



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 12:07 AM UTC

PDB ID : 7E4P / pdb_00007e4p
Title : Crystal structure of tubulin in complex with Ansamitocin P3
Authors : Wang, Y.; Li, W.
Deposited on : 2021-02-14
Resolution : 2.40 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:

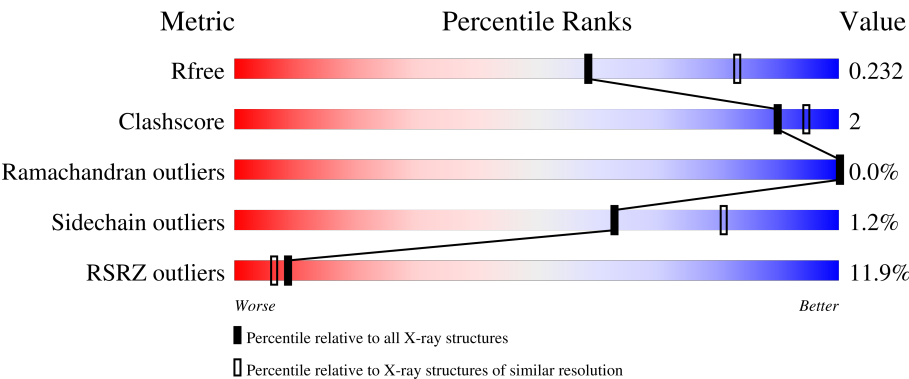
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal 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 i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	440	4% 95%
1	C	440	2% 96%
2	B	431	9% 95%
2	D	431	17% 91% 7%
3	E	138	12% 86% 12%

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Mol	Chain	Length	Quality of chain
4	F	380	27% 80% 8% 12%

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 35098 atoms, of which 16873 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Tubulin alpha-1B chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	437	Total	C	H	N	O	S	0	0	0
			6733	2163	3317	581	650	22			
1	C	440	Total	C	H	N	O	S	0	0	0
			6772	2175	3335	584	656	22			

- Molecule 2 is a protein called Tubulin beta-2B 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
			6488	2080	3179	562	640	27			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	E	121	Total	C	H	N	O	S	0	0	0
			2013	617	1013	181	197	5			

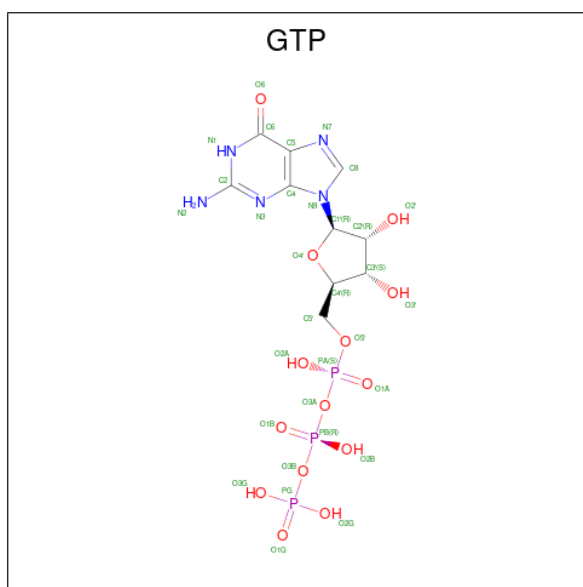
- Molecule 4 is a protein called Tubulin-Tyrosine Ligase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	F	336	Total	C	H	N	O	S	0	0	0
			5446	1773	2685	473	501	14			

There are 2 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

- Molecule 5 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).



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
			41	10	9	5	14	3		

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

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

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

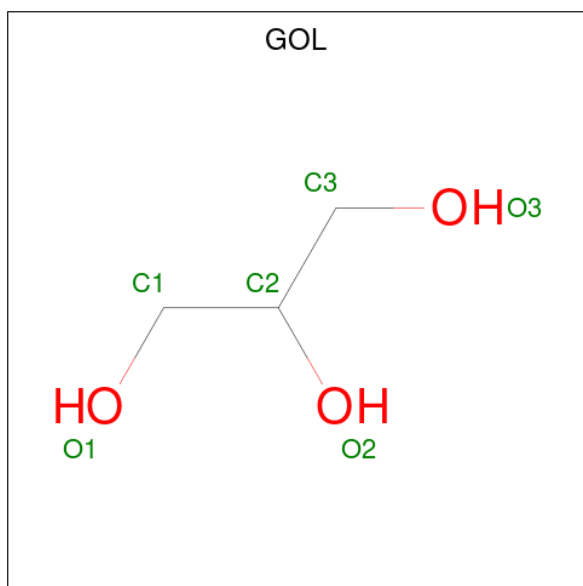
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Ca	0	0
			1	1		

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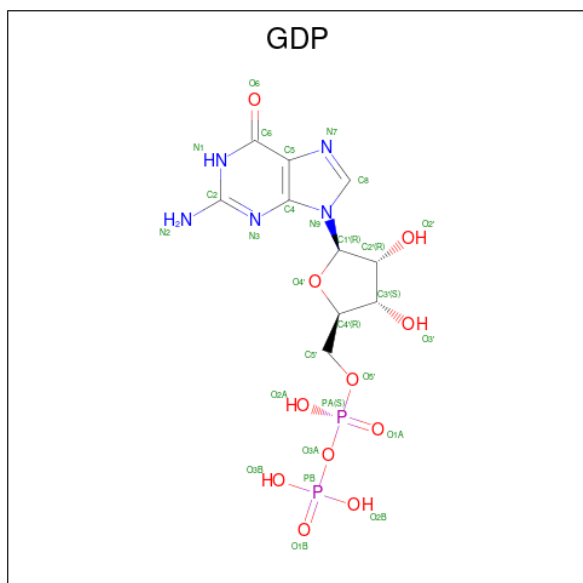
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	C	1	Total	Ca	0	0
			1	1		

- Molecule 8 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



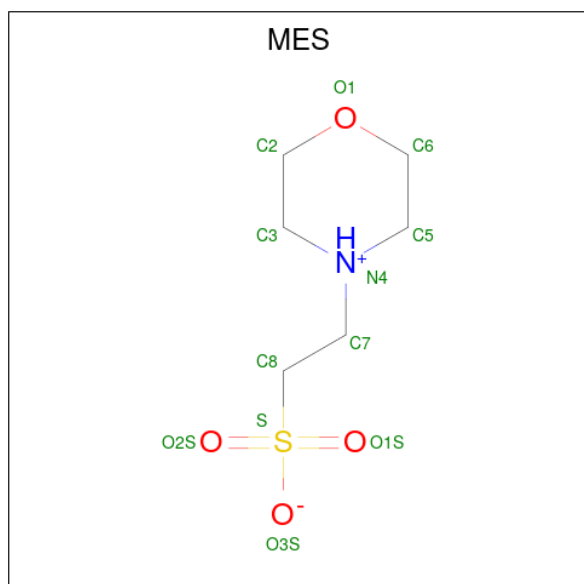
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 9 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



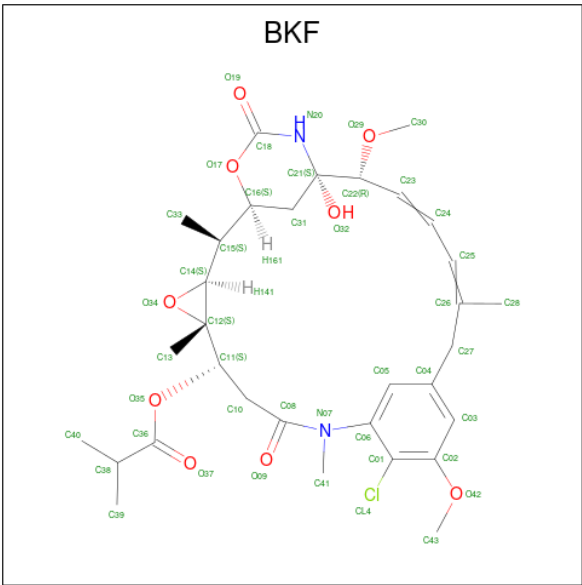
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
9	B	1	Total	C	H	N	O	P	0	0
			38	10	10	5	11	2		

- Molecule 10 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: C₆H₁₃NO₄S).



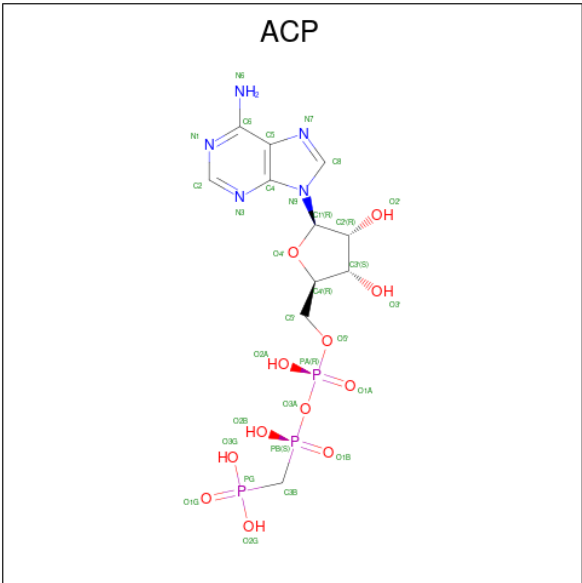
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
10	B	1	Total	C	H	N	O	S	0	0
			24	6	12	1	4	1		

