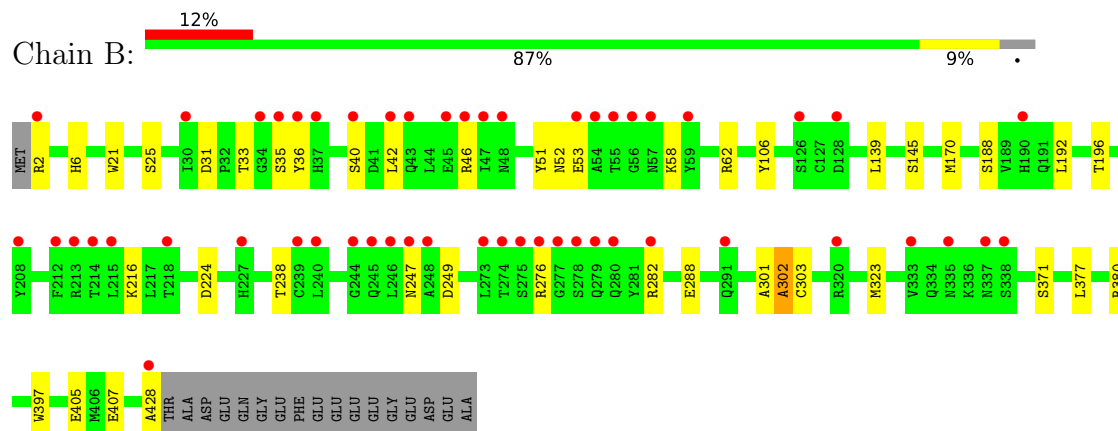
• Molecule 1: Tubulin alpha-1B chain



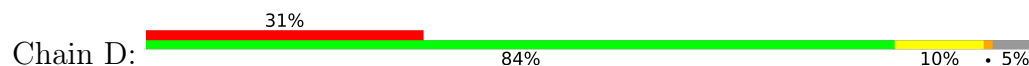
• Molecule 1: Tubulin alpha-1B chain

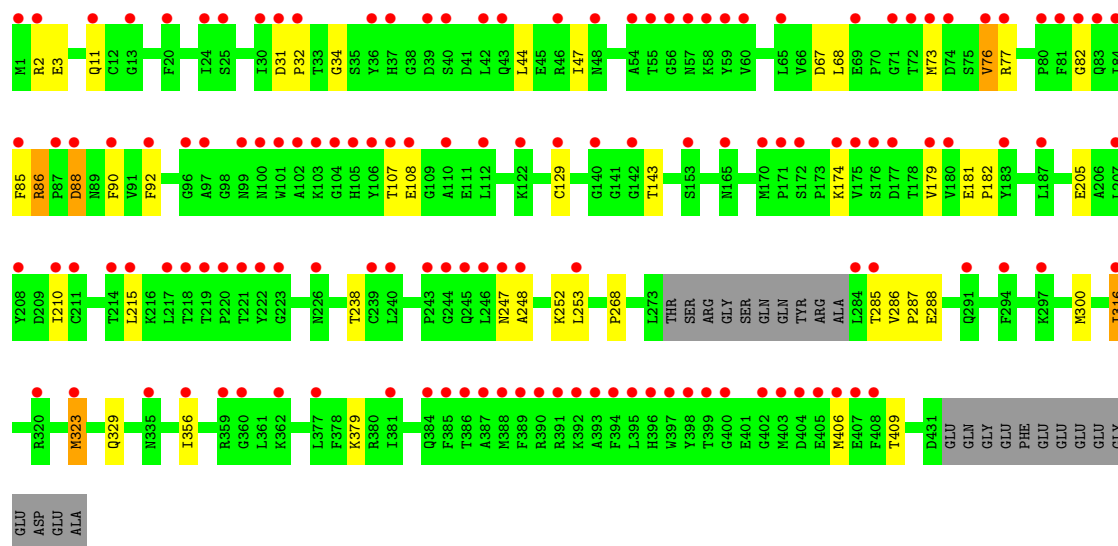


• Molecule 2: Tubulin beta chain

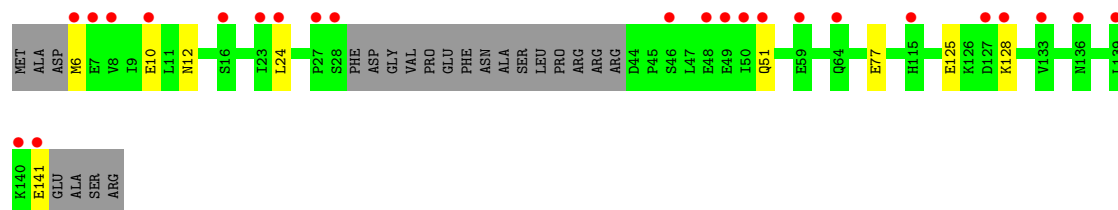
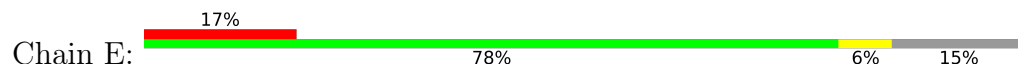


• Molecule 2: Tubulin beta chain

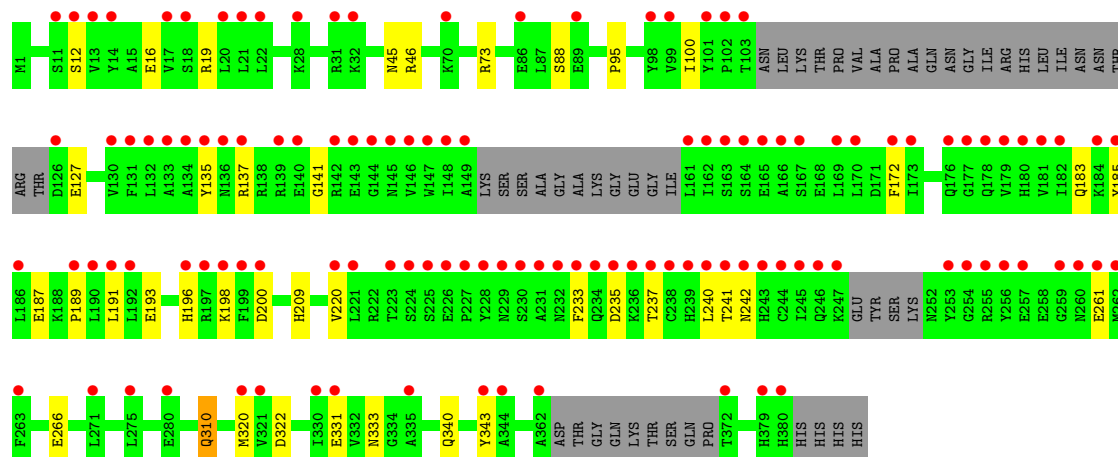
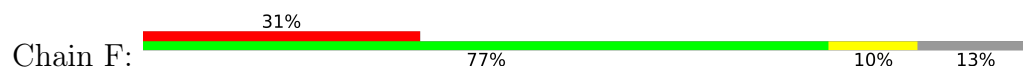




• Molecule 3: Stathmin-4



• 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	105.31Å 157.53Å 182.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.99 – 2.69 46.99 – 2.69	Depositor EDS
% Data completeness (in resolution range)	97.7 (46.99-2.69) 97.6 (46.99-2.69)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.05 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, R_{free}	0.224 , 0.248 0.227 , 0.249	Depositor DCC
R_{free} test set	806 reflections (0.95%)	wwPDB-VP
Wilson B-factor (Å ²)	42.2	Xtriage
Anisotropy	0.063	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 38.4	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	34712	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.62% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GDP, CA, MG, ACP, GOL, GTP, AF6, 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	0.37	0/3494	0.68	0/4743
1	C	0.38	0/3521	0.64	0/4781
2	B	0.36	0/3436	0.66	1/4654 (0.0%)
2	D	0.34	0/3382	0.69	0/4581
3	E	0.34	0/1008	0.64	0/1337
4	F	0.31	0/2806	0.65	1/3791 (0.0%)
All	All	0.35	0/17647	0.67	2/23887 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	172	PHE	N-CA-C	-5.54	105.64	112.90
2	B	42	LEU	N-CA-C	-5.07	106.93	113.01

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3416	3317	3330	15	0
1	C	3443	3340	3353	19	0
2	B	3361	3225	3238	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	3309	3179	3189	32	0
3	E	1000	1014	1018	5	0
4	F	2744	2698	2709	21	0
5	A	32	10	12	0	0
5	C	32	10	12	0	0
5	D	32	10	12	2	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	C	1	0	0	0	0
8	A	6	8	8	0	0
9	B	28	10	12	0	0
10	B	12	12	12	0	0
11	B	21	15	0	0	0
11	D	21	15	0	1	0
12	F	31	4	14	8	0
13	A	68	0	0	8	2
13	B	76	0	0	8	0
13	C	130	0	0	11	2
13	D	20	0	0	3	0
13	E	20	0	0	3	0
13	F	37	0	0	0	0
All	All	17845	16867	16919	116	2

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 3.

