



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 11:08 PM UTC

PDB ID : 5XP3 / pdb_00005xp3
Title : Crystal structure of apo T2R-TTL
Authors : Wang, Y.; Yang, J.; Wang, T.; Chen, L.
Deposited on : 2017-05-31
Resolution : 2.30 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

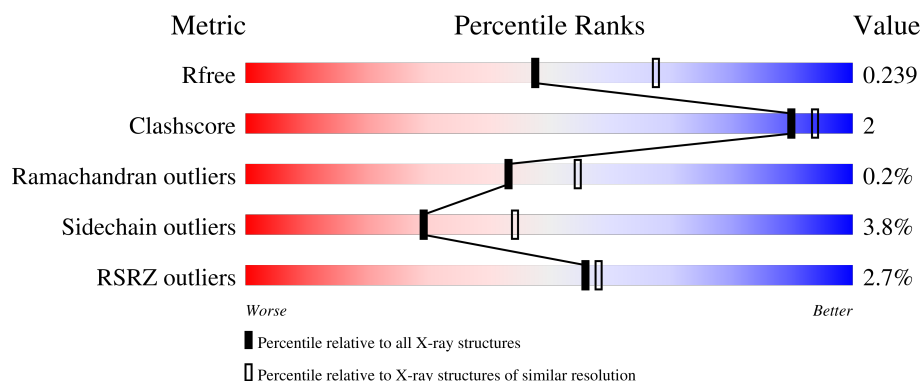
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	451	90% 6% ..
1	C	451	91% 6% ..
2	B	445	88% 8% .
2	D	445	87% 7% 5%
3	E	143	78% 6% • 15%

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Mol	Chain	Length	Quality of chain
4	F	384	8% 78% 9% 13%

2 Entry composition [i](#)

There are 12 unique types of molecules in this entry. The entry contains 17758 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 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	428	Total	C	N	O	S	0	0	0
			3369	2115	577	650	27			
2	D	421	Total	C	N	O	S	0	0	0
			3309	2080	562	640	27			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	440	GLY	GLU	conflict	UNP F2Z5B2
B	441	GLU	GLY	conflict	UNP F2Z5B2
D	440	GLY	GLU	conflict	UNP F2Z5B2
D	441	GLU	GLY	conflict	UNP F2Z5B2

- 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	-	expression tag	UNP P63043
E	4	ALA	-	expression tag	UNP P63043

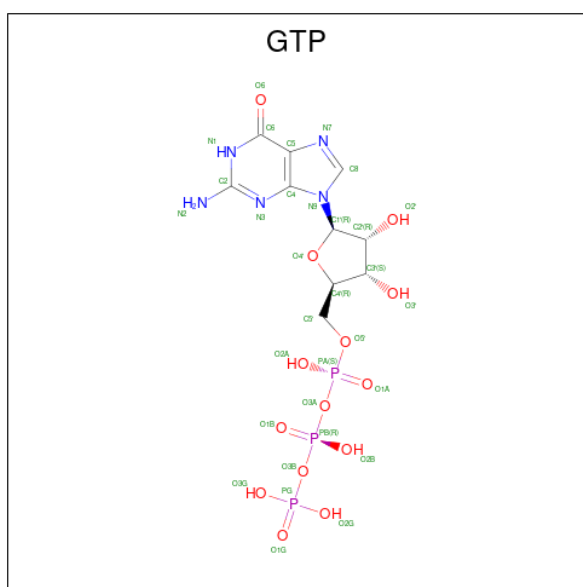
- Molecule 4 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	334	Total	C	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		

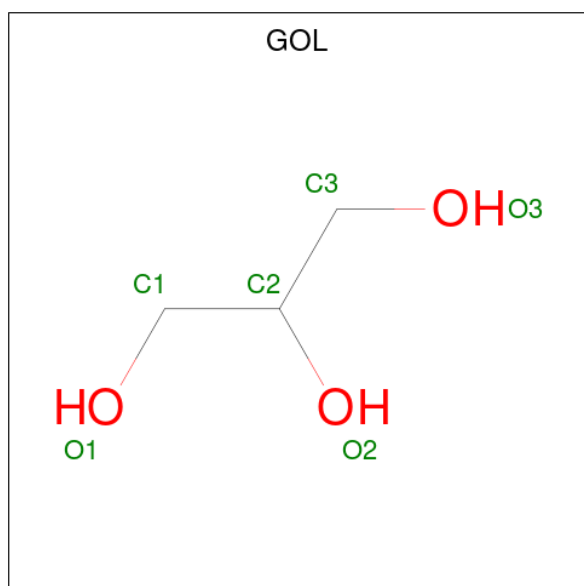
- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

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

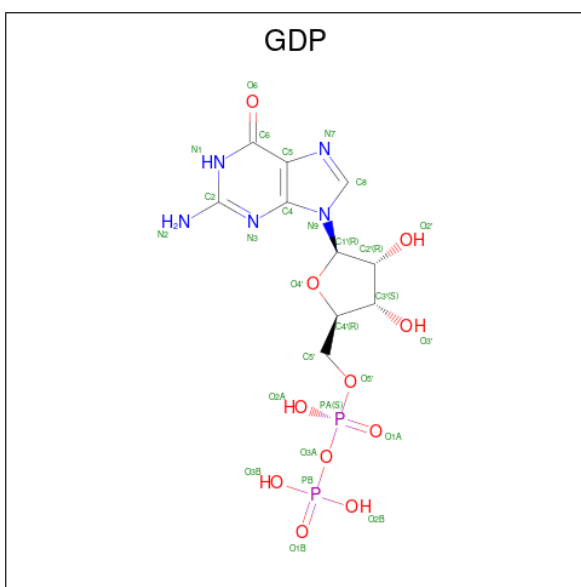
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total Ca 1 1	0	0
7	C	1	Total Ca 1 1	0	0

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



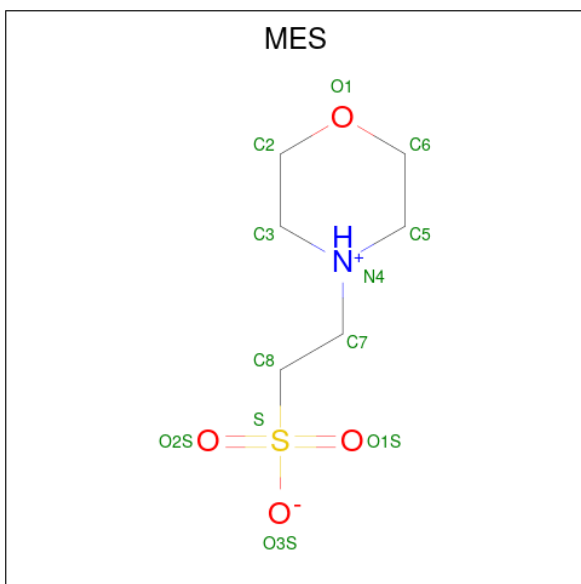
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C O 6 3 3	0	0

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



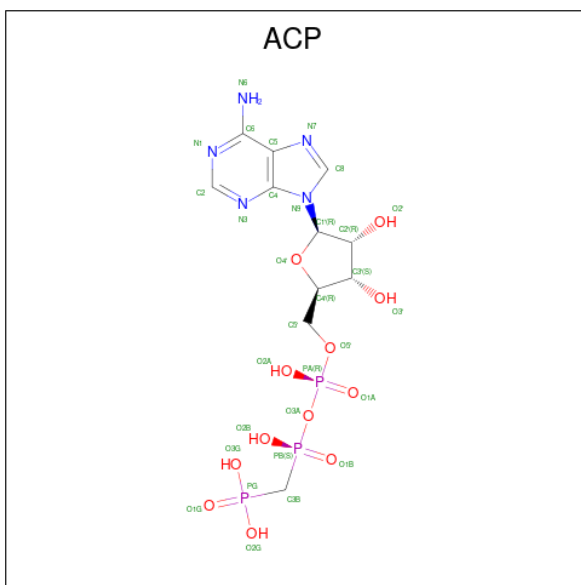
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	B	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

