



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:41 AM UTC

PDB ID : 5H7O / pdb_00005h7o
Title : Crystal structure of DJ-101 in complex with tubulin protein
Authors : Arnst, K.; Wang, Y.; Hwang, D.-J.; Xue, Y.; Costello, T.; Hamilton, D.; Chen, Q.; Yang, J.; Park, F.; Dalton, J.T.; Miller, D.D.; Li, W.
Deposited on : 2016-11-20
Resolution : 2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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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

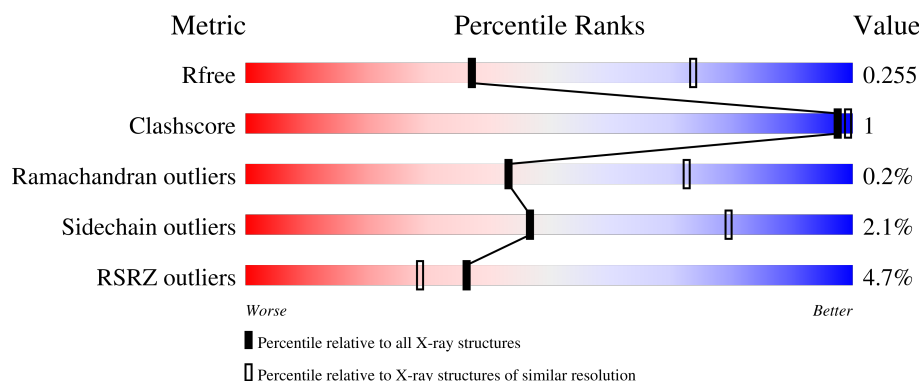
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	0% 93% • •
1	C	450	95% • •
2	B	445	2% 91% • •
2	D	445	8% 92% • 5%
3	E	143	6% 81% • 15%

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Mol	Chain	Length	Quality of chain
4	F	384	12% 84% • 13%

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 17517 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-1B chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	437	Total	C	N	O	S	0	0	0
			3416	2163	581	650	22			
1	C	440	Total	C	N	O	S	0	0	0
			3437	2175	584	656	22			

- Molecule 2 is a protein called Tubulin beta-2B chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	426	Total	C	N	O	S	0	0	0
			3350	2104	572	648	26			
2	D	421	Total	C	N	O	S	0	0	0
			3309	2080	562	640	27			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	121	Total	C	N	O	S	0	0	0
			1000	617	181	197	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	3	MET	-	initiating methionine	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	N	O	S	0	0	0
			2744	1761	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	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		

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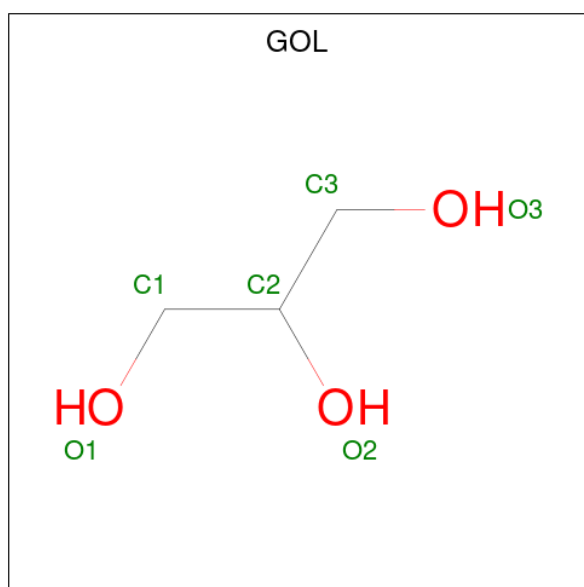
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	1	Total	Mg	0	0
			1	1		

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

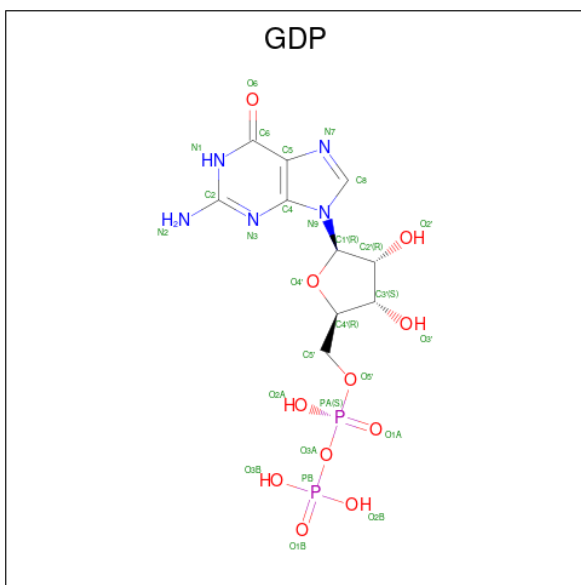
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Ca	0	0
			1	1		
7	C	1	Total	Ca	0	0
			1	1		

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



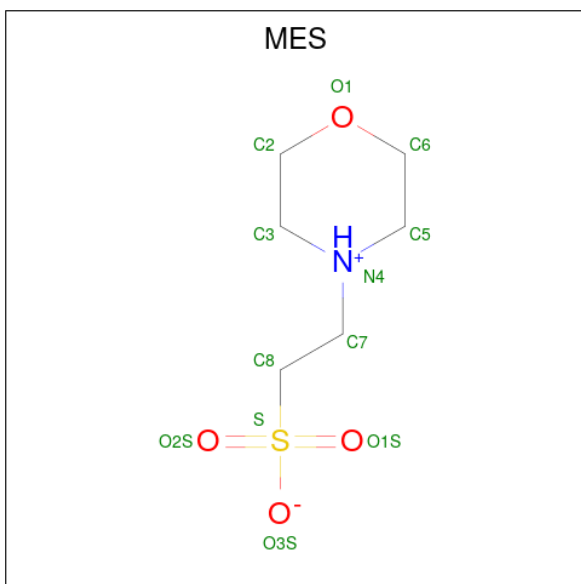
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			6	3	3		

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



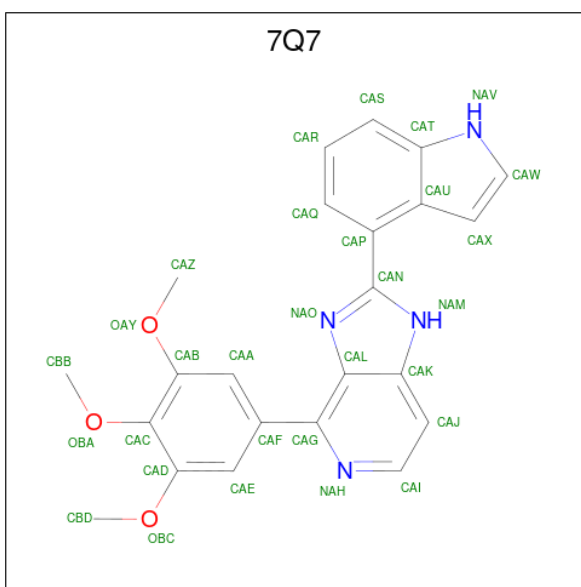
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	B	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

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



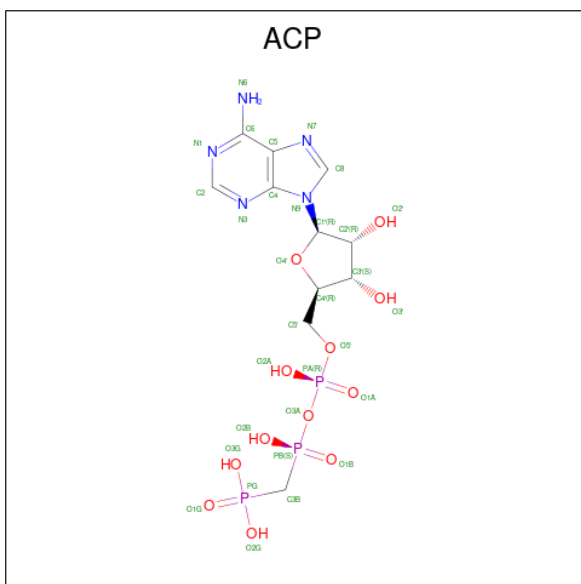
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 11 is 2-(1H-indol-4-yl)-4-(3,4,5-trimethoxyphenyl)-1H-imidazo[4,5-c]pyridine (CCD ID: 7Q7) (formula: C₂₃H₂₀N₄O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	B	1	Total 30	C 23	N 4	O 3	0	0
11	D	1	Total 30	C 23	N 4	O 3	0	0

- Molecule 12 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (CCD ID: ACP) (formula: $\text{C}_{11}\text{H}_{18}\text{N}_5\text{O}_{12}\text{P}_3$).