All (116) 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)
4:F:137:ARG:O	4:F:141:GLY:N	2.17	0.77
1:C:347[B]:CYS:O	13:C:601:HOH:O	2.08	0.69
2:B:428:ALA:O	13:B:601:HOH:O	2.12	0.68
1:A:207:GLU:OE2	13:A:601:HOH:O	2.11	0.68
1:C:327:ASP:OD2	13:C:602:HOH:O	2.12	0.68
2:D:86:ARG:NH1	2:D:88:ASP:OD2	2.27	0.68
1:C:368:LEU:O	13:C:603:HOH:O	2.13	0.67
3:E:6:MET:N	13:E:201:HOH:O	2.28	0.67
1:A:161:TYR:O	13:A:602:HOH:O	2.13	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:367:ASP:O	13:C:604:HOH:O	2.15	0.65
1:A:229:ARG:NH2	13:A:604:HOH:O	2.16	0.64
4:F:333:ASN:ND2	12:F:401:ACP:O2G	2.28	0.64
2:D:107:THR:OG1	2:D:108:GLU:N	2.29	0.63
2:B:31:ASP:OD1	2:B:35:SER:N	2.31	0.62
4:F:340:GLN:N	4:F:340:GLN:OE1	2.34	0.61
2:D:379:LYS:O	13:D:601:HOH:O	2.16	0.60
1:A:433:GLU:OE1	4:F:46:ARG:NH1	2.35	0.60
1:A:423:GLU:OE1	13:A:603:HOH:O	2.15	0.60
2:D:2:ARG:NH1	2:D:129:CYS:SG	2.71	0.59
4:F:200:ASP:OD1	4:F:241:THR:OG1	2.18	0.59
1:C:178:SER:OG	1:C:183:GLU:OE1	2.18	0.59
12:F:401:ACP:O1A	12:F:401:ACP:H3B2	2.02	0.59
2:B:302:ALA:O	2:B:380:ARG:NH2	2.36	0.58
4:F:185:TYR:OH	4:F:198:LYS:NZ	2.36	0.58
1:C:1:MET:N	13:C:613:HOH:O	2.34	0.58
1:C:215:ARG:NH1	13:C:614:HOH:O	2.36	0.57
2:D:31:ASP:O	2:D:34:GLY:N	2.37	0.57
2:B:301:ALA:O	2:B:303:CYS:N	2.37	0.56
1:C:221:ARG:NH1	2:D:323:MET:SD	2.78	0.56
2:D:88:ASP:OD1	2:D:88:ASP:N	2.39	0.56
4:F:331:GLU:OE2	12:F:401:ACP:H3B2	2.05	0.56
2:D:3:GLU:N	2:D:3:GLU:OE2	2.38	0.56
1:C:100:ALA:HA	2:D:252:LYS:HG2	1.88	0.55
2:D:73:MET:SD	2:D:76:VAL:HG22	2.46	0.55
2:D:253:LEU:HB3	11:D:502:AF6:C10	2.37	0.55
1:A:229:ARG:NE	13:A:604:HOH:O	2.24	0.55
2:B:33:THR:O	2:B:58:LYS:NZ	2.37	0.54
2:B:36:TYR:OH	2:B:40:SER:O	2.25	0.54
1:C:350:GLY:O	13:C:605:HOH:O	2.18	0.54
2:D:67:ASP:OD1	2:D:68:LEU:N	2.37	0.54
2:B:282:ARG:NH2	2:B:288:GLU:OE2	2.40	0.54
1:A:166:LYS:NZ	13:A:602:HOH:O	2.41	0.53
2:B:216:LYS:NZ	13:B:610:HOH:O	2.30	0.53
2:B:224:ASP:OD1	2:B:276:ARG:NH2	2.42	0.53
1:C:347[A]:CYS:O	13:C:601:HOH:O	2.18	0.52
2:D:406:MET:O	2:D:409:THR:N	2.42	0.52
2:B:405:GLU:OE2	13:B:602:HOH:O	2.19	0.52
1:C:179:THR:O	1:C:179:THR:OG1	2.27	0.52
1:C:414:GLU:OE1	13:C:606:HOH:O	2.19	0.51
2:B:397:TRP:O	13:B:603:HOH:O	2.19	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:331:GLU:OE2	12:F:401:ACP:O2G	2.28	0.51
4:F:241:THR:HG23	12:F:401:ACP:O2'	2.11	0.51
2:D:76:VAL:O	2:D:82:GLY:HA2	2.11	0.50
1:C:244:PHE:CD1	1:C:358:GLN:HG3	2.47	0.50
1:A:76:ASP:OD1	1:A:79:ARG:NH1	2.43	0.50
4:F:193:GLU:OE2	4:F:196:HIS:ND1	2.32	0.50
2:B:192:LEU:O	2:B:196:THR:OG1	2.30	0.50
2:D:85:PHE:HB2	2:D:90:PHE:HZ	1.76	0.49
1:A:263:PRO:O	1:A:266:HIS:ND1	2.42	0.49
1:A:417:GLU:OE1	13:A:605:HOH:O	2.20	0.49
2:D:287:PRO:HA	2:D:329:GLN:HG2	1.95	0.48
4:F:242:ASN:OD1	12:F:401:ACP:H5'1	2.14	0.48
4:F:331:GLU:OE2	12:F:401:ACP:C3B	2.61	0.48
2:D:73:MET:HG3	2:D:92:PHE:CE2	2.49	0.48
4:F:320:MET:HE1	12:F:401:ACP:H2	1.96	0.47
4:F:189:PRO:HA	4:F:322:ASP:HA	1.95	0.47
3:E:10:GLU:OE1	3:E:12:ASN:ND2	2.44	0.47
2:B:52:ASN:OD1	2:B:62:ARG:NH2	2.48	0.47
2:D:44:LEU:HA	2:D:47:ILE:HB	1.96	0.47
2:D:248:ALA:HB1	2:D:253:LEU:HD11	1.96	0.46
2:D:143:THR:N	5:D:501:GTP:O2B	2.46	0.46
2:D:73:MET:SD	2:D:90:PHE:CE2	3.09	0.46
4:F:193:GLU:OE1	4:F:196:HIS:N	2.49	0.46
2:D:31:ASP:HB3	2:D:32:PRO:HD2	1.99	0.45
2:D:73:MET:HE3	2:D:77:ARG:CZ	2.46	0.45
2:D:215:LEU:HG	13:D:602:HOH:O	2.17	0.45
2:B:2:ARG:NH1	2:B:249:ASP:OD2	2.50	0.45
2:D:174:LYS:NZ	2:D:205:GLU:OE2	2.50	0.45
4:F:95:PRO:HB2	4:F:183:GLN:CG	2.48	0.44
3:E:141:GLU:HA	13:E:204:HOH:O	2.17	0.44
2:B:216:LYS:CE	13:B:610:HOH:O	2.65	0.44
2:B:405:GLU:HG3	13:B:602:HOH:O	2.17	0.44
2:B:170:MET:HG3	2:B:377:LEU:HD11	1.99	0.44
2:B:371:SER:N	13:B:618:HOH:O	2.43	0.44
2:D:31:ASP:HB3	2:D:32:PRO:CD	2.47	0.44
2:D:181:GLU:N	2:D:182:PRO:HD2	2.32	0.44
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.36	0.43
3:E:24:LEU:CD2	13:E:201:HOH:O	2.66	0.43
2:D:238:THR:HB	2:D:316:ILE:HD13	2.01	0.43
2:B:21:TRP:O	2:B:25:SER:OG	2.35	0.43
2:B:247:ASN:O	2:B:247:ASN:ND2	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:209:HIS:HB2	4:F:310:GLN:CG	2.48	0.43
2:B:25:SER:OG	2:B:51:TYR:OH	2.36	0.43
1:C:229:ARG:HD2	13:C:630:HOH:O	2.18	0.42
2:D:268:PRO:HG2	2:D:300:MET:HB2	2.01	0.42
4:F:220:VAL:HG21	4:F:261:GLU:HG2	2.02	0.42
2:B:139:LEU:HD12	2:B:170:MET:SD	2.59	0.42
3:E:125:GLU:HG2	3:E:128:LYS:HE3	2.01	0.42
1:C:254:GLU:HA	13:C:651:HOH:O	2.19	0.42
1:A:209:ILE:HD11	1:A:302:MET:SD	2.60	0.42
2:D:181:GLU:OE1	5:D:501:GTP:O3'	2.33	0.41
4:F:209:HIS:HB2	4:F:310:GLN:HG3	2.01	0.41
1:A:180:ALA:HB3	1:A:183:GLU:HG3	2.01	0.41
1:A:229:ARG:CZ	13:A:604:HOH:O	2.54	0.41
1:C:71:GLU:OE2	1:C:73:THR:OG1	2.36	0.41
2:D:286:VAL:HB	2:D:287:PRO:HD3	2.02	0.41
2:B:145:SER:OG	2:B:188:SER:OG	2.36	0.41
1:C:71:GLU:HG2	1:C:72:PRO:HD2	2.03	0.41
1:C:244:PHE:CG	1:C:358:GLN:HG3	2.55	0.41
1:A:166:LYS:HE2	1:A:197:HIS:O	2.21	0.41
2:D:210:ILE:O	13:D:602:HOH:O	2.22	0.41
4:F:340:GLN:HA	4:F:343:TYR:HD2	1.86	0.41
2:B:2:ARG:NH1	13:B:628:HOH:O	2.53	0.40
4:F:16:GLU:OE2	4:F:19:ARG:NH1	2.54	0.40
1:A:221:ARG:HH11	2:B:323:MET:HB3	1.86	0.40
2:B:106:TYR:OH	2:B:407:GLU:OE2	2.38	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:A:633:HOH:O	13:C:718:HOH:O[3_545]	2.01	0.19
13:A:633:HOH:O	13:C:725:HOH:O[3_545]	2.13	0.07