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



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

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



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

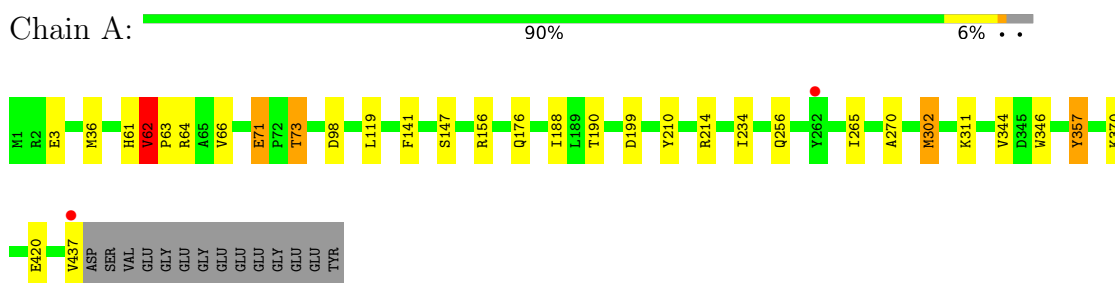
- Molecule 12 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	62	Total O 62 62	0	0
12	B	69	Total O 69 69	0	0
12	C	131	Total O 131 131	0	0
12	D	19	Total O 19 19	0	0
12	E	10	Total O 10 10	0	0
12	F	13	Total O 13 13	0	0

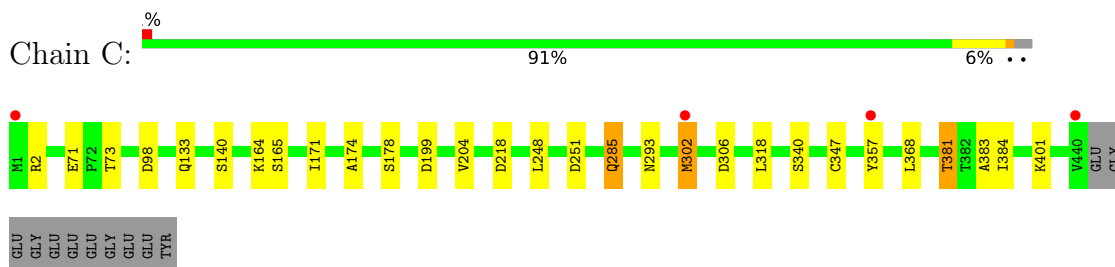
3 Residue-property plots [i](#)

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.

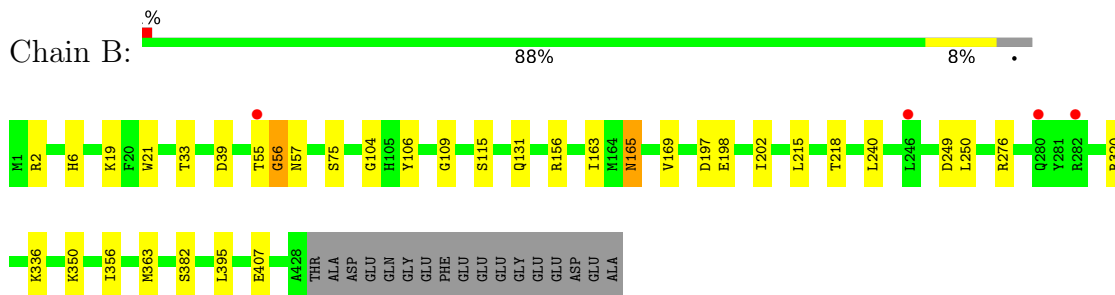
- Molecule 1: Tubulin alpha-1B chain



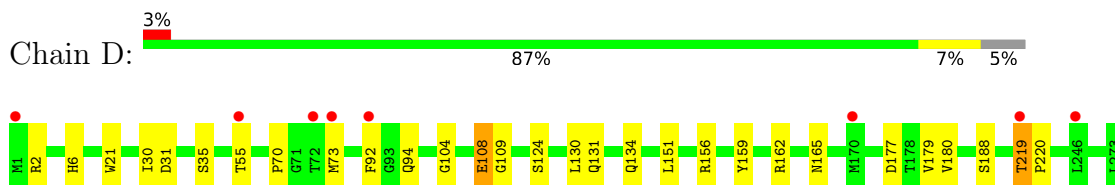
- Molecule 1: Tubulin alpha-1B chain

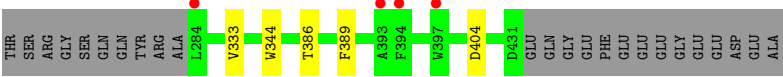


- Molecule 2: Tubulin beta chain

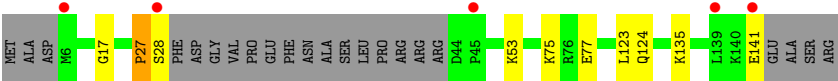
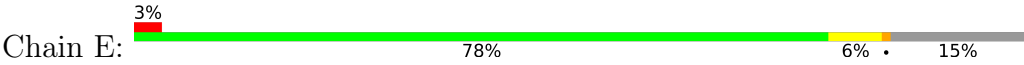


- Molecule 2: Tubulin beta chain

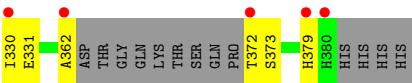
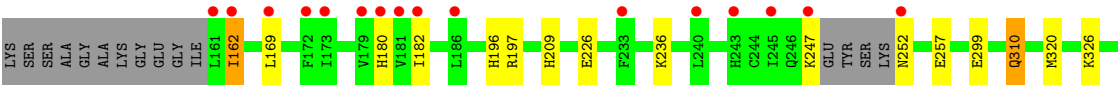
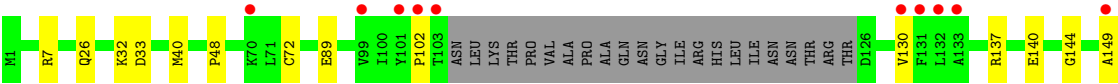
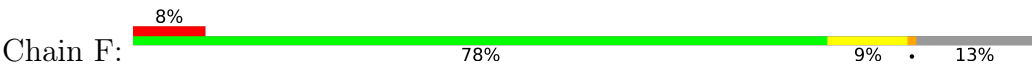




● Molecule 3: Stathmin-4



● Molecule 4: Uncharacterized protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	105.17Å 157.96Å 181.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.30 50.00 – 2.31	Depositor EDS
% Data completeness (in resolution range)	99.6 (50.00-2.30) 99.6 (50.00-2.31)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.34 (at 2.31Å)	Xtriage
Refinement program	REFMAC 5.8.0107	Depositor
R, R_{free}	0.189 , 0.240 0.190 , 0.239	Depositor DCC
R_{free} test set	6607 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	49.4	Xtriage
Anisotropy	0.062	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 26.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	17758	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.52% 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, ACP, GTP, GOL, MG, MES, CA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.81	1/3494 (0.0%)	1.03	3/4743 (0.1%)
1	C	0.87	0/3515	1.04	5/4772 (0.1%)
2	B	0.81	0/3444	1.04	0/4664
2	D	0.71	0/3382	1.03	2/4581 (0.0%)
3	E	0.80	0/1008	1.13	0/1337
4	F	0.70	0/2806	1.03	8/3791 (0.2%)
All	All	0.79	1/17649 (0.0%)	1.04	18/23888 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	62	VAL	CA-CB	7.25	1.60	1.54

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	162	ILE	N-CA-C	7.72	119.96	108.54
1	C	306	ASP	CA-C-N	6.55	126.17	119.56
1	C	306	ASP	C-N-CA	6.55	126.17	119.56
1	A	62	VAL	CB-CA-C	6.25	116.20	110.13
1	C	381	THR	CB-CA-C	-5.97	97.56	109.33
1	C	302	MET	CB-CG-SD	-5.86	95.13	112.70
1	A	62	VAL	N-CA-C	5.67	114.36	107.61
4	F	299	GLU	CA-C-N	-5.66	113.19	119.19
4	F	299	GLU	C-N-CA	-5.66	113.19	119.19
1	A	357	TYR	N-CA-C	5.62	118.34	111.82
2	D	124	SER	N-CA-C	5.54	117.76	111.11
4	F	226	GLU	CA-C-N	5.29	126.45	119.84
4	F	226	GLU	C-N-CA	5.29	126.45	119.84
1	C	73	THR	N-CA-C	5.27	117.94	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	373	SER	N-CA-C	5.24	117.83	110.23
2	D	389	PHE	N-CA-C	5.22	116.97	111.28
4	F	379	HIS	N-CA-C	5.13	116.67	108.41
4	F	72	CYS	N-CA-C	5.12	119.63	113.17

