



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:39 AM UTC

PDB ID : 5XKG / pdb_00005xkg
Title : Crystal structure of T2R-TTL-CH1 complex
Authors : Wang, Y.; Yang, J.; Wang, T.; Chen, L.
Deposited on : 2017-05-07
Resolution : 2.20 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

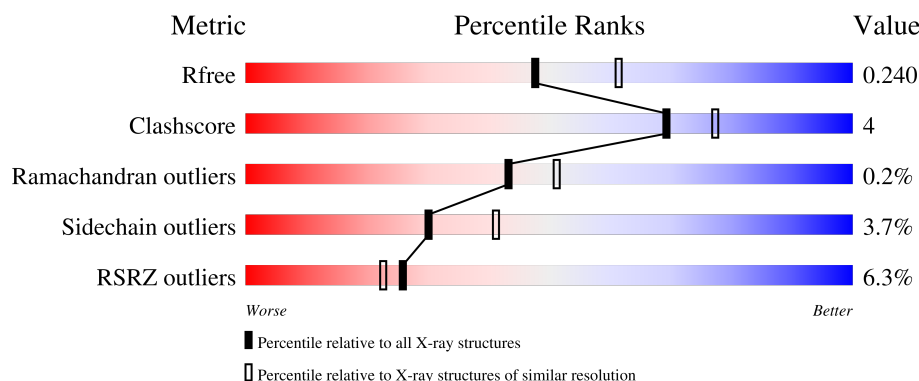
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	
1	C	451	
2	B	445	
2	D	445	
3	E	143	

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Mol	Chain	Length	Quality of chain
4	F	384	12% 77% 8% • 13%

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 18087 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	2	0
			3428	2169	583	652	24			
1	C	440	Total	C	N	O	S	0	1	0
			3446	2180	585	659	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	1	0
			3375	2118	578	651	28			
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	-	expression tag	UNP P63043
E	4	ALA	-	expression tag	UNP P63043

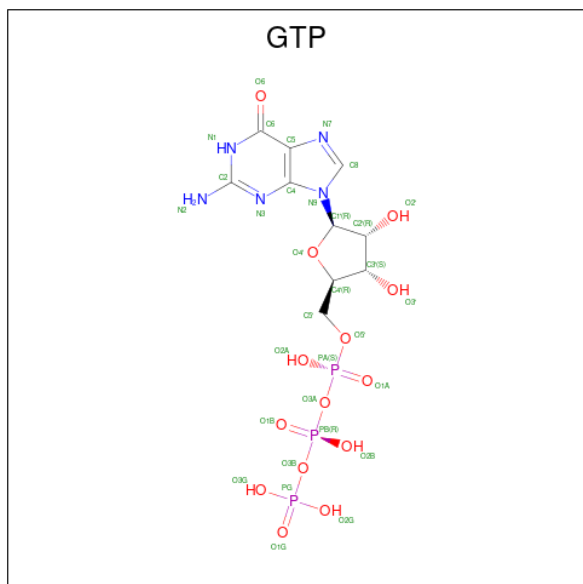
- Molecule 4 is a protein called Tubulin tyrosine ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	334	Total	C	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 32	C 10	N 5	O 14	P 3	0	0
5	C	1	Total 32	C 10	N 5	O 14	P 3	0	0
5	D	1	Total 32	C 10	N 5	O 14	P 3	0	0

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

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

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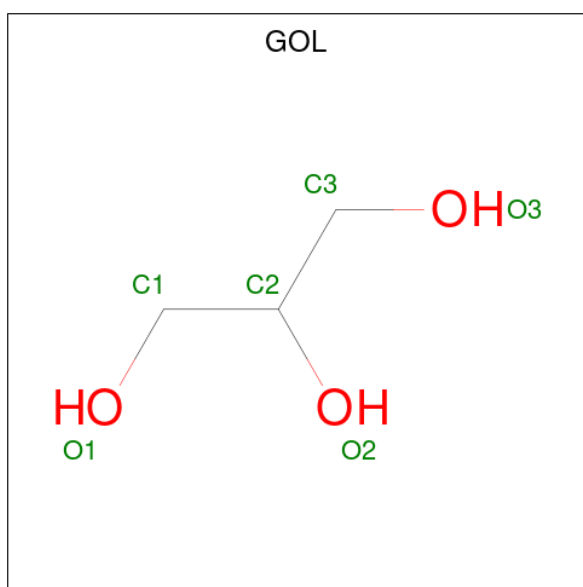
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	1	Total	Mg	0	0
			1	1		

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

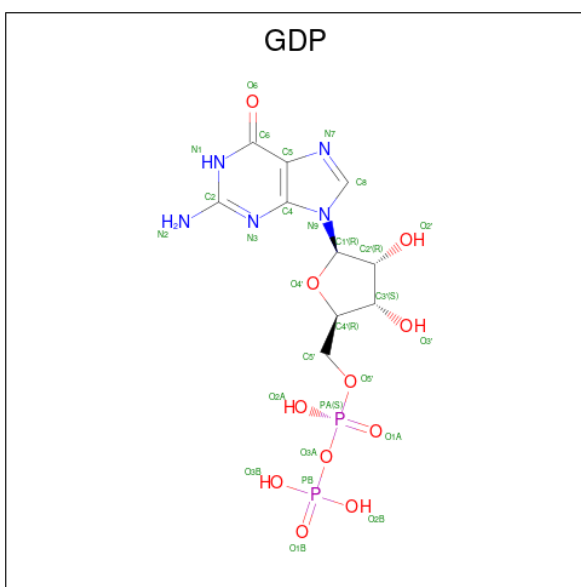
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Ca	0	0
			1	1		
7	C	1	Total	Ca	0	0
			1	1		

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



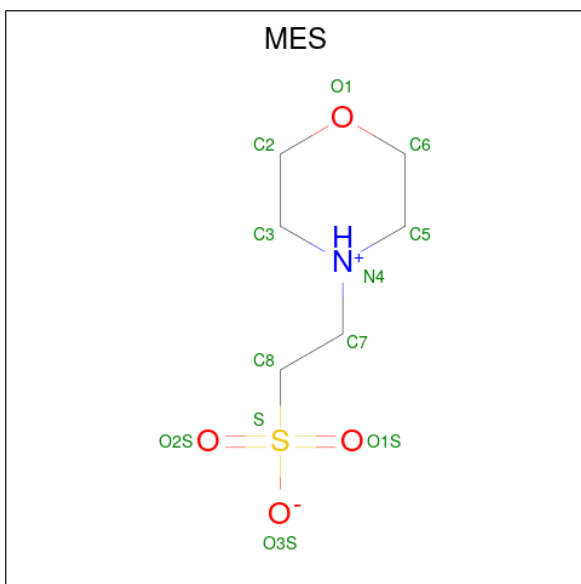
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			6	3	3		

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



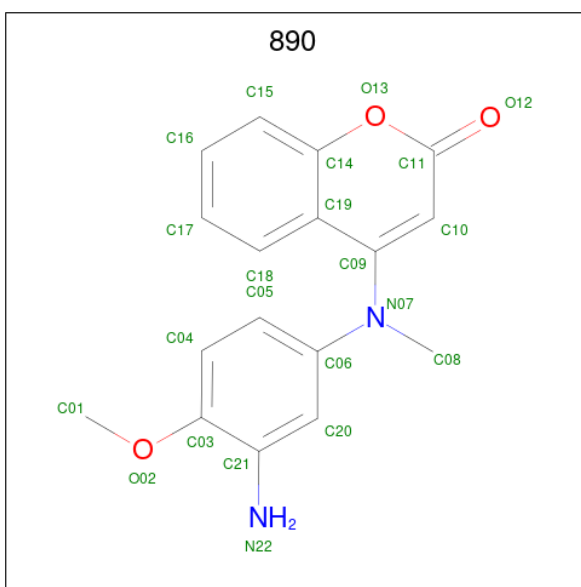
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	B	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

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



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

- Molecule 11 is 4-[(3-azanyl-4-methoxy-phenyl)-methyl-amino]chromen-2-one (CCD ID: 890) (formula: $C_{17}H_{16}N_2O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	B	1	Total	C	N	O	0	0
			22	17	2	3		
11	D	1	Total	C	N	O	0	0
			22	17	2	3		