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

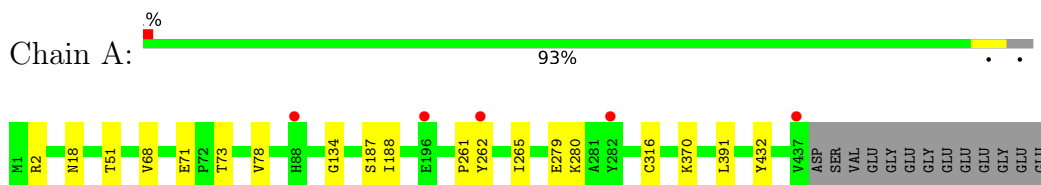
- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	6	Total 6	O 6	0	0
13	B	8	Total 8	O 8	0	0
13	C	8	Total 8	O 8	0	0

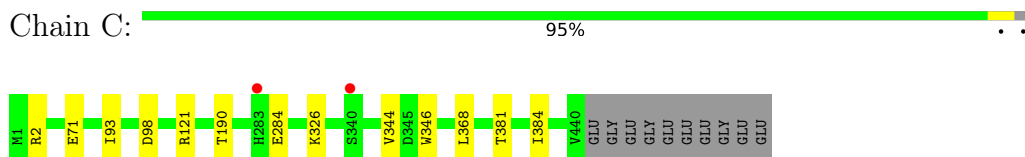
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

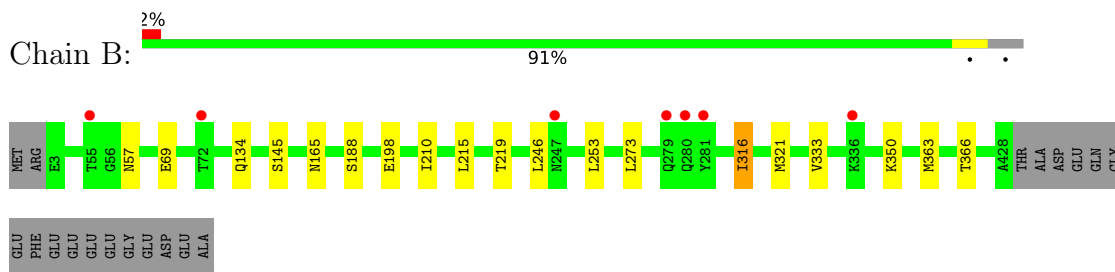
- Molecule 1: Tubulin alpha-1B chain



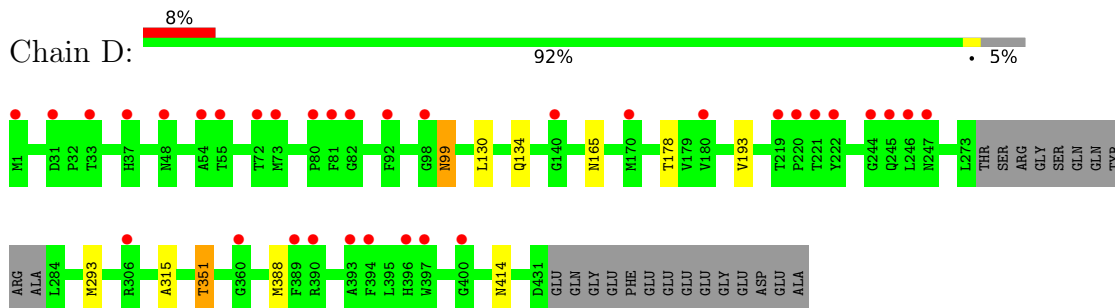
- Molecule 1: Tubulin alpha-1B chain



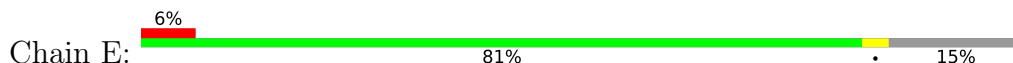
- Molecule 2: Tubulin beta-2B chain

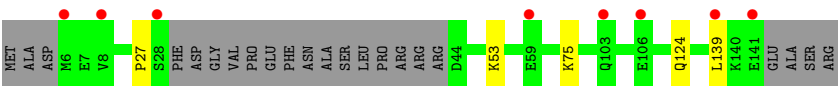


- Molecule 2: Tubulin beta-2B chain

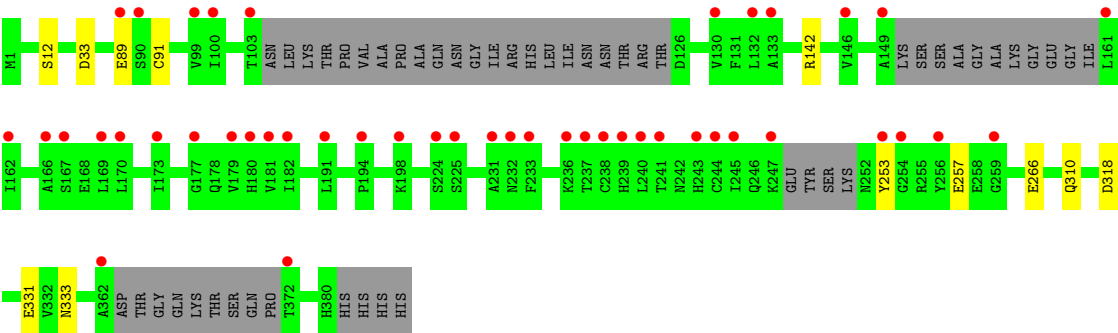
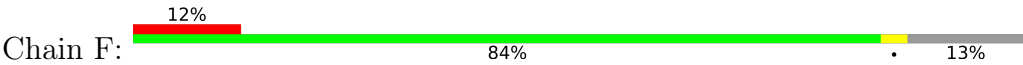


- Molecule 3: Stathmin-4





● 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	105.20Å 157.03Å 182.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.80 50.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.8 (50.00-2.80) 99.8 (50.00-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.12 (at 2.80Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.214 , 0.256 0.216 , 0.255	Depositor DCC
R_{free} test set	3809 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	48.9	Xtriage
Anisotropy	0.253	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 23.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	17517	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.56% 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: GTP, CA, MES, ACP, GOL, MG, GDP, 7Q7

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	0.56	0/3494	0.81	1/4743 (0.0%)
1	C	0.55	0/3515	0.81	0/4772
2	B	0.56	0/3425	0.80	0/4640
2	D	0.56	0/3382	0.79	0/4581
3	E	0.57	0/1008	0.83	0/1337
4	F	0.56	0/2806	0.76	0/3791
All	All	0.56	0/17630	0.80	1/23864 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	134	GLY	N-CA-C	5.95	118.00	110.38

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	0	3331	4	0
1	C	3437	0	3348	4	0
2	B	3350	0	3225	7	0
2	D	3309	0	3189	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	1000	0	1018	0	0
4	F	2744	0	2709	5	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	C	1	0	0	0	0
8	A	6	0	8	0	0
9	B	28	0	12	0	0
10	B	12	0	13	0	0
11	B	30	0	0	0	0
11	D	30	0	0	0	0
12	F	31	0	14	6	0
13	A	6	0	0	0	0
13	B	8	0	0	0	0
13	C	8	0	0	0	0
All	All	17517	0	16903	27	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 (27) 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:318:ASP:OD2	12:F:401:ACP:O1G	1.56	1.24
4:F:331:GLU:OE2	12:F:401:ACP:O1G	1.93	0.87
4:F:331:GLU:OE2	12:F:401:ACP:PG	2.34	0.85
4:F:331:GLU:OE2	12:F:401:ACP:O2G	2.01	0.79
2:D:315:ALA:HB3	2:D:351:THR:HG22	1.81	0.61
2:D:193:VAL:HG11	2:D:414:ASN:HD21	1.70	0.57
1:A:18:ASN:HD21	1:A:78:VAL:HG22	1.70	0.55
2:B:316:ILE:HG23	2:B:366:THR:HB	1.89	0.54
1:A:265:ILE:HG23	1:A:432:TYR:CE1	2.43	0.53
1:A:187:SER:HB3	1:A:391:LEU:HD21	1.90	0.53
12:F:401:ACP:H3B2	12:F:401:ACP:O2A	2.11	0.50
2:D:315:ALA:HB3	2:D:351:THR:CG2	2.44	0.48
4:F:331:GLU:OE1	12:F:401:ACP:O2B	2.31	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:210:ILE:HG23	2:B:273:LEU:HD13	1.96	0.48
2:B:219:THR:HG21	1:C:326:LYS:HA	1.98	0.45
1:C:344:VAL:HG21	1:C:346:TRP:CE2	2.52	0.45
2:D:134:GLN:HA	2:D:165:ASN:O	2.16	0.44
1:C:93:ILE:HD11	1:C:121:ARG:HG3	1.99	0.43
1:A:2:ARG:O	1:A:51:THR:HG23	2.18	0.43
2:B:145:SER:OG	2:B:188:SER:OG	2.36	0.43
2:B:321:MET:HE2	2:B:363:MET:HE1	2.01	0.43
1:C:71:GLU:HB2	1:C:98:ASP:HB3	2.01	0.42
2:D:99:ASN:HD22	2:D:99:ASN:N	2.18	0.42
2:B:134:GLN:HA	2:B:165:ASN:O	2.20	0.42
2:D:193:VAL:CG1	2:D:414:ASN:HD21	2.34	0.41
2:B:198:GLU:OE1	2:B:253:LEU:HD23	2.21	0.41
2:D:293:MET:HE1	2:D:315:ALA:HB1	2.03	0.41

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	435/450 (97%)	419 (96%)	15 (3%)	1 (0%)	43	72
1	C	438/450 (97%)	429 (98%)	9 (2%)	0	100	100
2	B	424/445 (95%)	411 (97%)	13 (3%)	0	100	100
2	D	417/445 (94%)	406 (97%)	11 (3%)	0	100	100
3	E	117/143 (82%)	115 (98%)	1 (1%)	1 (1%)	14	41
4	F	324/384 (84%)	304 (94%)	18 (6%)	2 (1%)	21	51
All	All	2155/2317 (93%)	2084 (97%)	67 (3%)	4 (0%)	43	72

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	F	253	TYR
3	E	27	PRO
4	F	91	CYS
1	A	261	PRO

