



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 9, 2022 – 12:11 PM JST

PDB ID : 7CE8
Title : Crystal structure of T2R-TTL-Compound11 complex
Authors : Chen, L.J.; Chen, Q.; Yu, Y.; Yang, J.H.
Deposited on : 2020-06-22
Resolution : 2.73 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.31.2
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) : 2.31.2

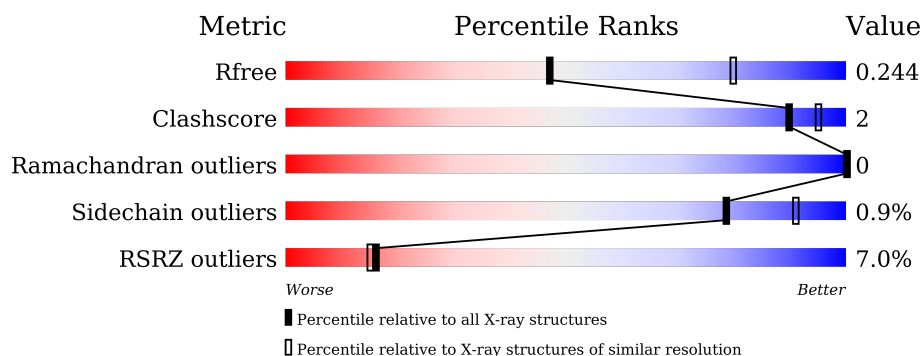
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.73 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	3359 (2.74-2.70)
Clashscore	141614	3686 (2.74-2.70)
Ramachandran outliers	138981	3622 (2.74-2.70)
Sidechain outliers	138945	3623 (2.74-2.70)
RSRZ outliers	127900	3276 (2.74-2.70)

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	<div> <div>95%</div> <div> <div></div> <div></div> <div></div> <div></div> </div> </div>
1	C	450	<div> <div>%</div> <div>95%</div> <div> <div></div> <div></div> <div></div> <div></div> </div> </div>
2	B	445	<div> <div>3%</div> <div>92%</div> <div> <div></div> <div></div> <div></div> <div></div> </div> </div>
2	D	445	<div> <div>10%</div> <div>89%</div> <div>6% 5%</div> <div> <div></div> <div></div> <div></div> <div></div> </div> </div>
3	E	143	<div> <div>6%</div> <div>83%</div> <div>15%</div> <div> <div></div> <div></div> <div></div> <div></div> </div> </div>
4	F	384	<div> <div>22%</div> <div>80%</div> <div>7% 13%</div> <div> <div></div> <div></div> <div></div> <div></div> </div> </div>

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 34705 atoms, of which 16903 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	3	0
			6755	2169	3327	583	652	24			
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
			6589	2110	3228	576	649	26			
2	D	421	Total	C	H	N	O	S	0	0	0
			6485	2080	3176	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	4	0
			2046	627	1028	186	200	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
			5441	1761	2697	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
5	A	1	Total	C	H	N	O	P	0	0
			42	10	10	5	14	3		
5	C	1	Total	C	H	N	O	P	0	0
			42	10	10	5	14	3		
5	D	1	Total	C	H	N	O	P	0	0
			42	10	10	5	14	3		

- Molecule 6 is MAGNESIUM ION (three-letter code: 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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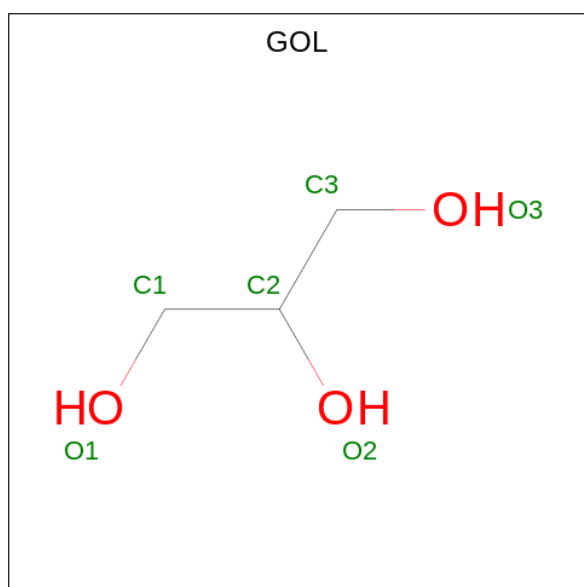
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	1	Total	Mg	0	0
			1	1		

- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

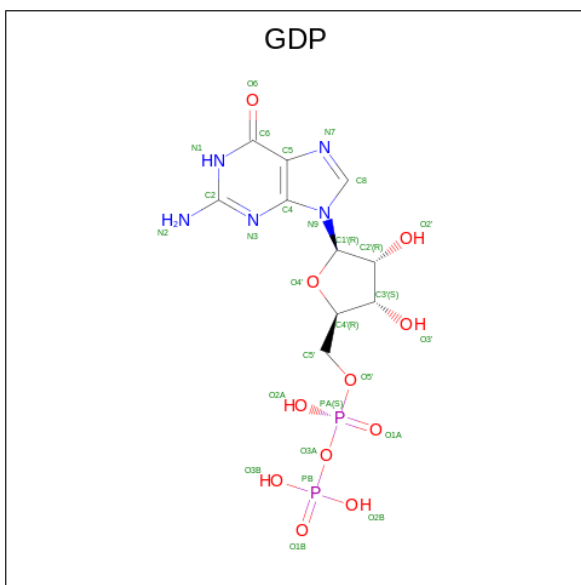
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Ca	0	0
			1	1		
7	C	1	Total	Ca	0	0
			1	1		

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



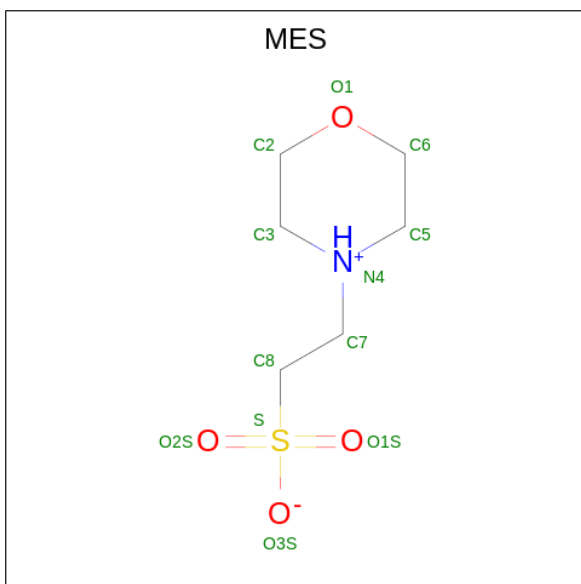
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 9 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



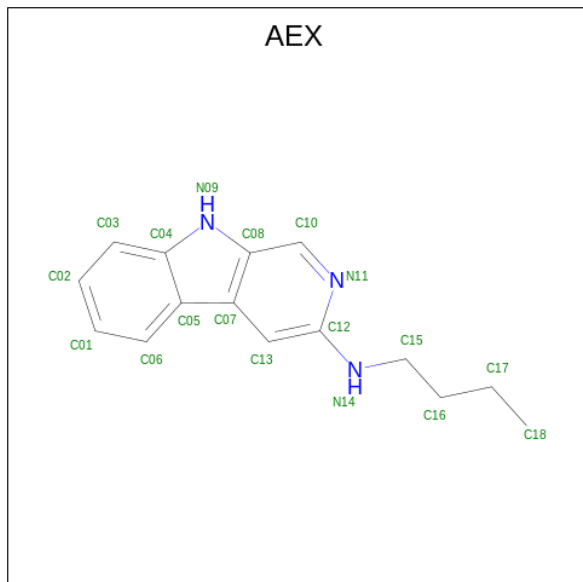
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	B	1	Total	C	H	N	O	P	
			38	10	10	5	11	2	

- Molecule 10 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



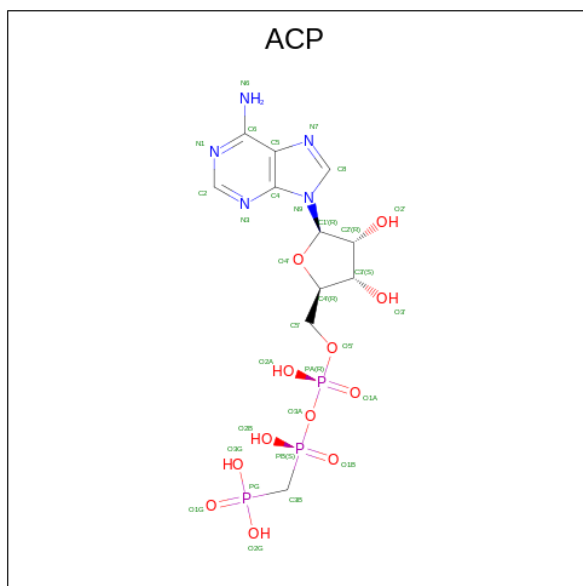
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	B	1	Total	C	H	N	O	S	
			24	6	12	1	4	1	
10	D	1	Total	C	H	N	O	S	
			25	6	13	1	4	1	

- Molecule 11 is N-butyl-9H-beta-carboline-3-amine (three-letter code: AEX) (formula: $C_{15}H_{17}N_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	B	1	Total	C	H	N	0	0
			35	15	17	3		
11	D	1	Total	C	H	N	0	0
			35	15	17	3		

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




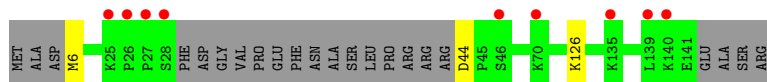
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
12	F	1	Total	C	N	O	P	0	0
			31	11	5	12	3		

- Molecule 13 is water.