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%)	421 (97%)	14 (3%)	0	100	100
1	C	439/450 (98%)	429 (98%)	10 (2%)	0	100	100
2	B	425/445 (96%)	415 (98%)	9 (2%)	1 (0%)	43	68
2	D	417/445 (94%)	402 (96%)	15 (4%)	0	100	100
3	E	117/143 (82%)	114 (97%)	3 (3%)	0	100	100
4	F	324/384 (84%)	314 (97%)	10 (3%)	0	100	100
All	All	2157/2317 (93%)	2095 (97%)	61 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	302	ALA

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%)	368 (100%)	0	100	100
1	C	372/378 (98%)	369 (99%)	3 (1%)	73	88
2	B	369/383 (96%)	366 (99%)	3 (1%)	73	88
2	D	364/383 (95%)	353 (97%)	11 (3%)	36	66
3	E	109/127 (86%)	107 (98%)	2 (2%)	51	78
4	F	301/342 (88%)	286 (95%)	15 (5%)	22	48
All	All	1883/1991 (95%)	1849 (98%)	34 (2%)	51	78

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	46	ARG

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Mol	Chain	Res	Type
2	B	53	GLU
2	B	238	THR
1	C	177	VAL
1	C	179	THR
1	C	251	ASP
2	D	11	GLN
2	D	76	VAL
2	D	86	ARG
2	D	88	ASP
2	D	179	VAL
2	D	247	ASN
2	D	285	THR
2	D	288	GLU
2	D	316	ILE
2	D	323	MET
2	D	356	ILE
3	E	51	GLN
3	E	77	GLU
4	F	12	SER
4	F	45	ASN
4	F	73	ARG
4	F	88	SER
4	F	100	ILE
4	F	127	GLU
4	F	135	TYR
4	F	187	GLU
4	F	191	LEU
4	F	233	PHE
4	F	235	ASP
4	F	237	THR
4	F	240	LEU
4	F	266	GLU
4	F	310	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	A	85	GLN
1	A	88	HIS
1	A	216	ASN
1	A	300	ASN

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Mol	Chain	Res	Type
1	A	342	GLN
1	A	393	HIS
2	B	165	ASN
2	B	191	GLN
2	B	245	GLN
2	B	332	ASN
2	B	375	GLN
1	C	15	GLN
1	C	342	GLN
1	C	356	ASN
1	C	393	HIS
2	D	191	GLN
2	D	247	ASN
2	D	347	ASN
4	F	178	GLN
4	F	239	HIS
4	F	269	GLN
4	F	306	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 6 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	$\# Z > 2$
8	GOL	A	504	-	5,5,5	0.40	0	5,5,5	0.17	0
11	AF6	D	502	-	24,24,24	1.84	5 (20%)	32,33,33	1.08	2 (6%)
10	MES	B	503	-	12,12,12	2.26	1 (8%)	15,16,16	2.14	4 (26%)
11	AF6	B	504	-	24,24,24	1.78	5 (20%)	32,33,33	1.11	3 (9%)
12	ACP	F	401	-	31,33,33	1.52	6 (19%)	47,52,52	2.18	18 (38%)
5	GTP	C	501	6	33,34,34	0.90	1 (3%)	50,54,54	1.52	10 (20%)
9	GDP	B	501	6	29,30,30	1.23	4 (13%)	45,47,47	1.63	6 (13%)
5	GTP	A	501	6	33,34,34	0.96	0	50,54,54	1.53	8 (16%)
5	GTP	D	501	6	33,34,34	0.92	1 (3%)	50,54,54	1.58	9 (18%)

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
8	GOL	A	504	-	-	2/4/4/4	-
11	AF6	D	502	-	-	0/5/5/5	0/4/4/4
10	MES	B	503	-	-	4/6/14/14	0/1/1/1
11	AF6	B	504	-	-	0/5/5/5	0/4/4/4
12	ACP	F	401	-	-	2/19/38/38	0/3/3/3
5	GTP	C	501	6	-	8/22/38/38	0/3/3/3
9	GDP	B	501	6	-	3/16/32/32	0/3/3/3
5	GTP	A	501	6	-	8/22/38/38	0/3/3/3
5	GTP	D	501	6	-	5/22/38/38	0/3/3/3

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	503	MES	C8-S	-7.61	1.66	1.77
11	D	502	AF6	C12-N14	7.00	1.46	1.36
11	B	504	AF6	C12-N14	6.69	1.46	1.36
9	B	501	GDP	C6-N1	-3.21	1.32	1.38
12	F	401	ACP	C5-C4	3.15	1.44	1.39
12	F	401	ACP	C5-N7	-3.09	1.33	1.39
12	F	401	ACP	C8-N9	-2.97	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	501	GDP	C5-C4	2.94	1.46	1.38
11	B	504	AF6	C06-C05	-2.61	1.37	1.41
12	F	401	ACP	PG-O2G	2.51	1.60	1.55
11	D	502	AF6	C06-C05	-2.46	1.37	1.41
11	B	504	AF6	C10-C08	2.40	1.43	1.39
11	D	502	AF6	C13-C07	2.35	1.43	1.39
11	D	502	AF6	C10-C08	2.35	1.43	1.39
5	D	501	GTP	C2-N3	2.29	1.38	1.33
11	B	504	AF6	C13-C07	2.24	1.43	1.39
12	F	401	ACP	C5-C6	2.18	1.47	1.41
9	B	501	GDP	C5-N7	-2.18	1.34	1.39
9	B	501	GDP	C4-N9	-2.09	1.32	1.38
11	B	504	AF6	C07-C08	-2.07	1.38	1.41
11	D	502	AF6	C07-C08	-2.06	1.38	1.41
5	C	501	GTP	C2-N3	2.00	1.38	1.33
12	F	401	ACP	PG-O3G	2.00	1.59	1.55

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	F	401	ACP	C5-C4-N3	-6.59	117.64	126.72
10	B	503	MES	C5-N4-C3	6.32	122.46	108.84
9	B	501	GDP	C5-C4-N3	-5.44	119.73	128.39
5	D	501	GTP	C5-C4-N3	-5.08	120.30	128.39
12	F	401	ACP	N3-C4-N9	4.78	135.29	127.17
5	A	501	GTP	C5-C4-N3	-4.72	120.88	128.39
5	C	501	GTP	C5-C4-N3	-4.67	120.96	128.39
5	C	501	GTP	C2-N3-C4	4.60	120.23	112.30
5	D	501	GTP	C2-N3-C4	4.58	120.18	112.30
5	A	501	GTP	C2-N3-C4	4.50	120.05	112.30
9	B	501	GDP	N9-C4-N3	4.44	134.84	125.95
9	B	501	GDP	C2-N3-C4	4.43	119.92	112.30
12	F	401	ACP	C4-C5-N7	-4.33	105.63	110.58
12	F	401	ACP	C2-N3-C4	4.18	122.04	111.83
11	D	502	AF6	C10-N11-C12	4.13	121.70	117.83
11	B	504	AF6	C10-N11-C12	4.04	121.62	117.83
12	F	401	ACP	N3-C2-N1	-3.78	122.86	128.58
12	F	401	ACP	O2G-PG-O1G	-3.77	102.63	112.39
5	D	501	GTP	N9-C4-N3	3.41	132.78	125.95
9	B	501	GDP	C6-C5-N7	3.26	136.21	130.29
12	F	401	ACP	C5-N7-C8	3.24	108.54	103.45
10	B	503	MES	C7-N4-C5	3.21	119.80	111.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	F	401	ACP	PB-O3A-PA	-3.15	122.11	132.37
5	A	501	GTP	N9-C4-N3	3.00	131.95	125.95
5	D	501	GTP	C2-N1-C6	-2.87	119.90	125.11
5	C	501	GTP	N9-C4-N3	2.79	131.53	125.95
5	D	501	GTP	N9-C8-N7	-2.72	108.36	113.40
5	A	501	GTP	N9-C8-N7	-2.70	108.40	113.40
5	C	501	GTP	N9-C8-N7	-2.63	108.53	113.40
5	D	501	GTP	C8-N7-C5	2.57	108.84	104.26
5	A	501	GTP	C2-N1-C6	-2.56	120.47	125.11
5	C	501	GTP	C2-N1-C6	-2.54	120.50	125.11
10	B	503	MES	O3S-S-C8	2.51	110.92	106.00
5	A	501	GTP	C8-N7-C5	2.50	108.71	104.26
5	D	501	GTP	C5-C6-N1	2.49	119.60	113.25
5	C	501	GTP	C5-C6-N1	2.43	119.45	113.25
11	B	504	AF6	C16-C15-N14	-2.41	106.91	113.60
5	A	501	GTP	O6-C6-C5	-2.41	120.18	126.53
5	C	501	GTP	C8-N7-C5	2.39	108.52	104.26
12	F	401	ACP	O2G-PG-C3B	2.39	112.19	106.40
5	D	501	GTP	O6-C6-C5	-2.38	120.24	126.53
5	A	501	GTP	C5-C6-N1	2.38	119.31	113.25
12	F	401	ACP	O3G-PG-C3B	2.27	111.90	106.40
12	F	401	ACP	C6-C5-N7	2.26	136.45	132.09
12	F	401	ACP	C2-N1-C6	2.26	122.44	118.73
5	C	501	GTP	O6-C6-C5	-2.26	120.57	126.53
12	F	401	ACP	N9-C8-N7	-2.24	110.76	113.94
12	F	401	ACP	O2A-PA-O3A	2.20	113.23	107.27
12	F	401	ACP	O1G-PG-C3B	-2.20	106.58	111.37
12	F	401	ACP	C4-N9-C8	2.15	108.00	105.74
9	B	501	GDP	O3B-PB-O3A	2.15	111.83	104.64
11	D	502	AF6	C13-C12-N11	-2.13	120.13	122.92
10	B	503	MES	O1S-S-C8	2.12	109.93	106.73
12	F	401	ACP	O3G-PG-O2G	2.12	114.00	107.96
9	B	501	GDP	C4-C5-N7	-2.12	107.31	110.67
5	D	501	GTP	O2B-PB-O3B	2.12	112.99	107.27
12	F	401	ACP	O1B-PB-C3B	-2.11	103.50	109.05
5	C	501	GTP	O2A-PA-O3A	2.09	112.93	107.27
11	B	504	AF6	C13-C12-N11	-2.02	120.27	122.92
5	C	501	GTP	N1-C2-N3	-2.00	119.65	123.32