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%)	359 (98%)	9 (2%)	43	77
1	C	371/378 (98%)	365 (98%)	6 (2%)	55	83
2	B	368/383 (96%)	361 (98%)	7 (2%)	50	81
2	D	364/383 (95%)	359 (99%)	5 (1%)	59	85
3	E	109/127 (86%)	105 (96%)	4 (4%)	30	65
4	F	301/342 (88%)	293 (97%)	8 (3%)	39	74
All	All	1881/1991 (94%)	1842 (98%)	39 (2%)	47	79

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	68	VAL
1	A	71	GLU
1	A	73	THR
1	A	188	ILE
1	A	262	TYR
1	A	279	GLU
1	A	280	LYS
1	A	316	CYS
1	A	370	LYS
2	B	57	ASN
2	B	69	GLU
2	B	215	LEU
2	B	246	LEU
2	B	316	ILE
2	B	333	VAL

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Mol	Chain	Res	Type
2	B	350	LYS
1	C	2	ARG
1	C	190	THR
1	C	284	GLU
1	C	368	LEU
1	C	381	THR
1	C	384	ILE
2	D	99	ASN
2	D	130	LEU
2	D	178	THR
2	D	351	THR
2	D	388	MET
3	E	53	LYS
3	E	75	LYS
3	E	124	GLN
3	E	139	LEU
4	F	12	SER
4	F	33	ASP
4	F	89	GLU
4	F	142	ARG
4	F	257	GLU
4	F	266	GLU
4	F	310	GLN
4	F	333	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	A	18	ASN
1	A	301	GLN
1	A	309	HIS
2	B	11	GLN
2	B	43	GLN
2	B	99	ASN
2	B	165	ASN
2	B	292	GLN
2	B	426	GLN
1	C	128	GLN
1	C	133	GLN
1	C	256	GLN
1	C	356	ASN

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Mol	Chain	Res	Type
1	C	393	HIS
2	D	37	HIS
2	D	43	GLN
2	D	83	GLN
2	D	99	ASN
2	D	375	GLN
2	D	414	ASN
3	E	12	ASN
3	E	92	ASN
3	E	124	GLN
4	F	176	GLN
4	F	252	ASN
4	F	260	ASN
4	F	306	HIS
4	F	333	ASN

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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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
5	GTP	A	501	6	33,34,34	1.32	5 (15%)	50,54,54	1.64	8 (16%)
9	GDP	B	501	6	29,30,30	1.18	4 (13%)	45,47,47	1.69	6 (13%)
8	GOL	A	504	-	5,5,5	0.28	0	5,5,5	0.28	0
5	GTP	C	501	6	33,34,34	1.28	7 (21%)	50,54,54	1.62	7 (14%)
12	ACP	F	401	-	31,33,33	2.32	11 (35%)	47,52,52	2.42	16 (34%)
5	GTP	D	501	6	33,34,34	1.18	3 (9%)	50,54,54	1.67	7 (14%)
11	7Q7	D	503	-	34,34,34	2.95	14 (41%)	46,49,49	1.87	10 (21%)
10	MES	B	503	-	12,12,12	2.22	1 (8%)	15,16,16	1.26	1 (6%)
11	7Q7	B	504	-	34,34,34	2.97	14 (41%)	46,49,49	1.88	11 (23%)

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	-	6/22/38/38	0/3/3/3
9	GDP	B	501	6	-	3/16/32/32	0/3/3/3
8	GOL	A	504	-	-	2/4/4/4	-
5	GTP	C	501	6	-	6/22/38/38	0/3/3/3
12	ACP	F	401	-	-	9/19/38/38	0/3/3/3
5	GTP	D	501	6	-	7/22/38/38	0/3/3/3
11	7Q7	D	503	-	-	4/14/14/14	0/5/5/5
10	MES	B	503	-	-	1/6/14/14	0/1/1/1
11	7Q7	B	504	-	-	4/14/14/14	0/5/5/5

All (59) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	D	503	7Q7	CAF-CAG	-7.97	1.40	1.49
11	B	504	7Q7	CAF-CAG	-7.70	1.40	1.49
10	B	503	MES	C8-S	-7.19	1.67	1.77
11	B	504	7Q7	CAP-CAN	-6.96	1.35	1.47
11	D	503	7Q7	CAP-CAN	-6.84	1.35	1.47
11	D	503	7Q7	CAU-CAT	-6.55	1.35	1.41
11	B	504	7Q7	CAU-CAT	-6.45	1.35	1.41
12	F	401	ACP	PG-O1G	5.45	1.61	1.50
12	F	401	ACP	PB-O1B	5.39	1.64	1.51
11	B	504	7Q7	CAG-CAL	-5.34	1.35	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	D	503	7Q7	CAK-CAL	-5.13	1.35	1.40
11	B	504	7Q7	CAK-CAL	-5.09	1.35	1.40
12	F	401	ACP	C5-C4	4.85	1.47	1.39
11	D	503	7Q7	CAG-CAL	-4.54	1.36	1.40
12	F	401	ACP	PB-O2B	4.40	1.67	1.56
11	D	503	7Q7	CAP-CAU	-3.92	1.36	1.41
11	B	504	7Q7	CAP-CAU	-3.80	1.36	1.41
11	D	503	7Q7	CAJ-CAK	-3.50	1.34	1.39
11	B	504	7Q7	CAS-CAT	-3.45	1.34	1.39
11	B	504	7Q7	CAJ-CAK	-3.43	1.34	1.39
11	D	503	7Q7	CAS-CAT	-3.39	1.34	1.39
12	F	401	ACP	PB-O3A	3.24	1.62	1.58
5	D	501	GTP	C5-C4	3.24	1.47	1.38
11	B	504	7Q7	CAL-NAO	-3.23	1.33	1.39
12	F	401	ACP	PG-O2G	-3.17	1.47	1.55
11	D	503	7Q7	CAK-NAM	-3.04	1.33	1.38
9	B	501	GDP	C5-C4	3.00	1.47	1.38
12	F	401	ACP	C5-C6	2.99	1.49	1.41
5	A	501	GTP	C5-C4	2.99	1.46	1.38
11	B	504	7Q7	CAK-NAM	-2.95	1.33	1.38
11	D	503	7Q7	CAW-NAV	-2.93	1.32	1.38
11	D	503	7Q7	CAL-NAO	-2.92	1.34	1.39
11	D	503	7Q7	CAU-CAX	-2.92	1.34	1.44
5	C	501	GTP	C5-C4	2.90	1.46	1.38
11	B	504	7Q7	CAU-CAX	-2.82	1.34	1.44
5	C	501	GTP	PB-O3B	2.81	1.62	1.59
12	F	401	ACP	PA-O3A	2.75	1.62	1.59
11	B	504	7Q7	CAW-NAV	-2.74	1.33	1.38
11	B	504	7Q7	CAI-NAH	2.72	1.40	1.34
11	D	503	7Q7	CAI-NAH	2.71	1.40	1.34
5	A	501	GTP	PB-O3B	2.70	1.62	1.59
11	B	504	7Q7	CAT-NAV	-2.50	1.33	1.37
12	F	401	ACP	C8-N7	2.50	1.36	1.31
5	A	501	GTP	PA-O3A	2.47	1.62	1.59
12	F	401	ACP	PG-O3G	2.46	1.60	1.55
5	A	501	GTP	C4-N9	-2.34	1.32	1.38
11	D	503	7Q7	CAT-NAV	-2.34	1.34	1.37
5	C	501	GTP	PA-O3A	2.34	1.62	1.59
5	A	501	GTP	C5-N7	-2.32	1.34	1.39
5	D	501	GTP	C5-N7	-2.26	1.34	1.39
9	B	501	GDP	C5-N7	-2.21	1.34	1.39
9	B	501	GDP	PA-O3A	2.16	1.61	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	F	401	ACP	C5-N7	-2.16	1.35	1.39
5	C	501	GTP	C6-N1	-2.16	1.34	1.38
5	C	501	GTP	C5-N7	-2.15	1.34	1.39
5	C	501	GTP	C4-N9	-2.12	1.32	1.38
9	B	501	GDP	C6-N1	-2.11	1.34	1.38
5	C	501	GTP	PB-O3A	2.05	1.61	1.59
5	D	501	GTP	PB-O3B	2.01	1.61	1.59