- Molecule 11 is (1S,2S,3S,5S,6S,16Z,18Z,20R,21S)-11-chloro-21-hydroxy-12,20-dimethoxy-2,5,9,16-tetramethyl-8,23-dioxo-4,24-dioxa-9,22-diazatetracyclo[19.3.1.1 10,14 .0 3,5] hexacosa-10(26),11,13,16,18-pentaen-6-yl 2-methylpropanoate (CCD ID: BKF) (formula: C₃₂H₄₃ClN₂O₉) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
11	D	1	Total	C	Cl	H	N	O	0	0
			87	32	1	43	2	9		

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



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
12	F	1	Total	C	H	N	O	P	0	0
			45	11	14	5	12	3		

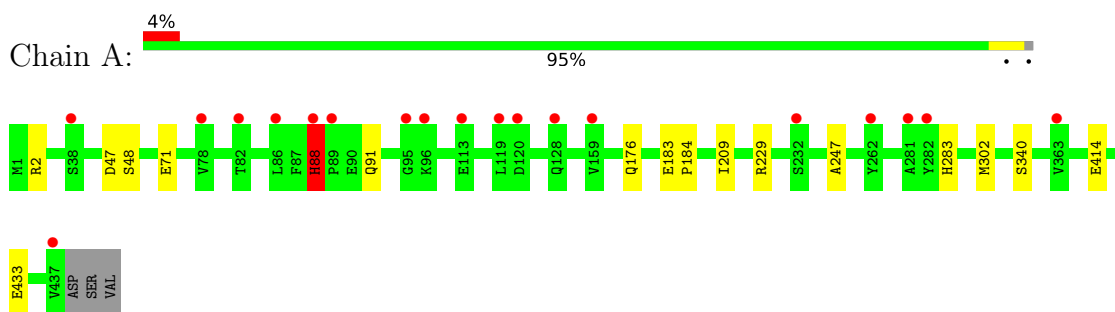
- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	162	Total 162	O 162	0	0
13	B	135	Total 135	O 135	0	0
13	C	260	Total 260	O 260	0	0
13	D	70	Total 70	O 70	0	0
13	E	21	Total 21	O 21	0	0
13	F	69	Total 69	O 69	0	0

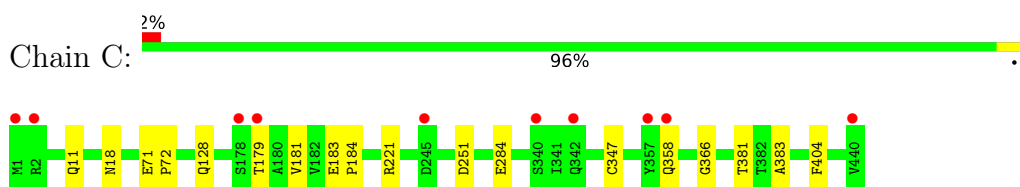
3 Residue-property plots [i](#)

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.

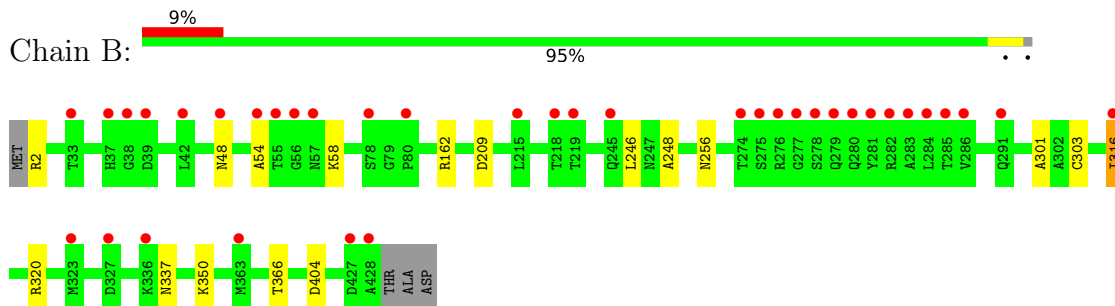
- Molecule 1: Tubulin alpha-1B chain



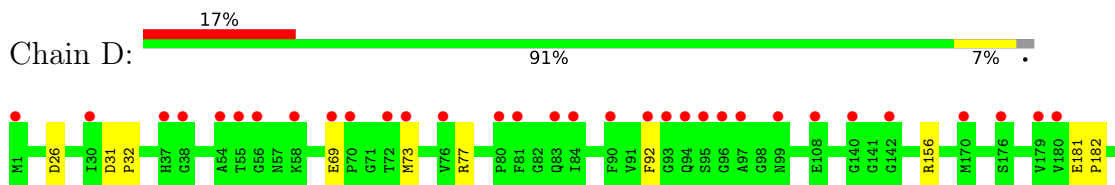
- Molecule 1: Tubulin alpha-1B chain

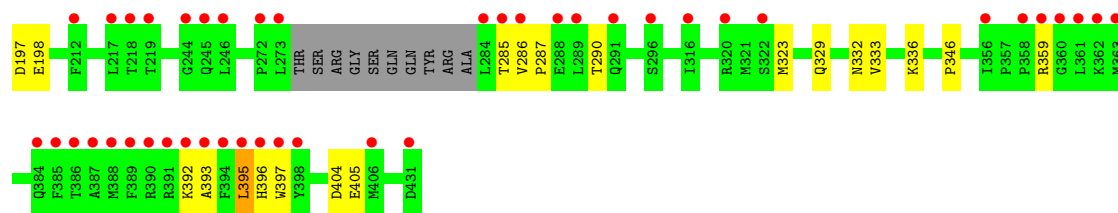


- Molecule 2: Tubulin beta-2B chain

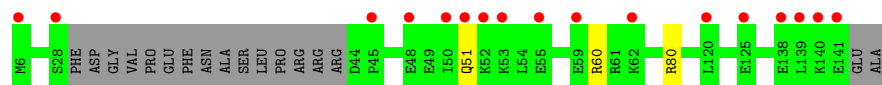
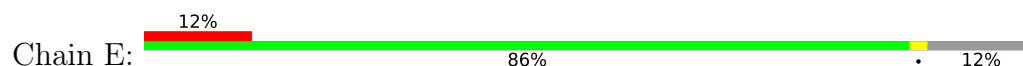


- Molecule 2: Tubulin beta-2B chain

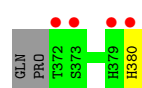
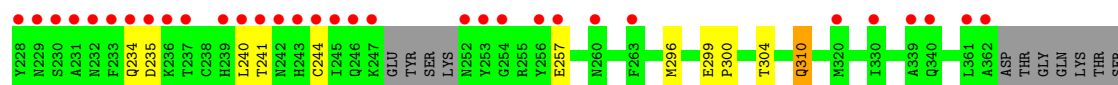
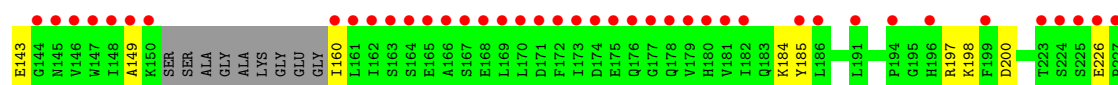
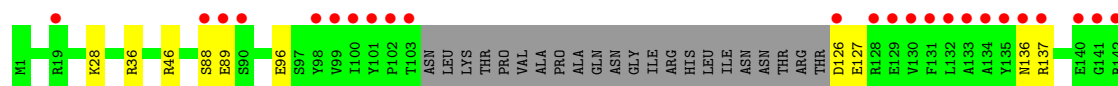
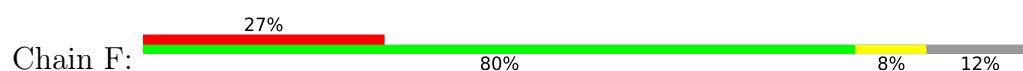




● Molecule 3: Stathmin-4



● 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	105.40Å 158.57Å 181.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.25 – 2.40 47.25 – 2.40	Depositor EDS
% Data completeness (in resolution range)	97.0 (47.25-2.40) 97.4 (47.25-2.40)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.02 (at 2.39Å)	Xtriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, R_{free}	0.213 , 0.229 0.218 , 0.232	Depositor DCC
R_{free} test set	1156 reflections (0.96%)	wwPDB-VP
Wilson B-factor (Å ²)	35.9	Xtriage
Anisotropy	0.065	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 36.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	35098	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.55% 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: GTP, MG, BKF, ACP, GOL, MES, CA, 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	0.33	0/3494	0.67	3/4743 (0.1%)
1	C	0.32	0/3515	0.65	0/4772
2	B	0.30	0/3436	0.63	1/4654 (0.0%)
2	D	0.32	1/3382 (0.0%)	0.66	1/4581 (0.0%)
3	E	0.27	0/1008	0.61	0/1337
4	F	0.29	0/2823	0.63	0/3813
All	All	0.31	1/17658 (0.0%)	0.65	5/23900 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
4	F	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	346	PRO	C-O	-5.06	1.17	1.23

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	395	LEU	N-CA-C	-7.00	104.55	113.23
2	B	248	ALA	N-CA-C	6.33	120.26	112.54
1	A	88	HIS	CA-C-N	5.76	127.04	119.84
1	A	88	HIS	C-N-CA	5.76	127.04	119.84
1	A	340	SER	CA-C-O	-5.04	115.68	120.92

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	F	88	SER	Mainchain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3416	3317	3330	11	0
1	C	3437	3335	3348	9	1
2	B	3361	3228	3238	11	0
2	D	3309	3179	3189	17	0
3	E	1000	1013	1018	1	1
4	F	2761	2685	2733	14	0
5	A	32	10	12	1	0
5	C	32	10	12	0	0
5	D	32	9	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
6	F	1	0	0	0	0
7	A	1	0	0	0	0
7	C	1	0	0	0	0
8	A	6	8	8	0	0
9	B	28	10	12	0	0
10	B	12	12	12	0	0
11	D	44	43	0	1	0
12	F	31	14	14	0	0
13	A	162	0	0	4	0
13	B	135	0	0	7	0
13	C	260	0	0	5	0
13	D	70	0	0	5	0
13	E	21	0	0	0	0
13	F	69	0	0	2	0
All	All	18225	16873	16938	63	1