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	58	Total	O	0	0
			58	58		
13	B	58	Total	O	0	0
			58	58		
13	C	89	Total	O	0	0
			89	89		
13	D	13	Total	O	0	0
			13	13		
13	E	17	Total	O	0	0
			17	17		
13	F	37	Total	O	0	0
			37	37		

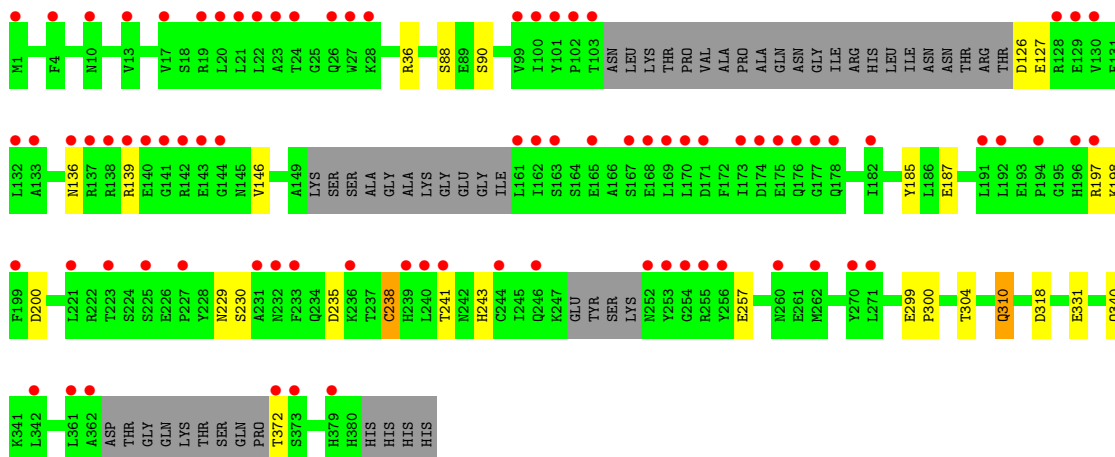
- Molecule 3: Stathmin-4

Chain E:  6% 83% 15%



- Molecule 4: Tubulin tyrosine ligase

Chain F:  22% 80% 7% 13%



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 157.68Å 181.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.13 – 2.73 48.13 – 2.73	Depositor EDS
% Data completeness (in resolution range)	98.5 (48.13-2.73) 98.4 (48.13-2.73)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.16 (at 2.73Å)	Xtriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, R_{free}	0.207 , 0.242 0.213 , 0.244	Depositor DCC
R_{free} test set	1181 reflections (1.48%)	wwPDB-VP
Wilson B-factor (Å ²)	45.5	Xtriage
Anisotropy	0.044	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 42.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	34705	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 2.46% 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: GOL, AEX, ACP, MES, GTP, CA, MG, GDP

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	0.24	0/3514	0.39	0/4770
1	C	0.25	0/3521	0.40	0/4781
2	B	0.24	0/3436	0.39	0/4654
2	D	0.23	0/3382	0.38	0/4581
3	E	0.22	0/1044	0.33	0/1385
4	F	0.23	0/2806	0.38	0/3791
All	All	0.24	0/17703	0.39	0/23962

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	3428	3327	3329	6	0
1	C	3443	3340	3353	7	0
2	B	3361	3228	3238	11	0
2	D	3309	3176	3189	16	0
3	E	1018	1028	1007	3	0
4	F	2744	2697	2709	20	0
5	A	32	10	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	32	10	12	0	0
5	D	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
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
10	D	12	13	13	0	0
11	B	18	17	0	0	0
11	D	18	17	0	2	0
12	F	31	0	14	7	0
13	A	58	0	0	0	0
13	B	58	0	0	6	0
13	C	89	0	0	3	0
13	D	13	0	0	3	0
13	E	17	0	0	2	0
13	F	37	0	0	3	0
All	All	17802	16903	16920	62	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (62) 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:331:GLU:OE2	12:F:401:ACP:O2G	1.97	0.82
2:B:46:ARG:NH1	2:B:242:PHE:O	2.12	0.80
1:C:251:ASP:OD2	13:C:601:HOH:O	2.02	0.77
12:F:401:ACP:O2G	12:F:401:ACP:O1B	2.05	0.75
2:D:2:ARG:NH1	2:D:129:CYS:SG	2.61	0.74
1:A:88:HIS:ND1	1:A:90:GLU:OE1	2.23	0.71
4:F:229:ASN:N	4:F:238:CYS:SG	2.67	0.67
4:F:241:THR:OG1	12:F:401:ACP:O3'	2.12	0.67
1:C:218:ASP:OD2	13:C:602:HOH:O	2.13	0.67
4:F:126:ASP:N	13:F:501:HOH:O	2.27	0.67
2:D:191:GLN:OE1	3:E:126:LYS:NZ	2.28	0.65
1:A:178:SER:OG	1:A:183:GLU:OE1	2.14	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:156:ARG:NH1	2:D:195:ASN:OD1	2.29	0.64
4:F:304:THR:O	4:F:310:GLN:NE2	2.32	0.63
4:F:126:ASP:OD1	4:F:127:GLU:N	2.30	0.63
4:F:185:TYR:OH	4:F:198:LYS:NZ	2.31	0.61
2:B:36:TYR:OH	2:B:40:SER:O	2.21	0.59
3:E:44:ASP:N	13:E:202:HOH:O	2.38	0.57
4:F:36:ARG:NH2	13:F:504:HOH:O	2.38	0.57
2:B:2:ARG:NH1	13:B:606:HOH:O	2.38	0.56
3:E:6:MET:N	13:E:203:HOH:O	2.40	0.55
4:F:372:THR:N	13:F:508:HOH:O	2.40	0.55
1:C:1:MET:N	13:C:613:HOH:O	2.39	0.54
4:F:197:ARG:NH1	4:F:257:GLU:OE2	2.28	0.54
4:F:331:GLU:OE2	12:F:401:ACP:O1B	2.26	0.54
4:F:331:GLU:OE2	12:F:401:ACP:PG	2.65	0.54
2:B:31:ASP:OD1	2:B:35:SER:N	2.37	0.52
2:D:404:ASP:OD1	2:D:405:GLU:N	2.43	0.51
4:F:200:ASP:OD1	4:F:241:THR:OG1	2.26	0.51
2:D:390:ARG:NH1	13:D:606:HOH:O	2.44	0.50
2:D:2:ARG:NH2	13:D:605:HOH:O	2.44	0.50
2:B:301:ALA:O	2:B:303:CYS:N	2.44	0.49
2:B:412:GLU:OE2	13:B:601:HOH:O	2.20	0.48
4:F:318:ASP:OD2	12:F:401:ACP:O3G	2.32	0.47
2:D:41:ASP:OD1	2:D:41:ASP:N	2.48	0.47
1:A:173:PRO:HB3	1:A:183:GLU:OE2	2.14	0.47
2:D:107:THR:OG1	2:D:108:GLU:N	2.46	0.47
4:F:146:VAL:N	4:F:187:GLU:OE2	2.48	0.47
1:A:263:PRO:O	1:A:266:HIS:ND1	2.34	0.46
2:D:51:TYR:O	2:D:62:ARG:NH2	2.49	0.46
2:D:19:LYS:NZ	2:D:223:GLY:HA2	2.31	0.45
2:B:380:ARG:NH1	13:B:617:HOH:O	2.49	0.45
2:D:141:GLY:O	2:D:184:ASN:ND2	2.50	0.45
1:A:183:GLU:N	1:A:184:PRO:CD	2.81	0.44
2:B:209:ASP:OD2	13:B:602:HOH:O	2.21	0.44
1:C:221:ARG:NH2	2:D:323:MET:SD	2.91	0.43
4:F:340:GLN:N	4:F:340:GLN:OE1	2.50	0.43
1:A:88:HIS:N	1:A:91:GLN:OE1	2.48	0.43
1:C:165:SER:HA	1:C:199:ASP:OD2	2.17	0.43
2:D:200:TYR:OH	11:D:504:AEX:N14	2.52	0.43
4:F:136:ASN:O	4:F:139:ARG:N	2.51	0.43
2:B:283:ALA:N	13:B:613:HOH:O	2.46	0.42
2:D:181:GLU:N	2:D:182:PRO:HD2	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:90:SER:O	4:F:90:SER:OG	2.34	0.42
1:C:183:GLU:N	1:C:184:PRO:CD	2.82	0.42
2:D:253:LEU:HB3	11:D:504:AEX:C10	2.50	0.41
2:B:392:LYS:NZ	13:B:614:HOH:O	2.47	0.41
4:F:331:GLU:OE2	12:F:401:ACP:O3G	2.38	0.41
2:D:251:ARG:NH1	13:D:607:HOH:O	2.46	0.41
4:F:299:GLU:N	4:F:300:PRO:HD2	2.36	0.41
2:B:209:ASP:O	2:B:213:ARG:N	2.54	0.40
1:C:36:MET:HB3	1:C:61:HIS:CE1	2.57	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	438/450 (97%)	423 (97%)	15 (3%)	0	100	100
1	C	439/450 (98%)	427 (97%)	12 (3%)	0	100	100
2	B	425/445 (96%)	411 (97%)	14 (3%)	0	100	100
2	D	417/445 (94%)	406 (97%)	11 (3%)	0	100	100
3	E	121/143 (85%)	119 (98%)	2 (2%)	0	100	100
4	F	324/384 (84%)	309 (95%)	15 (5%)	0	100	100
All	All	2164/2317 (93%)	2095 (97%)	69 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	371/378 (98%)	371 (100%)	0	100	100
1	C	372/378 (98%)	366 (98%)	6 (2%)	62	83
2	B	369/383 (96%)	368 (100%)	1 (0%)	92	97
2	D	364/383 (95%)	360 (99%)	4 (1%)	73	89
3	E	113/127 (89%)	113 (100%)	0	100	100
4	F	301/342 (88%)	295 (98%)	6 (2%)	55	80
All	All	1890/1991 (95%)	1873 (99%)	17 (1%)	78	91