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	F	401	ACP	O1B-PB-C3B	8.08	130.34	109.05
11	D	503	7Q7	CAL-CAK-NAM	6.42	108.78	105.13
11	B	504	7Q7	CAL-CAK-NAM	5.87	108.47	105.13
12	F	401	ACP	C5-C4-N3	-5.77	118.77	126.72
5	D	501	GTP	C5-C4-N3	-5.65	119.39	128.39
9	B	501	GDP	C5-C4-N3	-5.49	119.65	128.39
5	C	501	GTP	C5-C4-N3	-5.26	120.03	128.39
11	B	504	7Q7	CAJ-CAI-NAH	-5.16	117.65	123.97
5	A	501	GTP	C5-C4-N3	-5.07	120.32	128.39
9	B	501	GDP	C2-N3-C4	5.03	120.96	112.30
5	C	501	GTP	C2-N3-C4	4.82	120.59	112.30
5	D	501	GTP	C2-N3-C4	4.75	120.49	112.30
12	F	401	ACP	N3-C4-N9	4.51	134.83	127.17
5	A	501	GTP	C2-N3-C4	4.43	119.93	112.30
5	D	501	GTP	N9-C4-N3	4.42	134.79	125.95
11	D	503	7Q7	CAK-CAL-NAO	-4.41	106.49	110.31
11	D	503	7Q7	CAJ-CAI-NAH	-4.25	118.76	123.97
9	B	501	GDP	N9-C4-N3	4.23	134.41	125.95
12	F	401	ACP	O2B-PB-O1B	-4.19	96.30	109.95
12	F	401	ACP	C2-N3-C4	4.00	121.61	111.83
12	F	401	ACP	N3-C2-N1	-3.89	122.70	128.58
5	A	501	GTP	N9-C4-N3	3.87	133.69	125.95
5	C	501	GTP	N9-C4-N3	3.84	133.64	125.95
11	B	504	7Q7	CAK-CAL-NAO	-3.83	107.00	110.31
12	F	401	ACP	C4-C5-N7	-3.68	106.37	110.58
12	F	401	ACP	O2B-PB-C3B	3.64	121.79	106.73
5	C	501	GTP	C6-C5-N7	3.61	136.85	130.29
5	A	501	GTP	C6-C5-N7	3.45	136.57	130.29
9	B	501	GDP	C6-C5-N7	3.38	136.43	130.29
5	D	501	GTP	C6-C5-N7	3.23	136.17	130.29
11	B	504	7Q7	CAZ-OAY-CAB	-3.15	112.89	117.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	B	504	7Q7	CAU-CAX-CAW	3.11	109.85	106.64
11	D	503	7Q7	CAU-CAX-CAW	3.08	109.82	106.64
11	B	504	7Q7	CAU-CAT-NAV	3.04	108.83	107.09
12	F	401	ACP	PB-O3A-PA	-2.95	122.75	132.37
11	D	503	7Q7	CAU-CAT-NAV	2.92	108.75	107.09
12	F	401	ACP	C4-N9-C8	2.85	108.73	105.74
12	F	401	ACP	C5-N7-C8	2.80	107.85	103.45
10	B	503	MES	O3S-S-C8	2.60	111.09	106.00
11	D	503	7Q7	CAL-CAG-NAH	2.55	119.44	118.02
5	C	501	GTP	C4-C5-N7	-2.55	106.62	110.67
12	F	401	ACP	C6-C5-N7	2.51	136.93	132.09
5	A	501	GTP	C4-C5-N7	-2.48	106.74	110.67
12	F	401	ACP	O3G-PG-C3B	2.47	112.39	106.40
11	B	504	7Q7	CAX-CAW-NAV	-2.45	107.42	110.25
11	D	503	7Q7	CAX-CAW-NAV	-2.44	107.43	110.25
5	A	501	GTP	O6-C6-C5	-2.43	120.11	126.53
11	D	503	7Q7	NAM-CAN-NAO	-2.42	108.31	112.44
9	B	501	GDP	O6-C6-C5	-2.41	120.18	126.53
5	D	501	GTP	C4-C5-N7	-2.39	106.88	110.67
11	D	503	7Q7	CAZ-OAY-CAB	-2.38	114.02	117.51
5	A	501	GTP	O3B-PB-O1B	-2.37	103.58	110.70
12	F	401	ACP	C3'-C2'-C1'	2.34	105.90	101.46
12	F	401	ACP	N9-C8-N7	-2.31	110.65	113.94
5	D	501	GTP	O6-C6-C5	-2.31	120.44	126.53
11	B	504	7Q7	CAI-NAH-CAG	2.29	121.32	116.84
11	B	504	7Q7	NAM-CAN-NAO	-2.29	108.55	112.44
5	A	501	GTP	O2B-PB-O3B	2.26	113.39	107.27
9	B	501	GDP	C4-C5-N7	-2.26	107.09	110.67
5	C	501	GTP	O3G-PG-O2G	2.25	116.25	107.80
5	C	501	GTP	O6-C6-C5	-2.22	120.68	126.53
11	D	503	7Q7	CAL-NAO-CAN	2.15	108.61	105.09
12	F	401	ACP	C2-N1-C6	2.06	122.12	118.73
11	B	504	7Q7	CAL-NAO-CAN	2.05	108.45	105.09
11	B	504	7Q7	CAT-CAU-CAX	-2.05	105.53	107.02
5	D	501	GTP	O3B-PG-O1G	-2.02	100.44	111.04

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-O3A

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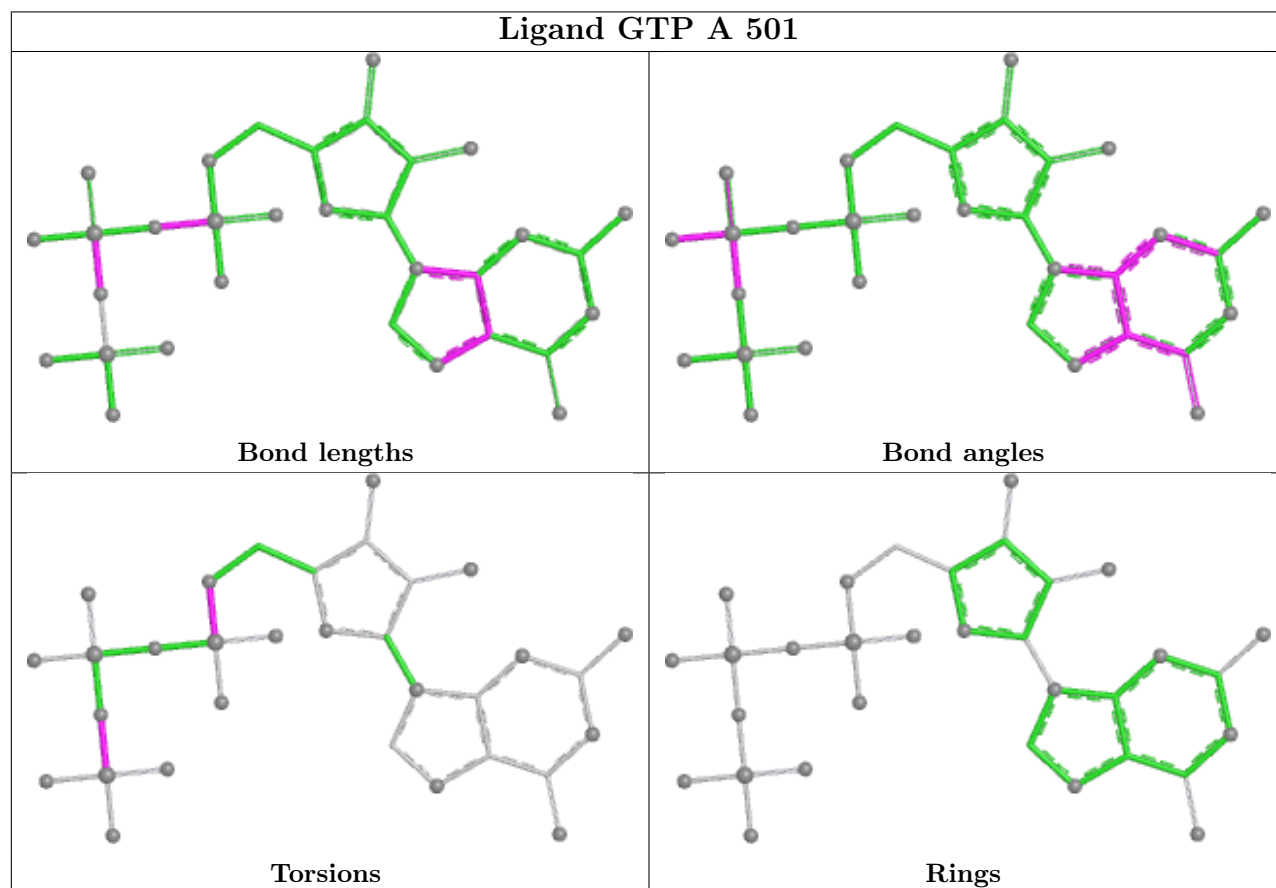
Mol	Chain	Res	Type	Atoms
5	A	501	GTP	C5'-O5'-PA-O1A
5	A	501	GTP	C5'-O5'-PA-O2A
5	C	501	GTP	PB-O3B-PG-O3G
5	C	501	GTP	C5'-O5'-PA-O3A
5	C	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O2A
5	D	501	GTP	C5'-O5'-PA-O3A
5	D	501	GTP	C5'-O5'-PA-O2A
8	A	504	GOL	C1-C2-C3-O3
9	B	501	GDP	C5'-O5'-PA-O3A
9	B	501	GDP	C5'-O5'-PA-O1A
9	B	501	GDP	C5'-O5'-PA-O2A
10	B	503	MES	N4-C7-C8-S
12	F	401	ACP	PB-C3B-PG-O1G
12	F	401	ACP	PB-C3B-PG-O3G
12	F	401	ACP	PG-C3B-PB-O1B
12	F	401	ACP	PG-C3B-PB-O3A
11	B	504	7Q7	CAC-CAB-OAY-CAZ
11	D	503	7Q7	CAC-CAD-OBC-CBD
11	D	503	7Q7	CAE-CAD-OBC-CBD
11	D	503	7Q7	CAC-CAB-OAY-CAZ
11	B	504	7Q7	CAA-CAB-OAY-CAZ
12	F	401	ACP	O4'-C4'-C5'-O5'
11	B	504	7Q7	CAC-CAD-OBC-CBD
11	D	503	7Q7	CAA-CAB-OAY-CAZ
11	B	504	7Q7	CAE-CAD-OBC-CBD
8	A	504	GOL	O2-C2-C3-O3
12	F	401	ACP	PB-O3A-PA-O1A
12	F	401	ACP	C3'-C4'-C5'-O5'
5	D	501	GTP	C5'-O5'-PA-O1A
12	F	401	ACP	PB-C3B-PG-O2G
5	D	501	GTP	PB-O3B-PG-O1G
5	D	501	GTP	PB-O3A-PA-O1A
12	F	401	ACP	PB-O3A-PA-O2A
5	A	501	GTP	PB-O3B-PG-O1G
5	A	501	GTP	PB-O3B-PG-O3G
5	D	501	GTP	C3'-C4'-C5'-O5'
5	C	501	GTP	PB-O3B-PG-O1G
5	C	501	GTP	PB-O3A-PA-O2A
5	D	501	GTP	PB-O3A-PA-O2A