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)
2:D:392:LYS:C	13:D:614:HOH:O	2.29	0.75
2:D:26:ASP:OD1	2:D:359:ARG:NH2	2.22	0.72
1:C:358:GLN:NE2	13:C:603:HOH:O	2.22	0.72
4:F:36:ARG:NH2	13:F:502:HOH:O	2.27	0.66
1:A:2:ARG:NH2	13:A:606:HOH:O	2.28	0.66
2:B:246:LEU:HD21	2:B:350:LYS:HB3	1.80	0.63
5:A:501:GTP:H5'	13:A:612:HOH:O	1.97	0.62
4:F:126:ASP:OD1	4:F:127:GLU:N	2.33	0.61
2:B:2:ARG:N	13:B:616:HOH:O	2.34	0.60
1:A:247:ALA:O	13:A:601:HOH:O	2.15	0.60
4:F:304:THR:O	4:F:310:GLN:NE2	2.37	0.58
1:A:414:GLU:OE1	3:E:60:ARG:NH1	2.37	0.58
4:F:197:ARG:NH1	4:F:257:GLU:OE2	2.37	0.57
2:D:404:ASP:OD1	2:D:405:GLU:N	2.37	0.57
1:A:88:HIS:H	1:A:88:HIS:HD1	1.54	0.56
2:B:48:ASN:ND2	13:B:616:HOH:O	2.41	0.54
4:F:160:ILE:HG21	4:F:240:LEU:HD21	1.90	0.53
1:A:433:GLU:OE2	4:F:46:ARG:NH1	2.43	0.51
2:D:69:GLU:OE2	13:D:601:HOH:O	2.20	0.51
2:D:393:ALA:C	13:D:614:HOH:O	2.55	0.49
2:D:287:PRO:HA	2:D:329:GLN:HG2	1.94	0.48
2:B:162:ARG:NH1	13:B:628:HOH:O	2.46	0.48
2:D:77:ARG:HG2	13:D:647:HOH:O	2.12	0.48
1:C:381:THR:HG22	1:C:383:ALA:H	1.79	0.48
2:B:301:ALA:O	2:B:303:CYS:N	2.47	0.47
2:B:337:ASN:OD1	13:B:601:HOH:O	2.20	0.46
2:B:256:ASN:OD1	13:B:602:HOH:O	2.21	0.46
4:F:296:MET:CE	4:F:380:HIS:CG	2.98	0.46
2:B:316:ILE:HG23	2:B:366:THR:HB	1.98	0.46
4:F:200:ASP:OD1	4:F:241:THR:OG1	2.26	0.45
11:D:502:BKF:C41	11:D:502:BKF:CL4	3.02	0.45
1:A:283:HIS:O	13:A:602:HOH:O	2.20	0.45
2:D:332:ASN:OD1	2:D:336:LYS:NZ	2.39	0.45
1:C:179:THR:HG21	13:C:647:HOH:O	2.16	0.45
4:F:28:LYS:NZ	13:F:510:HOH:O	2.41	0.45
2:D:156:ARG:NH1	2:D:197:ASP:OD2	2.50	0.44
1:A:88:HIS:ND1	1:A:91:GLN:OE1	2.51	0.44
2:D:393:ALA:N	13:D:614:HOH:O	2.45	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:18:ASN:OD1	13:C:601:HOH:O	2.21	0.44
2:B:209:ASP:OD2	13:B:603:HOH:O	2.21	0.44
4:F:185:TYR:OH	4:F:198:LYS:NZ	2.49	0.44
1:A:88:HIS:HD1	1:A:88:HIS:N	2.15	0.44
2:D:290:THR:HG22	2:D:333:VAL:HG21	1.99	0.43
1:C:71:GLU:HG2	1:C:72:PRO:HD2	1.99	0.43
2:D:181:GLU:N	2:D:182:PRO:HD2	2.33	0.43
4:F:149:ALA:O	4:F:160:ILE:HA	2.18	0.43
2:D:286:VAL:HB	2:D:287:PRO:HD3	2.01	0.43
2:D:396:HIS:NE2	2:D:397:TRP:NE1	2.67	0.43
4:F:226:GLU:OE1	4:F:226:GLU:N	2.52	0.42
2:D:73:MET:HG3	2:D:92:PHE:HB3	2.01	0.42
2:D:31:ASP:HB2	2:D:32:PRO:HD2	2.01	0.42
1:C:128:GLN:OE1	13:C:604:HOH:O	2.22	0.41
4:F:96:GLU:HB3	4:F:184:LYS:HE3	2.02	0.41
2:B:404:ASP:OD1	13:B:604:HOH:O	2.22	0.41
1:C:11:GLN:OE1	13:C:602:HOH:O	2.21	0.41
1:C:183:GLU:N	1:C:184:PRO:CD	2.83	0.41
1:A:209:ILE:HD11	1:A:302:MET:SD	2.60	0.41
1:A:183:GLU:N	1:A:184:PRO:CD	2.84	0.41
2:B:54:ALA:N	2:B:58:LYS:O	2.47	0.41
4:F:299:GLU:N	4:F:300:PRO:HD2	2.36	0.41
1:A:47:ASP:N	1:A:47:ASP:OD1	2.54	0.40
2:D:395:LEU:HD12	2:D:395:LEU:HA	1.97	0.40
1:C:181:VAL:HG11	1:C:404:PHE:CZ	2.57	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:366:GLY:O	3:E:80:ARG:NH2[4_545]	2.17	0.03

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	435/440 (99%)	424 (98%)	11 (2%)	0	100	100
1	C	438/440 (100%)	428 (98%)	10 (2%)	0	100	100
2	B	425/431 (99%)	414 (97%)	11 (3%)	0	100	100
2	D	417/431 (97%)	409 (98%)	8 (2%)	0	100	100
3	E	117/138 (85%)	115 (98%)	2 (2%)	0	100	100
4	F	326/380 (86%)	313 (96%)	12 (4%)	1 (0%)	36	50
All	All	2158/2260 (96%)	2103 (98%)	54 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	F	89	GLU

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	368/371 (99%)	363 (99%)	5 (1%)	59	79
1	C	371/371 (100%)	367 (99%)	4 (1%)	65	82
2	B	369/372 (99%)	367 (100%)	2 (0%)	81	91
2	D	364/372 (98%)	361 (99%)	3 (1%)	73	86
3	E	109/123 (89%)	108 (99%)	1 (1%)	70	85
4	F	303/338 (90%)	296 (98%)	7 (2%)	44	66
All	All	1884/1947 (97%)	1862 (99%)	22 (1%)	63	81

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	SER

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Mol	Chain	Res	Type
1	A	71	GLU
1	A	88	HIS
1	A	176	GLN
1	A	229	ARG
2	B	316	ILE
2	B	320	ARG
1	C	221	ARG
1	C	251	ASP
1	C	284	GLU
1	C	347	CYS
2	D	198	GLU
2	D	285	THR
2	D	323	MET
3	E	51	GLN
4	F	136	ASN
4	F	137	ARG
4	F	143	GLU
4	F	234	GLN
4	F	235	ASP
4	F	244	CYS
4	F	310	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	A	256	GLN
1	A	309	HIS
1	A	342	GLN
1	A	393	HIS
2	B	190	HIS
2	B	227	HIS
2	B	298	ASN
2	B	347	ASN
2	B	375	GLN
2	B	426	GLN
1	C	293	ASN
2	D	37	HIS
4	F	246	GLN
4	F	269	GLN
4	F	310	GLN
4	F	333	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 7 are monoatomic - leaving 8 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	C	501	6	33,34,34	0.94	1 (3%)	50,54,54	1.53	8 (16%)
9	GDP	B	501	6	29,30,30	1.19	2 (6%)	45,47,47	1.66	5 (11%)
5	GTP	D	501	6	33,34,34	0.94	1 (3%)	50,54,54	1.56	8 (16%)
12	ACP	F	401	6	31,33,33	4.31	10 (32%)	47,52,52	1.64	7 (14%)
10	MES	B	503	-	12,12,12	2.31	1 (8%)	15,16,16	2.36	3 (20%)
11	BKF	D	502	-	45,47,47	3.02	15 (33%)	53,71,71	3.07	27 (50%)
5	GTP	A	501	6	33,34,34	0.90	1 (3%)	50,54,54	1.56	8 (16%)
8	GOL	A	504	-	5,5,5	0.39	0	5,5,5	0.21	0

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	C	501	6	-	8/22/38/38	0/3/3/3
9	GDP	B	501	6	-	3/16/32/32	0/3/3/3
5	GTP	D	501	6	-	9/22/38/38	0/3/3/3
12	ACP	F	401	6	-	8/19/38/38	0/3/3/3
10	MES	B	503	-	-	1/6/14/14	0/1/1/1
11	BKF	D	502	-	-	19/50/76/76	0/2/4/4
5	GTP	A	501	6	-	7/22/38/38	0/3/3/3
8	GOL	A	504	-	-	2/4/4/4	-