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	501	GTP	PB-O3B-PG-O2G
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	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	A	504	GOL	O1-C1-C2-C3
9	B	501	GDP	C5'-O5'-PA-O3A
9	B	501	GDP	C5'-O5'-PA-O1A
9	B	501	GDP	C5'-O5'-PA-O2A
10	B	503	MES	C8-C7-N4-C5
10	B	503	MES	C7-C8-S-O1S
10	B	503	MES	C7-C8-S-O2S
10	B	503	MES	C7-C8-S-O3S
12	F	401	ACP	O4'-C4'-C5'-O5'
12	F	401	ACP	C3'-C4'-C5'-O5'
8	A	504	GOL	O1-C1-C2-O2
5	C	501	GTP	PB-O3B-PG-O1G
5	C	501	GTP	PB-O3A-PA-O2A
5	C	501	GTP	C4'-C5'-O5'-PA
5	D	501	GTP	PB-O3B-PG-O1G
5	C	501	GTP	PB-O3B-PG-O2G
5	C	501	GTP	PB-O3B-PG-O3G
5	D	501	GTP	PB-O3B-PG-O2G
5	A	501	GTP	PB-O3A-PA-O1A
5	A	501	GTP	PB-O3A-PA-O2A
5	A	501	GTP	PB-O3B-PG-O1G
5	A	501	GTP	C4'-C5'-O5'-PA

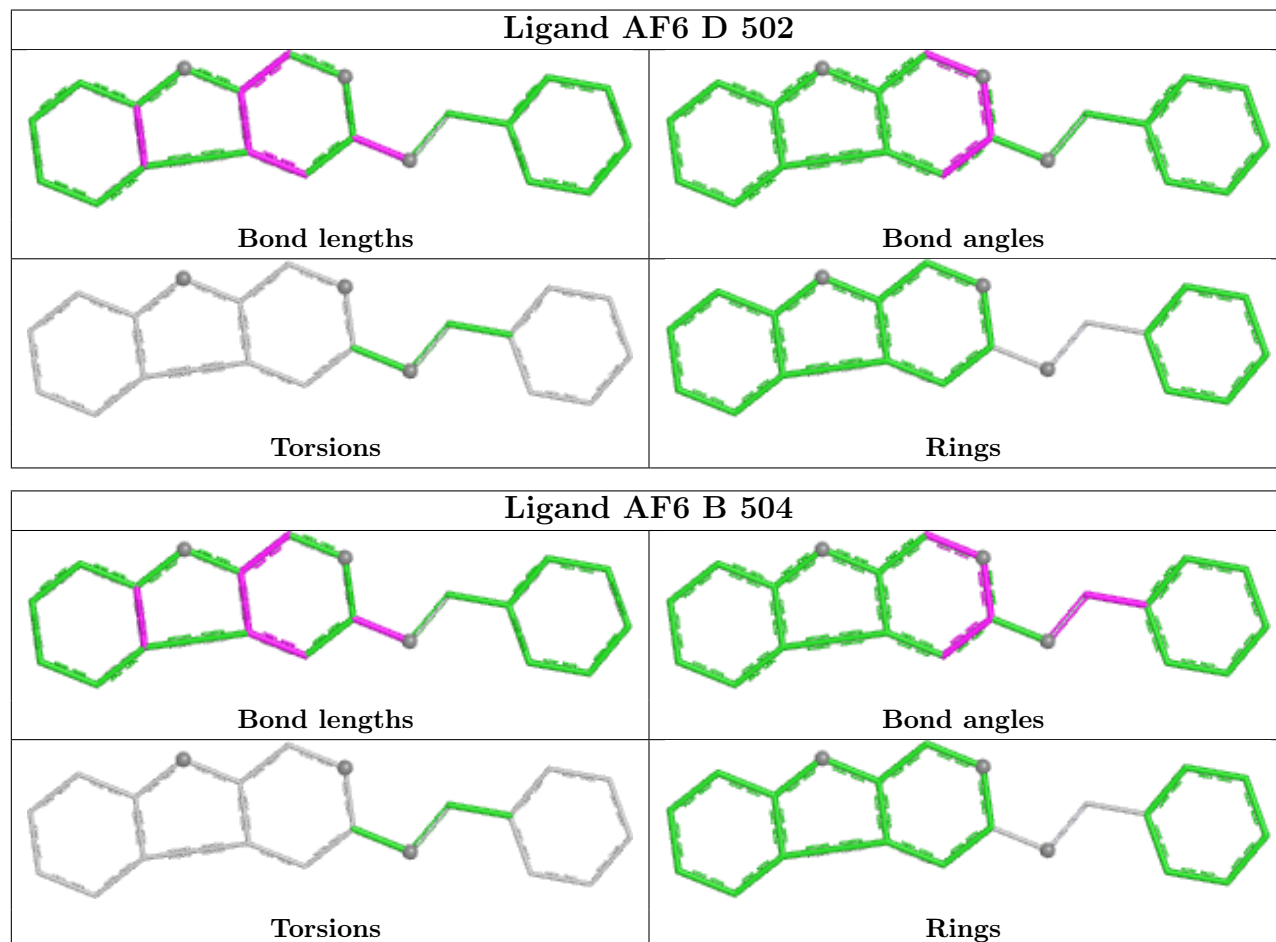
There are no ring outliers.

3 monomers are involved in 11 short contacts:

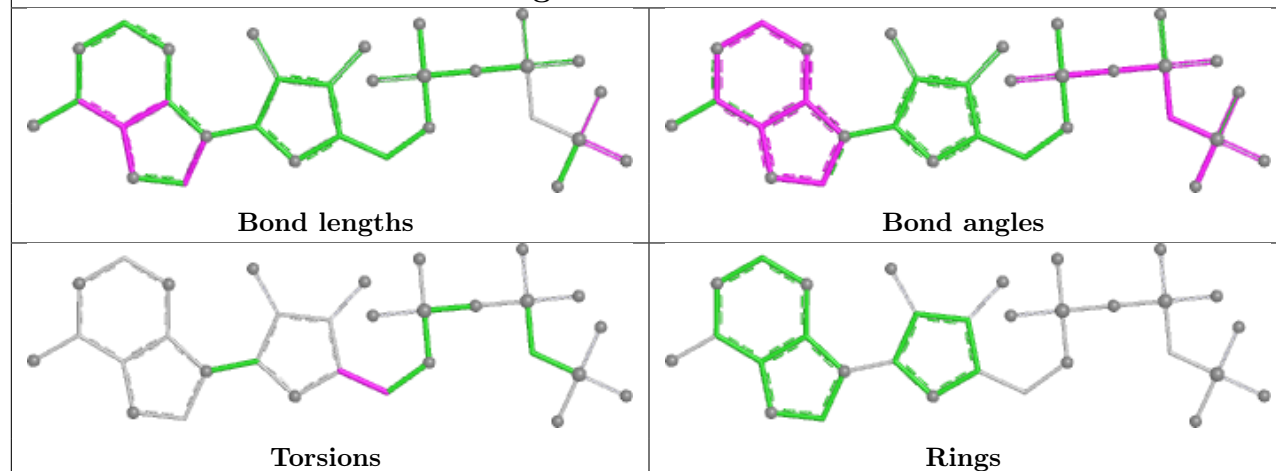
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	D	502	AF6	1	0
12	F	401	ACP	8	0
5	D	501	GTP	2	0