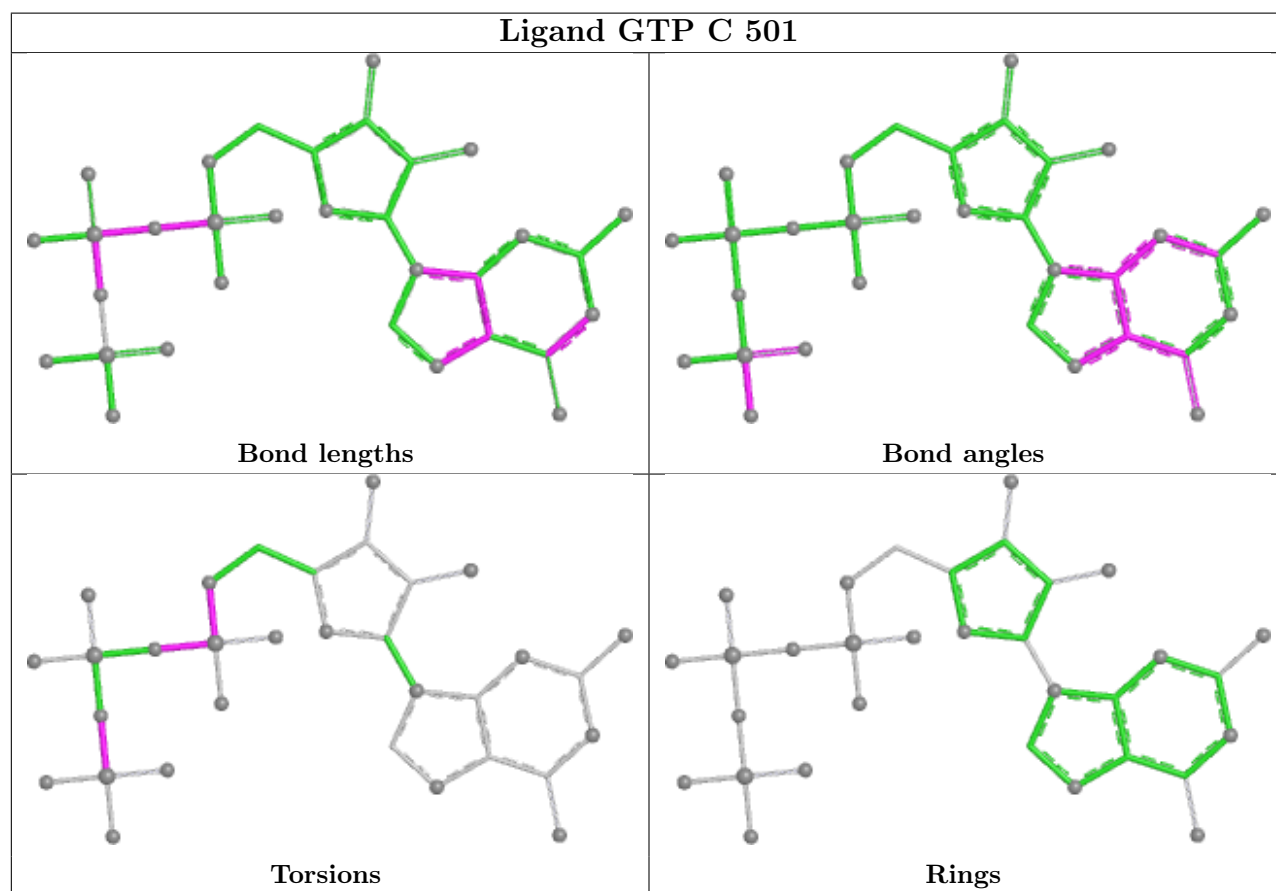
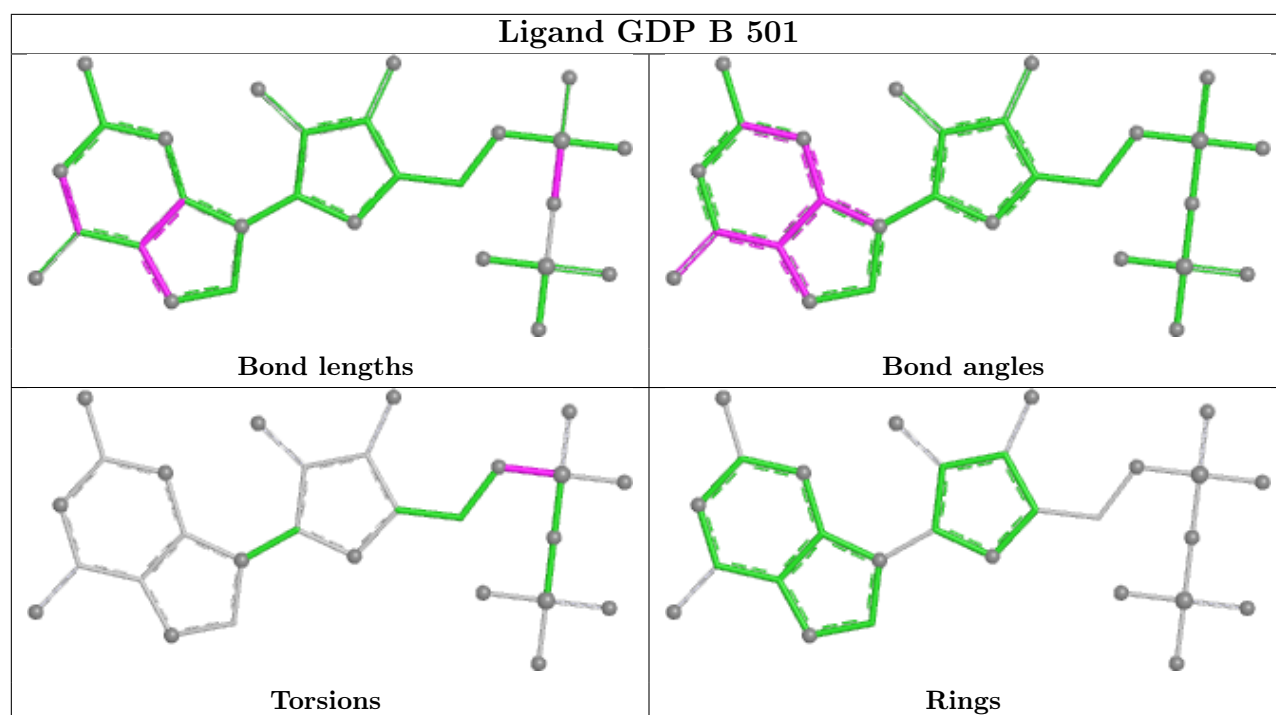
There are no ring outliers.

1 monomer is involved in 6 short contacts:

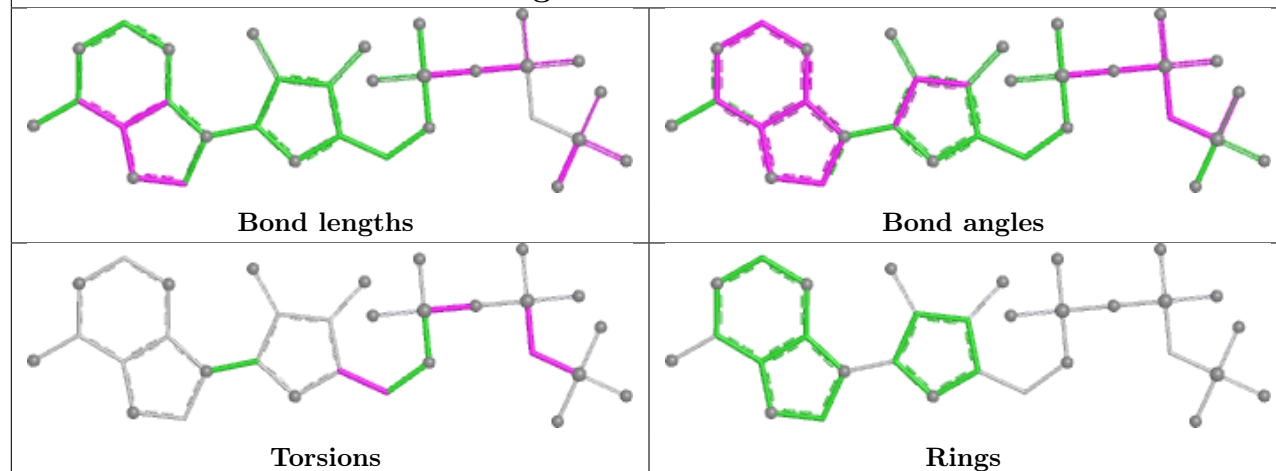
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	F	401	ACP	6	0

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.