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	F	401	ACP	PB-O3A	20.65	1.81	1.58
11	D	502	BKF	C08-N07	8.29	1.51	1.35
12	F	401	ACP	PA-O5'	7.91	1.90	1.59
10	B	503	MES	C8-S	-7.76	1.66	1.77
11	D	502	BKF	C10-C11	7.33	1.62	1.52
11	D	502	BKF	C12-C14	7.08	1.56	1.47
11	D	502	BKF	C06-N07	6.91	1.52	1.44
11	D	502	BKF	C15-C16	6.84	1.69	1.53
11	D	502	BKF	C27-C26	-5.33	1.48	1.52
11	D	502	BKF	C06-C01	4.80	1.45	1.40
11	D	502	BKF	C41-N07	4.06	1.53	1.46
12	F	401	ACP	C5'-C4'	3.96	1.63	1.51
11	D	502	BKF	C21-N20	3.84	1.52	1.45
11	D	502	BKF	C10-C08	3.55	1.57	1.51
12	F	401	ACP	O5'-C5'	-3.03	1.33	1.44
9	B	501	GDP	C5-C4	3.02	1.47	1.38
9	B	501	GDP	C6-N1	-2.91	1.33	1.38
12	F	401	ACP	C8-N7	2.90	1.37	1.31
12	F	401	ACP	C8-N9	2.71	1.42	1.37
12	F	401	ACP	C2-N1	2.63	1.38	1.33
12	F	401	ACP	PA-O3A	-2.59	1.56	1.59
11	D	502	BKF	C18-N20	2.52	1.40	1.34
11	D	502	BKF	C02-C01	2.45	1.44	1.40
11	D	502	BKF	O42-C02	2.32	1.40	1.37
11	D	502	BKF	O35-C11	-2.29	1.42	1.46
12	F	401	ACP	C5-C4	2.29	1.43	1.39
5	D	501	GTP	C2-N3	2.24	1.38	1.33
12	F	401	ACP	C4-N3	2.23	1.38	1.34
5	C	501	GTP	C2-N3	2.18	1.38	1.33
11	D	502	BKF	O19-C18	2.06	1.25	1.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	501	GTP	C2-N3	2.00	1.38	1.33

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	D	502	BKF	C05-C06-C01	-8.69	111.99	122.54
11	D	502	BKF	C12-O34-C14	7.08	64.83	60.81
11	D	502	BKF	O35-C36-C38	5.96	122.13	111.14
11	D	502	BKF	O09-C08-C10	-5.74	111.34	122.07
11	D	502	BKF	O35-C36-O37	-5.63	113.78	123.95
9	B	501	GDP	C5-C4-N3	-5.62	119.45	128.39
10	B	503	MES	C5-N4-C3	5.44	120.56	108.84
5	D	501	GTP	C5-C4-N3	-4.97	120.48	128.39
5	C	501	GTP	C5-C4-N3	-4.93	120.54	128.39
5	A	501	GTP	C5-C4-N3	-4.83	120.71	128.39
9	B	501	GDP	C2-N3-C4	4.76	120.50	112.30
5	D	501	GTP	C2-N3-C4	4.71	120.41	112.30
5	A	501	GTP	C2-N3-C4	4.68	120.37	112.30
12	F	401	ACP	O2A-PA-O3A	4.68	119.93	107.27
11	D	502	BKF	O42-C02-C01	4.68	120.57	115.44
5	C	501	GTP	C2-N3-C4	4.61	120.24	112.30
11	D	502	BKF	C28-C26-C25	-4.53	102.94	122.50
11	D	502	BKF	O34-C14-C15	4.52	122.82	117.41
10	B	503	MES	C7-N4-C5	4.46	123.13	111.24
12	F	401	ACP	O1B-PB-C3B	4.34	120.47	109.05
11	D	502	BKF	C06-C05-C04	4.25	126.91	120.28
9	B	501	GDP	N9-C4-N3	4.25	134.44	125.95
11	D	502	BKF	C28-C26-C27	-4.10	112.09	115.53
12	F	401	ACP	O5'-PA-O1A	-3.92	93.39	108.94
11	D	502	BKF	C43-O42-C02	3.92	123.27	117.51
9	B	501	GDP	C6-C5-N7	3.53	136.72	130.29
11	D	502	BKF	C41-N07-C08	-3.53	113.47	119.14
11	D	502	BKF	C33-C15-C16	3.32	116.22	111.39
11	D	502	BKF	O34-C12-C14	-3.24	57.33	59.38
11	D	502	BKF	C11-O35-C36	3.22	123.82	118.20
11	D	502	BKF	O09-C08-N07	-3.22	116.50	121.94
5	D	501	GTP	N9-C4-N3	3.21	132.38	125.95
10	B	503	MES	C6-C5-N4	-3.18	105.28	110.12
11	D	502	BKF	C13-C12-C11	3.13	122.84	114.62
5	C	501	GTP	N9-C4-N3	3.10	132.15	125.95
5	A	501	GTP	N9-C4-N3	2.93	131.81	125.95
11	D	502	BKF	O34-C14-C12	-2.91	57.84	59.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	D	502	BKF	C02-C01-CL4	-2.91	114.91	120.27
5	A	501	GTP	C2-N1-C6	-2.86	119.93	125.11
5	C	501	GTP	C2-N1-C6	-2.82	120.00	125.11
5	D	501	GTP	C2-N1-C6	-2.71	120.19	125.11
5	D	501	GTP	N9-C8-N7	-2.70	108.40	113.40
12	F	401	ACP	O1G-PG-C3B	-2.68	105.52	111.37
5	A	501	GTP	N9-C8-N7	-2.65	108.48	113.40
5	C	501	GTP	N9-C8-N7	-2.63	108.53	113.40
12	F	401	ACP	PB-O3A-PA	-2.60	123.90	132.37
11	D	502	BKF	C03-C02-C01	-2.60	117.87	120.99
5	D	501	GTP	C8-N7-C5	2.55	108.80	104.26
12	F	401	ACP	C5-C4-N3	-2.52	123.25	126.72
5	D	501	GTP	C5-C6-N1	2.51	119.64	113.25
5	C	501	GTP	C5-C6-N1	2.49	119.60	113.25
5	A	501	GTP	C8-N7-C5	2.48	108.67	104.26
5	C	501	GTP	C8-N7-C5	2.48	108.67	104.26
5	A	501	GTP	C5-C6-N1	2.47	119.54	113.25
11	D	502	BKF	O32-C21-C31	-2.44	103.19	109.98
9	B	501	GDP	C4-C5-N7	-2.42	106.84	110.67
5	D	501	GTP	O6-C6-C5	-2.41	120.16	126.53
5	A	501	GTP	O6-C6-C5	-2.36	120.30	126.53
5	C	501	GTP	O6-C6-C5	-2.34	120.35	126.53
12	F	401	ACP	O2A-PA-O5'	-2.33	96.99	107.57
11	D	502	BKF	O29-C22-C23	-2.29	104.50	111.08
11	D	502	BKF	O35-C11-C10	2.23	109.40	105.09
11	D	502	BKF	C16-C15-C14	2.16	116.74	111.19
11	D	502	BKF	O17-C16-C15	2.12	109.75	105.68
11	D	502	BKF	O17-C18-N20	2.10	122.69	118.78
11	D	502	BKF	O34-C12-C11	2.00	118.64	114.62

There are no chirality outliers.

All (57) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	501	GTP	PB-O3B-PG-O2G
5	A	501	GTP	PB-O3B-PG-O3G
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

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Mol	Chain	Res	Type	Atoms
5	D	501	GTP	C5'-O5'-PA-O1A
5	D	501	GTP	C5'-O5'-PA-O2A
8	A	504	GOL	O1-C1-C2-C3
9	B	501	GDP	C5'-O5'-PA-O3A
9	B	501	GDP	C5'-O5'-PA-O1A
9	B	501	GDP	C5'-O5'-PA-O2A
10	B	503	MES	C8-C7-N4-C5
11	D	502	BKF	C08-C10-C11-C12
11	D	502	BKF	O34-C14-C15-C33
11	D	502	BKF	C33-C15-C16-O17
11	D	502	BKF	C33-C15-C16-C31
11	D	502	BKF	C21-C22-C23-C24
11	D	502	BKF	C21-C22-O29-C30
11	D	502	BKF	C22-C23-C24-C25
11	D	502	BKF	C23-C24-C25-C26
11	D	502	BKF	C24-C25-C26-C27
11	D	502	BKF	C28-C26-C27-C04
11	D	502	BKF	C01-C06-N07-C08
11	D	502	BKF	C01-C06-N07-C41
11	D	502	BKF	C05-C06-N07-C08
11	D	502	BKF	C05-C06-N07-C41
11	D	502	BKF	O37-C36-O35-C11
11	D	502	BKF	C38-C36-O35-C11
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-O2B
12	F	401	ACP	PG-C3B-PB-O3A
12	F	401	ACP	O4'-C4'-C5'-O5'
8	A	504	GOL	O1-C1-C2-O2
5	D	501	GTP	PB-O3B-PG-O1G
5	C	501	GTP	PB-O3B-PG-O1G
5	D	501	GTP	PB-O3B-PG-O2G
5	A	501	GTP	PB-O3A-PA-O2A
5	C	501	GTP	PB-O3A-PA-O2A
11	D	502	BKF	O29-C22-C23-C24
5	D	501	GTP	C3'-C4'-C5'-O5'
12	F	401	ACP	C3'-C4'-C5'-O5'
5	A	501	GTP	C5'-O5'-PA-O2A
12	F	401	ACP	PB-C3B-PG-O2G
11	D	502	BKF	O37-C36-C38-C40
11	D	502	BKF	O35-C36-C38-C40