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	16	0
1	C	3437	0	3348	11	0
2	B	3369	0	3250	14	0
2	D	3309	0	3189	12	0
3	E	1000	0	1018	3	0
4	F	2744	0	2709	10	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	4	0
11	F	31	0	14	0	0
12	A	62	0	0	0	0
12	B	69	0	0	0	0
12	C	131	0	0	1	0
12	D	19	0	0	0	0
12	E	10	0	0	0	0
12	F	13	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	17758	0	16928	63	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 (63) 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:7:ARG:HD3	4:F:40:MET:HE3	1.63	0.80
1:C:71:GLU:HB2	1:C:98:ASP:HB3	1.66	0.75
2:B:197:ASP:OD1	10:B:503:MES:H32	1.92	0.69
4:F:209:HIS:HB2	4:F:310:GLN:HG3	1.74	0.68
1:C:381:THR:HG23	12:C:618:HOH:O	1.95	0.66
1:C:381:THR:HG22	1:C:383:ALA:H	1.62	0.65
2:B:197:ASP:OD2	10:B:503:MES:H52	1.97	0.64
1:C:204:VAL:HG22	1:C:302:MET:CE	2.28	0.63
2:D:156:ARG:HG2	3:E:123:LEU:HD11	1.81	0.63
2:B:165:ASN:HB2	2:B:198:GLU:HG3	1.80	0.62
1:A:265:ILE:HG22	1:A:265:ILE:O	2.04	0.58
1:C:248:LEU:HD12	1:C:357:TYR:OH	2.03	0.58
2:D:31:ASP:HB2	2:D:35:SER:H	1.68	0.58
2:B:131:GLN:HE22	2:B:250:LEU:H	1.53	0.57
2:B:131:GLN:NE2	2:B:250:LEU:H	2.03	0.55
4:F:149:ALA:O	4:F:180:HIS:CD2	2.60	0.55
4:F:197:ARG:NH1	4:F:257:GLU:OE1	2.41	0.54
2:D:73:MET:HG3	2:D:92:PHE:HB3	1.91	0.53
2:B:156:ARG:HG3	10:B:503:MES:H62	1.90	0.53
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.26	0.52
2:B:104:GLY:O	2:B:109:GLY:HA3	2.10	0.52
4:F:40:MET:HE1	4:F:48:PRO:HD2	1.91	0.52
1:A:234:ILE:HD13	1:A:302:MET:SD	2.49	0.52
2:B:156:ARG:CZ	10:B:503:MES:H21	2.40	0.51
2:D:6:HIS:CD2	2:D:21:TRP:HE1	2.29	0.51
4:F:7:ARG:CD	4:F:40:MET:HE3	2.37	0.50
4:F:137:ARG:HA	4:F:140:GLU:HG3	1.94	0.50
4:F:320:MET:HB2	4:F:330:ILE:HD11	1.94	0.50
1:C:165:SER:HA	1:C:199:ASP:OD2	2.13	0.49
2:B:56:GLY:N	2:B:57:ASN:HA	2.27	0.49
2:D:2:ARG:HB3	2:D:131:GLN:HG2	1.95	0.49
2:B:106:TYR:OH	2:B:407:GLU:OE2	2.30	0.48
2:D:104:GLY:O	2:D:109:GLY:HA3	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:GLU:HB2	1:A:98:ASP:HB3	1.96	0.47
1:A:199:ASP:HB3	1:A:256:GLN:HG2	1.97	0.47
1:A:147:SER:HB2	1:A:190:THR:HB	1.97	0.47
1:A:357:TYR:CE2	3:E:17:GLY:HA2	2.51	0.46
2:D:134:GLN:HA	2:D:165:ASN:O	2.16	0.46
1:A:3:GLU:HG2	1:A:64:ARG:CZ	2.46	0.46
2:D:108:GLU:H	2:D:108:GLU:HG2	1.58	0.46
1:A:119:LEU:HD11	1:A:156:ARG:HB3	1.98	0.45
1:A:210:TYR:CE2	1:A:214:ARG:HD2	2.51	0.45
2:B:131:GLN:NE2	2:B:249:ASP:HB2	2.32	0.45
4:F:169:LEU:HD13	4:F:182:ILE:HD11	1.98	0.45
1:A:141:PHE:O	1:A:147:SER:HB3	2.17	0.45
1:A:270:ALA:HB3	1:A:302:MET:HG2	2.00	0.44
1:C:174:ALA:O	1:C:178:SER:HB3	2.18	0.44
2:D:70:PRO:HD3	2:D:94:GLN:HA	2.00	0.44
4:F:26:GLN:HE22	4:F:362:ALA:H	1.66	0.44
1:A:36:MET:HB3	1:A:61:HIS:CE1	2.53	0.43
1:A:71:GLU:CD	1:A:73:THR:HG1	2.26	0.43
2:B:169:VAL:HA	2:B:202:ILE:O	2.18	0.43
1:C:401:LYS:HG3	2:D:344:TRP:CE3	2.54	0.43
2:D:219:THR:HA	2:D:220:PRO:HD3	1.80	0.42
2:D:159:TYR:HB3	2:D:162:ARG:HG3	2.01	0.42
2:B:163:ILE:HG21	2:B:250:LEU:HB3	2.02	0.41
1:C:140:SER:HA	1:C:171:ILE:HB	2.02	0.41
1:A:346:TRP:CD1	1:A:346:TRP:H	2.38	0.41
1:A:311:LYS:HD3	1:A:344:VAL:HG12	2.02	0.41
1:A:62:VAL:HA	1:A:63:PRO:HD3	1.97	0.41
1:C:204:VAL:HG22	1:C:302:MET:HE2	2.00	0.41
1:C:285:GLN:H	1:C:285:GLN:HG3	1.75	0.40
3:E:27:PRO:HB2	3:E:28:SER:H	1.72	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	435/451 (96%)	427 (98%)	8 (2%)	0	100	100
1	C	438/451 (97%)	430 (98%)	8 (2%)	0	100	100
2	B	426/445 (96%)	413 (97%)	12 (3%)	1 (0%)	43	55
2	D	417/445 (94%)	402 (96%)	15 (4%)	0	100	100
3	E	117/143 (82%)	115 (98%)	1 (1%)	1 (1%)	14	17
4	F	324/384 (84%)	307 (95%)	14 (4%)	3 (1%)	14	17
All	All	2157/2319 (93%)	2094 (97%)	58 (3%)	5 (0%)	43	55

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	E	27	PRO
4	F	32	LYS
4	F	144	GLY
4	F	102	PRO
2	B	56	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	368/379 (97%)	358 (97%)	10 (3%)	39	58
1	C	371/379 (98%)	359 (97%)	12 (3%)	34	51
2	B	370/383 (97%)	351 (95%)	19 (5%)	21	32
2	D	364/383 (95%)	351 (96%)	13 (4%)	31	47
3	E	109/127 (86%)	103 (94%)	6 (6%)	19	28
4	F	301/342 (88%)	289 (96%)	12 (4%)	28	42
All	All	1883/1993 (94%)	1811 (96%)	72 (4%)	29	44