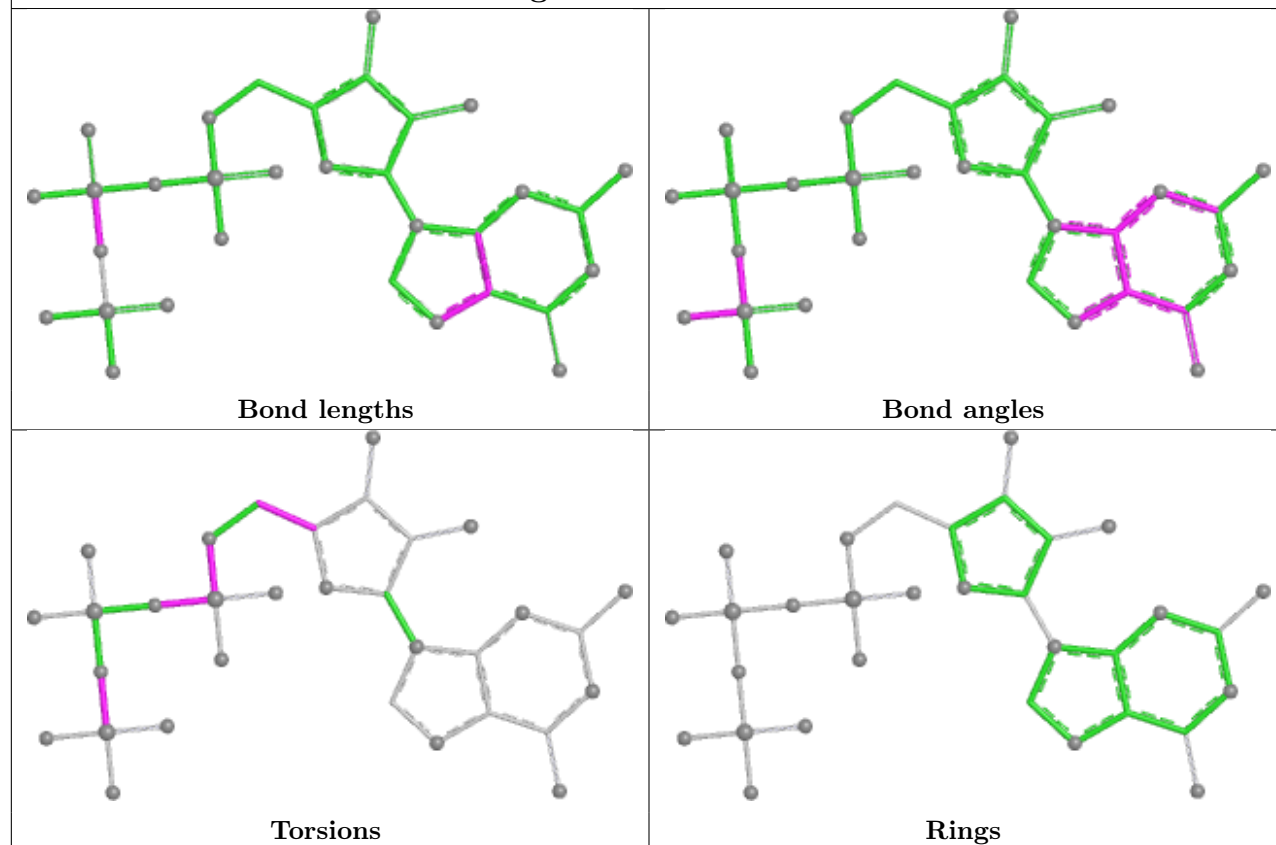




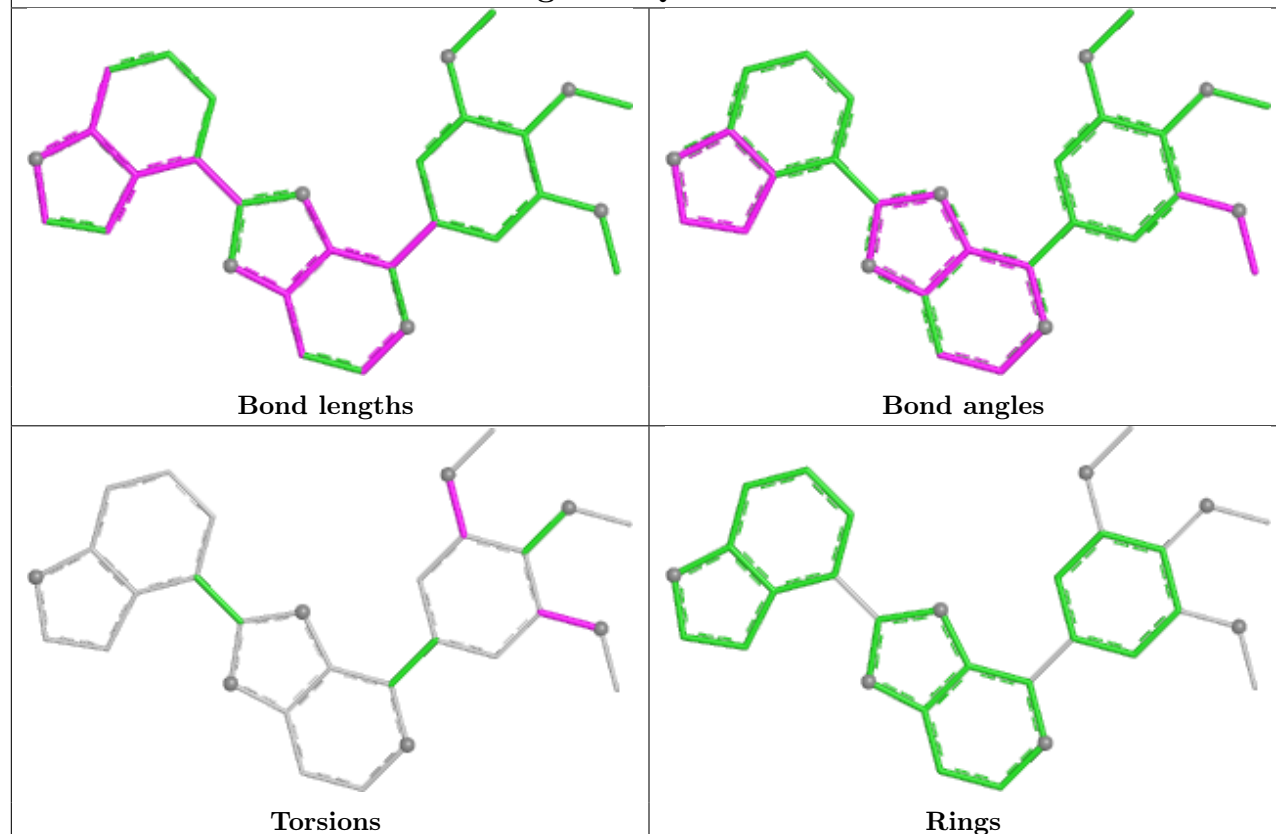
Ligand ACP F 401



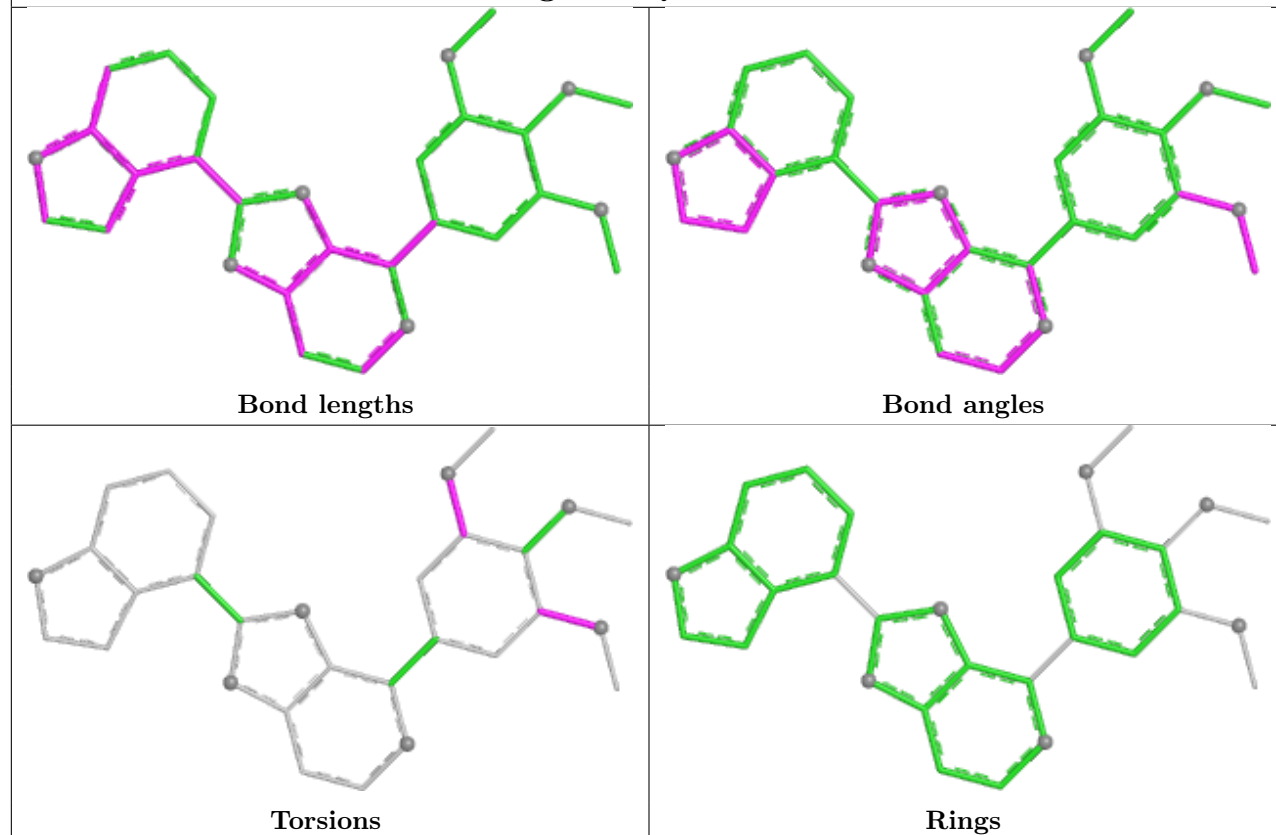
Ligand GTP D 501



Ligand 7Q7 D 503



Ligand 7Q7 B 504



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%)	0.06	5 (1%) 78 70	26, 46, 74, 96	0
1	C	440/450 (97%)	-0.23	2 (0%) 87 82	20, 36, 60, 78	0
2	B	426/445 (95%)	-0.00	7 (1%) 70 61	23, 43, 79, 112	0
2	D	421/445 (94%)	0.67	34 (8%) 18 13	33, 64, 101, 120	0
3	E	121/143 (84%)	0.75	8 (6%) 24 18	38, 65, 92, 105	0
4	F	334/384 (86%)	0.92	46 (13%) 6 5	35, 74, 129, 145	0
All	All	2179/2317 (94%)	0.28	102 (4%) 36 29	20, 52, 101, 145	0