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	300	MET
1	C	177	VAL
1	C	221	ARG
1	C	245	ASP
1	C	251	ASP
1	C	283	HIS
1	C	358	GLN
2	D	137	HIS
2	D	179	VAL
2	D	247	ASN
2	D	289	LEU
4	F	88	SER
4	F	230	SER
4	F	235	ASP
4	F	238	CYS
4	F	243	HIS
4	F	310	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	414	ASN

5.3.3 RNA ⓘ

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 6 are monoatomic - leaving 10 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
10	MES	D	502	-	12,12,12	2.20	1 (8%)	14,16,16	1.69	5 (35%)
11	AEX	B	504	-	19,20,20	1.14	1 (5%)	25,27,27	0.95	2 (8%)
5	GTP	A	501	6	26,34,34	1.13	2 (7%)	32,54,54	1.41	6 (18%)
5	GTP	D	501	6	26,34,34	1.15	2 (7%)	32,54,54	1.58	6 (18%)
10	MES	B	503	-	12,12,12	2.18	1 (8%)	14,16,16	2.21	5 (35%)
5	GTP	C	501	6	26,34,34	1.15	1 (3%)	32,54,54	1.42	5 (15%)
9	GDP	B	501	6	24,30,30	0.98	1 (4%)	30,47,47	1.04	3 (10%)
11	AEX	D	504	-	19,20,20	1.24	2 (10%)	25,27,27	0.95	2 (8%)
8	GOL	A	504	-	5,5,5	0.36	0	5,5,5	0.25	0
12	ACP	F	401	-	27,33,33	1.37	5 (18%)	32,52,52	1.39	5 (15%)

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
10	MES	D	502	-	-	5/6/14/14	0/1/1/1
11	AEX	B	504	-	-	0/5/5/5	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GTP	A	501	6	-	7/18/38/38	0/3/3/3
5	GTP	D	501	6	-	6/18/38/38	0/3/3/3
10	MES	B	503	-	-	4/6/14/14	0/1/1/1
5	GTP	C	501	6	-	7/18/38/38	0/3/3/3
9	GDP	B	501	6	-	3/12/32/32	0/3/3/3
11	AEX	D	504	-	-	0/5/5/5	0/3/3/3
8	GOL	A	504	-	-	2/4/4/4	-
12	ACP	F	401	-	-	8/15/38/38	0/3/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	D	502	MES	C8-S	-7.34	1.67	1.77
10	B	503	MES	C8-S	-7.31	1.67	1.77
5	C	501	GTP	C5-C6	-4.21	1.38	1.47
5	D	501	GTP	C5-C6	-4.16	1.39	1.47
5	A	501	GTP	C5-C6	-4.01	1.39	1.47
11	D	504	AEX	C12-N14	4.00	1.42	1.36
11	B	504	AEX	C12-N14	3.54	1.41	1.36
12	F	401	ACP	C2'-C1'	-2.95	1.49	1.53
9	B	501	GDP	C6-N1	-2.94	1.33	1.37
12	F	401	ACP	PG-O2G	2.44	1.60	1.54
5	D	501	GTP	C2-N3	2.22	1.38	1.33
12	F	401	ACP	C4-N3	-2.21	1.32	1.35
11	D	504	AEX	C12-N11	2.13	1.38	1.34
12	F	401	ACP	O4'-C4'	-2.09	1.40	1.45
12	F	401	ACP	C5-N7	-2.08	1.32	1.39
5	A	501	GTP	C2-N3	2.02	1.38	1.33

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	503	MES	C5-N4-C3	5.11	120.33	108.83
5	D	501	GTP	PB-O3B-PG	-3.81	119.77	132.83
5	D	501	GTP	PA-O3A-PB	-3.50	120.82	132.83
12	F	401	ACP	PB-O3A-PA	-3.36	121.91	132.56
12	F	401	ACP	C3'-C2'-C1'	3.35	106.02	100.98
5	C	501	GTP	PB-O3B-PG	-3.27	121.61	132.83
10	B	503	MES	O3S-S-C8	3.25	111.02	105.77
5	D	501	GTP	C5-C6-N1	3.12	119.47	113.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	501	GTP	C5-C6-N1	3.05	119.34	113.95
5	D	501	GTP	C8-N7-C5	3.03	108.76	102.99
5	C	501	GTP	PA-O3A-PB	-3.01	122.50	132.83
5	A	501	GTP	C8-N7-C5	2.99	108.69	102.99
10	D	502	MES	O2S-S-C8	2.97	110.50	106.92
5	C	501	GTP	C8-N7-C5	2.94	108.58	102.99
5	C	501	GTP	C5-C6-N1	2.91	119.09	113.95
9	B	501	GDP	PA-O3A-PB	-2.81	123.19	132.83
5	A	501	GTP	C2-N1-C6	-2.80	119.94	125.10
10	B	503	MES	C7-N4-C5	2.80	118.40	111.23
5	D	501	GTP	C2-N1-C6	-2.74	120.05	125.10
12	F	401	ACP	C4-C5-N7	-2.65	106.64	109.40
5	A	501	GTP	PB-O3B-PG	-2.64	123.76	132.83
12	F	401	ACP	N3-C2-N1	-2.63	124.56	128.68
5	C	501	GTP	C2-N1-C6	-2.59	120.33	125.10
5	A	501	GTP	PA-O3A-PB	-2.56	124.05	132.83
10	D	502	MES	O1S-S-C8	2.43	109.84	106.92
10	D	502	MES	C5-N4-C3	2.43	114.30	108.83
11	B	504	AEX	C13-C07-C05	2.40	135.60	132.28
11	D	504	AEX	C13-C07-C05	2.35	135.53	132.28
10	B	503	MES	O1S-S-C8	2.32	109.70	106.92
10	D	502	MES	C2-C3-N4	-2.29	106.63	110.10
9	B	501	GDP	C5-C6-N1	2.28	117.99	113.95
9	B	501	GDP	C8-N7-C5	2.26	107.30	102.99
5	D	501	GTP	O6-C6-C5	-2.15	120.17	124.37
10	D	502	MES	O3S-S-C8	2.10	109.16	105.77
11	B	504	AEX	C02-C03-C04	-2.06	117.12	120.08
12	F	401	ACP	O2A-PA-O1A	2.05	122.35	112.24
11	D	504	AEX	C02-C03-C04	-2.04	117.15	120.08
10	B	503	MES	C7-N4-C3	2.03	116.43	111.23
5	A	501	GTP	O6-C6-C5	-2.02	120.43	124.37

There are no chirality outliers.