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	62	VAL
1	A	66	VAL
1	A	71	GLU
1	A	73	THR
1	A	176	GLN
1	A	188	ILE
1	A	302	MET
1	A	370	LYS
1	A	420	GLU
1	A	437	VAL
2	B	2	ARG
2	B	19	LYS
2	B	33	THR
2	B	39	ASP
2	B	55	THR
2	B	75	SER
2	B	115	SER
2	B	165	ASN
2	B	215	LEU
2	B	218	THR
2	B	240	LEU
2	B	276	ARG
2	B	320	ARG
2	B	336	LYS
2	B	350	LYS
2	B	356	ILE
2	B	363	MET
2	B	382	SER
2	B	395	LEU
1	C	2	ARG
1	C	133	GLN
1	C	164	LYS
1	C	218	ASP
1	C	251	ASP
1	C	285	GLN
1	C	293	ASN
1	C	318	LEU
1	C	340	SER
1	C	347	CYS
1	C	368	LEU
1	C	384	ILE
2	D	30	ILE
2	D	55	THR

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Mol	Chain	Res	Type
2	D	108	GLU
2	D	130	LEU
2	D	151	LEU
2	D	177	ASP
2	D	179	VAL
2	D	180	VAL
2	D	188	SER
2	D	219	THR
2	D	333	VAL
2	D	386	THR
2	D	404	ASP
3	E	53	LYS
3	E	75	LYS
3	E	77	GLU
3	E	124	GLN
3	E	135	LYS
3	E	141	GLU
4	F	33	ASP
4	F	89	GLU
4	F	130	VAL
4	F	162	ILE
4	F	196	HIS
4	F	236	LYS
4	F	247	LYS
4	F	252	ASN
4	F	310	GLN
4	F	326	LYS
4	F	331	GLU
4	F	372	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	258	ASN
1	A	300	ASN
1	A	301	GLN
1	A	393	HIS
2	B	15	GLN
2	B	83	GLN
2	B	131	GLN
2	B	298	ASN
2	B	347	ASN

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Mol	Chain	Res	Type
2	B	375	GLN
1	C	11	GLN
1	C	50	ASN
1	C	85	GLN
1	C	101	ASN
1	C	356	ASN
1	C	393	HIS
2	D	165	ASN
2	D	245	GLN
2	D	426	GLN
3	E	18	GLN
3	E	78	HIS
3	E	92	ASN
3	E	124	GLN
4	F	26	GLN
4	F	180	HIS
4	F	229	ASN
4	F	232	ASN
4	F	260	ASN
4	F	269	GLN
4	F	333	ASN
4	F	380	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 13 ligands modelled in this entry, 6 are monoatomic - leaving 7 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	D	501	6	33,34,34	1.31	5 (15%)	50,54,54	1.71	6 (12%)
9	GDP	B	501	6	29,30,30	1.28	4 (13%)	45,47,47	1.81	11 (24%)
10	MES	B	503	-	12,12,12	2.16	2 (16%)	15,16,16	5.70	8 (53%)
8	GOL	A	504	-	5,5,5	0.37	0	5,5,5	0.35	0
11	ACP	F	401	-	31,33,33	1.89	9 (29%)	47,52,52	1.78	9 (19%)
5	GTP	A	501	6	33,34,34	1.39	6 (18%)	50,54,54	1.76	9 (18%)
5	GTP	C	501	6	33,34,34	1.19	4 (12%)	50,54,54	1.72	10 (20%)

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

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	503	MES	C8-S	-6.49	1.68	1.77
11	F	401	ACP	C5-C4	5.29	1.48	1.39
11	F	401	ACP	PB-O3A	4.09	1.62	1.58
5	D	501	GTP	PB-O3B	3.49	1.63	1.59
5	A	501	GTP	PA-O3A	3.41	1.63	1.59
9	B	501	GDP	PA-O3A	3.40	1.63	1.59
5	D	501	GTP	C5-C4	3.21	1.47	1.38
5	A	501	GTP	PB-O3B	3.02	1.62	1.59
11	F	401	ACP	PG-O3G	2.98	1.61	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	F	401	ACP	C5-C6	2.93	1.49	1.41
9	B	501	GDP	C5-C4	2.93	1.46	1.38
11	F	401	ACP	PA-O3A	2.80	1.62	1.59
5	A	501	GTP	C5-C4	2.76	1.46	1.38
11	F	401	ACP	PG-O2G	2.72	1.61	1.55
5	C	501	GTP	C6-N1	-2.70	1.33	1.38
5	A	501	GTP	C5-N7	-2.67	1.33	1.39
11	F	401	ACP	C5-N7	-2.66	1.34	1.39
5	A	501	GTP	C6-N1	-2.61	1.34	1.38
5	C	501	GTP	C5-C4	2.52	1.45	1.38
10	B	503	MES	O2S-S	2.49	1.52	1.45
5	D	501	GTP	PA-O3A	2.30	1.62	1.59
5	A	501	GTP	C4-N9	-2.29	1.32	1.38
11	F	401	ACP	C8-N7	2.25	1.36	1.31
5	C	501	GTP	PB-O3B	2.21	1.61	1.59
9	B	501	GDP	C4-N9	-2.20	1.32	1.38
5	C	501	GTP	C5-N7	-2.17	1.34	1.39
11	F	401	ACP	PB-O2B	2.12	1.61	1.56
5	D	501	GTP	C5-N7	-2.11	1.34	1.39
9	B	501	GDP	C6-N1	-2.10	1.34	1.38
5	D	501	GTP	PB-O3A	2.02	1.61	1.59

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	503	MES	O3S-S-O2S	-11.33	83.05	111.40
10	B	503	MES	O3S-S-C8	-10.73	85.01	106.00
10	B	503	MES	O3S-S-O1S	-9.75	87.00	111.40
10	B	503	MES	O2S-S-C8	8.71	119.89	106.73
10	B	503	MES	O1S-S-C8	7.01	117.33	106.73
5	D	501	GTP	C5-C4-N3	-5.95	118.91	128.39
11	F	401	ACP	C5-C4-N3	-5.86	118.65	126.72
5	A	501	GTP	C5-C4-N3	-5.77	119.21	128.39
5	A	501	GTP	C2-N3-C4	5.26	121.36	112.30
5	C	501	GTP	C5-C4-N3	-5.23	120.07	128.39
5	D	501	GTP	C2-N3-C4	5.22	121.29	112.30
11	F	401	ACP	N3-C4-N9	4.83	135.38	127.17
9	B	501	GDP	C2-N3-C4	4.68	120.36	112.30
9	B	501	GDP	C5-C4-N3	-4.67	120.96	128.39
5	C	501	GTP	C2-N3-C4	4.63	120.27	112.30
5	D	501	GTP	N9-C4-N3	4.33	134.61	125.95
5	C	501	GTP	N9-C4-N3	4.22	134.40	125.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	501	GDP	N9-C4-N3	4.01	133.97	125.95
5	A	501	GTP	N9-C4-N3	3.95	133.85	125.95
11	F	401	ACP	C2-N3-C4	3.75	120.99	111.83
5	A	501	GTP	C6-C5-N7	3.54	136.72	130.29
11	F	401	ACP	N3-C2-N1	-3.53	123.25	128.58
9	B	501	GDP	C6-C5-N7	3.47	136.60	130.29
5	C	501	GTP	C6-C5-N7	3.27	136.24	130.29
5	D	501	GTP	C6-C5-N7	3.25	136.21	130.29
10	B	503	MES	C6-O1-C2	3.11	119.92	109.88
11	F	401	ACP	C4-C5-N7	-2.96	107.20	110.58
9	B	501	GDP	O6-C6-C5	-2.94	118.78	126.53
9	B	501	GDP	O4'-C1'-N9	-2.90	101.79	108.36
5	A	501	GTP	C4-C5-N7	-2.65	106.47	110.67
5	D	501	GTP	C4-C5-N7	-2.63	106.51	110.67
10	B	503	MES	C5-N4-C3	2.54	114.31	108.84
5	C	501	GTP	C4-C5-N7	-2.53	106.67	110.67
5	C	501	GTP	C8-N7-C5	2.45	108.62	104.26
5	C	501	GTP	O3G-PG-O1G	2.41	120.23	110.83
5	D	501	GTP	O6-C6-C5	-2.39	120.22	126.53
5	C	501	GTP	N9-C8-N7	-2.37	109.00	113.40
9	B	501	GDP	C6-C5-C4	-2.33	115.33	118.83
5	C	501	GTP	O3A-PB-O1B	-2.30	103.78	110.70
11	F	401	ACP	C3'-C2'-C1'	2.25	105.73	101.46
5	A	501	GTP	O6-C6-C5	-2.24	120.61	126.53
5	A	501	GTP	O3G-PG-O3B	-2.23	97.15	104.64
5	A	501	GTP	O2A-PA-O1A	2.22	122.76	112.44
11	F	401	ACP	C5-N7-C8	2.21	106.93	103.45
5	C	501	GTP	C8-N9-C4	2.21	110.17	106.03
9	B	501	GDP	O2A-PA-O3A	2.16	113.11	107.27
9	B	501	GDP	O3A-PA-O1A	-2.10	104.39	110.70
9	B	501	GDP	C8-N9-C4	2.08	109.93	106.03
10	B	503	MES	O2S-S-O1S	2.06	120.52	113.82
9	B	501	GDP	C5-C6-N1	2.04	118.45	113.25
11	F	401	ACP	C4-N9-C8	2.02	107.86	105.74
11	F	401	ACP	C2-N1-C6	2.02	122.04	118.73
5	A	501	GTP	O3G-PG-O2G	2.00	115.31	107.80