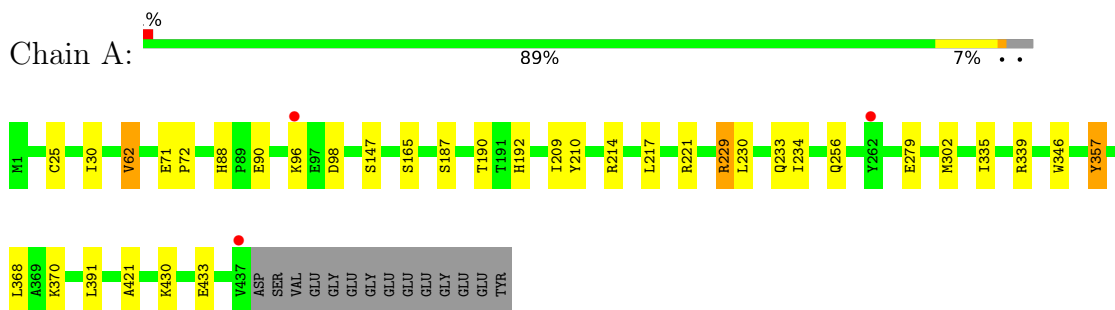
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	143	Total	O	0	0
			143	143		
12	B	121	Total	O	0	0
			121	121		
12	C	234	Total	O	0	0
			234	234		
12	D	30	Total	O	0	0
			30	30		
12	E	27	Total	O	0	0
			27	27		
12	F	38	Total	O	0	0
			38	38		

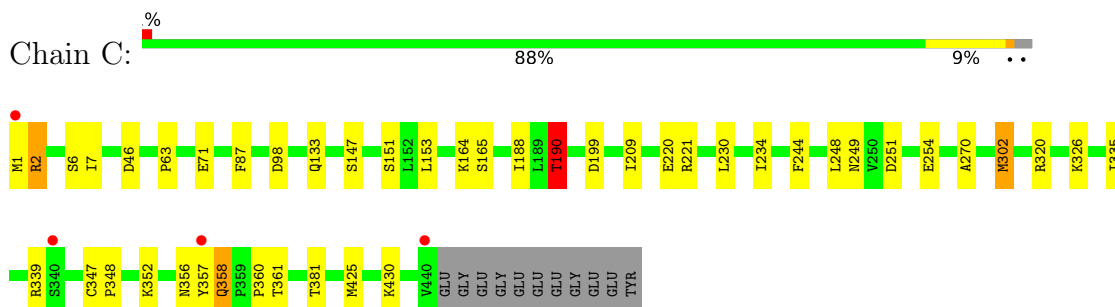
3 Residue-property plots [i](#)

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.

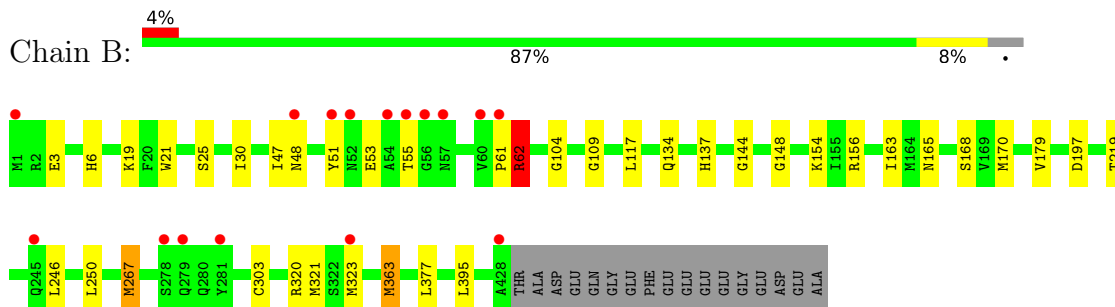
- Molecule 1: Tubulin alpha-1B chain



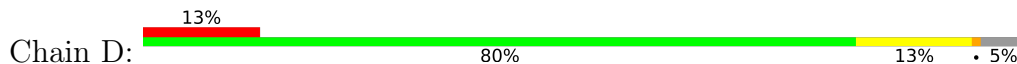
- Molecule 1: Tubulin alpha-1B chain

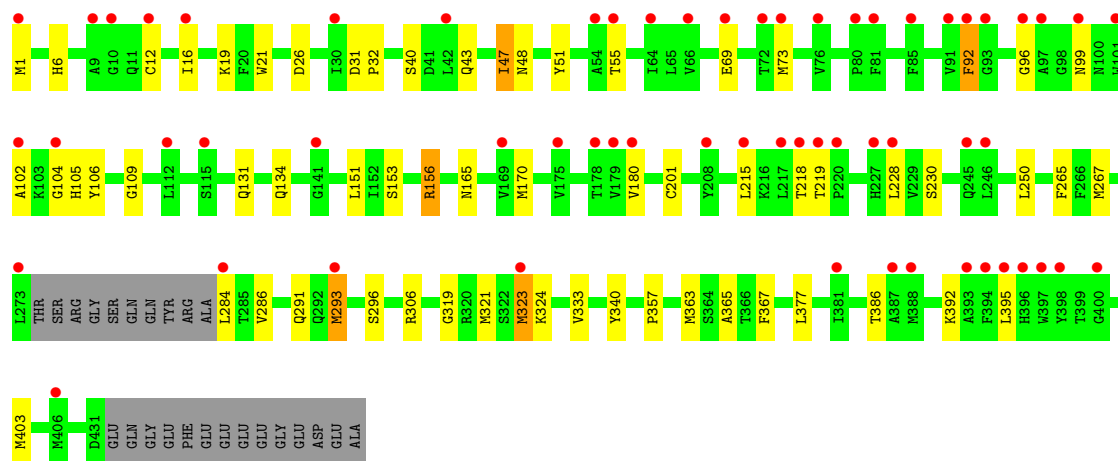


- Molecule 2: Tubulin beta chain

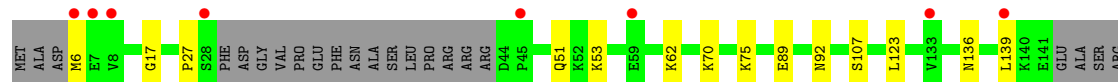
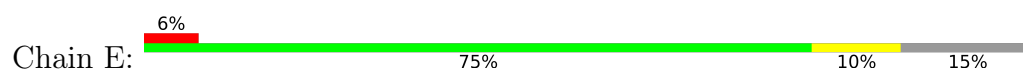


- Molecule 2: Tubulin beta chain

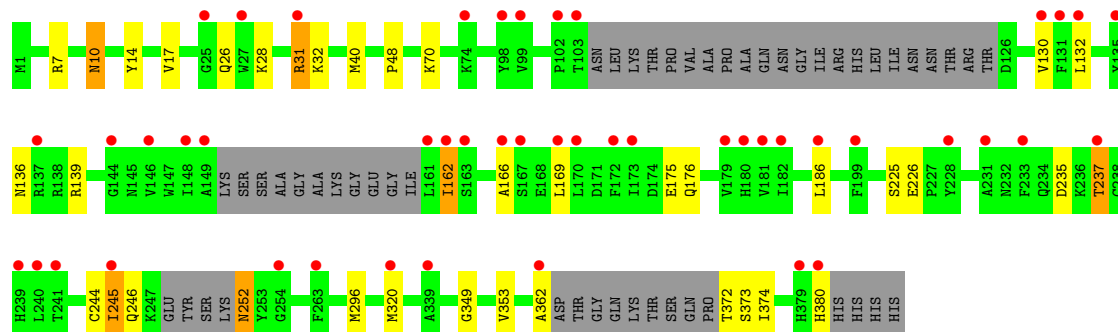
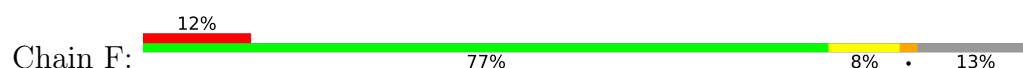




• Molecule 3: Stathmin-4



• Molecule 4: 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	105.12Å 157.66Å 181.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.68 – 2.20 39.68 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.9 (39.68-2.20) 99.9 (39.68-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.12 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.8.0107	Depositor
R, R_{free}	0.196 , 0.240 0.197 , 0.240	Depositor DCC
R_{free} test set	7554 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	39.8	Xtriage
Anisotropy	0.039	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 35.7	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	18087	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.47% 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: 890, MES, CA, GOL, GTP, MG, GDP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.78	0/3506	1.01	3/4759 (0.1%)
1	C	0.85	1/3524 (0.0%)	0.99	4/4785 (0.1%)
2	B	0.78	0/3450	0.99	2/4672 (0.0%)
2	D	0.70	1/3382 (0.0%)	1.02	3/4581 (0.1%)
3	E	0.71	0/1008	1.05	0/1337
4	F	0.67	0/2806	0.96	2/3791 (0.1%)
All	All	0.76	2/17676 (0.0%)	1.00	14/23925 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	6	SER	C-O	-5.97	1.16	1.23
2	D	286	VAL	CA-CB	5.88	1.57	1.54