All (42) 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-O1A
5	A	501	GTP	C5'-O5'-PA-O2A
5	C	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O2A
5	D	501	GTP	C5'-O5'-PA-O1A

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Mol	Chain	Res	Type	Atoms
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	D	502	MES	C7-C8-S-O3S
12	F	401	ACP	PG-C3B-PB-O1B
12	F	401	ACP	PG-C3B-PB-O2B
12	F	401	ACP	PG-C3B-PB-O3A
12	F	401	ACP	O4'-C4'-C5'-O5'
12	F	401	ACP	C3'-C4'-C5'-O5'
10	B	503	MES	C7-C8-S-O3S
8	A	504	GOL	O1-C1-C2-C3
8	A	504	GOL	O1-C1-C2-O2
5	D	501	GTP	C3'-C4'-C5'-O5'
10	D	502	MES	C8-C7-N4-C5
12	F	401	ACP	PB-O3A-PA-O1A
5	D	501	GTP	C5'-O5'-PA-O3A
5	D	501	GTP	O4'-C4'-C5'-O5'
5	A	501	GTP	PB-O3A-PA-O2A
5	D	501	GTP	C4'-C5'-O5'-PA
5	D	501	GTP	C5'-O5'-PA-O2A
10	B	503	MES	C7-C8-S-O1S
10	B	503	MES	C7-C8-S-O2S
10	D	502	MES	C7-C8-S-O1S
10	D	502	MES	C7-C8-S-O2S
12	F	401	ACP	PB-C3B-PG-O2G
5	A	501	GTP	C4'-C5'-O5'-PA
5	C	501	GTP	PB-O3A-PA-O2A
5	C	501	GTP	C4'-C5'-O5'-PA
10	D	502	MES	C8-C7-N4-C3
12	F	401	ACP	PB-C3B-PG-O1G
5	A	501	GTP	PB-O3B-PG-O3G
5	C	501	GTP	PB-O3B-PG-O2G
5	A	501	GTP	C5'-O5'-PA-O3A
5	C	501	GTP	C5'-O5'-PA-O3A
9	B	501	GDP	C5'-O5'-PA-O3A
5	C	501	GTP	PB-O3B-PG-O1G

There are no ring outliers.

2 monomers are involved in 9 short contacts:

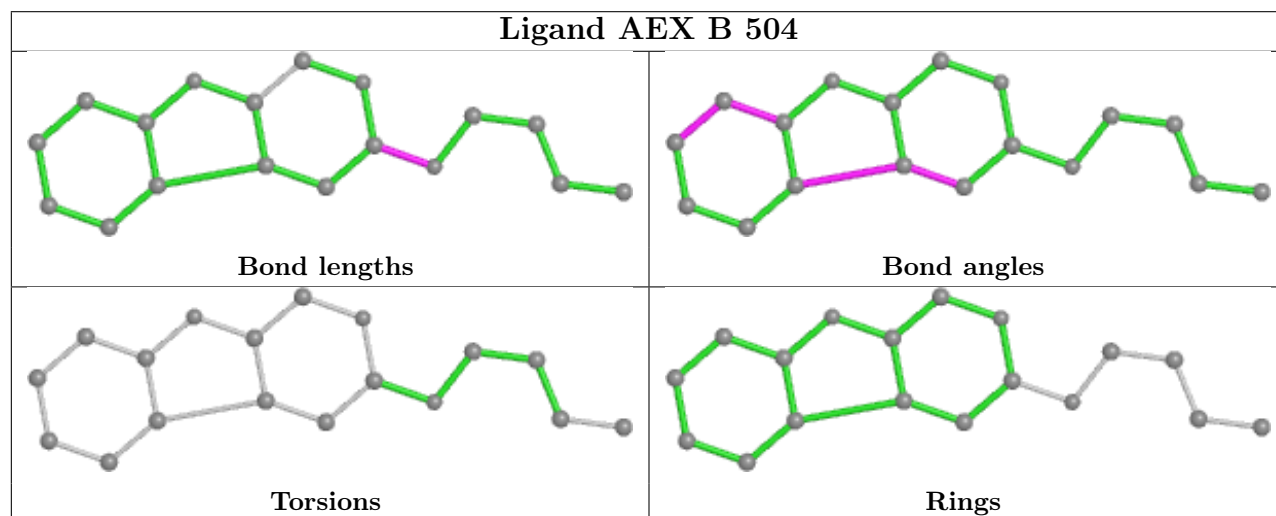
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	D	504	AEX	2	0

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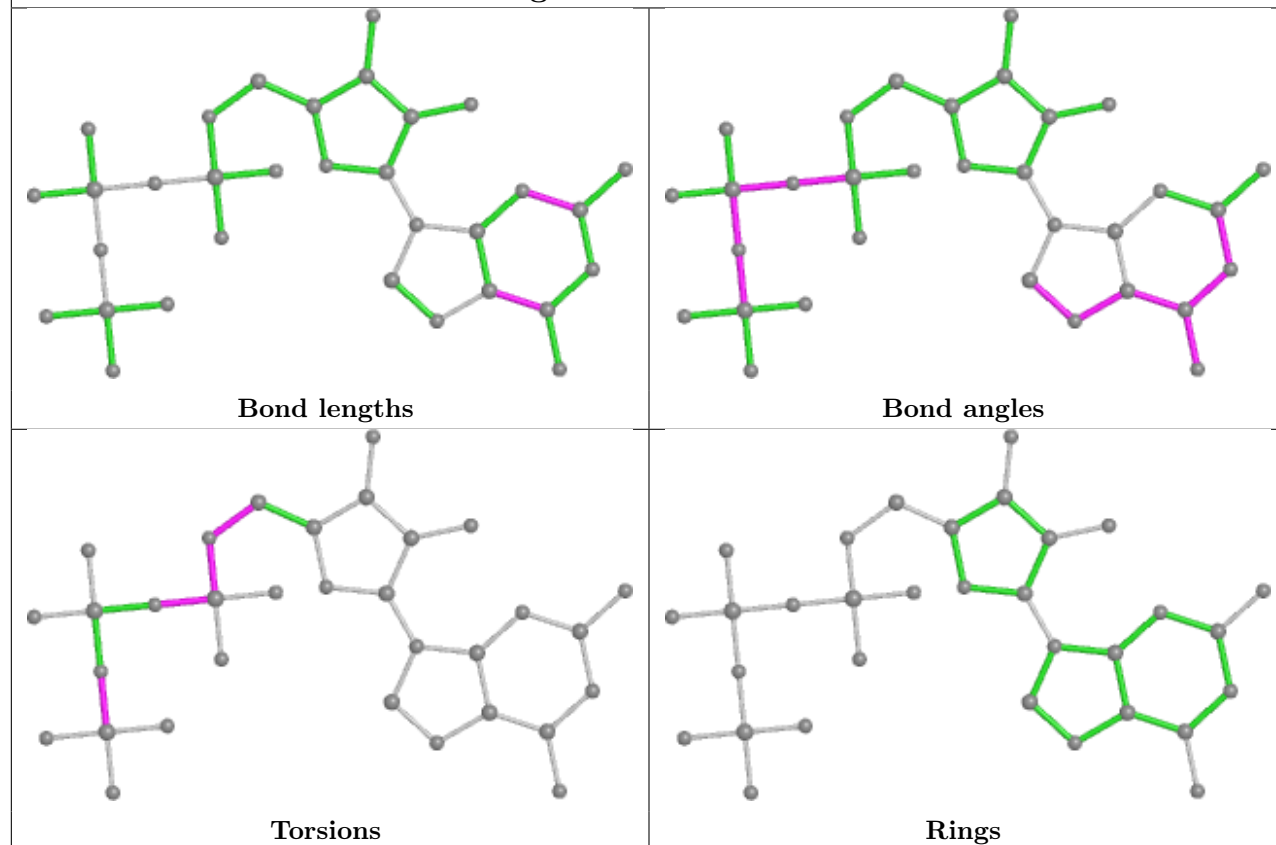
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	F	401	ACP	7	0