All (102) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	161	LEU	7.7
4	F	149	ALA	5.3
4	F	233	PHE	5.2
4	F	243	HIS	4.8
4	F	180	HIS	4.7
2	D	81	PHE	4.3
4	F	245	ILE	4.1
4	F	181	VAL	3.7
2	D	397	TRP	3.6
4	F	179	VAL	3.6
3	E	28	SER	3.6
1	A	262	TYR	3.6
2	D	246	LEU	3.6
4	F	162	ILE	3.4
2	D	247	ASN	3.4
1	A	437	VAL	3.3
4	F	244	CYS	3.3
2	D	219	THR	3.3
2	D	55	THR	3.3

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Mol	Chain	Res	Type	RSRZ
4	F	90	SER	3.3
2	D	394	PHE	3.1
2	D	389	PHE	3.1
3	E	6	MET	3.1
4	F	169	LEU	3.1
2	D	80	PRO	3.0
2	D	396	HIS	3.0
4	F	173	ILE	3.0
2	D	72	THR	3.0
4	F	247	LYS	2.8
4	F	132	LEU	2.8
4	F	237	THR	2.8
2	D	140	GLY	2.8
4	F	362	ALA	2.8
1	C	283	HIS	2.8
2	D	306	ARG	2.7
3	E	141	GLU	2.7
4	F	182	ILE	2.7
1	A	88	HIS	2.7
2	D	1	MET	2.7
2	D	73	MET	2.7
2	D	220	PRO	2.7
4	F	236	LYS	2.7
2	D	360	GLY	2.7
2	B	280	GLN	2.7
4	F	231	ALA	2.7
2	D	170	MET	2.7
4	F	259	GLY	2.6
4	F	372	THR	2.6
2	B	55	THR	2.6
4	F	253	TYR	2.6
1	A	282	TYR	2.5
3	E	8	VAL	2.5
2	D	245	GLN	2.5
2	D	33	THR	2.5
2	D	221	THR	2.5
4	F	241	THR	2.5
4	F	224	SER	2.4
2	B	247	ASN	2.4
4	F	254	GLY	2.4
4	F	89	GLU	2.4
2	D	54	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
4	F	166	ALA	2.3
1	C	340	SER	2.3
4	F	103	THR	2.3
2	D	393	ALA	2.3
3	E	139	LEU	2.3
4	F	225	SER	2.3
4	F	100	ILE	2.3
4	F	99	VAL	2.3
3	E	106	GLU	2.3
2	D	180	VAL	2.3
2	B	72	THR	2.2
2	B	279	GLN	2.2
2	D	37	HIS	2.2
4	F	167	SER	2.2
1	A	196	GLU	2.2
4	F	232	ASN	2.2
4	F	191	LEU	2.2
4	F	240	LEU	2.2
2	D	390	ARG	2.1
2	D	82	GLY	2.1
2	D	400	GLY	2.1
4	F	256	TYR	2.1
3	E	103	GLN	2.1
2	D	244	GLY	2.1
4	F	170	LEU	2.1
4	F	238	CYS	2.1
4	F	239	HIS	2.1
2	B	336	LYS	2.1
4	F	198	LYS	2.1
2	D	31	ASP	2.1
4	F	177	GLY	2.1
4	F	133	ALA	2.1
2	B	281	TYR	2.1
2	D	222	TYR	2.1
4	F	130	VAL	2.0
4	F	194	PRO	2.0
2	D	48	ASN	2.0
2	D	92	PHE	2.0
2	D	98	GLY	2.0
3	E	59	GLU	2.0
4	F	146	VAL	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](#)

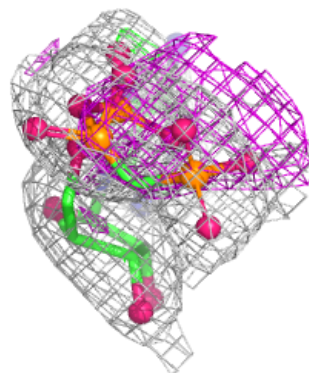
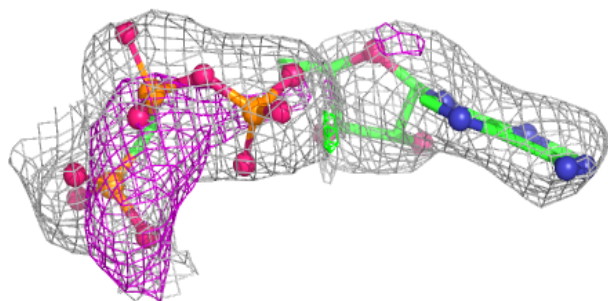
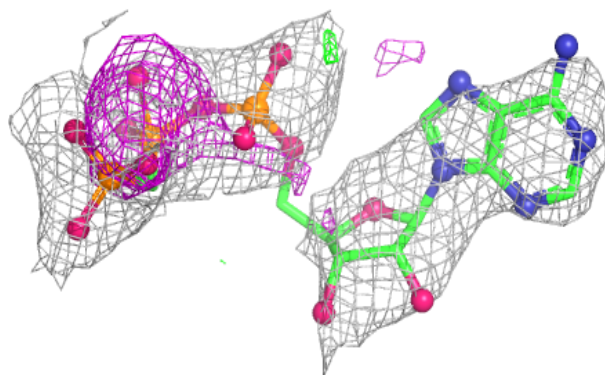
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
12	ACP	F	401	31/31	0.76	0.14	82,89,104,110	0
10	MES	B	503	12/12	0.78	0.23	97,103,107,107	0
8	GOL	A	504	6/6	0.84	0.19	57,61,63,66	0
11	7Q7	D	503	30/30	0.85	0.18	73,78,85,88	0
6	MG	D	502	1/1	0.85	0.18	49,49,49,49	0
5	GTP	D	501	32/32	0.89	0.11	50,54,64,73	0
7	CA	C	503	1/1	0.91	0.08	66,66,66,66	0
7	CA	A	503	1/1	0.93	0.10	73,73,73,73	0
6	MG	B	502	1/1	0.94	0.07	33,33,33,33	0
11	7Q7	B	504	30/30	0.94	0.09	38,42,51,53	0
5	GTP	A	501	32/32	0.96	0.07	30,32,34,34	0
6	MG	A	502	1/1	0.97	0.10	32,32,32,32	0
9	GDP	B	501	28/28	0.97	0.06	26,30,30,32	0
5	GTP	C	501	32/32	0.98	0.05	24,26,27,28	0
6	MG	C	502	1/1	1.00	0.02	29,29,29,29	0

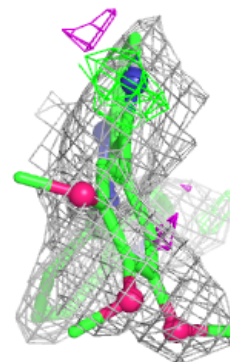
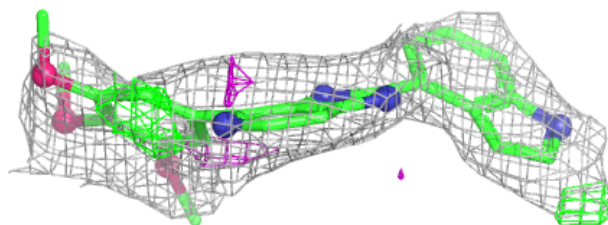
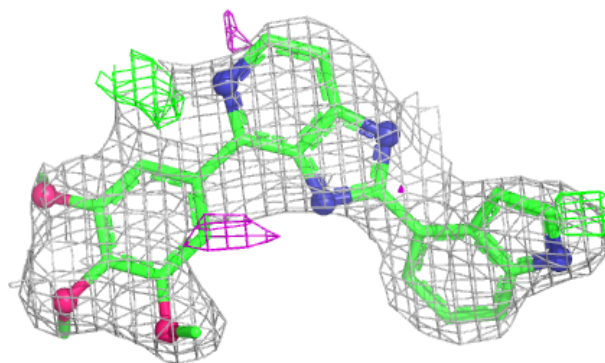
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