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	190	THR	CB-CA-C	-9.13	95.33	110.85
2	D	105	HIS	N-CA-C	7.90	119.67	111.14
2	B	246	LEU	N-CA-C	7.26	119.19	111.28
1	C	190	THR	N-CA-CB	6.47	119.73	110.16
1	C	2	ARG	N-CA-C	6.26	119.69	110.30
4	F	162	ILE	N-CA-C	6.12	117.59	108.54
2	D	106	TYR	N-CA-C	5.98	120.71	113.41
1	A	357	TYR	N-CA-C	5.90	118.50	111.71
4	F	373	SER	N-CA-C	5.90	119.03	110.42
2	D	267	MET	CB-CA-C	-5.55	103.70	110.08
1	A	62	VAL	N-CA-C	5.38	113.76	107.89
1	C	361	THR	N-CA-C	-5.32	101.89	110.14
2	B	267	MET	CB-CA-C	-5.19	104.11	110.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	62	VAL	CB-CA-C	5.14	115.87	110.37

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	3428	0	3340	21	0
1	C	3446	0	3354	22	0
2	B	3375	0	3254	35	0
2	D	3309	0	3189	30	0
3	E	1000	0	1018	3	0
4	F	2744	0	2709	18	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	B	22	0	0	1	0
11	D	22	0	0	0	0
12	A	143	0	0	0	0
12	B	121	0	0	0	0
12	C	234	0	0	2	0
12	D	30	0	0	0	0
12	E	27	0	0	0	0
12	F	38	0	0	0	0
All	All	18087	0	16933	122	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 4.

All (122) 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:B:21:TRP:CZ3	2:B:61:PRO:HB3	1.87	1.10
1:C:234:ILE:HD13	1:C:302:MET:SD	2.17	0.83
2:B:25:SER:HA	2:B:51:TYR:OH	1.78	0.82
2:B:197:ASP:OD2	10:B:503:MES:H52	1.83	0.78
2:B:21:TRP:CZ3	2:B:61:PRO:CB	2.70	0.74
1:C:147:SER:O	1:C:190:THR:HG23	1.90	0.72
4:F:31:ARG:HH11	4:F:31:ARG:HG3	1.58	0.68
2:D:156:ARG:HG2	3:E:123:LEU:HD11	1.75	0.67
2:D:131:GLN:NE2	2:D:250:LEU:H	1.93	0.67
2:B:156:ARG:CZ	10:B:503:MES:H21	2.26	0.66
2:B:51:TYR:HA	2:B:61:PRO:HA	1.78	0.65
2:B:156:ARG:HG3	10:B:503:MES:H62	1.77	0.65
2:B:197:ASP:OD1	10:B:503:MES:H32	1.96	0.65
2:D:92:PHE:O	2:D:92:PHE:HD1	1.80	0.64
1:C:71:GLU:HB2	1:C:98:ASP:HB3	1.80	0.63
2:B:62:ARG:HH11	2:B:62:ARG:HB2	1.64	0.60
4:F:186:LEU:HD13	4:F:320:MET:HG2	1.83	0.59
2:B:25:SER:CA	2:B:51:TYR:OH	2.51	0.58
1:C:248:LEU:HD12	1:C:357:TYR:OH	2.03	0.58
1:A:209:ILE:HD11	1:A:302:MET:SD	2.43	0.58
2:B:30:ILE:HG13	2:B:51:TYR:CE2	2.38	0.58
2:B:62:ARG:HB2	2:B:62:ARG:NH1	2.19	0.56
2:B:21:TRP:CH2	2:B:61:PRO:HB3	2.40	0.55
1:A:229:ARG:HH11	1:A:229:ARG:HG2	1.73	0.53
1:A:221:ARG:HG3	2:B:323:MET:HB3	1.90	0.53
2:B:179:VAL:HG12	1:C:348:PRO:HG2	1.91	0.53
1:C:244:PHE:CD1	1:C:358:GLN:HG3	2.44	0.53
2:B:267:MET:SD	2:B:303[B]:CYS:SG	3.06	0.53
2:B:104:GLY:O	2:B:109:GLY:HA3	2.09	0.52
4:F:40:MET:HE1	4:F:48:PRO:HD2	1.91	0.52
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.27	0.52
2:D:104:GLY:O	2:D:109:GLY:HA3	2.10	0.51
1:A:210:TYR:CE2	1:A:214:ARG:HD2	2.46	0.51
1:C:209:ILE:HG23	1:C:230:LEU:HD23	1.92	0.51
4:F:7:ARG:HD3	4:F:40:MET:HE3	1.93	0.51
2:B:51:TYR:CD2	2:B:61:PRO:HG3	2.46	0.51
2:B:134:GLN:HA	2:B:165:ASN:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:99:ASN:HD22	2:D:99:ASN:N	2.08	0.51
2:B:170:MET:HG3	2:B:377:LEU:HD11	1.94	0.50
1:A:229:ARG:HH11	1:A:229:ARG:CG	2.25	0.50
2:B:321:MET:HB3	2:B:363:MET:HE1	1.93	0.50
4:F:31:ARG:HG3	4:F:31:ARG:NH1	2.27	0.49
1:A:147:SER:HB2	1:A:190:THR:HB	1.94	0.49
4:F:226:GLU:HG3	4:F:237:THR:HB	1.94	0.49
2:B:219:THR:HG22	12:C:780:HOH:O	2.12	0.49
1:A:71:GLU:HB2	1:A:98:ASP:HB3	1.94	0.48
4:F:10:ASN:HD22	4:F:10:ASN:N	2.11	0.48
2:D:69:GLU:HG2	2:D:96:GLY:CA	2.43	0.48
2:D:134:GLN:HA	2:D:165:ASN:O	2.13	0.48
1:A:88:HIS:CD2	1:A:90:GLU:HB2	2.49	0.48
1:C:320:ARG:HG3	1:C:360:PRO:HD3	1.96	0.48
2:D:170:MET:HG3	2:D:377:LEU:HD11	1.94	0.47
4:F:225:SER:HB3	4:F:252:ASN:HB3	1.96	0.47
2:B:137:HIS:HE1	2:B:168:SER:OG	1.97	0.47
1:A:71:GLU:HG2	1:A:72:PRO:HD2	1.96	0.47
1:A:357:TYR:CE2	3:E:17:GLY:HA2	2.50	0.47
2:D:92:PHE:C	2:D:92:PHE:CD1	2.93	0.47
4:F:136:ASN:HA	4:F:139:ARG:HB3	1.97	0.47
2:B:267:MET:HE2	2:B:267:MET:HB3	1.68	0.47
2:D:215:LEU:HD11	2:D:228:LEU:HD21	1.96	0.47
2:D:40:SER:HB3	2:D:43:GLN:HG3	1.96	0.47
2:B:219:THR:HG21	1:C:326:LYS:HB2	1.97	0.46
2:D:92:PHE:HD1	2:D:92:PHE:C	2.23	0.46
4:F:166:ALA:HA	4:F:169:LEU:HD12	1.98	0.46
2:D:69:GLU:OE2	2:D:96:GLY:HA3	2.16	0.45
1:A:187:SER:HB3	1:A:391:LEU:HD21	1.99	0.45
2:B:137:HIS:HD2	2:B:144:GLY:O	1.99	0.45
1:A:335:ILE:HG23	1:A:339:ARG:HG3	1.98	0.45
1:A:346:TRP:CD1	1:A:346:TRP:H	2.34	0.45
2:D:47:ILE:HD13	2:D:51:TYR:CD2	2.52	0.45
4:F:349:GLY:HA3	4:F:374:ILE:HD11	1.98	0.44
1:A:25:CYS:HB3	1:A:30:ILE:O	2.17	0.44
1:A:233:GLN:HG3	1:A:368:LEU:CD1	2.47	0.44
11:B:504:890:C06	11:B:504:890:C18	2.95	0.44
1:C:221:ARG:HD3	2:D:323:MET:HG3	2.00	0.44
1:C:254:GLU:HG2	1:C:352:LYS:HE2	2.00	0.44
1:C:1:MET:HA	1:C:46:ASP:OD1	2.17	0.44
2:D:73:MET:HG3	2:D:92:PHE:HB3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:357:TYR:CZ	3:E:17:GLY:HA2	2.53	0.43
1:C:220:GLU:HG2	2:D:324:LYS:HD2	2.01	0.43
1:A:217:LEU:HD21	1:A:368:LEU:HD23	2.00	0.43
1:A:234:ILE:HD13	1:A:302:MET:SD	2.58	0.43
1:A:165:SER:OG	1:A:256:GLN:NE2	2.51	0.43
2:B:117:LEU:HD11	2:B:154:LYS:HD3	2.01	0.43
4:F:245:ILE:HG22	4:F:245:ILE:O	2.18	0.43
1:C:249:ASN:OD1	1:C:356:ASN:ND2	2.52	0.43
2:D:321:MET:HE2	2:D:363:MET:HG2	2.01	0.43
2:D:319:GLY:HA2	2:D:357:PRO:HG3	1.99	0.43
4:F:14:TYR:HA	4:F:17:VAL:HB	2.01	0.43
2:B:163:ILE:HG21	2:B:250:LEU:HB3	2.00	0.43
1:C:151:SER:HB3	1:C:190:THR:HG22	1.99	0.42
1:C:270:ALA:HB3	1:C:302:MET:HG2	2.01	0.42
2:D:102:ALA:HB2	2:D:403:MET:SD	2.60	0.42
2:D:99:ASN:N	2:D:99:ASN:ND2	2.67	0.42
2:B:144:GLY:O	2:B:148:GLY:HA3	2.19	0.42
2:D:12:CYS:O	2:D:16:ILE:HG12	2.20	0.42
2:D:134:GLN:HB3	2:D:165:ASN:HD22	1.84	0.42
2:B:21:TRP:HZ3	2:B:61:PRO:HB3	1.67	0.42
2:D:31:ASP:HB2	2:D:32:PRO:CD	2.50	0.42
2:D:19:LYS:HB3	2:D:230:SER:HB3	2.03	0.41
1:A:209:ILE:HG23	1:A:230:LEU:HD23	2.01	0.41
1:C:335:ILE:HG23	1:C:339:ARG:HG3	2.02	0.41
2:D:6:HIS:CD2	2:D:21:TRP:HE1	2.38	0.41
2:B:47:ILE:HG12	2:B:51:TYR:HB2	2.02	0.41
2:B:179:VAL:HG11	12:C:774:HOH:O	2.21	0.41
2:D:306:ARG:HG2	2:D:340:TYR:CZ	2.55	0.41
4:F:296:MET:HE3	4:F:380:HIS:CG	2.55	0.41
1:C:188:ILE:HG13	1:C:425:MET:HG3	2.02	0.41
1:C:165:SER:HA	1:C:199:ASP:OD2	2.21	0.41
4:F:26:GLN:HE22	4:F:362:ALA:H	1.69	0.41
2:B:51:TYR:N	2:B:51:TYR:CD1	2.89	0.41
1:C:209:ILE:HD11	1:C:302:MET:SD	2.61	0.41
4:F:244:CYS:SG	4:F:245:ILE:HG13	2.60	0.41
2:B:3:GLU:HG2	2:B:62:ARG:NH2	2.37	0.40
1:C:7:ILE:HG21	1:C:153:LEU:HD21	2.02	0.40
1:C:63:PRO:HG2	1:C:87:PHE:CE1	2.56	0.40
2:D:201:CYS:SG	2:D:265:PHE:HB3	2.62	0.40
1:A:192:HIS:CG	1:A:421:ALA:HA	2.57	0.40
2:D:293:MET:HE3	2:D:365:ALA:HB1	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:244:CYS:C	4:F:246:GLN:H	2.29	0.40
2:D:293:MET:HE2	2:D:367:PHE:HB2	2.03	0.40
4:F:10:ASN:N	4:F:10:ASN:ND2	2.68	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	437/451 (97%)	428 (98%)	9 (2%)	0	100	100
1	C	439/451 (97%)	430 (98%)	9 (2%)	0	100	100
2	B	427/445 (96%)	410 (96%)	16 (4%)	1 (0%)	43	51
2	D	417/445 (94%)	408 (98%)	8 (2%)	1 (0%)	43	51
3	E	117/143 (82%)	115 (98%)	1 (1%)	1 (1%)	14	14
4	F	324/384 (84%)	302 (93%)	20 (6%)	2 (1%)	21	23
All	All	2161/2319 (93%)	2093 (97%)	63 (3%)	5 (0%)	43	51