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

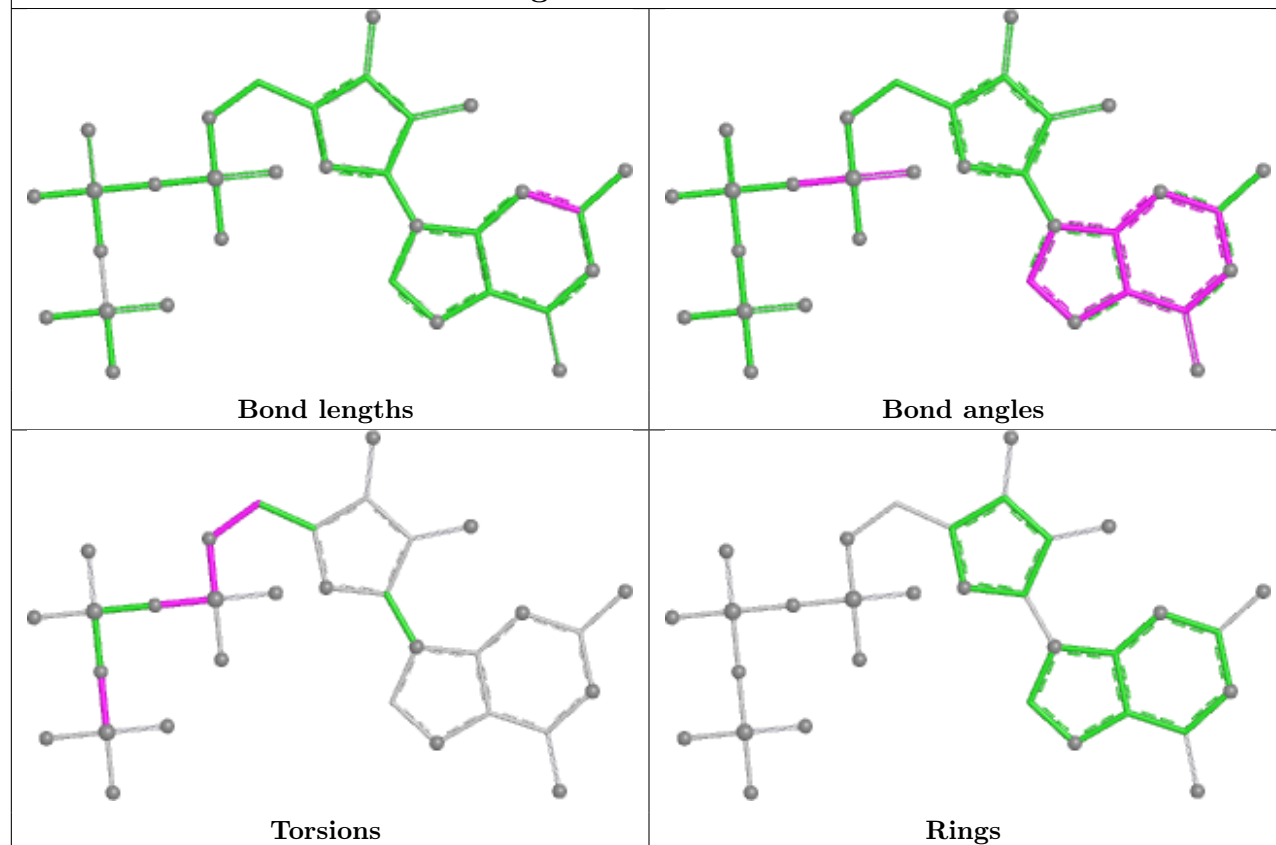
addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. 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.

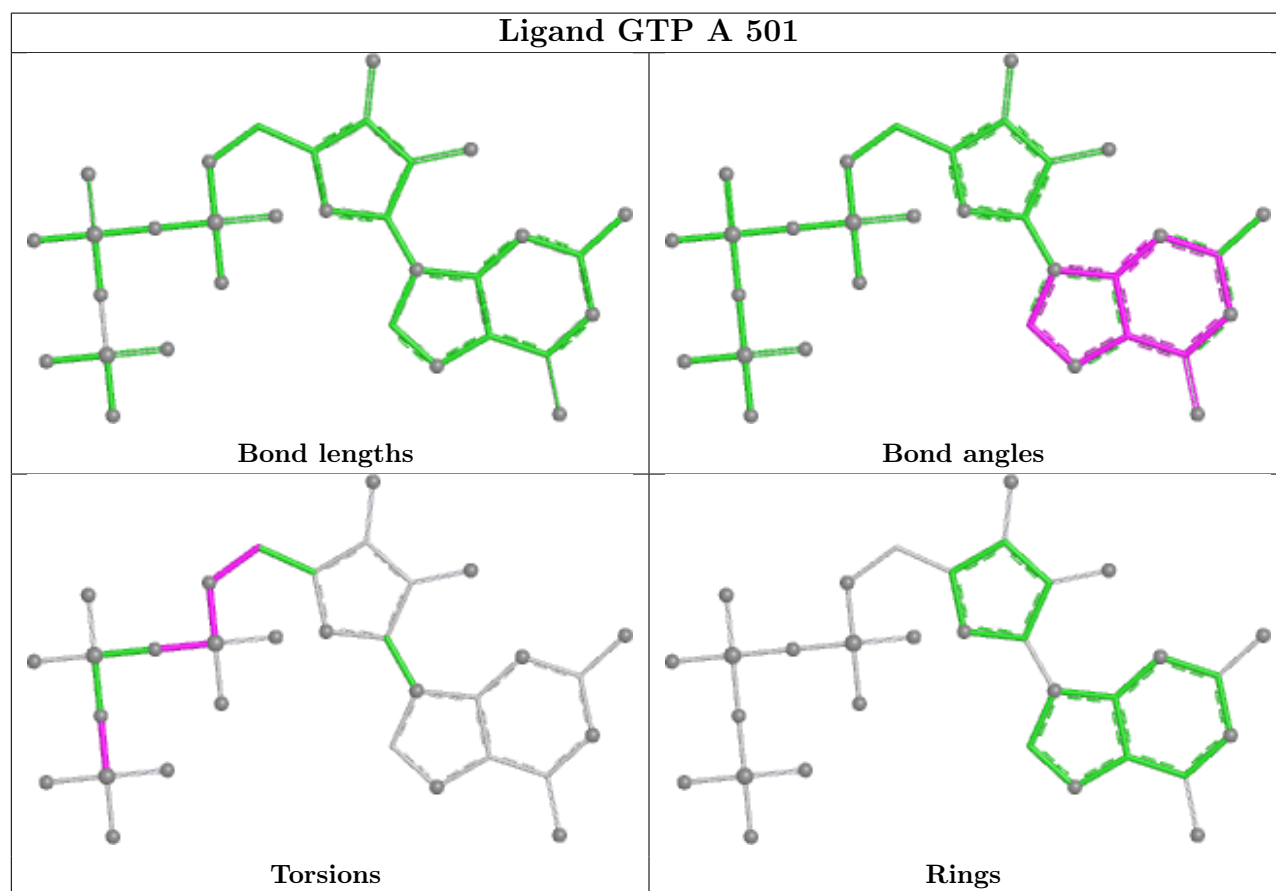
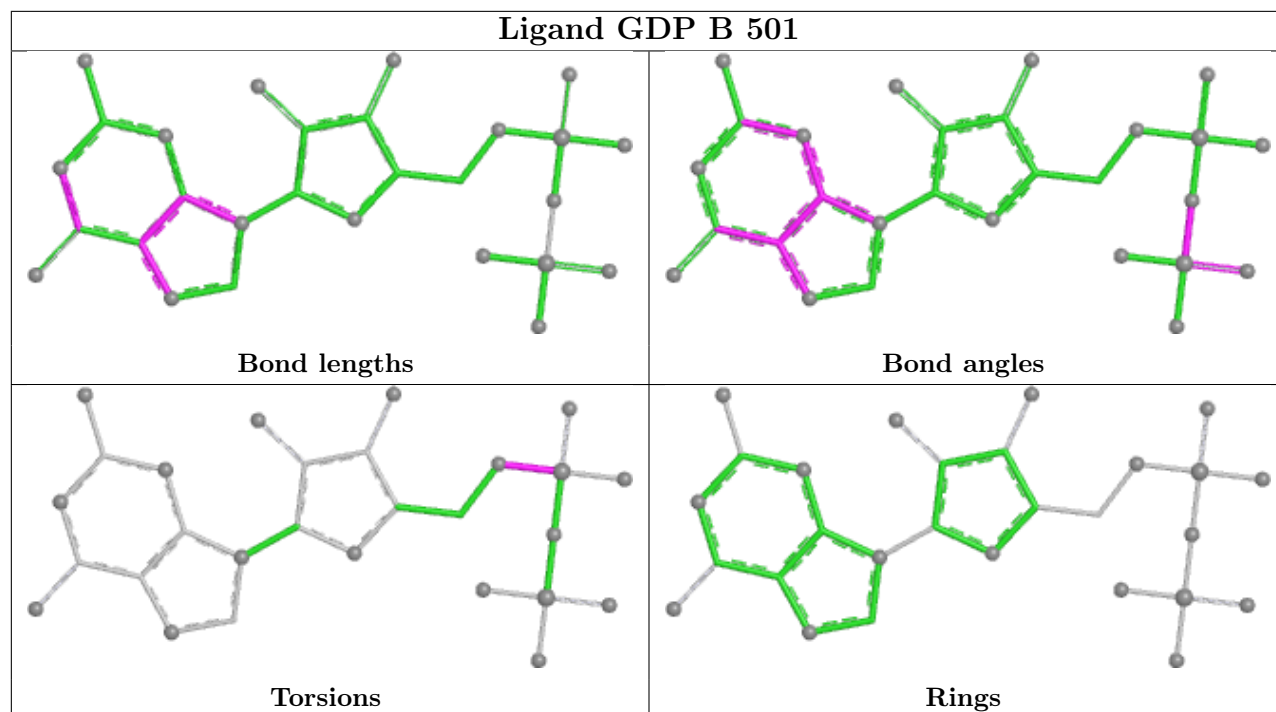