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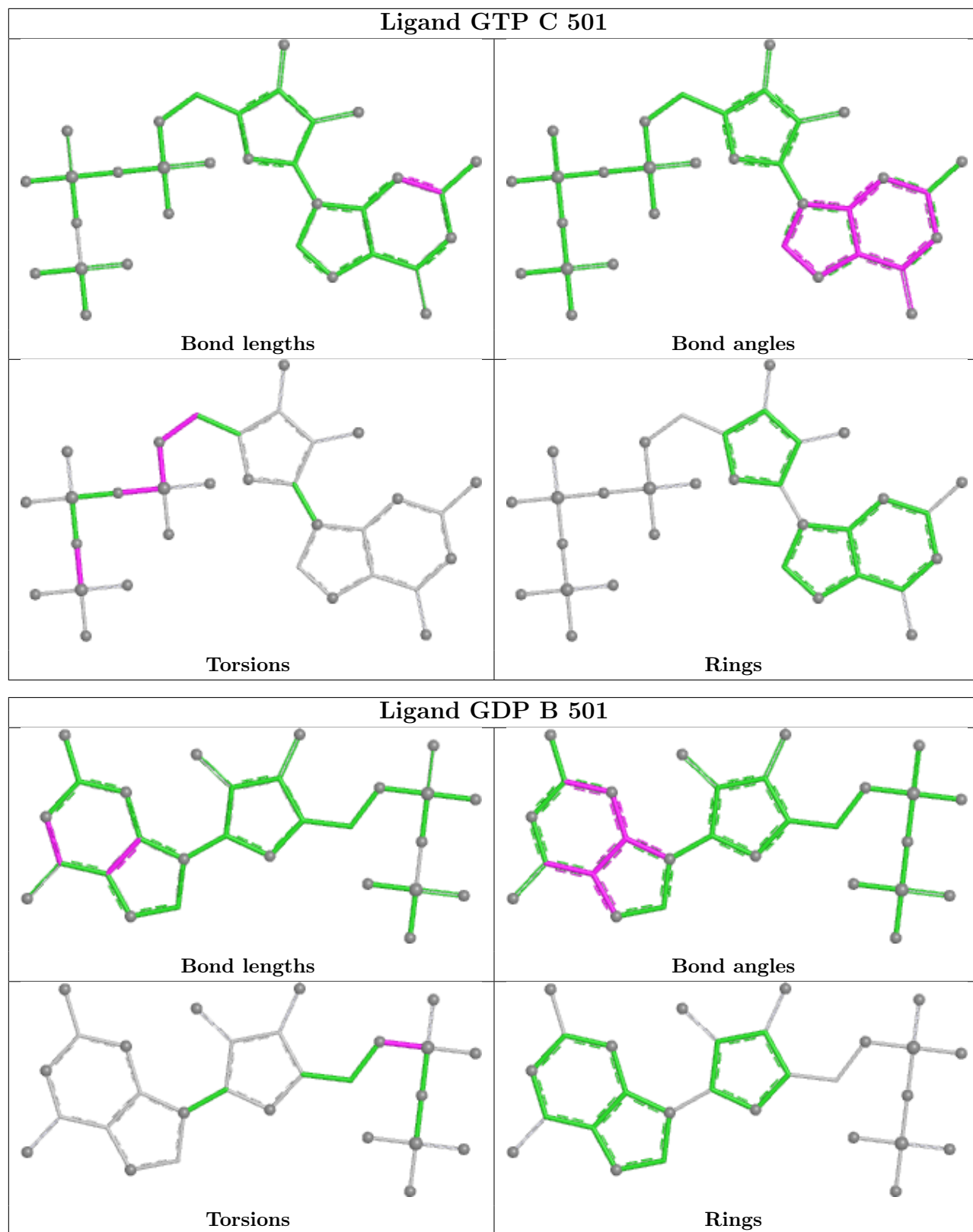
Mol	Chain	Res	Type	Atoms
5	D	501	GTP	C4'-C5'-O5'-PA
5	D	501	GTP	O4'-C4'-C5'-O5'
5	A	501	GTP	PB-O3B-PG-O1G
5	C	501	GTP	PB-O3B-PG-O2G
5	C	501	GTP	PB-O3B-PG-O3G
5	D	501	GTP	PB-O3A-PA-O2A
5	C	501	GTP	C4'-C5'-O5'-PA

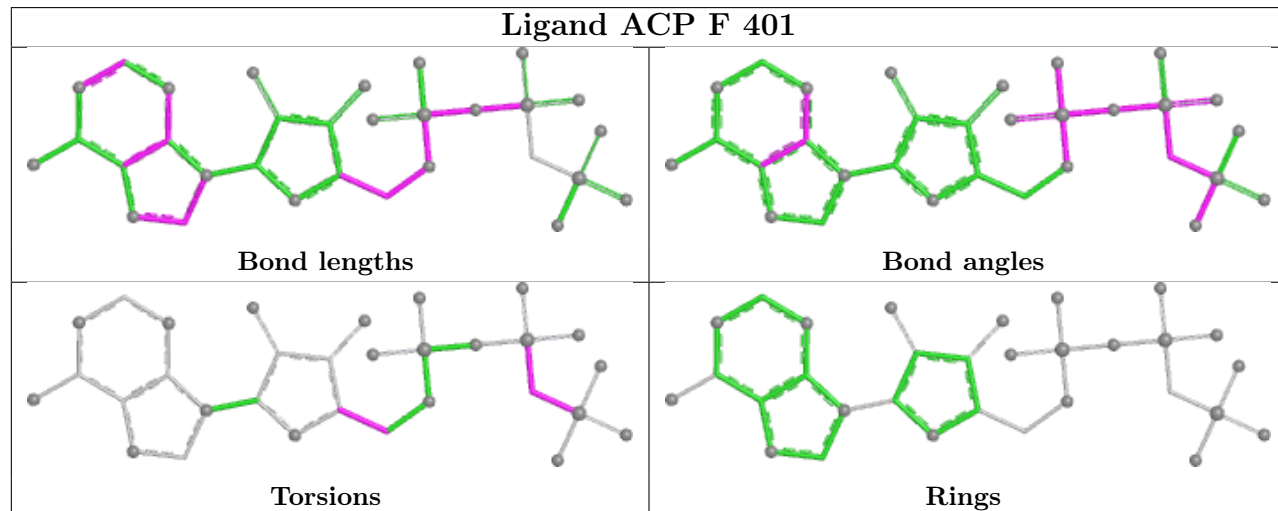
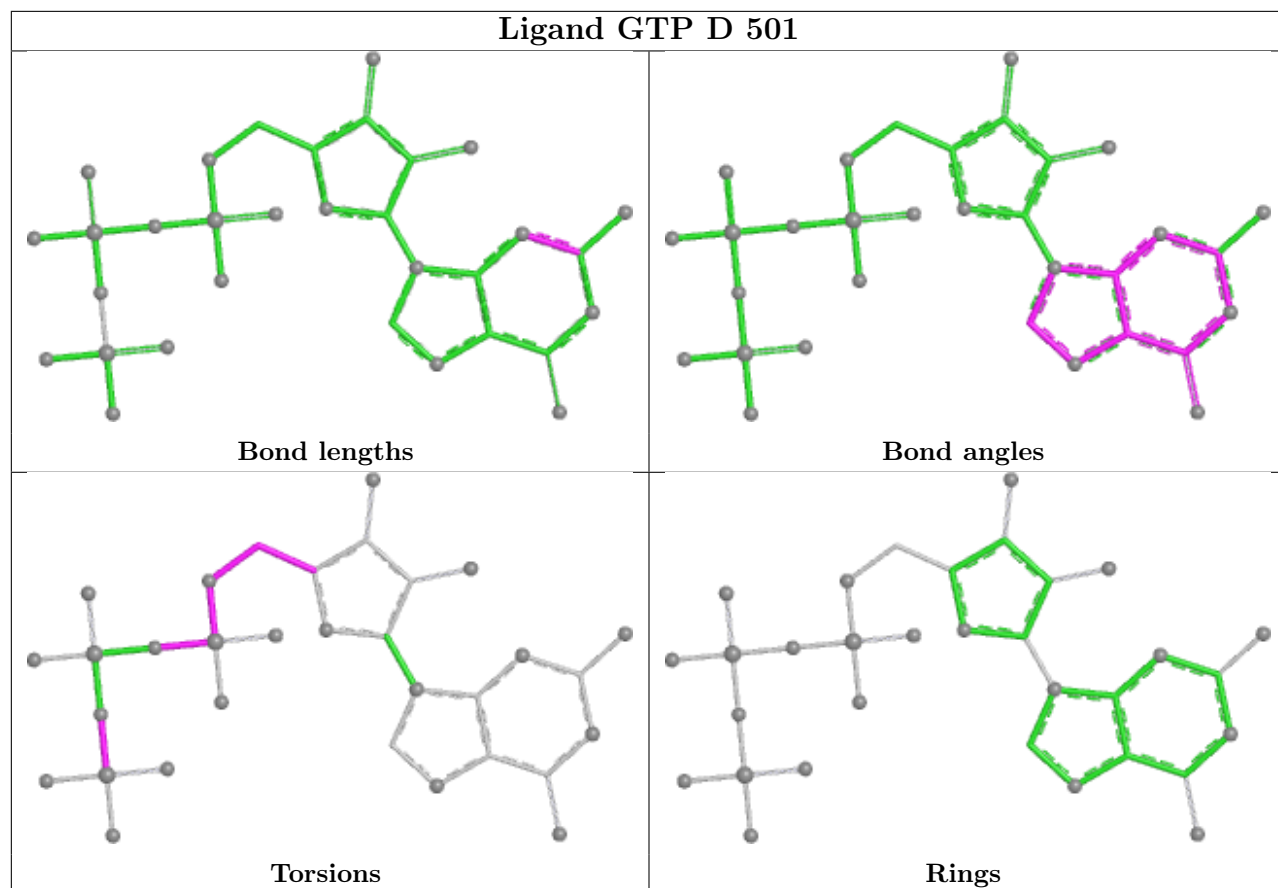
There are no ring outliers.