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	392	LYS
2	B	62	ARG
4	F	245	ILE
4	F	32	LYS
3	E	27	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	370/379 (98%)	363 (98%)	7 (2%)	50	66
1	C	372/379 (98%)	362 (97%)	10 (3%)	39	53
2	B	371/383 (97%)	363 (98%)	8 (2%)	45	61
2	D	364/383 (95%)	344 (94%)	20 (6%)	19	24
3	E	109/127 (86%)	98 (90%)	11 (10%)	7	7
4	F	301/342 (88%)	287 (95%)	14 (5%)	23	31
All	All	1887/1993 (95%)	1817 (96%)	70 (4%)	30	41

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	62	VAL
1	A	96	LYS
1	A	229	ARG
1	A	279	GLU
1	A	370	LYS
1	A	430	LYS
1	A	433	GLU
2	B	19	LYS
2	B	48	ASN
2	B	53	GLU
2	B	55	THR
2	B	62	ARG
2	B	320	ARG
2	B	363	MET
2	B	395	LEU
1	C	2	ARG
1	C	133	GLN
1	C	164	LYS
1	C	190	THR
1	C	251	ASP
1	C	302	MET
1	C	347	CYS

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Mol	Chain	Res	Type
1	C	358	GLN
1	C	381	THR
1	C	430	LYS
2	D	1	MET
2	D	26	ASP
2	D	47	ILE
2	D	48	ASN
2	D	55	THR
2	D	92	PHE
2	D	151	LEU
2	D	153	SER
2	D	156	ARG
2	D	180	VAL
2	D	218	THR
2	D	219	THR
2	D	284	LEU
2	D	291	GLN
2	D	293	MET
2	D	296	SER
2	D	323	MET
2	D	333	VAL
2	D	386	THR
2	D	395	LEU
3	E	6	MET
3	E	51	GLN
3	E	53	LYS
3	E	62	LYS
3	E	70	LYS
3	E	75	LYS
3	E	89	GLU
3	E	92	ASN
3	E	107	SER
3	E	136	ASN
3	E	139	LEU
4	F	10	ASN
4	F	28	LYS
4	F	31	ARG
4	F	70	LYS
4	F	130	VAL
4	F	132	LEU
4	F	162	ILE
4	F	175	GLU

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Mol	Chain	Res	Type
4	F	176	GLN
4	F	235	ASP
4	F	237	THR
4	F	252	ASN
4	F	353	VAL
4	F	372	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	256	GLN
1	A	301	GLN
2	B	8	GLN
2	B	14	ASN
2	B	48	ASN
2	B	134	GLN
2	B	137	HIS
2	B	247	ASN
2	B	329	GLN
2	B	332	ASN
1	C	256	GLN
1	C	393	HIS
2	D	11	GLN
2	D	99	ASN
2	D	131	GLN
2	D	292	GLN
2	D	329	GLN
2	D	347	ASN
2	D	426	GLN
4	F	10	ASN
4	F	136	ASN
4	F	209	HIS
4	F	229	ASN
4	F	232	ASN
4	F	269	GLN
4	F	310	GLN
4	F	348	GLN
4	F	379	HIS

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 14 ligands modelled in this entry, 6 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	$\# Z > 2$
10	MES	B	503	-	12,12,12	1.74	2 (16%)	15,16,16	5.57	9 (60%)
11	890	D	503	-	24,24,24	2.09	10 (41%)	29,34,34	1.66	7 (24%)
9	GDP	B	501	6	29,30,30	1.35	3 (10%)	45,47,47	1.78	8 (17%)
8	GOL	A	504	-	5,5,5	0.42	0	5,5,5	0.50	0
5	GTP	C	501	6	33,34,34	1.15	4 (12%)	50,54,54	1.58	7 (14%)
5	GTP	A	501	6	33,34,34	1.10	2 (6%)	50,54,54	1.79	9 (18%)
5	GTP	D	501	6	33,34,34	1.32	5 (15%)	50,54,54	1.66	6 (12%)
11	890	B	504	-	24,24,24	2.06	10 (41%)	29,34,34	1.50	7 (24%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	MES	B	503	-	-	4/6/14/14	0/1/1/1
11	890	D	503	-	-	2/10/10/10	0/3/3/3
9	GDP	B	501	6	-	5/16/32/32	0/3/3/3
8	GOL	A	504	-	-	1/4/4/4	-
5	GTP	C	501	6	-	8/22/38/38	0/3/3/3
5	GTP	A	501	6	-	7/22/38/38	0/3/3/3
5	GTP	D	501	6	-	6/22/38/38	0/3/3/3
11	890	B	504	-	-	0/10/10/10	0/3/3/3