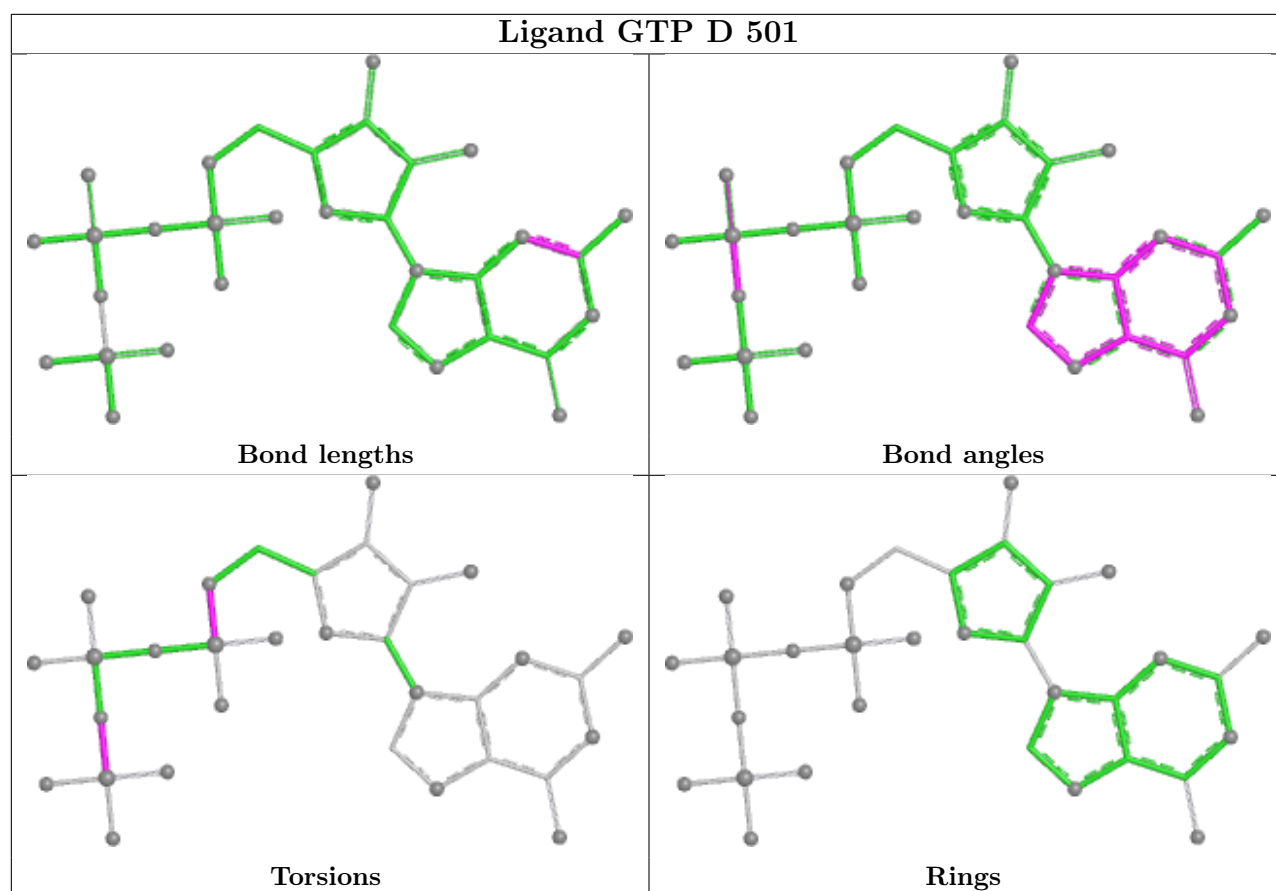
Ligand ACP F 401



Ligand GTP C 501







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%)	0.28	9 (2%) 63 61	21, 39, 70, 98	0
1	C	440/450 (97%)	-0.04	16 (3%) 46 42	16, 29, 59, 79	1 (0%)
2	B	427/445 (95%)	0.54	52 (12%) 8 7	18, 39, 90, 137	0
2	D	421/445 (94%)	1.57	136 (32%) 1 1	27, 68, 106, 122	0
3	E	121/143 (84%)	1.09	24 (19%) 3 2	28, 61, 99, 115	0
4	F	334/384 (86%)	1.56	120 (35%) 1 0	33, 72, 139, 156	0
All	All	2180/2317 (94%)	0.76	357 (16%) 4 4	16, 48, 107, 156	1 (0%)

All (357) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	161	LEU	7.9
2	D	394	PHE	7.0
2	D	1	MET	6.1
4	F	240	LEU	6.0
2	D	246	LEU	5.9
4	F	233	PHE	5.8
1	C	179	THR	5.7
4	F	170	LEU	5.7
2	D	247	ASN	5.6
2	D	245	GLN	5.3
4	F	169	LEU	5.1
2	D	396	HIS	5.1
2	B	42	LEU	5.0
2	D	393	ALA	4.9
2	B	239	CYS	4.9
2	B	280	GLN	4.8
2	D	73	MET	4.8
4	F	166	ALA	4.7
2	D	172	SER	4.7

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Mol	Chain	Res	Type	RSRZ
2	D	90	PHE	4.5
4	F	199	PHE	4.5
2	B	248	ALA	4.5
2	B	246	LEU	4.5
2	B	57	ASN	4.5
4	F	186	LEU	4.4
2	B	275	SER	4.3
2	D	248	ALA	4.3
4	F	130	VAL	4.3
4	F	253	TYR	4.3
2	D	176	SER	4.2
4	F	245	ILE	4.2
2	D	48	ASN	4.2
2	D	54	ALA	4.2
2	D	403	MET	4.2
4	F	184	LYS	4.1
4	F	149	ALA	4.0
4	F	144	GLY	4.0
4	F	133	ALA	3.9
4	F	380	HIS	3.9
2	D	55	THR	3.9
2	B	56	GLY	3.9
4	F	163	SER	3.9
2	D	81	PHE	3.9
4	F	362	ALA	3.9
3	E	6	MET	3.9
3	E	50	ILE	3.8
4	F	235	ASP	3.8
1	C	340	SER	3.8
4	F	238	CYS	3.7
4	F	237	THR	3.7
2	D	108	GLU	3.7
4	F	177	GLY	3.7
2	D	210	ILE	3.7
4	F	225	SER	3.6
2	D	377	LEU	3.6
4	F	232	ASN	3.6
4	F	320	MET	3.6
2	D	407	GLU	3.6
2	D	395	LEU	3.6
2	B	247	ASN	3.5
4	F	230	SER	3.5

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Mol	Chain	Res	Type	RSRZ
4	F	162	ILE	3.5
2	D	214	THR	3.5
2	B	2	ARG	3.5
3	E	141	GLU	3.5
1	A	262	TYR	3.5
2	D	97	ALA	3.5
4	F	181	VAL	3.5
4	F	243	HIS	3.5
4	F	98	TYR	3.4
1	A	437	VAL	3.4
4	F	182	ILE	3.4
2	D	106	TYR	3.4
2	D	398	TYR	3.4
2	D	220	PRO	3.4
4	F	247	LYS	3.4
2	D	399	THR	3.4
2	B	277	GLY	3.4
2	D	88	ASP	3.4
2	D	408	PHE	3.4
2	B	126	SER	3.3
2	B	278	SER	3.3
2	D	217	LEU	3.3
4	F	172	PHE	3.3
2	D	219	THR	3.3
2	D	207	LEU	3.3
2	B	34	GLY	3.3
2	D	400	GLY	3.3
2	D	140	GLY	3.3
2	D	390	ARG	3.3
4	F	231	ALA	3.3
2	D	170	MET	3.2
3	E	115	HIS	3.2
4	F	173	ILE	3.2
2	D	177	ASP	3.2
2	B	245	GLN	3.2
2	D	36	TYR	3.2
2	D	99	ASN	3.2
2	D	100	ASN	3.2
4	F	176	GLN	3.2
2	D	59	TYR	3.2
2	D	179	VAL	3.1
4	F	228	TYR	3.1

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Mol	Chain	Res	Type	RSRZ
2	B	45	GLU	3.1
2	D	87	PRO	3.1
4	F	103	THR	3.1
1	C	341	ILE	3.1
2	B	212	PHE	3.1
4	F	185	TYR	3.1
2	D	389	PHE	3.1
4	F	189	PRO	3.1
2	D	60	VAL	3.1
2	D	92	PHE	3.1
2	D	175	VAL	3.1
4	F	224	SER	3.1
4	F	239	HIS	3.0
4	F	242	ASN	3.0
2	D	85	PHE	3.0
4	F	165	GLU	3.0
2	D	404	ASP	3.0
2	D	359	ARG	3.0
2	B	215	LEU	3.0
2	D	215	LEU	3.0
4	F	236	LYS	3.0
4	F	256	TYR	3.0
2	D	107	THR	3.0
4	F	241	THR	3.0
2	D	37	HIS	2.9
2	D	129	CYS	2.9
2	D	56	GLY	2.9
2	D	244	GLY	2.9
4	F	254	GLY	2.9
2	D	76	VAL	2.9
2	B	190	HIS	2.9
4	F	102	PRO	2.9
2	D	323	MET	2.9
2	D	2	ARG	2.9
2	D	142	GLY	2.9
2	D	360	GLY	2.9
2	D	218	THR	2.9
2	D	253	LEU	2.9
4	F	13	VAL	2.9
4	F	260	ASN	2.9
4	F	126	ASP	2.9
2	D	82	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
2	D	180	VAL	2.9
2	B	279	GLN	2.8
2	D	65	LEU	2.8
2	D	284	LEU	2.8
4	F	275	LEU	2.8
3	E	8	VAL	2.8
2	D	30	ILE	2.8
2	D	84	ILE	2.8
2	D	31	ASP	2.8
2	D	42	LEU	2.8
1	A	179	THR	2.8
2	B	214	THR	2.8
2	D	243	PRO	2.8
2	B	338	SER	2.8
3	E	46	SER	2.8
2	D	385	PHE	2.8
2	D	384	GLN	2.8
4	F	178	GLN	2.8
2	D	316	ILE	2.8
3	E	23	ILE	2.8
4	F	148	ILE	2.8
2	D	57	ASN	2.8
2	D	39	ASP	2.8
1	A	71	GLU	2.8
3	E	48	GLU	2.8
4	F	372	THR	2.8
2	D	24	ILE	2.7
4	F	167	SER	2.7
4	F	196	HIS	2.7
2	D	102	ALA	2.7
4	F	226	GLU	2.7
4	F	335	ALA	2.7
2	B	276	ARG	2.7
2	D	46	ARG	2.7
2	D	391	ARG	2.7
4	F	190	LEU	2.7
4	F	145	ASN	2.7
2	D	285	THR	2.7
4	F	137	ARG	2.7
2	D	381	ILE	2.7
4	F	17	VAL	2.7
2	D	171	PRO	2.7