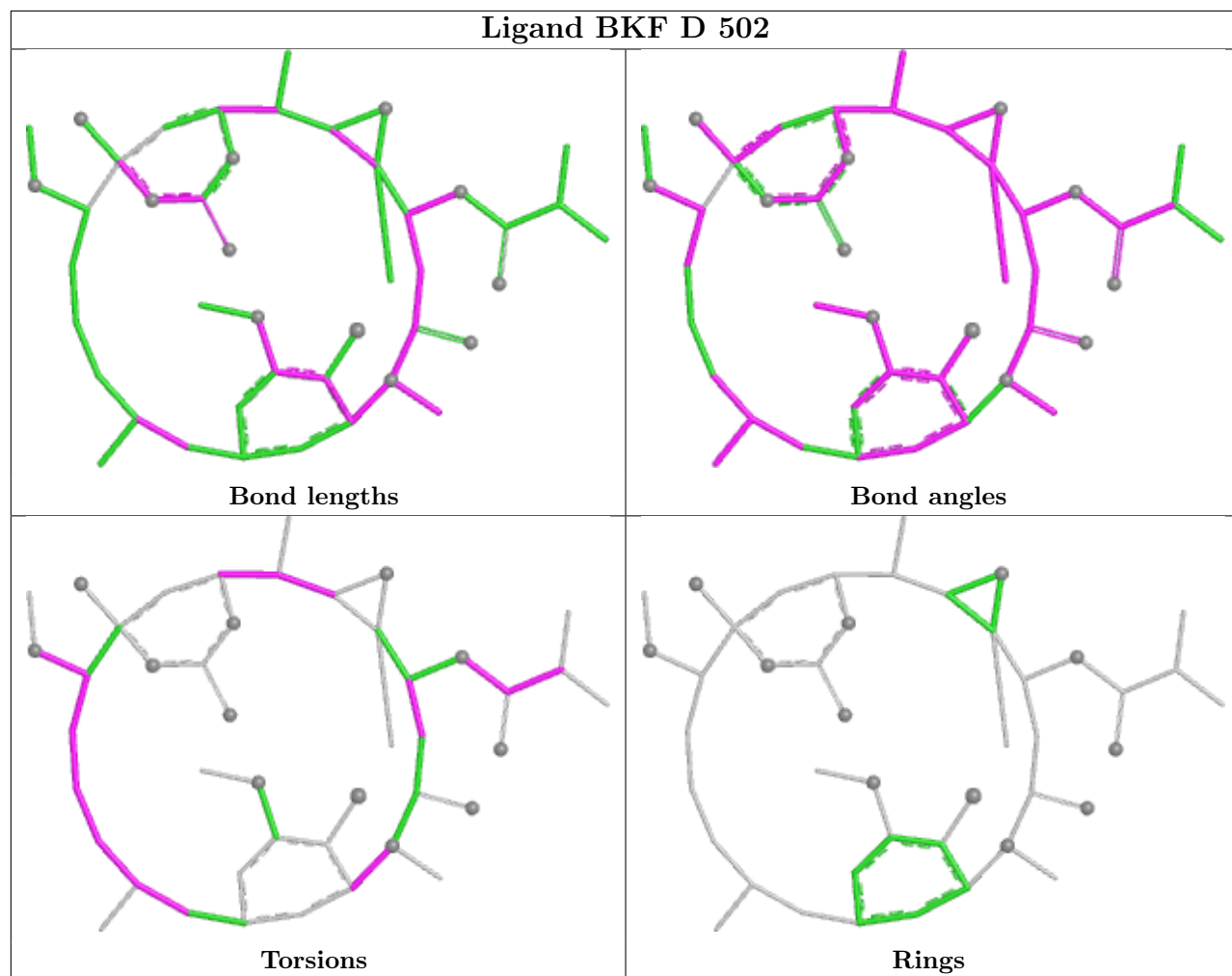
2 monomers are involved in 2 short contacts:

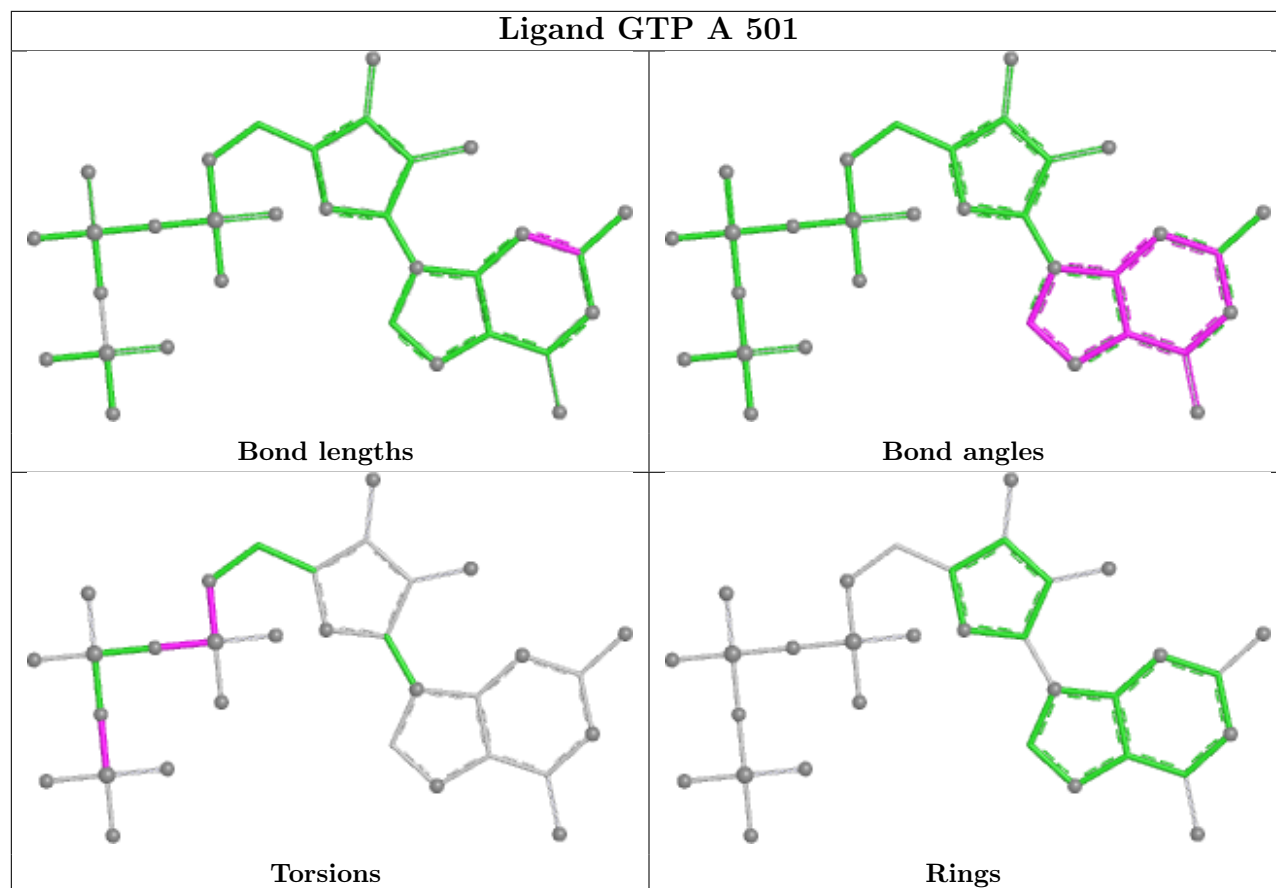
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	D	502	BKF	1	0
5	A	501	GTP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









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	437/440 (99%)	0.38	19 (4%) 40 36	23, 40, 69, 98	0
1	C	440/440 (100%)	-0.11	10 (2%) 61 57	17, 31, 54, 73	0
2	B	427/431 (99%)	0.39	37 (8%) 16 13	19, 40, 73, 126	0
2	D	421/431 (97%)	1.07	75 (17%) 4 3	28, 54, 89, 117	0
3	E	121/138 (87%)	1.02	17 (14%) 6 5	28, 55, 88, 103	0
4	F	336/380 (88%)	1.34	101 (30%) 1 1	31, 62, 131, 152	0
All	All	2182/2260 (96%)	0.60	259 (11%) 9 6	17, 44, 92, 152	0

All (259) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	380	HIS	6.6
2	D	284	LEU	5.9
2	D	55	THR	5.7
4	F	253	TYR	5.5
4	F	161	LEU	5.3
4	F	162	ILE	5.1
4	F	147	TRP	4.9
2	D	389	PHE	4.9
2	D	394	PHE	4.9
4	F	103	THR	4.8
2	D	386	THR	4.7
4	F	257	GLU	4.5
1	A	282	TYR	4.4
4	F	182	ILE	4.3
4	F	234	GLN	4.3
4	F	101	TYR	4.3
2	D	58	LYS	4.3
4	F	230	SER	4.3
4	F	254	GLY	4.3

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Mol	Chain	Res	Type	RSRZ
4	F	236	LYS	4.3
4	F	231	ALA	4.3
4	F	240	LEU	4.2
4	F	160	ILE	4.2
2	D	396	HIS	4.2
2	D	1	MET	4.1
2	B	282	ARG	4.1
2	D	316	ILE	4.0
4	F	233	PHE	4.0
4	F	133	ALA	4.0
4	F	173	ILE	4.0
4	F	142	ARG	4.0
2	D	246	LEU	4.0
2	D	320	ARG	3.9
4	F	172	PHE	3.9
4	F	246	GLN	3.9
1	C	1	MET	3.8
4	F	247	LYS	3.8
2	B	279	GLN	3.8
2	D	391	ARG	3.8
4	F	170	LEU	3.8
4	F	224	SER	3.8
3	E	55	GLU	3.8
4	F	150	LYS	3.7
4	F	177	GLY	3.7
2	D	288	GLU	3.7
4	F	260	ASN	3.7
2	D	72	THR	3.7
4	F	223	THR	3.7
4	F	379	HIS	3.7
1	A	262	TYR	3.7
2	B	428	ALA	3.7
3	E	141	GLU	3.7
4	F	362	ALA	3.7
2	B	278	SER	3.6
2	D	431	ASP	3.6
2	D	387	ALA	3.6
2	B	280	GLN	3.6
2	D	360	GLY	3.6
1	A	96	LYS	3.6
2	D	244	GLY	3.6
2	D	30	ILE	3.6