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	503	MES	C8-S	-4.98	1.70	1.77
9	B	501	GDP	PA-O3A	4.20	1.64	1.59
11	B	504	890	C18-C19	3.88	1.45	1.39
11	D	503	890	C18-C19	3.49	1.45	1.39
11	B	504	890	C10-C09	3.42	1.43	1.37
11	B	504	890	C05-C06	3.42	1.45	1.39
11	D	503	890	C15-C14	3.35	1.46	1.39
11	D	503	890	C17-C18	3.34	1.44	1.38
5	D	501	GTP	C5-C4	3.28	1.47	1.38
11	D	503	890	O02-C03	3.25	1.42	1.37
11	B	504	890	O02-C03	3.17	1.42	1.37
11	B	504	890	C15-C14	3.08	1.45	1.39
5	C	501	GTP	C6-N1	-3.08	1.33	1.38
11	D	503	890	C05-C06	2.99	1.44	1.39
5	A	501	GTP	C5-C4	2.95	1.46	1.38
9	B	501	GDP	C5-C4	2.91	1.46	1.38
11	B	504	890	C17-C18	2.75	1.43	1.38
5	C	501	GTP	C5-C4	2.70	1.46	1.38
11	D	503	890	C10-C09	2.68	1.42	1.37
5	D	501	GTP	PB-O3B	2.68	1.62	1.59
5	D	501	GTP	PA-O3A	2.66	1.62	1.59
5	D	501	GTP	PB-O3A	2.51	1.62	1.59
11	D	503	890	C21-N22	2.50	1.46	1.38
10	B	503	MES	O2S-S	2.49	1.52	1.45
11	D	503	890	C20-C06	2.42	1.43	1.39
5	C	501	GTP	C5-N7	-2.40	1.34	1.39
11	D	503	890	C05-C04	2.25	1.42	1.38
11	B	504	890	C05-C04	2.23	1.42	1.38
5	D	501	GTP	C5-N7	-2.22	1.34	1.39
11	D	503	890	C20-C21	2.19	1.43	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	B	504	890	C21-N22	2.16	1.45	1.38
9	B	501	GDP	C4-N9	-2.16	1.32	1.38
5	C	501	GTP	PG-O3G	-2.09	1.47	1.54
11	B	504	890	C10-C11	-2.08	1.40	1.44
11	B	504	890	C04-C03	2.04	1.43	1.39
5	A	501	GTP	C4-N9	-2.03	1.32	1.38

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	503	MES	O3S-S-O1S	-12.28	80.68	111.40
10	B	503	MES	O3S-S-O2S	-9.84	86.77	111.40
10	B	503	MES	O3S-S-C8	-8.18	90.01	106.00
10	B	503	MES	O1S-S-C8	7.61	118.22	106.73
10	B	503	MES	O2S-S-C8	6.96	117.25	106.73
5	D	501	GTP	C5-C4-N3	-5.94	118.93	128.39
5	C	501	GTP	C5-C4-N3	-5.17	120.16	128.39
5	A	501	GTP	C5-C4-N3	-5.12	120.24	128.39
5	D	501	GTP	C2-N3-C4	4.95	120.82	112.30
9	B	501	GDP	C2-N3-C4	4.92	120.78	112.30
5	A	501	GTP	C2-N3-C4	4.90	120.74	112.30
9	B	501	GDP	C5-C4-N3	-4.86	120.65	128.39
5	D	501	GTP	N9-C4-N3	4.34	134.63	125.95
5	C	501	GTP	C2-N3-C4	4.25	119.62	112.30
5	C	501	GTP	N9-C4-N3	4.20	134.36	125.95
9	B	501	GDP	N9-C4-N3	4.06	134.07	125.95
5	A	501	GTP	N9-C4-N3	3.80	133.56	125.95
9	B	501	GDP	C6-C5-N7	3.78	137.17	130.29
5	A	501	GTP	C6-C5-N7	3.64	136.92	130.29
10	B	503	MES	C6-O1-C2	3.58	121.46	109.88
5	D	501	GTP	C6-C5-N7	3.33	136.36	130.29
11	D	503	890	C01-O02-C03	3.25	122.28	117.51
11	B	504	890	C20-C06-N07	-3.11	116.73	119.59
11	D	503	890	O12-C11-C10	-3.11	119.67	125.92
11	B	504	890	O13-C11-O12	2.99	120.29	116.40
11	D	503	890	C03-C21-N22	-2.94	116.49	119.53
9	B	501	GDP	O6-C6-C5	-2.87	118.95	126.53
11	D	503	890	C21-C20-C06	-2.86	118.54	122.13
5	A	501	GTP	O6-C6-C5	-2.85	119.02	126.53
5	D	501	GTP	C4-C5-N7	-2.83	106.18	110.67
11	D	503	890	O13-C11-O12	2.83	120.08	116.40
5	C	501	GTP	C6-C5-N7	2.80	135.38	130.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	503	MES	O2S-S-O1S	2.79	122.88	113.82
11	B	504	890	O12-C11-C10	-2.71	120.46	125.92
11	D	503	890	C20-C21-C03	2.64	121.22	118.34
9	B	501	GDP	C6-C5-C4	-2.54	115.00	118.83
11	D	503	890	O13-C11-C10	2.54	120.25	117.16
11	B	504	890	C21-C20-C06	-2.51	118.98	122.13
10	B	503	MES	C5-N4-C3	2.47	114.17	108.84
5	A	501	GTP	O3G-PG-O2G	2.45	116.99	107.80
5	C	501	GTP	O3G-PG-O1G	2.39	120.17	110.83
5	A	501	GTP	C4-C5-N7	-2.37	106.91	110.67
5	A	501	GTP	N2-C2-N1	2.33	121.69	116.76
9	B	501	GDP	C5-C6-N1	2.32	119.17	113.25
11	B	504	890	C01-O02-C03	-2.31	114.12	117.51
5	C	501	GTP	C4-C5-N7	-2.25	107.11	110.67
5	D	501	GTP	C8-N7-C5	2.22	108.21	104.26
11	B	504	890	O13-C14-C15	2.19	119.16	116.25
5	C	501	GTP	C8-N7-C5	2.17	108.12	104.26
5	A	501	GTP	O3G-PG-O1G	2.16	119.23	110.83
10	B	503	MES	C7-N4-C5	2.12	116.88	111.24
9	B	501	GDP	C8-N9-C4	2.07	109.90	106.03
11	B	504	890	C20-C21-C03	2.04	120.56	118.34

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	501	GTP	C5'-O5'-PA-O3A
5	A	501	GTP	C5'-O5'-PA-O1A
5	A	501	GTP	C5'-O5'-PA-O2A
5	C	501	GTP	C5'-O5'-PA-O3A
5	C	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O2A
5	D	501	GTP	C5'-O5'-PA-O3A
5	D	501	GTP	C5'-O5'-PA-O1A
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	D	503	890	C10-C09-N07-C08
11	D	503	890	C19-C09-N07-C08
10	B	503	MES	N4-C7-C8-S
10	B	503	MES	C8-C7-N4-C3
10	B	503	MES	C7-C8-S-O1S

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Mol	Chain	Res	Type	Atoms
5	A	501	GTP	PB-O3B-PG-O1G
5	C	501	GTP	PB-O3B-PG-O1G
5	D	501	GTP	C5'-O5'-PA-O2A
9	B	501	GDP	C5'-O5'-PA-O2A
9	B	501	GDP	PB-O3A-PA-O1A
5	C	501	GTP	C4'-C5'-O5'-PA
5	A	501	GTP	C4'-C5'-O5'-PA
8	A	504	GOL	O1-C1-C2-C3
5	A	501	GTP	PB-O3B-PG-O3G
5	C	501	GTP	PB-O3B-PG-O2G
5	C	501	GTP	PB-O3B-PG-O3G
5	D	501	GTP	PB-O3A-PA-O2A
9	B	501	GDP	PB-O3A-PA-O2A
5	D	501	GTP	C4'-C5'-O5'-PA
5	A	501	GTP	PB-O3A-PA-O1A
5	C	501	GTP	PB-O3A-PA-O1A
5	D	501	GTP	PB-O3A-PA-O1A