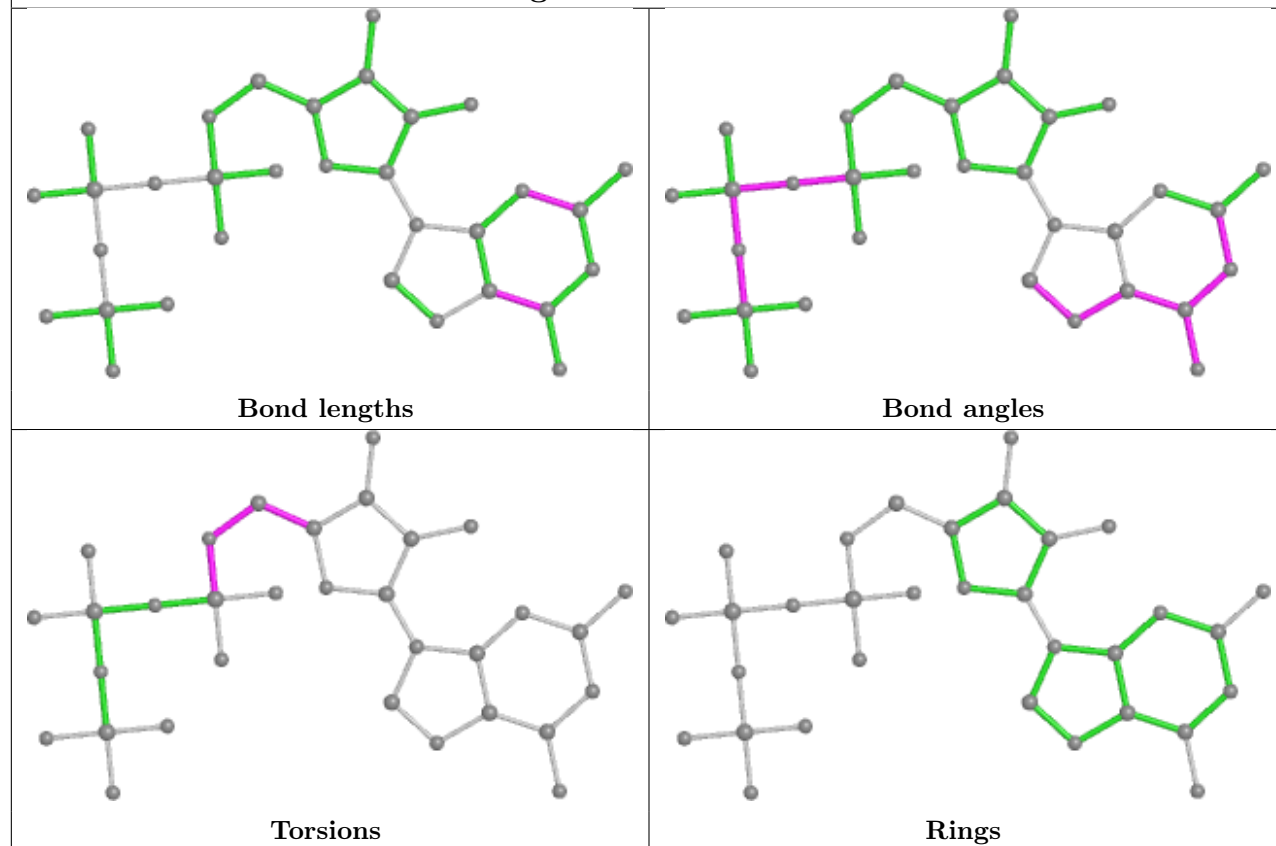
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