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	501	GTP	PB-O3B-PG-O3G

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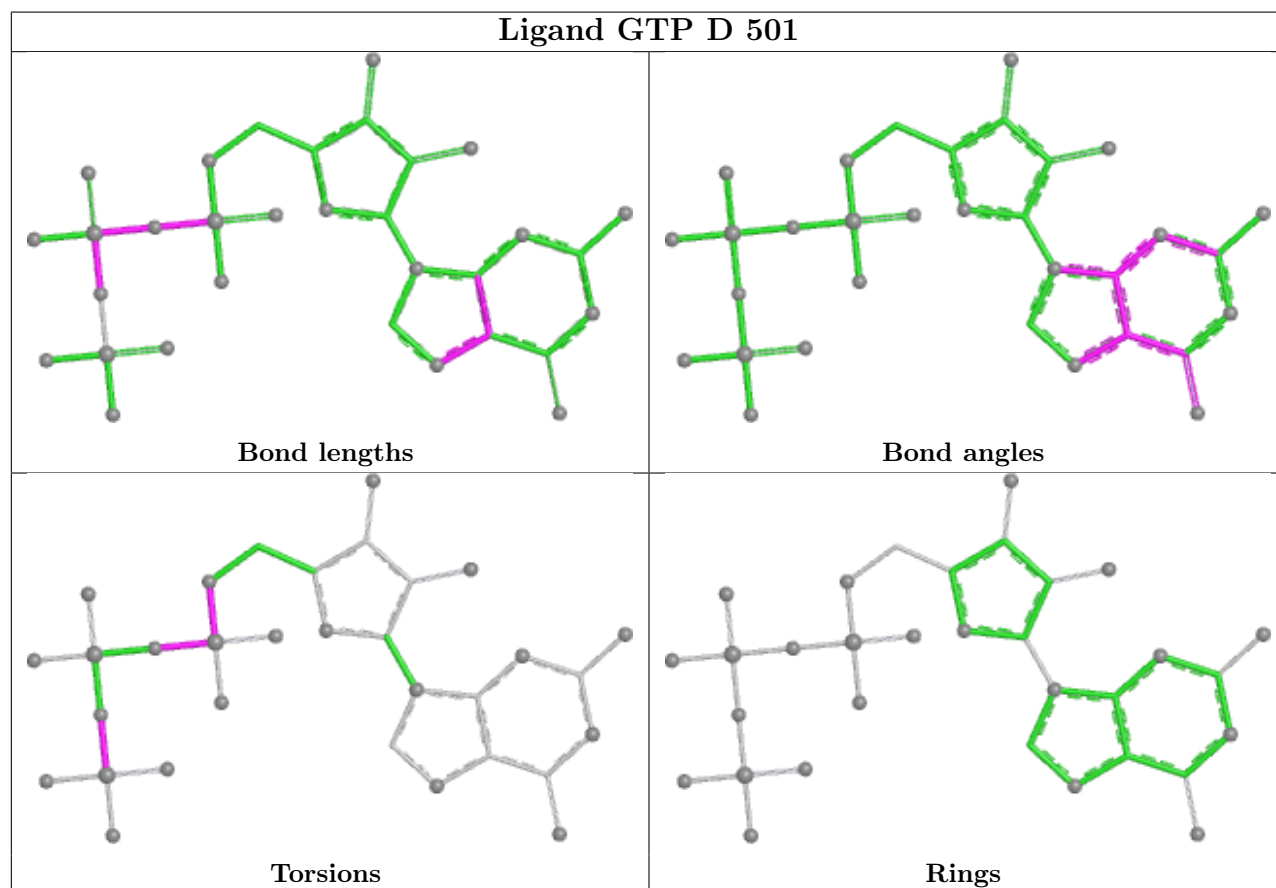
Mol	Chain	Res	Type	Atoms
5	A	501	GTP	C5'-O5'-PA-O3A
5	A	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O3A
5	C	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O2A
5	D	501	GTP	C5'-O5'-PA-O3A
5	D	501	GTP	C5'-O5'-PA-O1A
8	A	504	GOL	C1-C2-C3-O3
9	B	501	GDP	C5'-O5'-PA-O3A
9	B	501	GDP	C5'-O5'-PA-O1A
10	B	503	MES	C8-C7-N4-C5
11	F	401	ACP	PG-C3B-PB-O1B
11	F	401	ACP	PG-C3B-PB-O2B
11	F	401	ACP	PG-C3B-PB-O3A
11	F	401	ACP	C5'-O5'-PA-O1A
11	F	401	ACP	C5'-O5'-PA-O2A
11	F	401	ACP	C5'-O5'-PA-O3A
8	A	504	GOL	O2-C2-C3-O3
10	B	503	MES	C7-C8-S-O3S
11	F	401	ACP	O4'-C4'-C5'-O5'
10	B	503	MES	C8-C7-N4-C3
11	F	401	ACP	PB-O3A-PA-O5'
10	B	503	MES	C7-C8-S-O1S
5	D	501	GTP	PB-O3B-PG-O2G
10	B	503	MES	N4-C7-C8-S
5	A	501	GTP	C5'-O5'-PA-O2A
5	D	501	GTP	C5'-O5'-PA-O2A
9	B	501	GDP	C5'-O5'-PA-O2A
5	C	501	GTP	PB-O3B-PG-O3G
5	C	501	GTP	C4'-C5'-O5'-PA
5	D	501	GTP	PB-O3A-PA-O1A
5	D	501	GTP	PB-O3A-PA-O2A
9	B	501	GDP	PB-O3A-PA-O2A
5	C	501	GTP	PB-O3A-PA-O1A
9	B	501	GDP	PB-O3A-PA-O1A