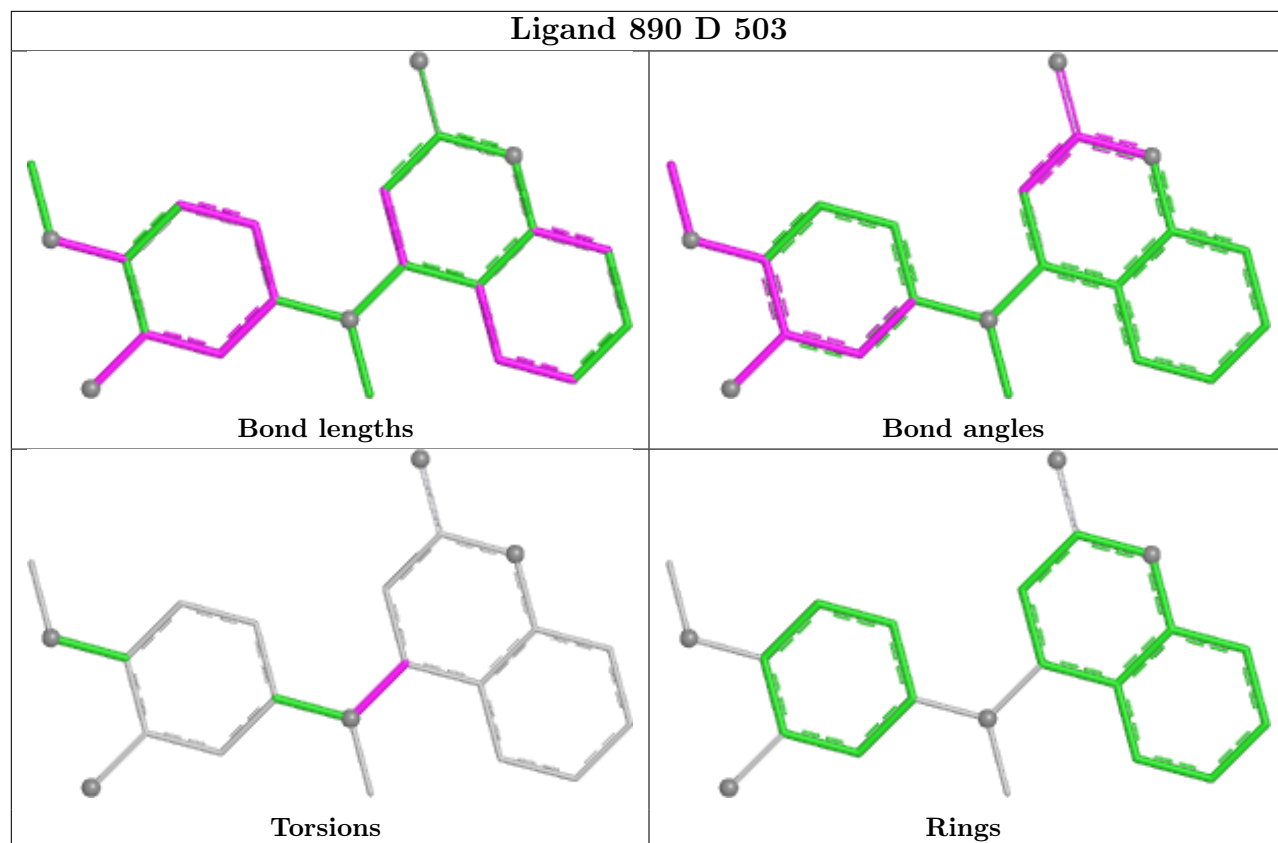
There are no ring outliers.

2 monomers are involved in 5 short contacts:

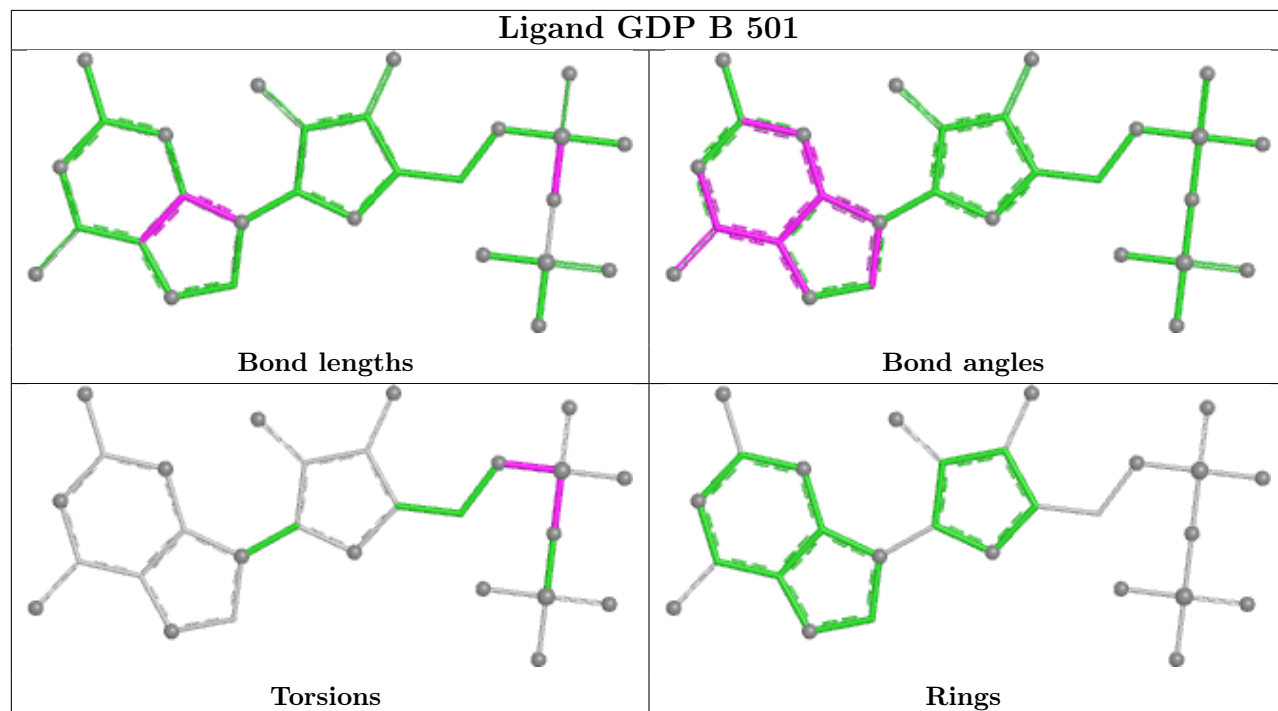
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	B	503	MES	4	0
11	B	504	890	1	0

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.