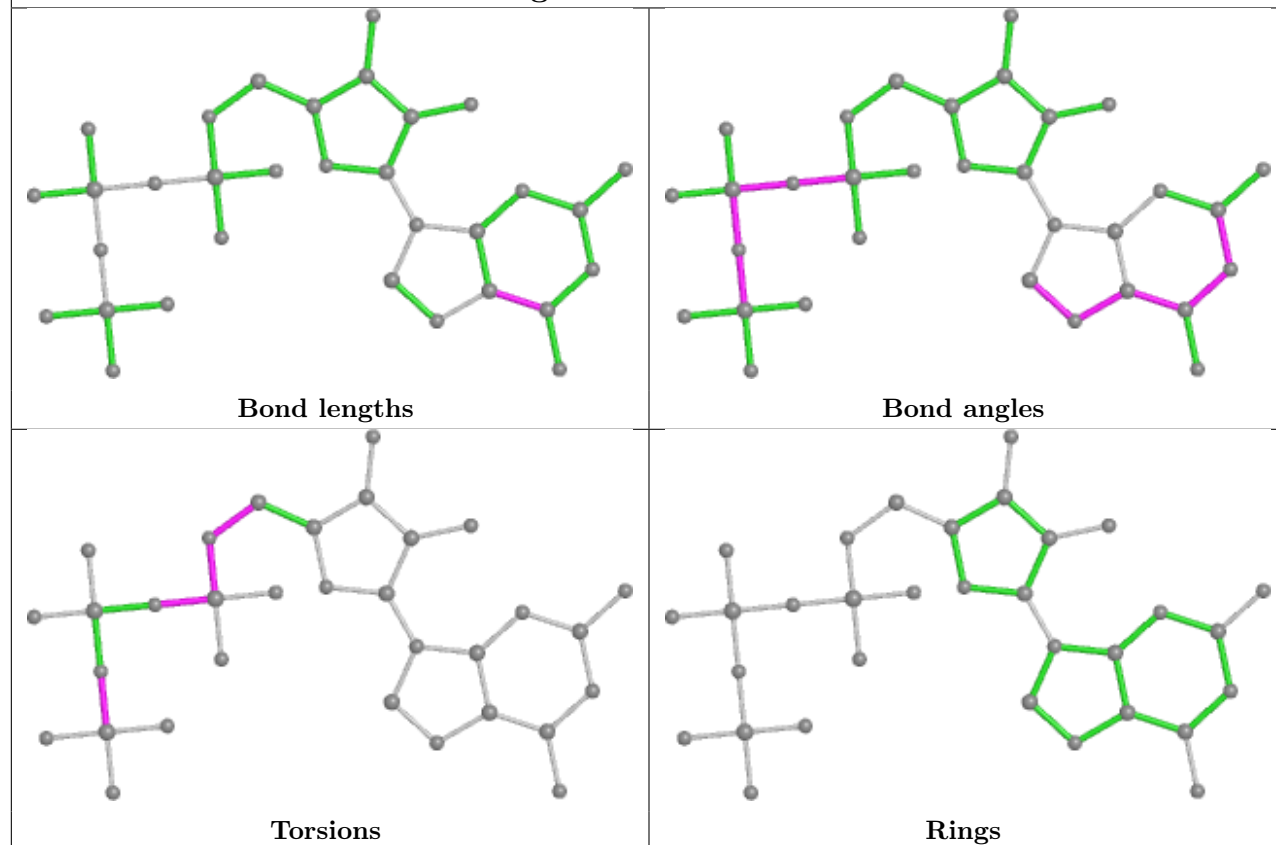
Ligand GTP A 501



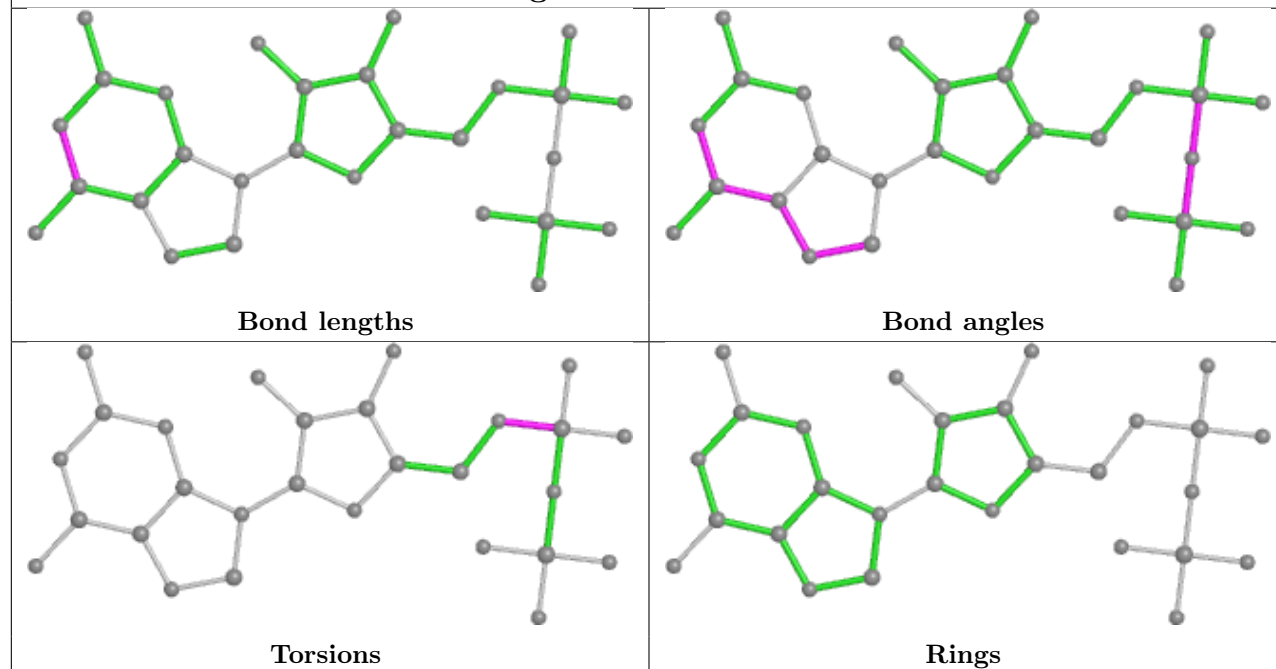
Ligand GTP D 501

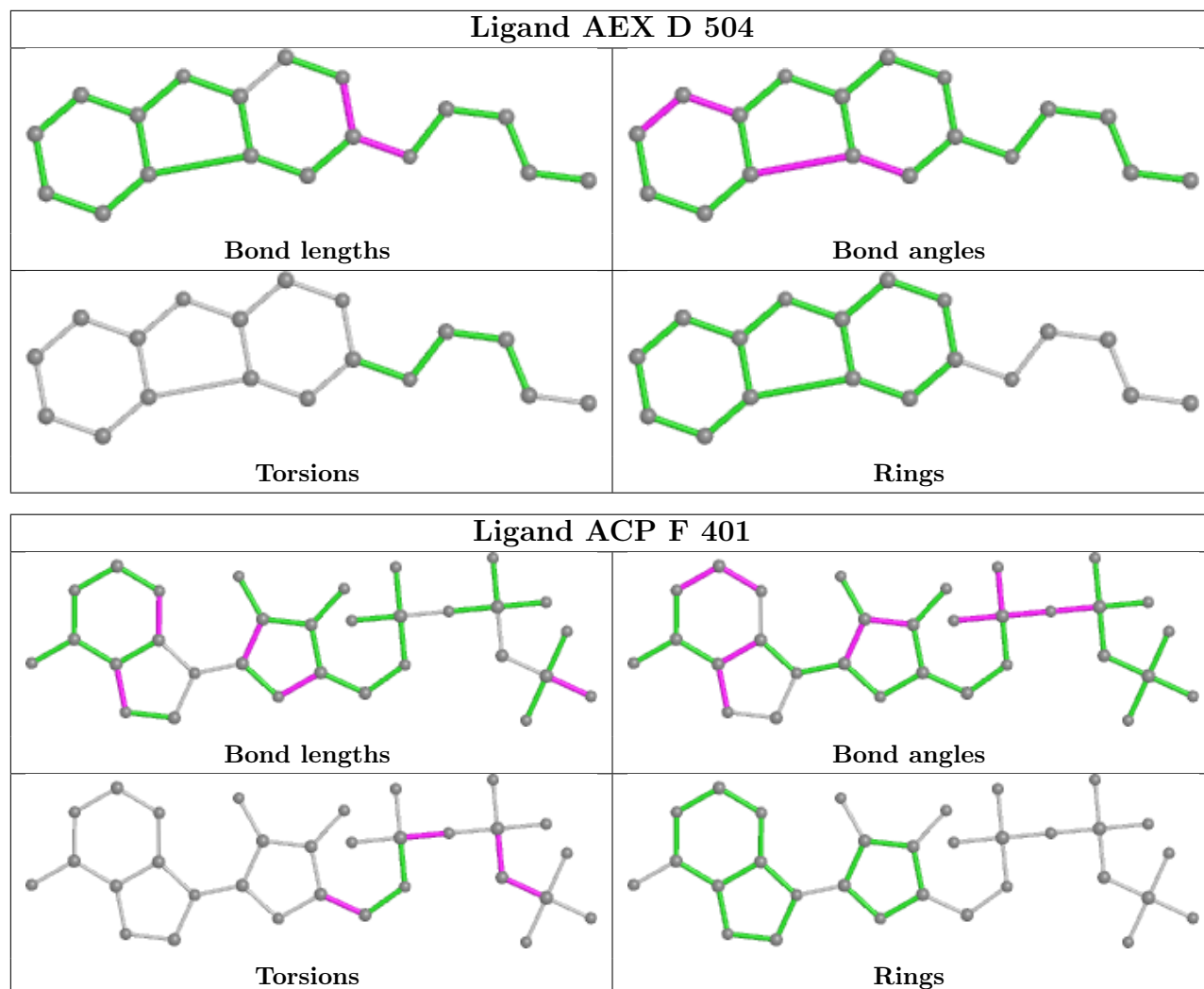


Ligand GTP C 501



Ligand GDP B 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%)	0.07	2 (0%) 91 92	19, 36, 65, 87	0
1	C	440/450 (97%)	-0.25	3 (0%) 87 89	14, 27, 55, 99	0
2	B	427/445 (95%)	0.02	13 (3%) 50 51	16, 37, 77, 116	0
2	D	421/445 (94%)	0.61	43 (10%) 6 5	25, 57, 94, 112	0
3	E	121/143 (84%)	0.53	9 (7%) 14 13	26, 58, 93, 109	0
4	F	334/384 (86%)	1.05	83 (24%) 0 0	30, 65, 123, 142	0
All	All	2180/2317 (94%)	0.27	153 (7%) 16 15	14, 44, 93, 142	0

All (153) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	170	LEU	7.6
4	F	173	ILE	7.4
2	D	245	GLN	6.2
4	F	142	ARG	6.0
2	B	279	GLN	5.2
4	F	21	LEU	5.2
4	F	130	VAL	5.1
4	F	20	LEU	5.0
4	F	101	TYR	5.0
4	F	141	GLY	4.9
2	B	57	ASN	4.8
4	F	240	LEU	4.8
4	F	100	ILE	4.7
2	D	391	ARG	4.7
4	F	102	PRO	4.7
4	F	233	PHE	4.7
2	D	55	THR	4.6
4	F	191	LEU	4.6
2	D	217	LEU	4.5

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Mol	Chain	Res	Type	RSRZ
2	D	92	PHE	4.4
4	F	138	ARG	4.4
4	F	103	THR	4.3
4	F	244	CYS	4.3
4	F	99	VAL	4.3
4	F	231	ALA	4.2
4	F	256	TYR	4.1
4	F	27	TRP	3.9
2	D	37	HIS	3.9
2	B	55	THR	3.9
4	F	254	GLY	3.8
4	F	253	TYR	3.8
3	E	140	LYS	3.8
2	D	394	PHE	3.8
4	F	372	THR	3.7
2	D	1	MET	3.7
4	F	192	LEU	3.7
4	F	225	SER	3.6
4	F	223	THR	3.6
2	D	219	THR	3.6
4	F	17	VAL	3.6
2	D	390	ARG	3.5
4	F	22	LEU	3.5
4	F	167	SER	3.5
4	F	194	PRO	3.5
4	F	137	ARG	3.5
2	B	280	GLN	3.4
1	A	262	TYR	3.4
4	F	236	LYS	3.3
2	D	42	LEU	3.3
2	D	57	ASN	3.3
4	F	196	HIS	3.3
4	F	232	ASN	3.2
4	F	1	MET	3.2
2	D	180	VAL	3.2
4	F	133	ALA	3.2
4	F	174	ASP	3.2
4	F	19	ARG	3.1
2	D	177	ASP	3.1
3	E	139	LEU	3.1
4	F	221	LEU	3.1
2	B	275	SER	3.1