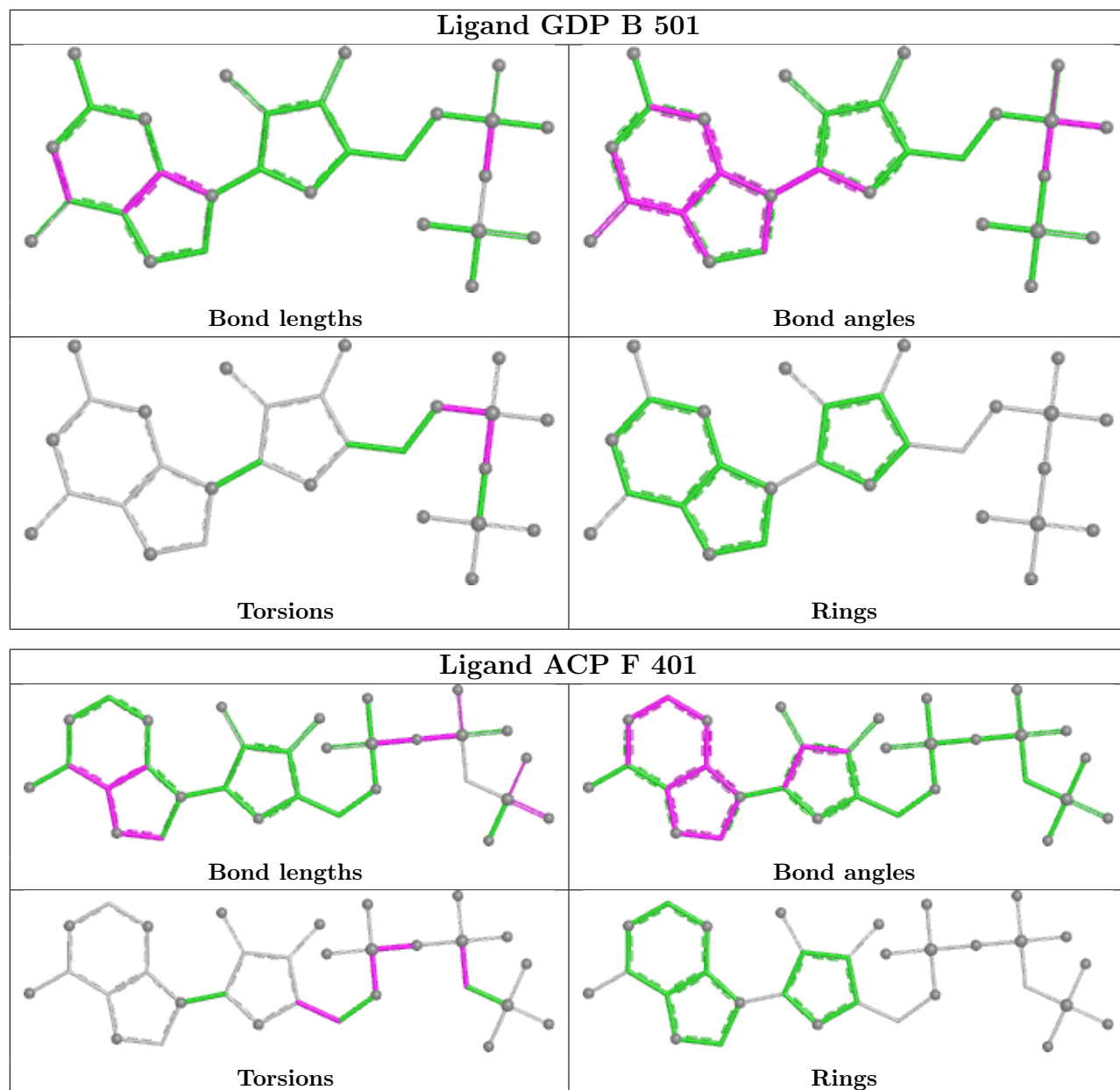
There are no ring outliers.

1 monomer is involved in 4 short contacts:

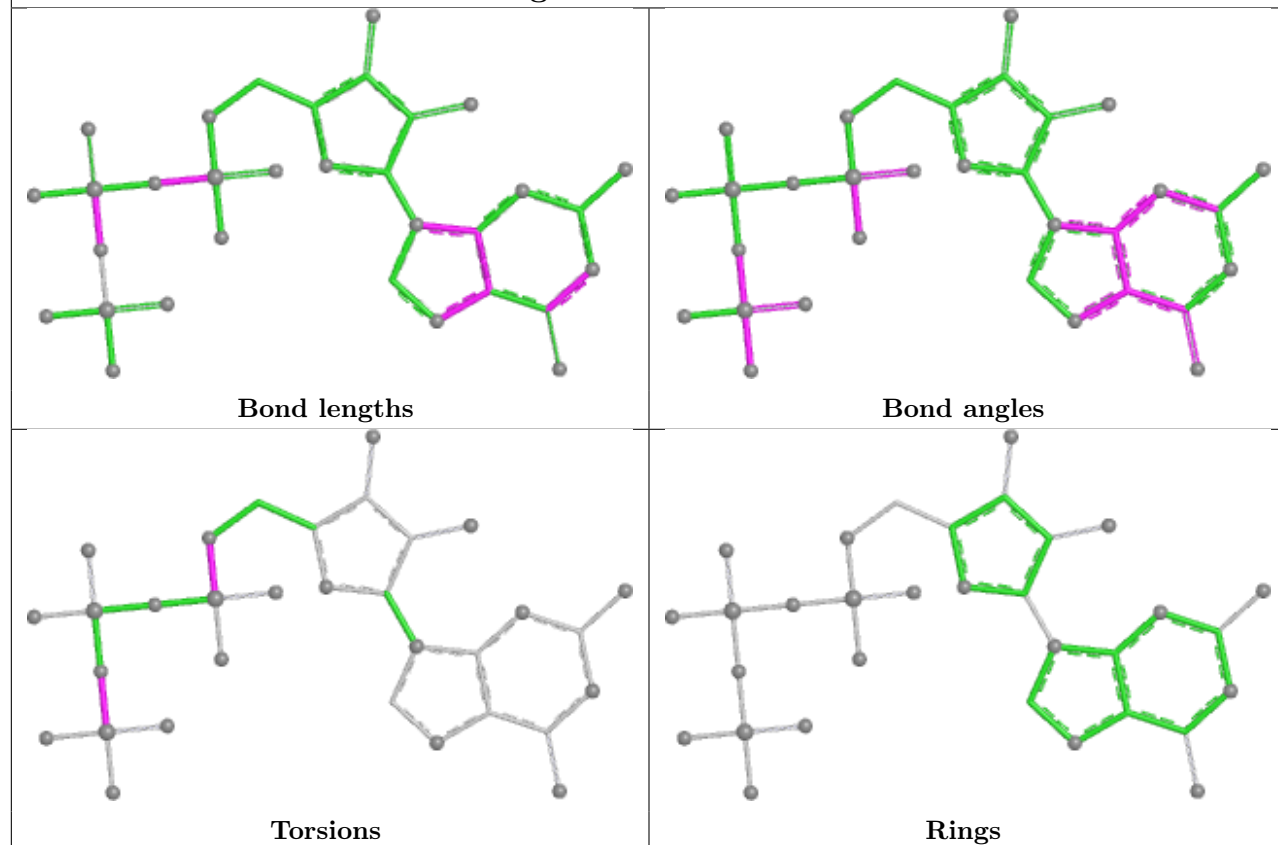
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	B	503	MES	4	0

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.