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Mol	Chain	Res	Type	RSRZ
2	B	46	ARG	2.7
2	B	55	THR	2.7
2	D	320	ARG	2.6
2	D	110	ALA	2.6
4	F	146	VAL	2.6
4	F	101	TYR	2.6
2	D	388	MET	2.6
4	F	134	ALA	2.6
2	B	218	THR	2.6
2	B	274	THR	2.6
2	D	104	GLY	2.6
2	D	211	CYS	2.6
4	F	143	GLU	2.6
4	F	99	VAL	2.6
4	F	229	ASN	2.6
2	B	35	SER	2.6
2	B	43	GLN	2.6
2	D	221	THR	2.6
4	F	20	LEU	2.6
4	F	191	LEU	2.6
4	F	192	LEU	2.6
4	F	180	HIS	2.6
2	D	40	SER	2.5
3	E	28	SER	2.5
3	E	49	GLU	2.5
2	D	101	TRP	2.5
1	C	357	TYR	2.5
2	D	222	TYR	2.5
4	F	257	GLU	2.5
2	D	83	GLN	2.5
4	F	246	GLN	2.5
4	F	263	PHE	2.5
2	D	103	LYS	2.5
2	D	174	LYS	2.5
2	D	240	LEU	2.5
4	F	140	GLU	2.5
2	B	428	ALA	2.5
4	F	234	GLN	2.5
2	B	282	ARG	2.5
4	F	164	SER	2.5
2	B	128	ASP	2.5
4	F	259	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
2	D	291	GLN	2.5
4	F	179	VAL	2.5
2	D	226	ASN	2.4
4	F	244	CYS	2.4
2	B	37	HIS	2.4
2	D	13	GLY	2.4
2	D	80	PRO	2.4
4	F	227	PRO	2.4
2	D	112	LEU	2.4
4	F	330	ILE	2.4
1	C	347[A]	CYS	2.4
2	D	239	CYS	2.4
4	F	147	TRP	2.4
4	F	280	GLU	2.4
2	B	36	TYR	2.4
2	B	59	TYR	2.4
2	B	54	ALA	2.4
2	D	20	PHE	2.4
2	B	213	ARG	2.4
2	D	387	ALA	2.4
4	F	379	HIS	2.4
1	C	284	GLU	2.4
4	F	200	ASP	2.4
4	F	261	GLU	2.4
1	C	280	LYS	2.4
4	F	131	PHE	2.4
2	D	392	LYS	2.4
2	D	223	GLY	2.4
2	B	240	LEU	2.3
2	D	183	TYR	2.3
1	C	283	HIS	2.3
4	F	18	SER	2.3
2	D	187	LEU	2.3
2	D	208	TYR	2.3
1	A	88	HIS	2.3
4	F	262	MET	2.3
2	B	40	SER	2.3
2	B	244	GLY	2.3
1	A	250	VAL	2.3
4	F	221	LEU	2.3
1	A	282	TYR	2.3
4	F	223	THR	2.3

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Mol	Chain	Res	Type	RSRZ
2	D	297	LYS	2.3
2	D	335	ASN	2.3
2	D	405	GLU	2.3
4	F	331	GLU	2.3
1	C	46	ASP	2.3
1	C	178	SER	2.3
4	F	12	SER	2.3
2	D	11	GLN	2.3
2	D	32	PRO	2.3
4	F	197	ARG	2.3
4	F	32	LYS	2.2
2	D	69	GLU	2.2
4	F	136	ASN	2.2
1	C	342	GLN	2.2
4	F	11	SER	2.2
2	D	402	GLY	2.2
2	D	397	TRP	2.2
3	E	139	LEU	2.2
3	E	128	LYS	2.2
4	F	343	TYR	2.2
2	B	320	ARG	2.2
2	D	165	ASN	2.2
3	E	136	ASN	2.2
3	E	51	GLN	2.2
4	F	132	LEU	2.2
1	A	281	ALA	2.2
4	F	344	ALA	2.2
2	B	53	GLU	2.2
2	D	72	THR	2.2
1	C	285	GLN	2.2
3	E	16	SER	2.2
1	A	1	MET	2.2
1	C	1	MET	2.2
3	E	10	GLU	2.2
2	D	362	LYS	2.2
4	F	198	LYS	2.2
2	B	273	LEU	2.2
2	D	153	SER	2.2
4	F	139	ARG	2.1
4	F	70	LYS	2.1
2	B	30	ILE	2.1
2	D	105	HIS	2.1

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Mol	Chain	Res	Type	RSRZ
3	E	133	VAL	2.1
3	E	7	GLU	2.1
4	F	89	GLU	2.1
4	F	255	ARG	2.1
2	D	386	THR	2.1
4	F	28	LYS	2.1
2	D	356	ILE	2.1
4	F	86	GLU	2.1
2	D	43	GLN	2.1
2	B	335	ASN	2.1
2	D	96	GLY	2.1
4	F	135	TYR	2.1
2	D	294	PHE	2.1
4	F	31	ARG	2.1
2	D	58	LYS	2.1
3	E	140	LYS	2.1
2	D	406	MET	2.1
2	B	291	GLN	2.1
4	F	271	LEU	2.1
2	B	208	TYR	2.1
4	F	321	VAL	2.1
3	E	59	GLU	2.0
4	F	142	ARG	2.0
2	D	25	SER	2.0
3	E	27	PRO	2.0
4	F	21	LEU	2.0
2	B	337	ASN	2.0
2	D	71	GLY	2.0
1	C	440	VAL	2.0
2	B	333	VAL	2.0
4	F	14	TYR	2.0
4	F	220	VAL	2.0
1	C	87	PHE	2.0
2	D	74	ASP	2.0
3	E	127	ASP	2.0
2	D	122	LYS	2.0
3	E	24	LEU	2.0
3	E	64	GLN	2.0
4	F	22	LEU	2.0
2	B	227	HIS	2.0
2	B	47	ILE	2.0
2	B	48	ASN	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	2	ARG	2.0
2	D	77	ARG	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

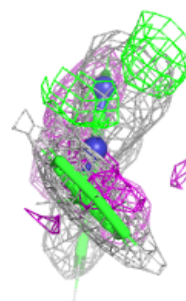
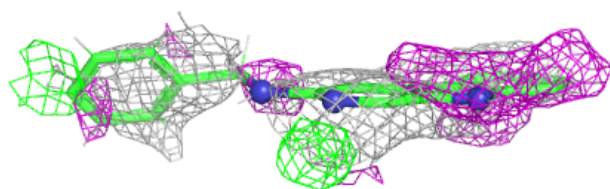
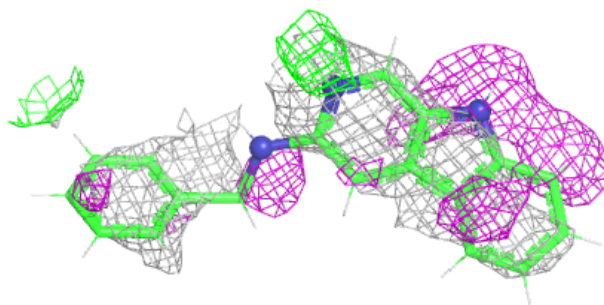
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	MG	D	503	1/1	0.59	0.24	89,89,89,89	0
11	AF6	D	502	21/21	0.69	0.20	48,58,70,72	0
12	ACP	F	401	31/31	0.77	0.17	83,91,118,118	0
5	GTP	D	501	32/32	0.88	0.15	51,61,87,128	0
8	GOL	A	504	6/6	0.93	0.13	32,53,64,65	0
11	AF6	B	504	21/21	0.93	0.11	29,34,44,48	0
10	MES	B	503	12/12	0.94	0.10	30,37,44,44	0
7	CA	A	503	1/1	0.94	0.07	57,57,57,57	0
6	MG	C	502	1/1	0.95	0.07	23,23,23,23	0
6	MG	B	502	1/1	0.95	0.07	23,23,23,23	0
9	GDP	B	501	28/28	0.96	0.08	15,23,29,35	0
5	GTP	A	501	32/32	0.97	0.08	19,26,34,36	0
6	MG	A	502	1/1	0.97	0.05	28,28,28,28	0
5	GTP	C	501	32/32	0.98	0.06	15,20,29,32	0
7	CA	C	503	1/1	0.99	0.02	40,40,40,40	0