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Mol	Chain	Res	Type	RSRZ
2	D	215	LEU	3.0
4	F	199	PHE	3.0
4	F	139	ARG	3.0
4	F	143	GLU	3.0
4	F	227	PRO	3.0
4	F	246	GLN	3.0
2	D	356	ILE	2.9
2	D	53	GLU	2.9
4	F	24	THR	2.9
3	E	27	PRO	2.9
2	D	389	PHE	2.9
4	F	182	ILE	2.9
4	F	171	ASP	2.9
4	F	132	LEU	2.8
4	F	178	GLN	2.8
2	D	73	MET	2.8
2	D	77	ARG	2.8
4	F	161	LEU	2.7
2	B	54	ALA	2.7
2	D	54	ALA	2.7
4	F	175	GLU	2.7
4	F	136	ASN	2.7
4	F	177	GLY	2.7
4	F	169	LEU	2.6
4	F	165	GLU	2.6
4	F	241	THR	2.6
2	D	216	LYS	2.5
4	F	362	ALA	2.5
2	D	84	ILE	2.5
2	B	36	TYR	2.5
4	F	197	ARG	2.5
2	D	176	SER	2.5
2	B	336	LYS	2.5
2	D	208	TYR	2.5
2	D	213	ARG	2.5
2	D	405	GLU	2.5
4	F	163	SER	2.5
4	F	129	GLU	2.4
3	E	26	PRO	2.4
3	E	28	SER	2.4
4	F	379	HIS	2.4
4	F	361	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
2	B	39	ASP	2.4
4	F	255	ARG	2.4
4	F	140	GLU	2.4
2	D	44	LEU	2.4
4	F	373	SER	2.4
4	F	128	ARG	2.4
4	F	13	VAL	2.4
3	E	46	SER	2.4
4	F	168	GLU	2.4
2	D	36	TYR	2.3
4	F	270	TYR	2.3
4	F	342	LEU	2.3
4	F	26	GLN	2.3
4	F	28	LYS	2.3
2	B	38	GLY	2.3
4	F	23	ALA	2.3
2	D	38	GLY	2.3
2	D	94	GLN	2.3
2	D	81	PHE	2.3
4	F	271	LEU	2.3
3	E	135	LYS	2.3
1	C	357	TYR	2.3
2	D	31	ASP	2.3
4	F	162	ILE	2.3
4	F	252	ASN	2.2
3	E	70	LYS	2.2
4	F	262	MET	2.2
2	D	30	ILE	2.2
2	D	175	VAL	2.2
4	F	239	HIS	2.2
2	D	108	GLU	2.2
2	D	39	ASP	2.1
4	F	4	PHE	2.1
4	F	260	ASN	2.1
2	B	248	ALA	2.1
4	F	176	GLN	2.1
1	C	340	SER	2.1
2	D	400	GLY	2.1
3	E	25	LYS	2.1
4	F	144	GLY	2.1
2	D	199	THR	2.1
4	F	10	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
2	D	83	GLN	2.1
1	C	179	THR	2.1
2	D	406	MET	2.1
2	B	245	GLN	2.0
1	A	163	LYS	2.0
2	D	59	TYR	2.0
2	B	278	SER	2.0
2	D	388	MET	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 monosaccharides in this entry.

6.4 Ligands [i](#)

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

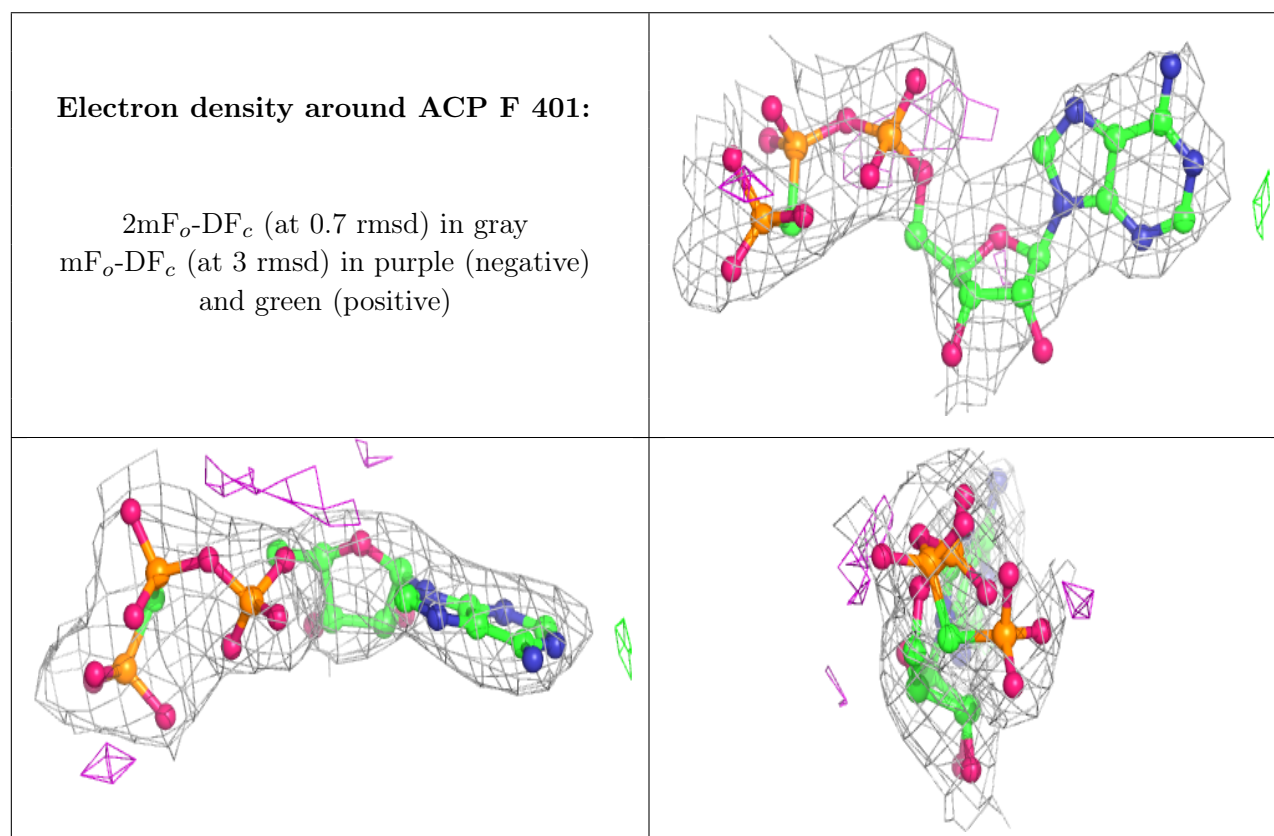
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	MG	D	503	1/1	0.87	0.14	60,60,60,60	0
12	ACP	F	401	31/31	0.87	0.19	67,92,121,133	0
10	MES	D	502	12/12	0.88	0.26	60,80,113,121	0
8	GOL	A	504	6/6	0.88	0.24	33,57,69,70	0
11	AEX	D	504	18/18	0.89	0.32	54,75,96,99	0
6	MG	C	502	1/1	0.94	0.20	26,26,26,26	0
5	GTP	D	501	32/32	0.94	0.15	37,53,70,76	0
7	CA	A	503	1/1	0.96	0.05	58,58,58,58	0
11	AEX	B	504	18/18	0.96	0.16	24,32,44,50	0
6	MG	B	502	1/1	0.96	0.19	27,27,27,27	0
10	MES	B	503	12/12	0.96	0.15	26,40,47,52	0
9	GDP	B	501	28/28	0.97	0.21	15,24,36,44	0
7	CA	C	503	1/1	0.98	0.09	40,40,40,40	0
5	GTP	A	501	32/32	0.98	0.23	16,26,34,35	0
6	MG	A	502	1/1	0.98	0.18	22,22,22,22	0

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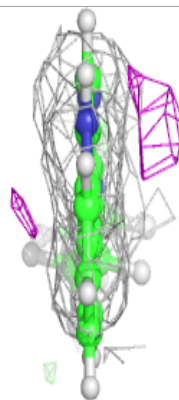
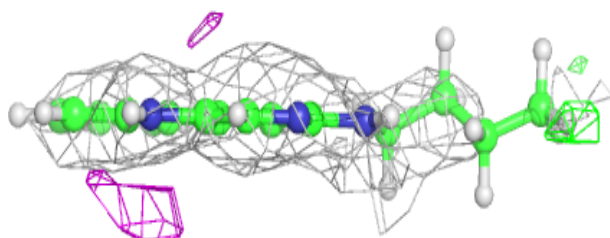
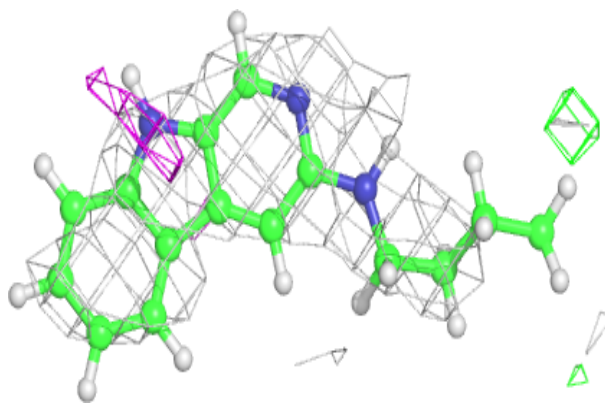
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	GTP	C	501	32/32	0.98	0.19	13,19,25,31	0

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.