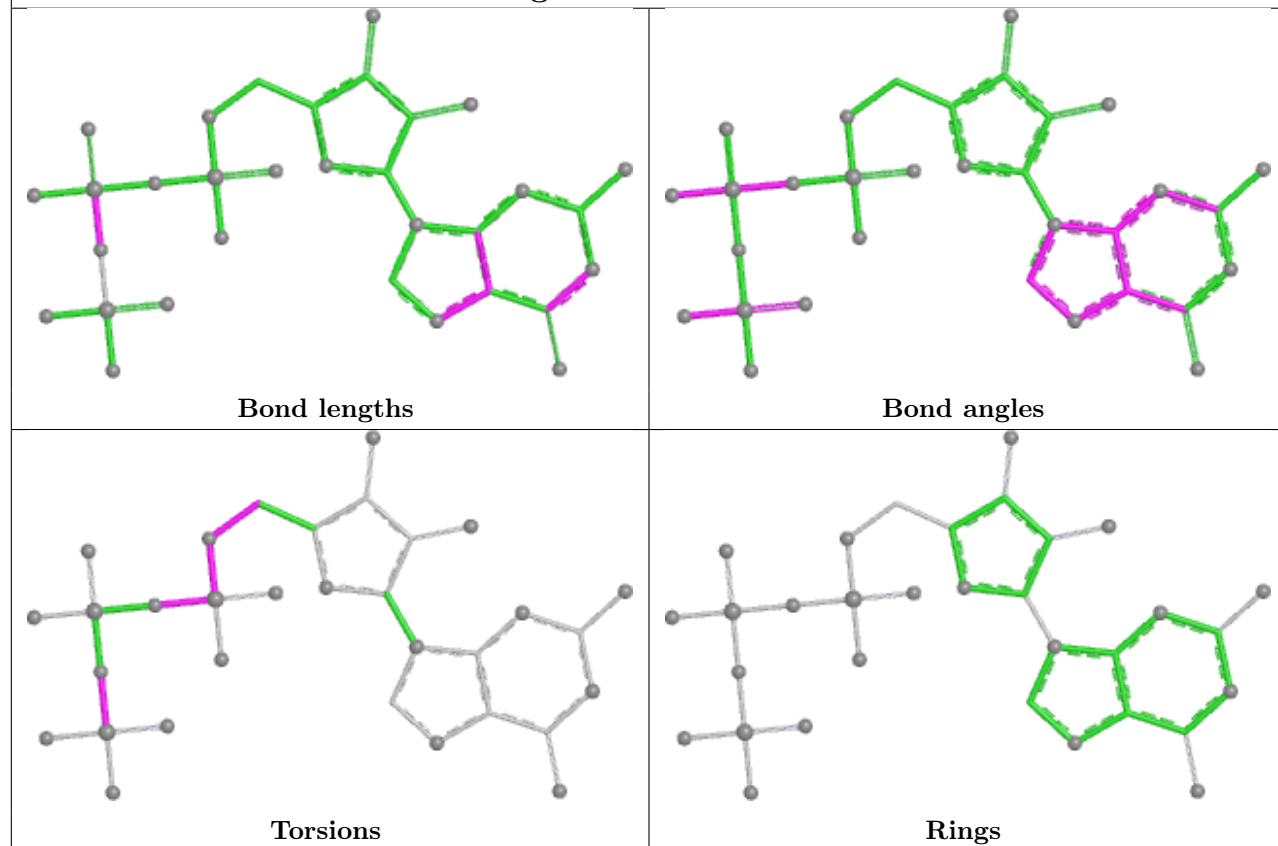




Ligand GTP A 501



Ligand GTP 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	437/451 (96%)	-0.09	2 (0%) 87 87	36, 51, 78, 98	0
1	C	440/451 (97%)	-0.37	4 (0%) 81 82	30, 42, 67, 92	0
2	B	428/445 (96%)	-0.09	4 (0%) 81 82	32, 50, 83, 129	0
2	D	421/445 (94%)	0.27	12 (2%) 53 56	38, 62, 99, 119	0
3	E	121/143 (84%)	0.45	5 (4%) 41 43	37, 64, 96, 131	0
4	F	334/384 (86%)	0.59	31 (9%) 14 16	40, 71, 134, 150	0
All	All	2181/2319 (94%)	0.06	58 (2%) 56 58	30, 54, 100, 150	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	161	LEU	6.7
1	C	440	VAL	4.6
1	A	437	VAL	4.5
1	A	262	TYR	4.2
4	F	130	VAL	4.1
3	E	6	MET	3.9
2	D	72	THR	3.9
4	F	362	ALA	3.8
4	F	103	THR	3.7
4	F	132	LEU	3.7
4	F	372	THR	3.6
2	B	246	LEU	3.5
4	F	181	VAL	3.4
4	F	182	ILE	3.2
4	F	133	ALA	3.1
2	D	55	THR	3.1
4	F	149	ALA	3.1
2	D	394	PHE	3.1
1	C	1	MET	3.0

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Mol	Chain	Res	Type	RSRZ
3	E	28	SER	3.0
2	D	284	LEU	3.0
4	F	169	LEU	3.0
4	F	180	HIS	2.9
4	F	186	LEU	2.9
2	D	1	MET	2.9
4	F	243	HIS	2.8
3	E	139	LEU	2.7
2	D	92	PHE	2.6
4	F	131	PHE	2.6
4	F	172	PHE	2.6
4	F	102	PRO	2.5
2	B	55	THR	2.5
4	F	245	ILE	2.5
3	E	141	GLU	2.5
2	D	170	MET	2.5
4	F	233	PHE	2.4
2	D	73	MET	2.4
4	F	240	LEU	2.4
2	D	397	TRP	2.4
3	E	45	PRO	2.3
4	F	70	LYS	2.3
2	D	219	THR	2.3
2	B	282	ARG	2.3
4	F	179	VAL	2.3
4	F	379	HIS	2.2
4	F	101	TYR	2.2
4	F	162	ILE	2.2
1	C	302	MET	2.2
2	D	246	LEU	2.2
4	F	252	ASN	2.2
2	D	393	ALA	2.2
4	F	99	VAL	2.1
1	C	357	TYR	2.1
4	F	330	ILE	2.1
4	F	380	HIS	2.1
4	F	173	ILE	2.0
2	B	280	GLN	2.0
4	F	247	LYS	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](#)

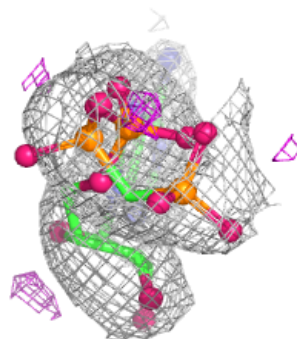
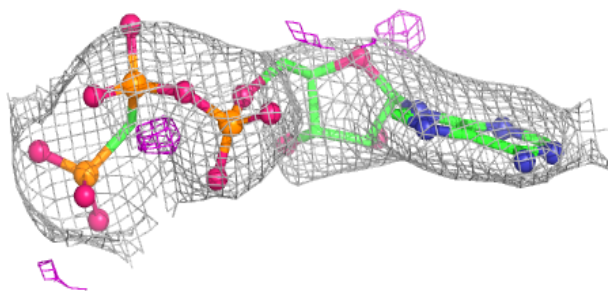
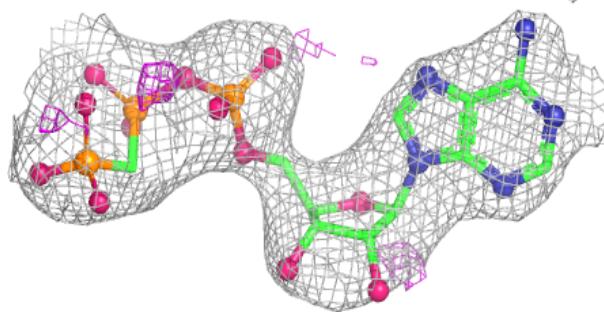
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	502	1/1	0.80	0.17	69,69,69,69	0
11	ACP	F	401	31/31	0.89	0.09	71,93,117,124	0
10	MES	B	503	12/12	0.91	0.12	61,71,77,79	0
5	GTP	D	501	32/32	0.94	0.08	48,58,77,87	0
8	GOL	A	504	6/6	0.94	0.08	53,61,64,68	0
7	CA	A	503	1/1	0.98	0.04	66,66,66,66	0
6	MG	B	502	1/1	0.99	0.03	37,37,37,37	0
9	GDP	B	501	28/28	0.99	0.04	30,36,40,44	0
5	GTP	C	501	32/32	0.99	0.04	31,33,38,38	0
5	GTP	A	501	32/32	0.99	0.04	34,38,43,45	0
6	MG	C	502	1/1	1.00	0.03	36,36,36,36	0
7	CA	C	503	1/1	1.00	0.02	49,49,49,49	0
6	MG	A	502	1/1	1.00	0.03	42,42,42,42	0

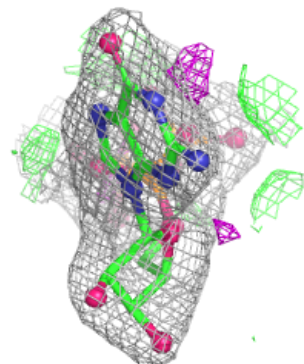
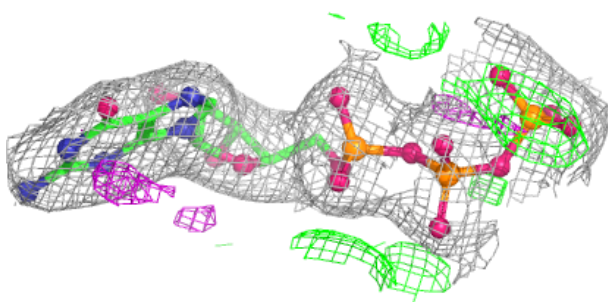
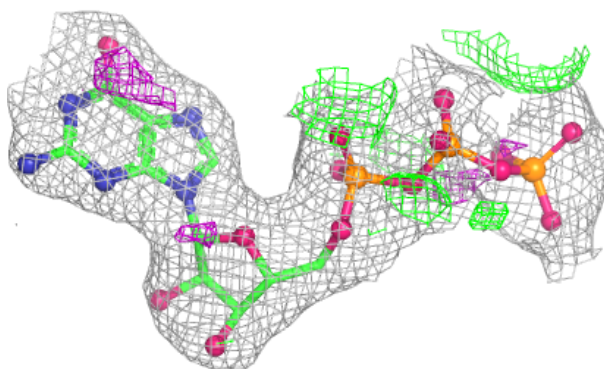
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