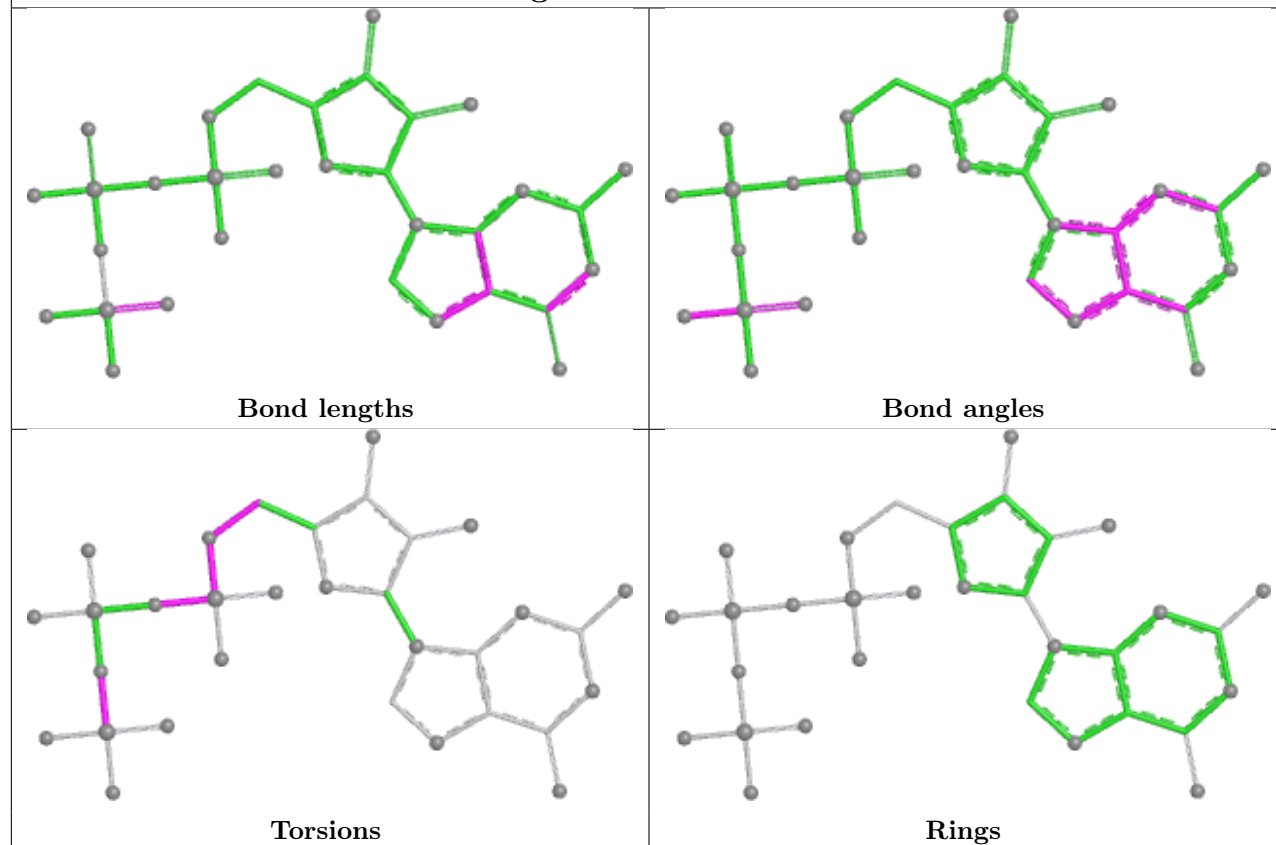
Ligand 890 D 503



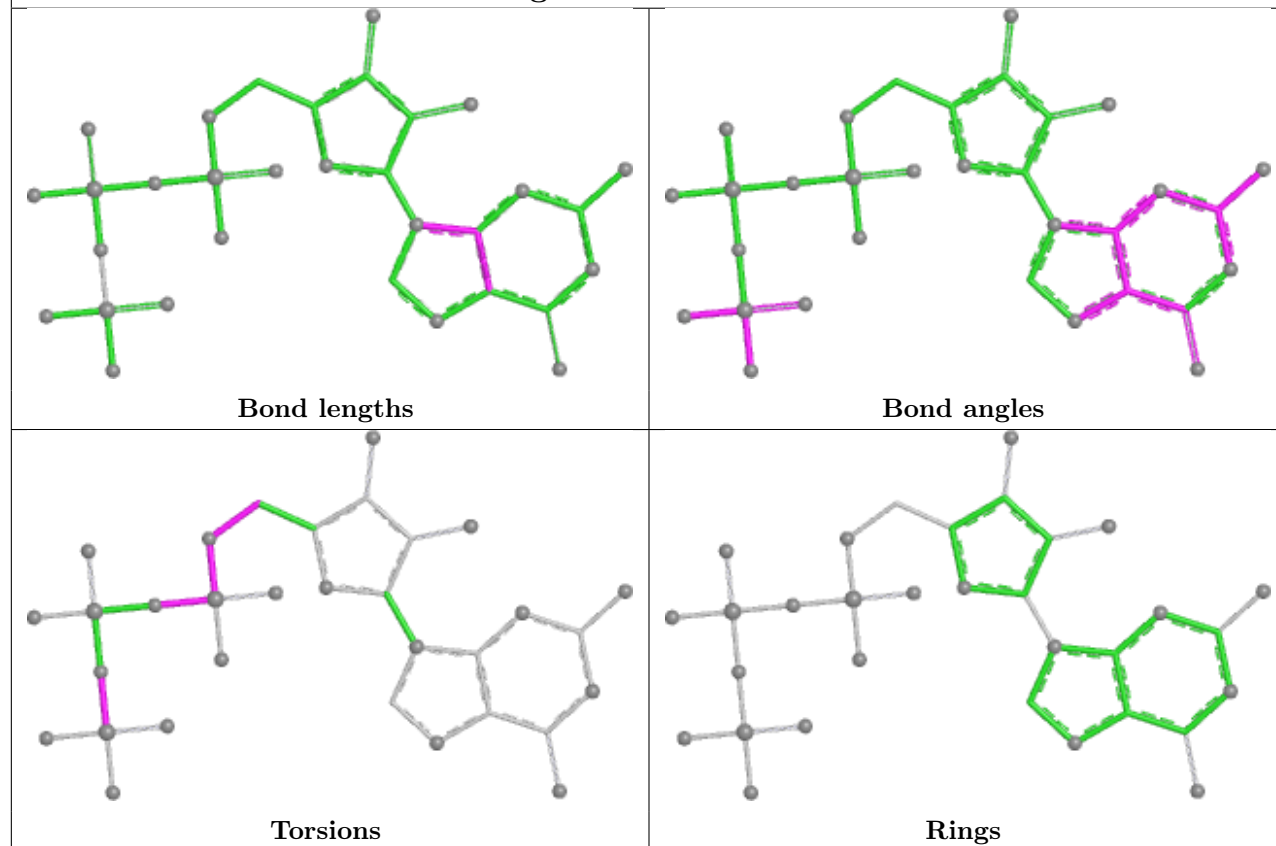
Ligand GDP B 501

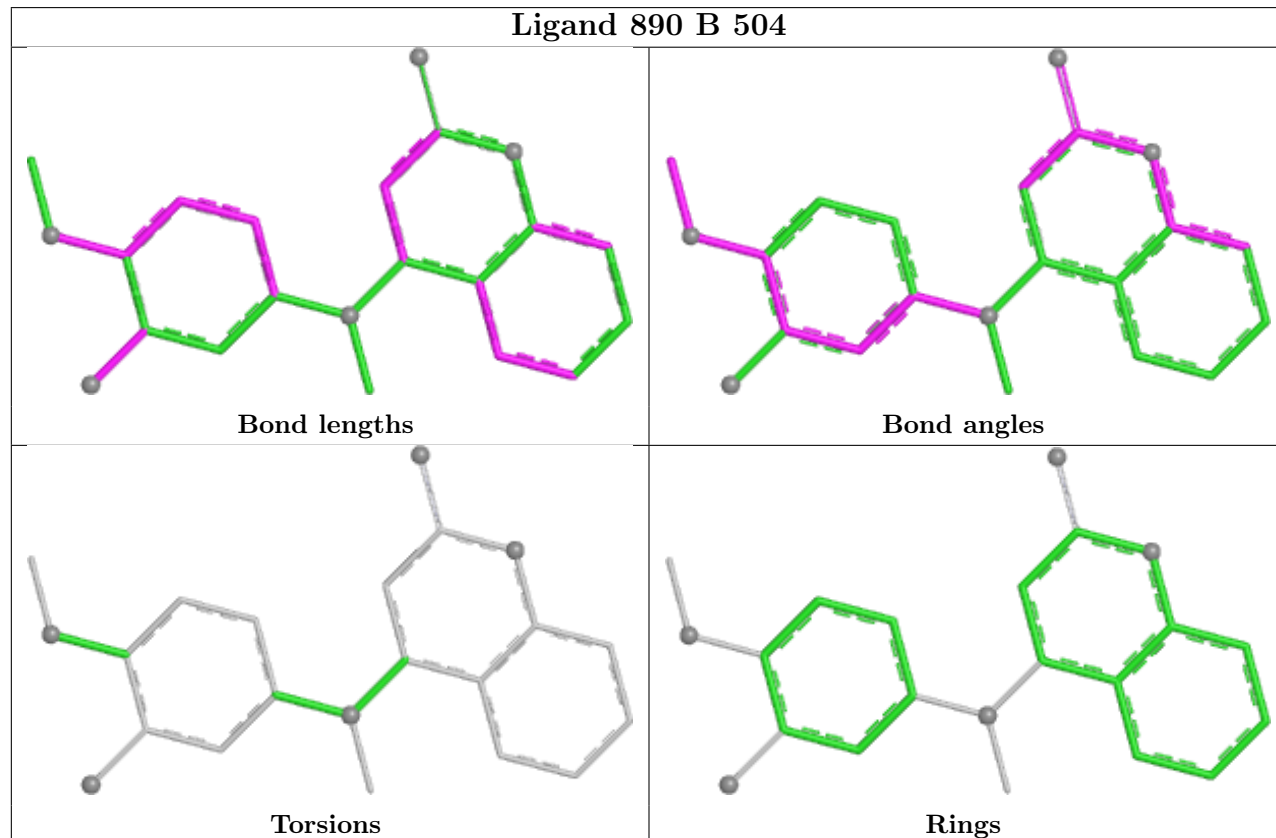
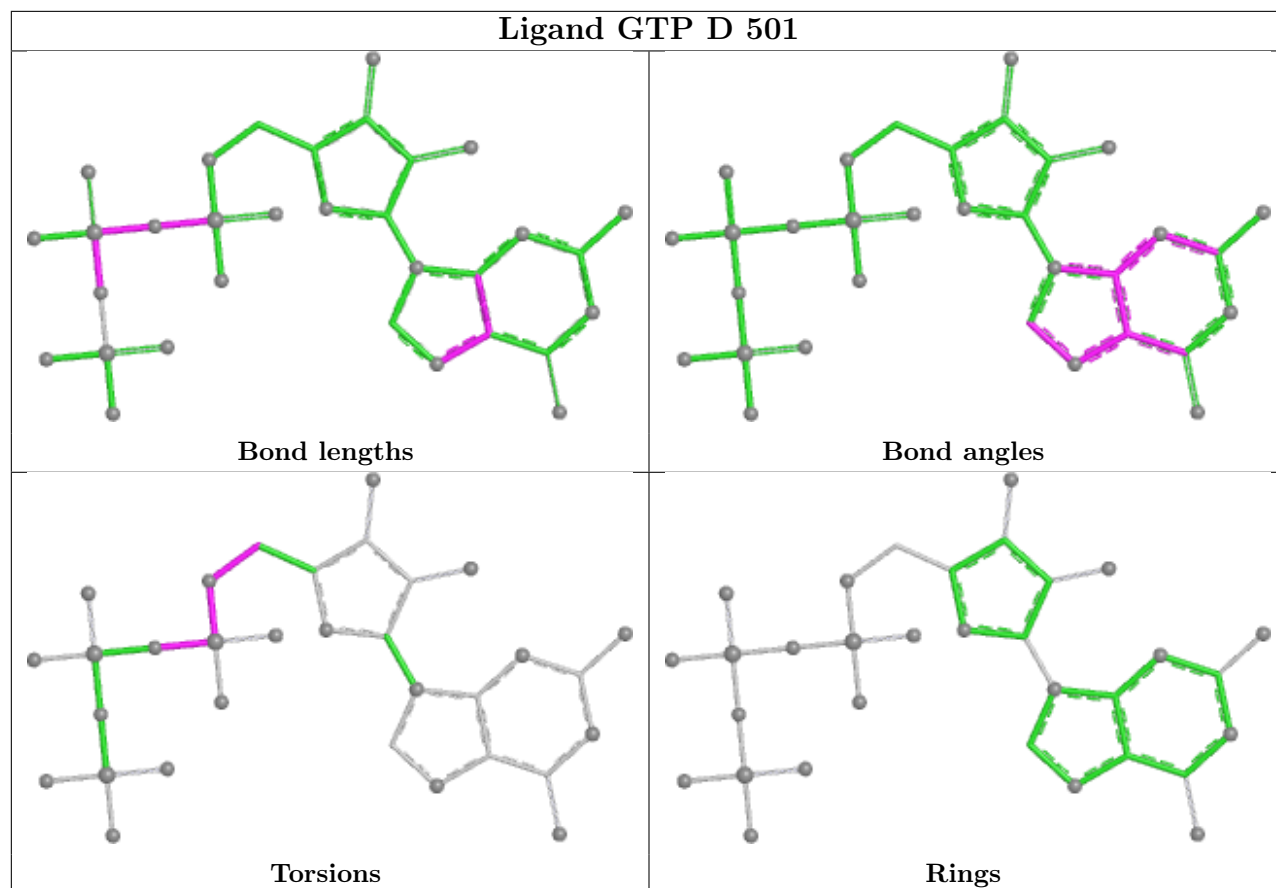