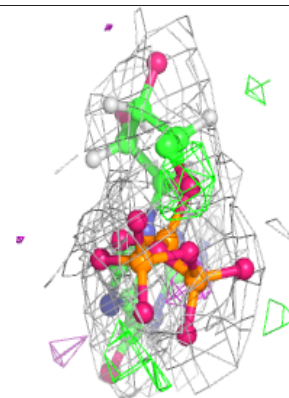
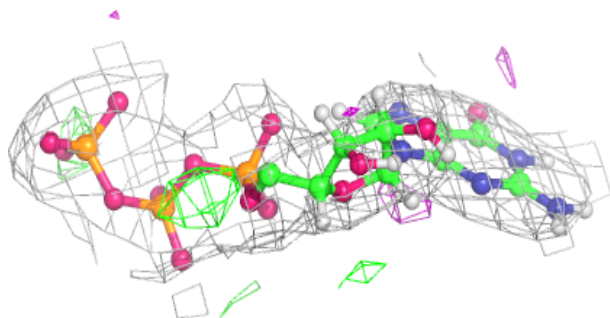
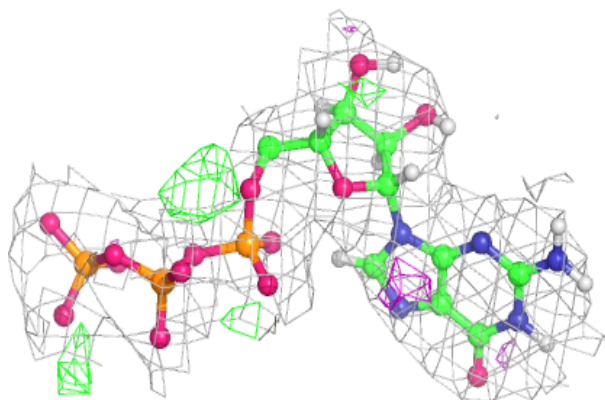


Electron density around AEX D 504:

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

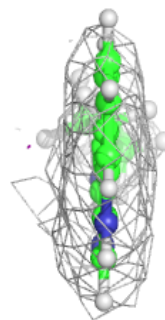
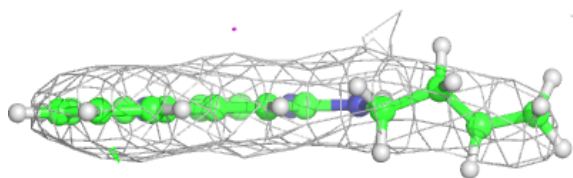
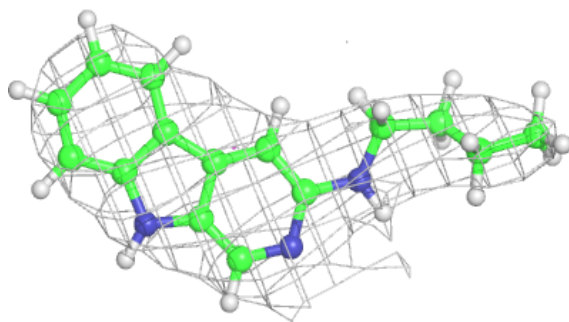
**Electron density around GTP D 501:**

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



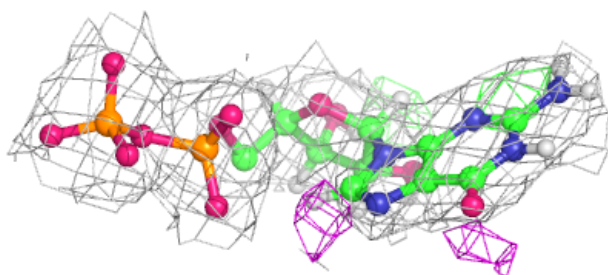
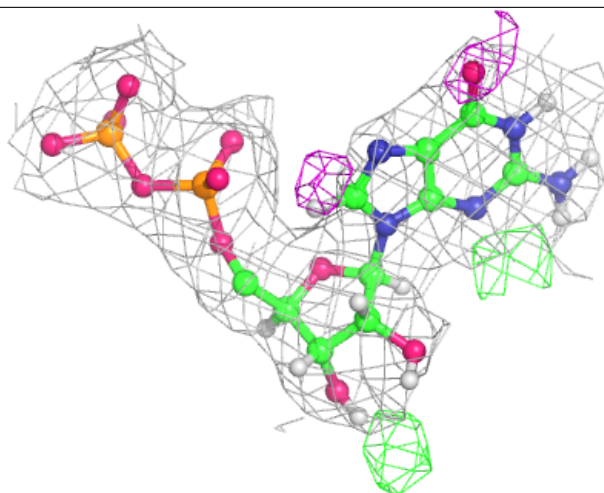
Electron density around AEX B 504:

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



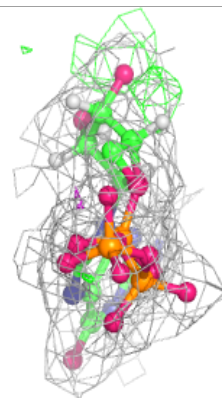
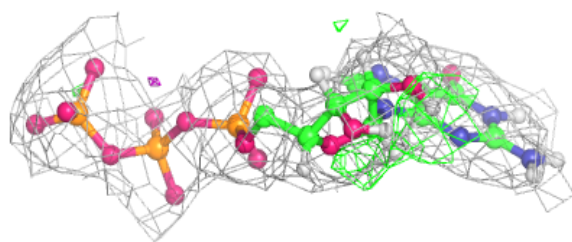
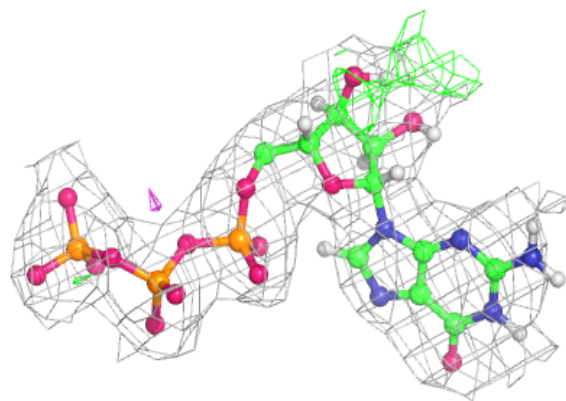
Electron density around GDP B 501:

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

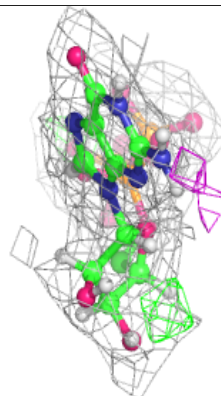
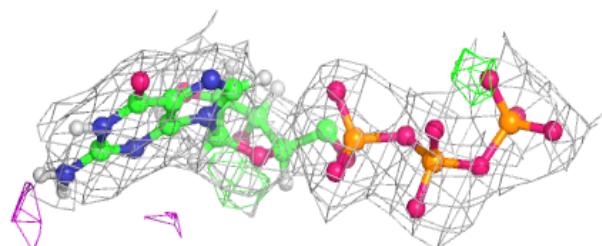
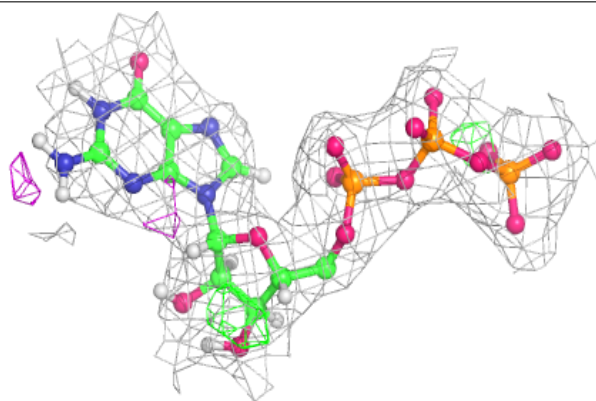


Electron density around GTP A 501:

$2mF_o-DF_c$ (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.