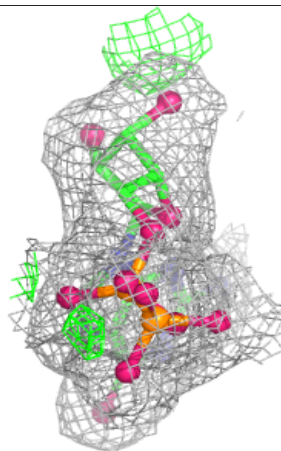
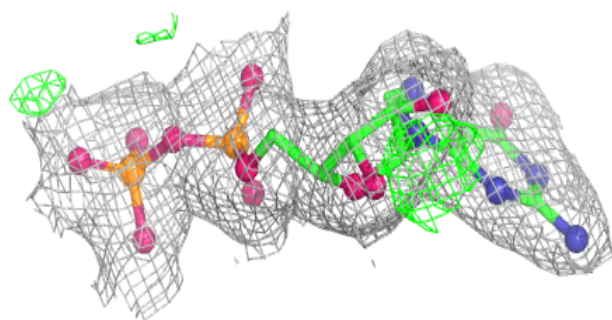
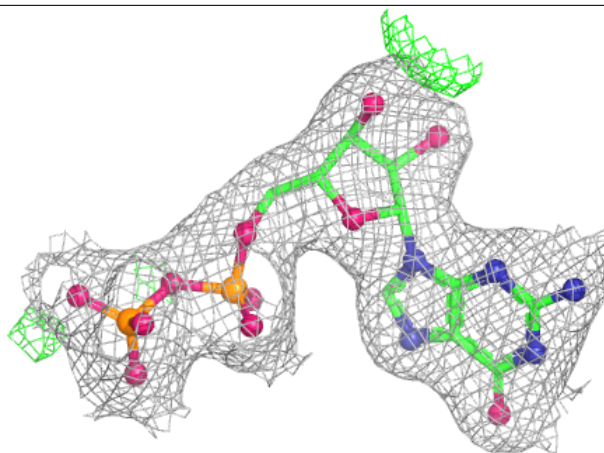
**Electron density around GTP D 501:**

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

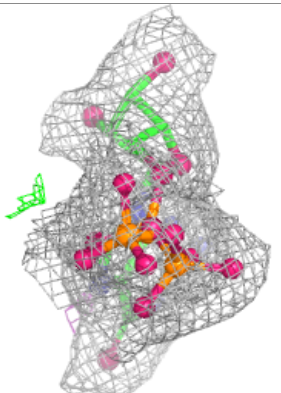
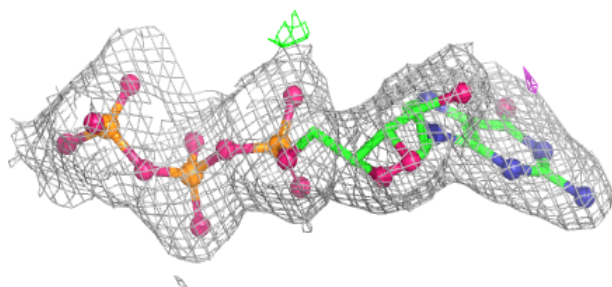
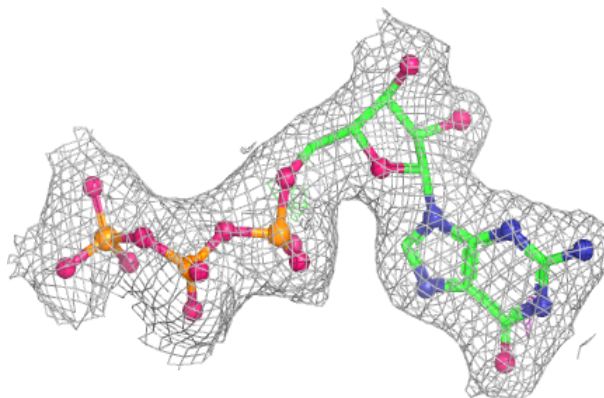


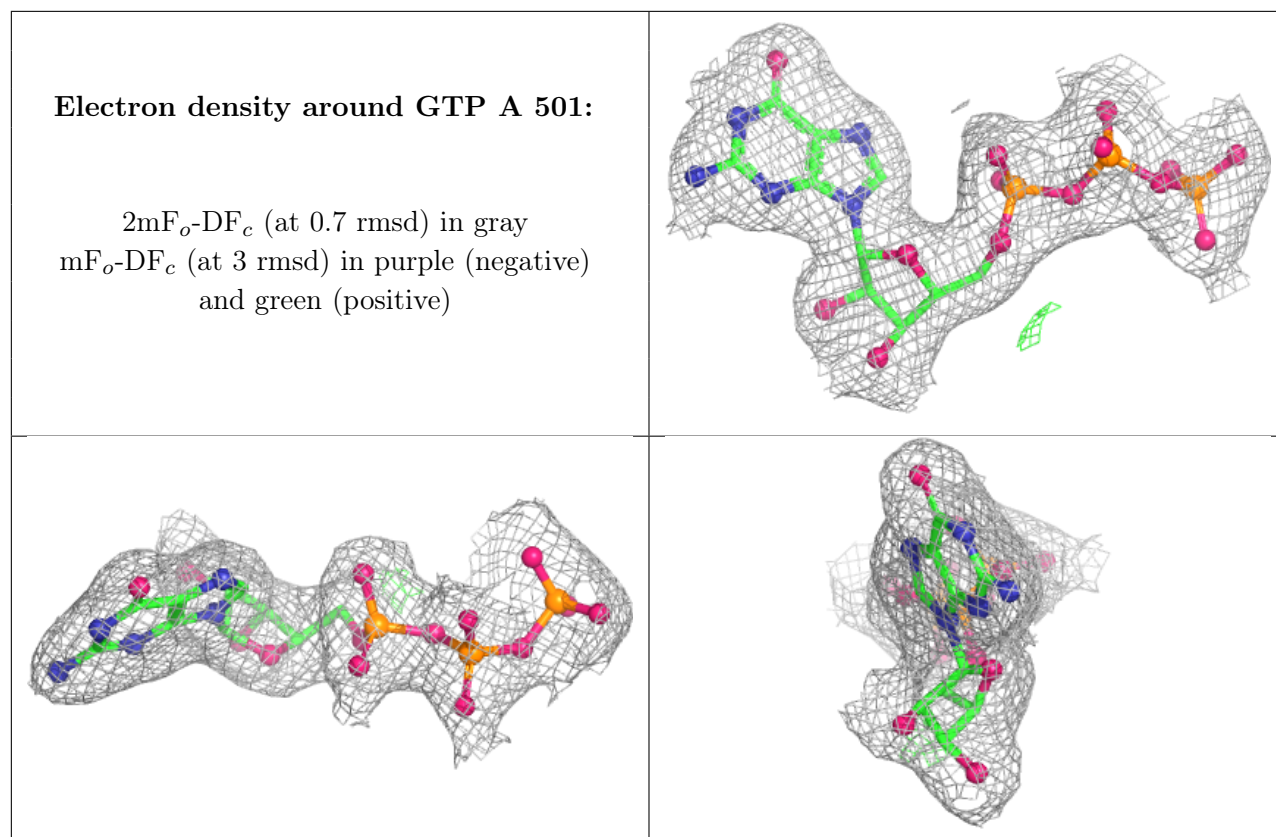
Electron density around GDP B 501:

$2mF_o-DF_c$ (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.