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Mol	Chain	Res	Type	RSRZ
3	E	59	GLU	3.5
4	F	166	ALA	3.5
2	B	57	ASN	3.5
2	D	285	THR	3.5
2	D	361	LEU	3.5
4	F	135	TYR	3.5
4	F	235	ASP	3.4
4	F	245	ILE	3.4
4	F	169	LEU	3.4
4	F	134	ALA	3.4
4	F	244	CYS	3.4
4	F	225	SER	3.4
2	D	92	PHE	3.3
2	D	388	MET	3.3
2	D	390	ARG	3.3
4	F	180	HIS	3.3
2	D	392	LYS	3.3
4	F	146	VAL	3.3
4	F	176	GLN	3.3
2	D	180	VAL	3.3
4	F	148	ILE	3.3
2	D	362	LYS	3.3
2	D	95	SER	3.2
2	B	55	THR	3.2
2	B	54	ALA	3.2
2	D	291	GLN	3.2
2	D	80	PRO	3.2
3	E	139	LEU	3.2
4	F	131	PHE	3.2
3	E	53	LYS	3.2
4	F	239	HIS	3.2
2	D	179	VAL	3.2
2	D	97	ALA	3.1
2	D	245	GLN	3.1
2	B	275	SER	3.1
4	F	226	GLU	3.1
2	B	281	TYR	3.1
3	E	140	LYS	3.1
2	D	385	PHE	3.1
4	F	88	SER	3.1
2	D	356	ILE	3.1
4	F	178	GLN	3.0

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Mol	Chain	Res	Type	RSRZ
2	B	42	LEU	3.0
4	F	252	ASN	3.0
2	B	245	GLN	3.0
4	F	237	THR	3.0
3	E	6	MET	3.0
4	F	372	THR	3.0
2	D	69	GLU	3.0
4	F	171	ASP	3.0
2	B	336	LYS	3.0
4	F	232	ASN	3.0
2	B	218	THR	3.0
4	F	229	ASN	3.0
4	F	181	VAL	2.9
2	D	397	TRP	2.9
4	F	102	PRO	2.9
2	B	323	MET	2.9
4	F	149	ALA	2.9
4	F	339	ALA	2.9
1	C	340	SER	2.9
2	D	96	GLY	2.9
1	A	437	VAL	2.9
1	C	440	VAL	2.9
2	D	37	HIS	2.9
4	F	89	GLU	2.9
1	A	88	HIS	2.8
2	D	83	GLN	2.8
2	B	277	GLY	2.8
2	D	93	GLY	2.8
4	F	228	TYR	2.8
3	E	48	GLU	2.8
4	F	98	TYR	2.8
2	B	80	PRO	2.8
1	C	357	TYR	2.7
2	B	316	ILE	2.7
4	F	90	SER	2.7
4	F	163	SER	2.7
4	F	164	SER	2.7
2	D	273	LEU	2.7
2	D	54	ALA	2.7
2	D	170	MET	2.7
2	D	363	MET	2.7
1	C	178	SER	2.7

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Mol	Chain	Res	Type	RSRZ
3	E	120	LEU	2.7
1	A	120	ASP	2.6
2	D	176	SER	2.6
2	B	56	GLY	2.6
2	D	81	PHE	2.6
1	A	86	LEU	2.6
2	D	384	GLN	2.6
2	D	359	ARG	2.6
4	F	263	PHE	2.6
4	F	99	VAL	2.6
4	F	196	HIS	2.6
1	C	245	ASP	2.6
2	D	73	MET	2.6
2	D	296	SER	2.6
2	D	219	THR	2.6
4	F	242	ASN	2.5
2	D	393	ALA	2.5
4	F	167	SER	2.5
4	F	241	THR	2.5
4	F	320	MET	2.5
2	D	140	GLY	2.5
4	F	126	ASP	2.5
3	E	125	GLU	2.5
4	F	136	ASN	2.5
1	A	281	ALA	2.5
2	D	406	MET	2.5
2	B	327	ASP	2.5
4	F	130	VAL	2.5
4	F	243	HIS	2.5
4	F	140	GLU	2.5
4	F	165	GLU	2.4
3	E	50	ILE	2.4
4	F	174	ASP	2.4
2	B	291	GLN	2.4
3	E	51	GLN	2.4
2	D	76	VAL	2.4
4	F	194	PRO	2.4
2	D	56	GLY	2.4
2	D	217	LEU	2.4
4	F	186	LEU	2.4
4	F	168	GLU	2.4
2	B	33	THR	2.4

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Mol	Chain	Res	Type	RSRZ
3	E	52	LYS	2.4
3	E	138	GLU	2.4
2	D	70	PRO	2.3
3	E	45	PRO	2.3
2	B	38	GLY	2.3
2	D	142	GLY	2.3
1	A	128	GLN	2.3
2	D	218	THR	2.3
2	D	395	LEU	2.3
4	F	330	ILE	2.3
2	B	363	MET	2.3
4	F	199	PHE	2.3
1	A	78	VAL	2.3
4	F	191	LEU	2.3
3	E	62	LYS	2.3
4	F	185	TYR	2.3
4	F	145	ASN	2.3
2	B	284	LEU	2.3
4	F	129	GLU	2.3
2	D	398	TYR	2.3
1	C	342	GLN	2.2
4	F	141	GLY	2.2
4	F	144	GLY	2.2
4	F	340	GLN	2.2
4	F	100	ILE	2.2
2	B	39	ASP	2.2
2	D	212	PHE	2.2
4	F	227	PRO	2.2
2	B	219	THR	2.2
2	B	274	THR	2.2
4	F	361	LEU	2.2
1	C	358	GLN	2.2
2	B	37	HIS	2.2
1	A	38	SER	2.2
3	E	28	SER	2.2
4	F	137	ARG	2.2
1	A	89	PRO	2.2
1	C	179	THR	2.2
2	D	289	LEU	2.2
4	F	132	LEU	2.2
4	F	373	SER	2.2
1	A	363	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	283	ALA	2.1
2	D	94	GLN	2.1
2	B	215	LEU	2.1
2	D	108	GLU	2.1
2	D	322	SER	2.1
1	C	2	ARG	2.1
4	F	175	GLU	2.1
2	B	78	SER	2.1
2	D	272	PRO	2.1
1	A	159	VAL	2.1
2	B	286	VAL	2.1
2	D	84	ILE	2.1
4	F	256	TYR	2.1
2	D	286	VAL	2.1
2	B	48	ASN	2.1
2	B	276	ARG	2.1
2	D	38	GLY	2.1
2	B	285	THR	2.1
2	D	358	PRO	2.1
4	F	179	VAL	2.0
4	F	19	ARG	2.0
4	F	128	ARG	2.0
1	A	82	THR	2.0
2	B	427	ASP	2.0
1	A	232	SER	2.0
2	D	90	PHE	2.0
1	A	113	GLU	2.0
1	A	119	LEU	2.0
1	A	95	GLY	2.0
2	D	99	ASN	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

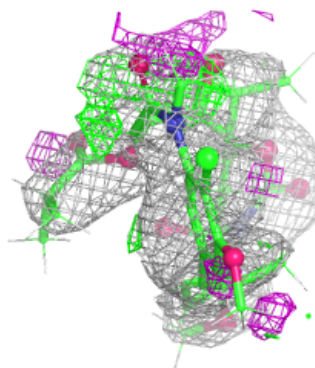
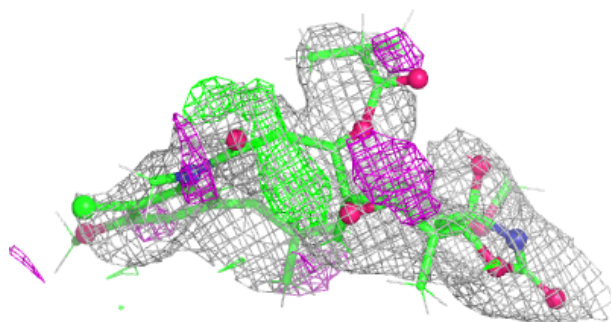
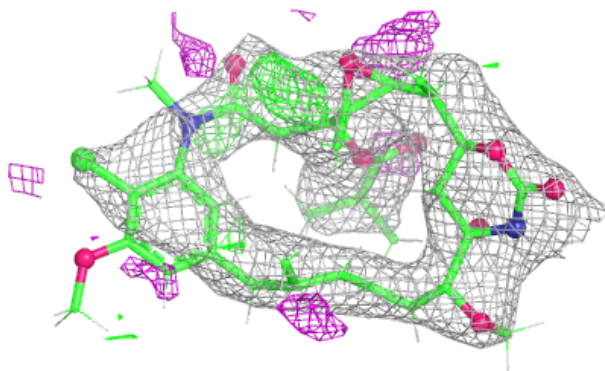
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
11	BKF	D	502	44/44	0.75	0.25	51,73,97,149	0
6	MG	F	402	1/1	0.80	0.17	69,69,69,69	0
6	MG	C	502	1/1	0.86	0.11	27,27,27,27	0
6	MG	D	503	1/1	0.87	0.13	69,69,69,69	0
8	GOL	A	504	6/6	0.88	0.13	36,49,58,59	0
12	ACP	F	401	31/31	0.88	0.14	61,79,100,116	0
5	GTP	D	501	32/32	0.91	0.13	44,53,69,79	0
10	MES	B	503	12/12	0.91	0.11	33,41,50,57	0
6	MG	B	502	1/1	0.93	0.12	24,24,24,24	0
7	CA	A	503	1/1	0.93	0.07	56,56,56,56	0
9	GDP	B	501	28/28	0.97	0.08	18,26,32,38	0
5	GTP	C	501	32/32	0.97	0.07	18,23,30,31	0
7	CA	C	503	1/1	0.97	0.03	37,37,37,37	0
5	GTP	A	501	32/32	0.97	0.07	22,27,34,38	0
6	MG	A	502	1/1	0.99	0.03	25,25,25,25	0