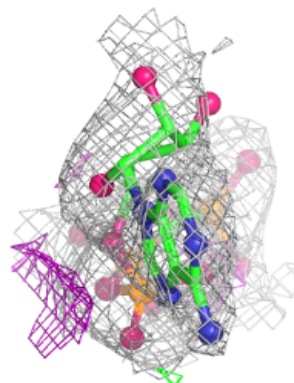
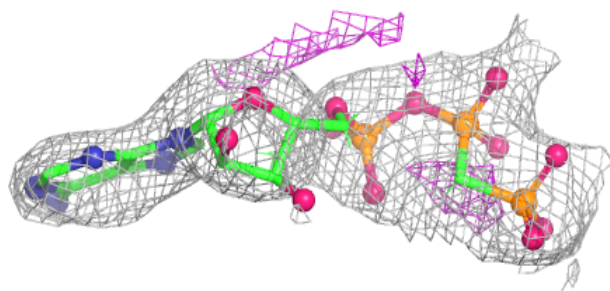
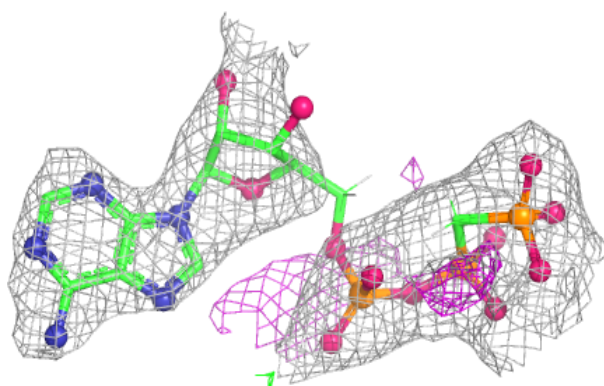
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around AF6 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)

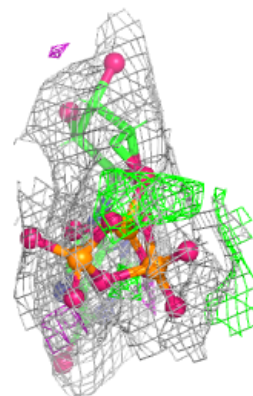
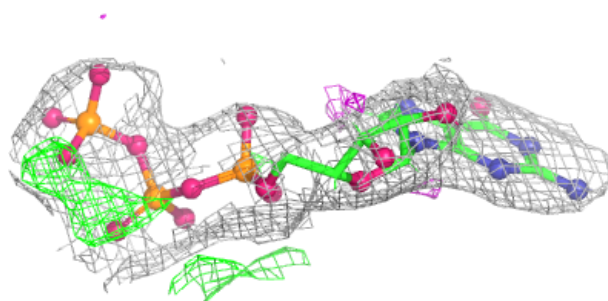
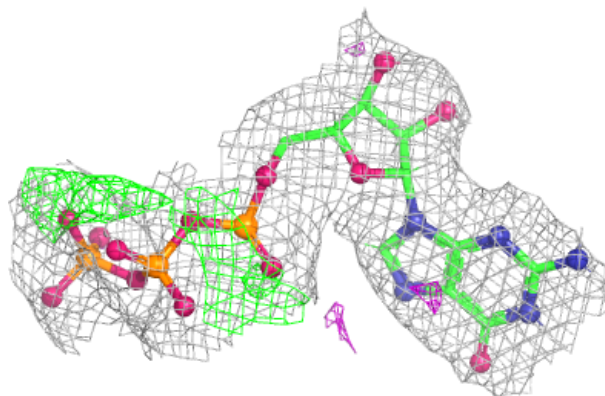
**Electron density around ACP F 401:**

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

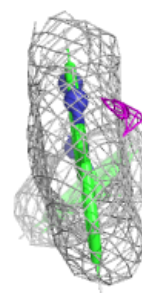
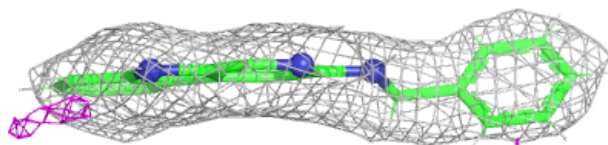
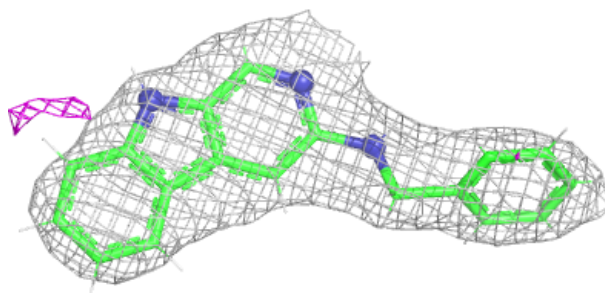


Electron density around GTP D 501:

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

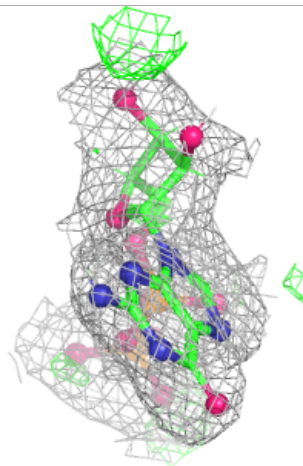
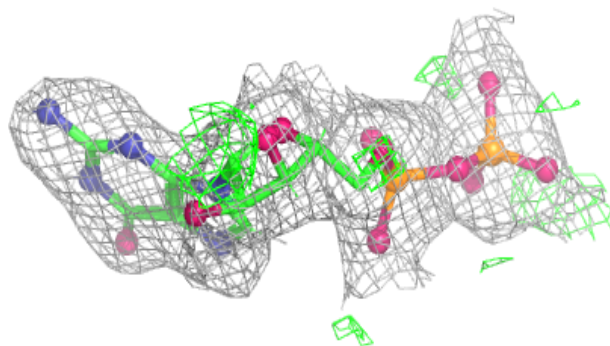
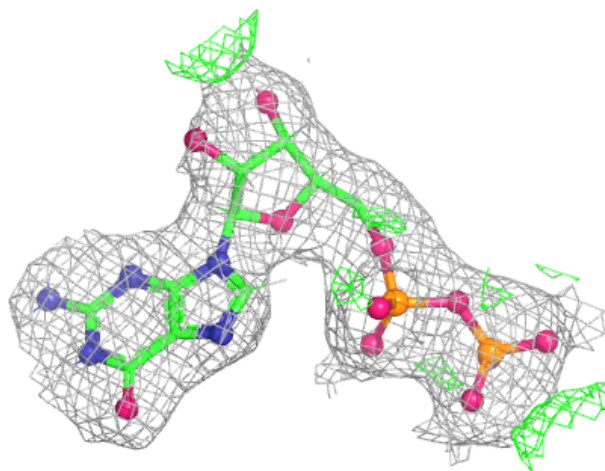
**Electron density around AF6 B 504:**

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



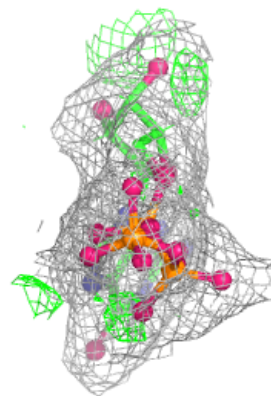
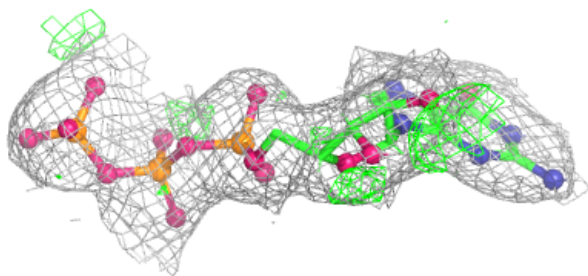
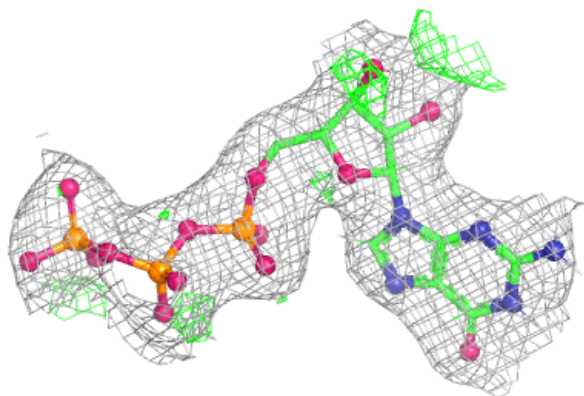
Electron density around GDP B 501:

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

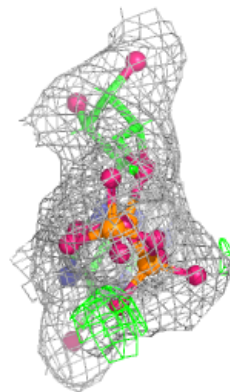
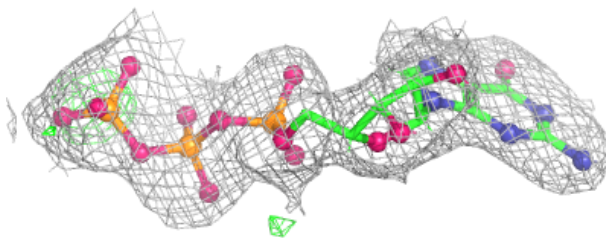
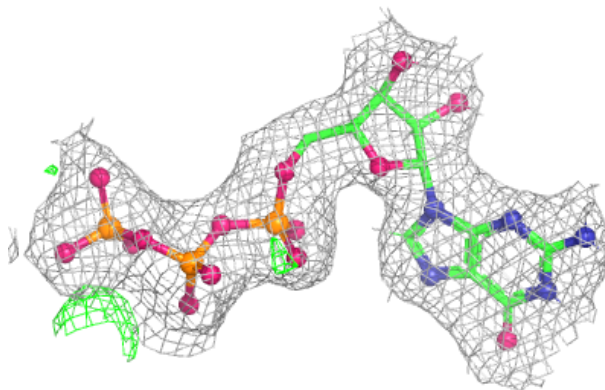


Electron density around GTP A 501:

$2mF_o-DF_c$ (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 ⓘ

There are no such residues in this entry.