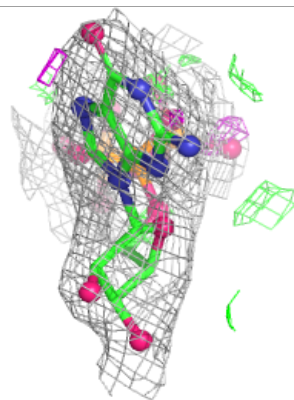
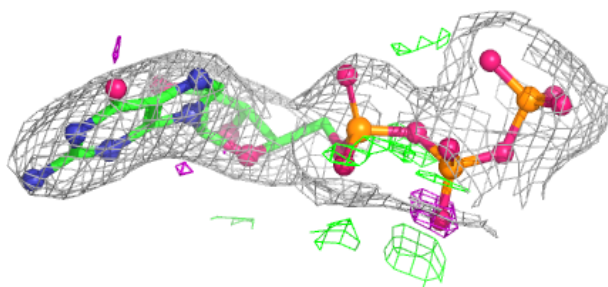
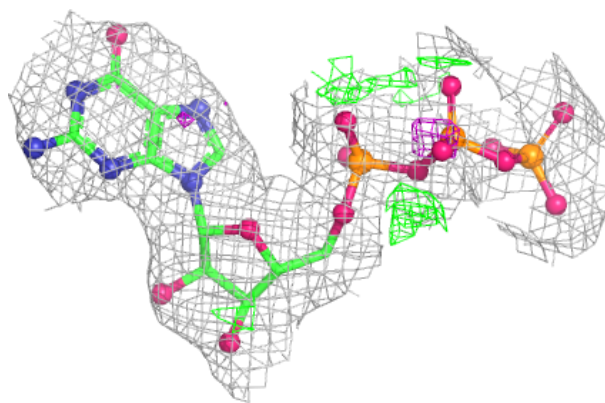
**Electron density around 7Q7 D 503:**

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

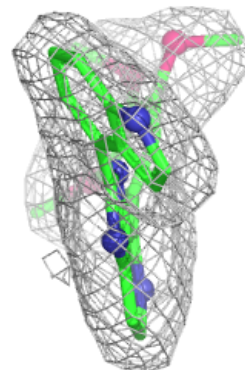
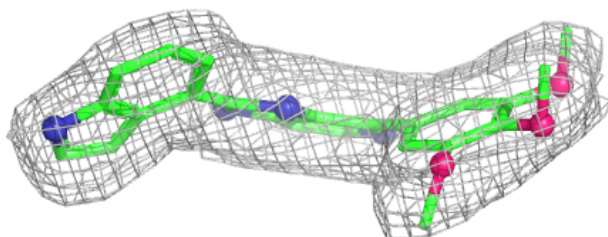
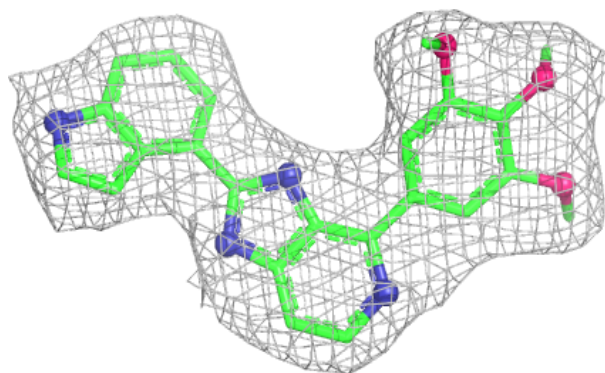


Electron density around GTP D 501:

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

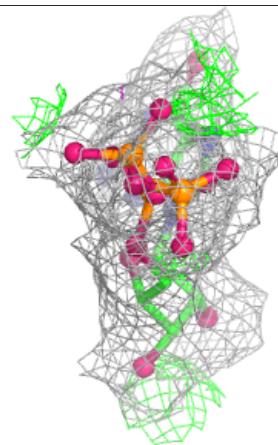
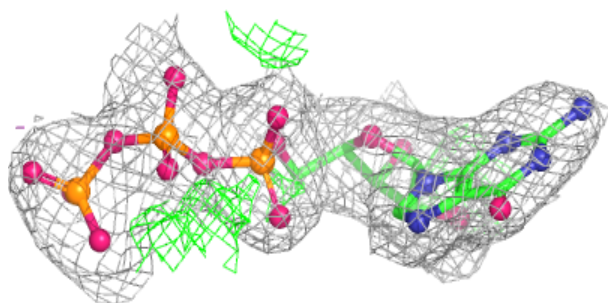
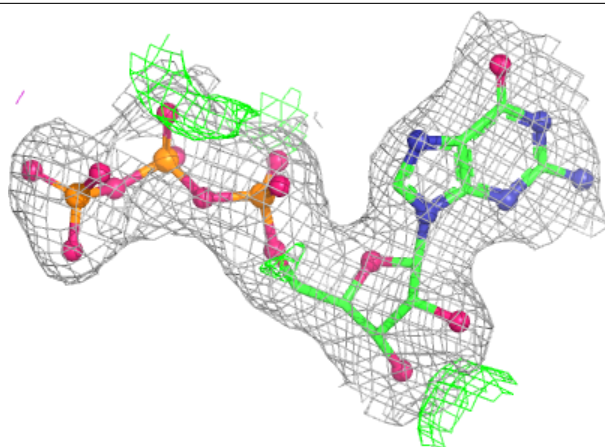
**Electron density around 7Q7 B 504:**

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



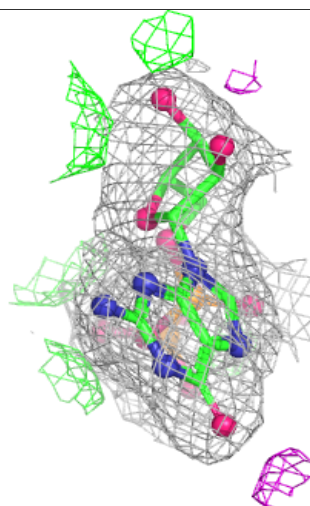
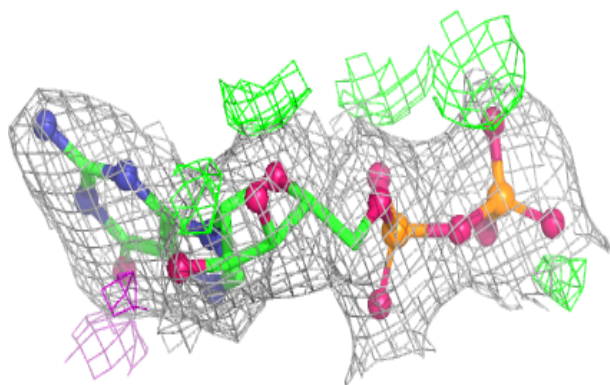
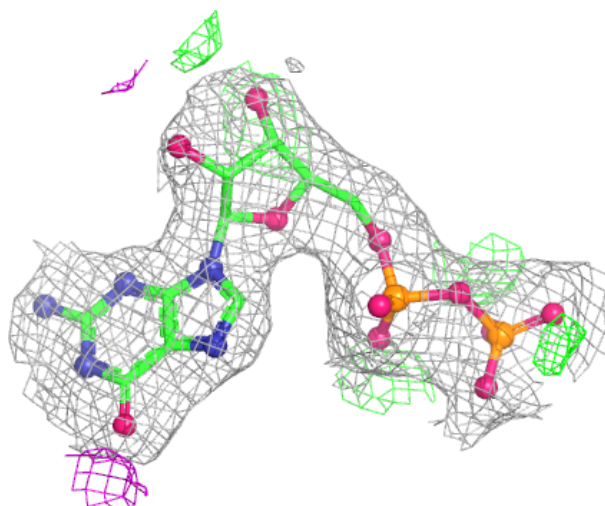
Electron density around GTP A 501:

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



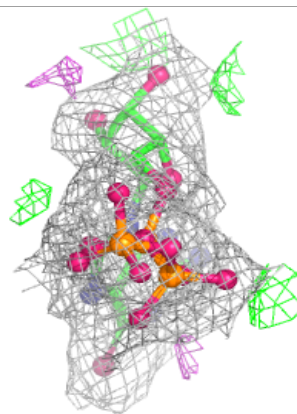
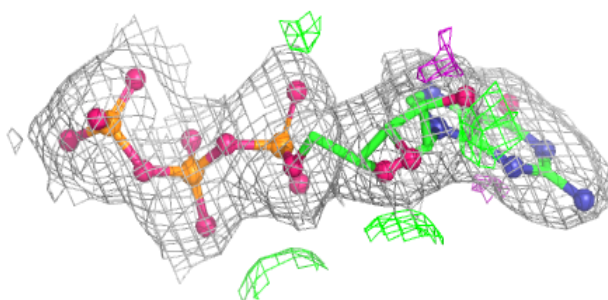
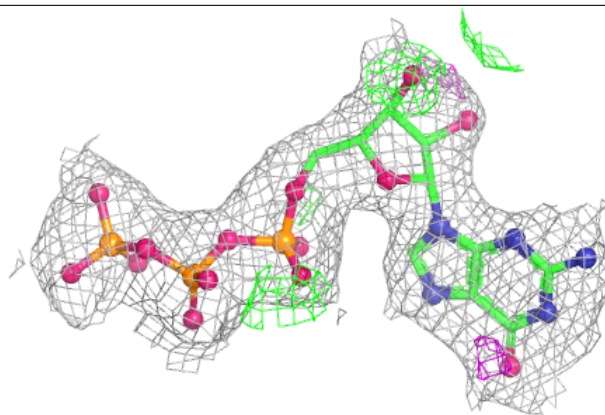
Electron density around GDP B 501:

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



Electron density around GTP C 501:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.