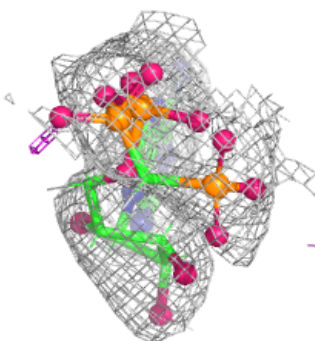
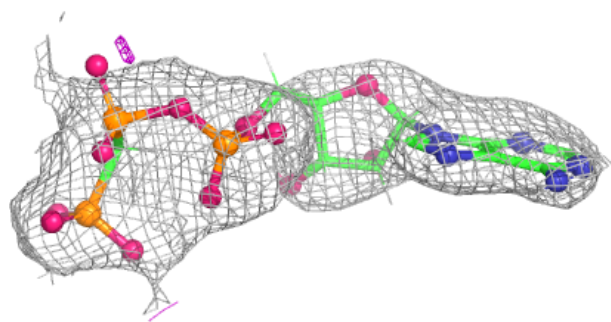
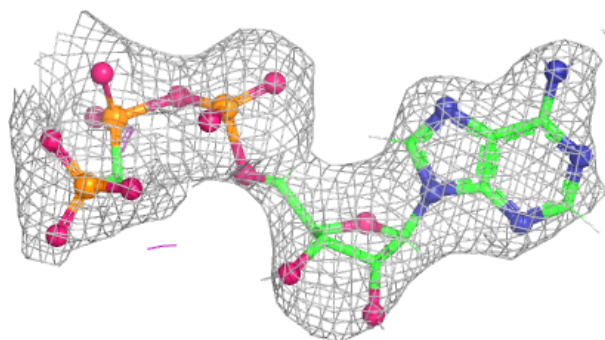
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around BKF D 502:

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

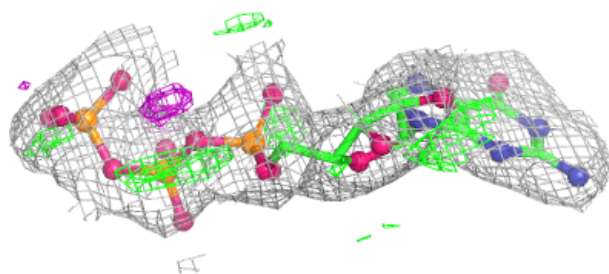
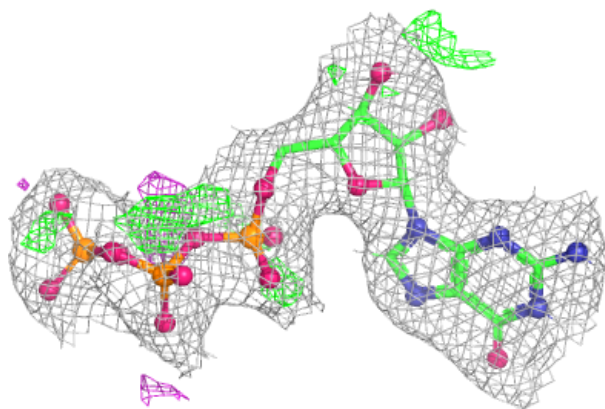
**Electron density around ACP F 401:**

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



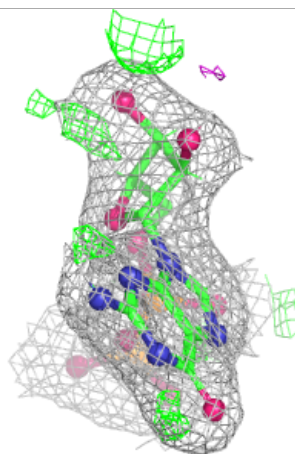
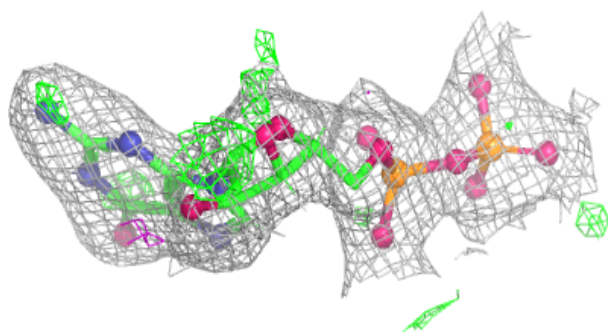
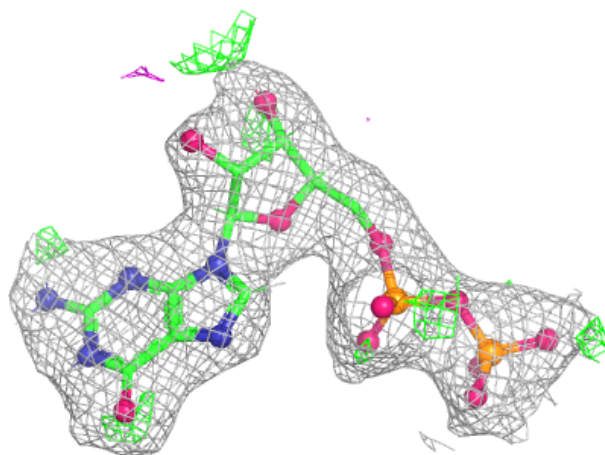
Electron density around GTP D 501:

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



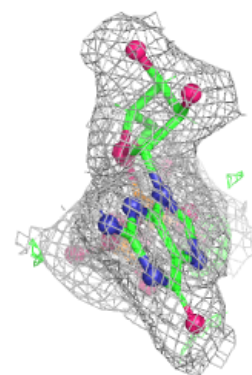
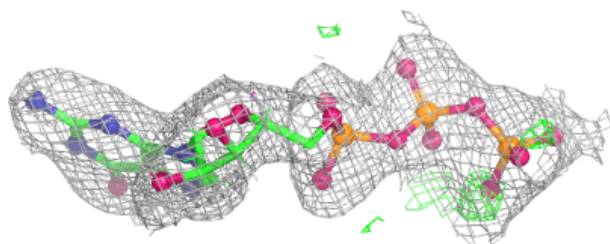
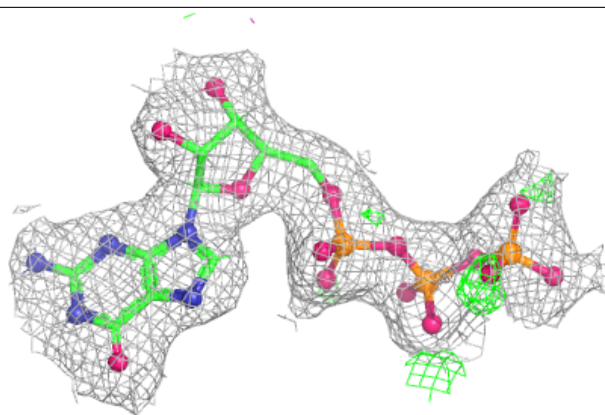
Electron density around GDP B 501:

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

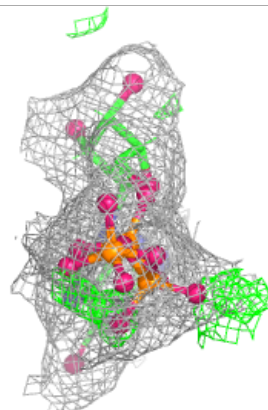
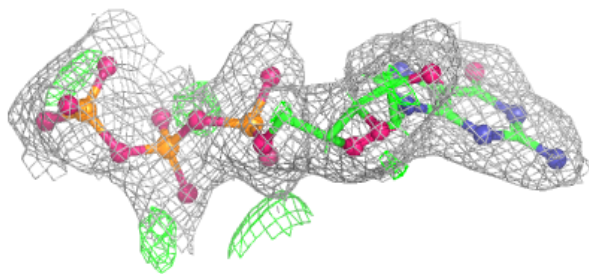
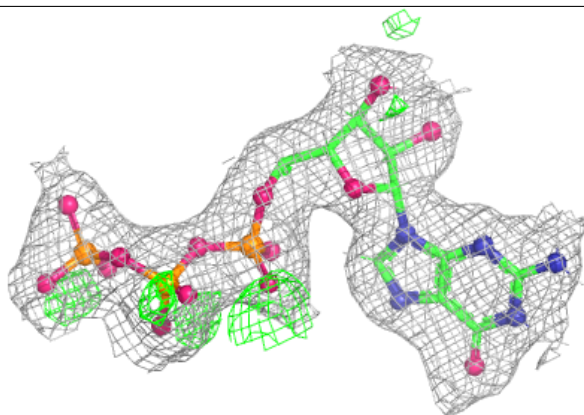


Electron density around GTP C 501:

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

**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)



6.5 Other polymers [i](#)

There are no such residues in this entry.