Ligand GTP C 501



Ligand GTP A 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%)	-0.01	3 (0%) 84 82	18, 41, 64, 85	2 (0%)
1	C	440/451 (97%)	-0.34	4 (0%) 81 79	18, 33, 58, 78	1 (0%)
2	B	428/445 (96%)	0.10	16 (3%) 45 42	20, 41, 76, 119	1 (0%)
2	D	421/445 (94%)	0.95	60 (14%) 6 4	30, 64, 98, 126	0
3	E	121/143 (84%)	0.67	8 (6%) 24 21	31, 55, 92, 114	0
4	F	334/384 (86%)	0.91	47 (14%) 6 4	35, 64, 129, 147	0
All	All	2181/2319 (94%)	0.31	138 (6%) 26 23	18, 46, 97, 147	4 (0%)

All (138) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	61	PRO	8.1
4	F	161	LEU	6.1
2	B	51	TYR	5.6
4	F	169	LEU	5.1
2	B	1	MET	5.1
2	B	60	VAL	5.0
4	F	380	HIS	4.6
2	B	52	ASN	4.5
1	A	437	VAL	4.4
4	F	132	LEU	4.2
3	E	6	MET	3.9
4	F	233	PHE	3.9
1	C	1	MET	3.9
2	D	394	PHE	3.9
4	F	166	ALA	3.7
4	F	182	ILE	3.7
4	F	130	VAL	3.7
4	F	179	VAL	3.7
2	D	73	MET	3.6

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Mol	Chain	Res	Type	RSRZ
4	F	180	HIS	3.6
4	F	74	LYS	3.5
2	B	57	ASN	3.5
1	C	440	VAL	3.5
2	D	179	VAL	3.5
4	F	181	VAL	3.5
2	D	55	THR	3.5
4	F	173	ILE	3.5
2	D	81	PHE	3.5
4	F	103	THR	3.4
4	F	149	ALA	3.4
2	D	180	VAL	3.3
2	D	393	ALA	3.3
4	F	245	ILE	3.3
2	D	92	PHE	3.3
2	B	428	ALA	3.2
2	D	217	LEU	3.2
2	D	323	MET	3.2
4	F	170	LEU	3.1
2	D	80	PRO	3.1
2	D	406	MET	3.0
2	D	218	THR	3.0
2	B	279	GLN	3.0
4	F	240	LEU	3.0
2	D	1	MET	3.0
4	F	131	PHE	2.9
4	F	99	VAL	2.9
2	D	219	THR	2.9
2	D	64	ILE	2.8
2	D	284	LEU	2.7
2	D	72	THR	2.7
2	D	93	GLY	2.7
2	D	12	CYS	2.7
2	D	397	TRP	2.7
2	D	228	LEU	2.7
1	C	357	TYR	2.7
2	D	395	LEU	2.7
4	F	162	ILE	2.6
4	F	254	GLY	2.6
4	F	146	VAL	2.6
2	D	400	GLY	2.6
1	C	340	SER	2.6

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Mol	Chain	Res	Type	RSRZ
2	B	323	MET	2.6
3	E	28	SER	2.6
2	D	54	ALA	2.6
3	E	45	PRO	2.6
4	F	241	THR	2.5
2	D	388	MET	2.5
4	F	27	TRP	2.5
2	D	69	GLU	2.5
1	A	262	TYR	2.5
2	D	85	PHE	2.4
2	D	91	VAL	2.4
2	D	42	LEU	2.4
2	B	55	THR	2.4
4	F	163	SER	2.4
4	F	172	PHE	2.4
4	F	199	PHE	2.4
2	D	273	LEU	2.4
2	B	281	TYR	2.4
2	D	396	HIS	2.4
4	F	135	TYR	2.4
2	D	10	GLY	2.4
2	D	387	ALA	2.4
4	F	379	HIS	2.4
3	E	7	GLU	2.4
2	D	398	TYR	2.3
2	D	104	GLY	2.3
4	F	144	GLY	2.3
4	F	339	ALA	2.3
2	D	178	THR	2.3
2	D	96	GLY	2.3
2	D	141	GLY	2.3
2	D	115	SER	2.3
4	F	167	SER	2.3
2	B	48	ASN	2.3
4	F	228	TYR	2.3
2	D	16	ILE	2.3
2	D	215	LEU	2.2
2	D	227	HIS	2.2
2	B	245	GLN	2.2
2	D	381	ILE	2.2
2	D	175	VAL	2.2
3	E	133	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
4	F	320	MET	2.2
2	D	30	ILE	2.2
4	F	186	LEU	2.2
4	F	362	ALA	2.2
2	D	112	LEU	2.2
2	D	97	ALA	2.2
4	F	231	ALA	2.2
4	F	263	PHE	2.1
4	F	239	HIS	2.1
2	B	54	ALA	2.1
2	D	9	ALA	2.1
4	F	237	THR	2.1
2	D	99	ASN	2.1
2	D	245	GLN	2.1
2	D	102	ALA	2.1
4	F	98	TYR	2.1
2	D	66	VAL	2.1
2	D	76	VAL	2.1
4	F	25	GLY	2.1
2	D	220	PRO	2.1
2	D	169	VAL	2.1
2	B	56	GLY	2.1
3	E	59	GLU	2.0
2	D	246	LEU	2.0
3	E	139	LEU	2.0
4	F	148	ILE	2.0
2	D	208	TYR	2.0
3	E	8	VAL	2.0
4	F	31	ARG	2.0
2	D	101	TRP	2.0
2	D	293	MET	2.0
2	B	278	SER	2.0
4	F	102	PRO	2.0
4	F	137	ARG	2.0
1	A	96	LYS	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 [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

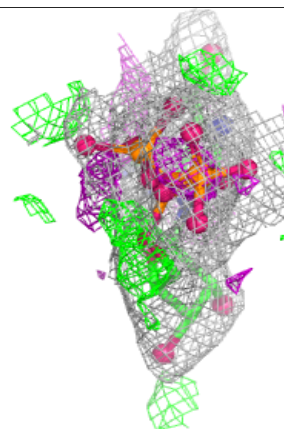
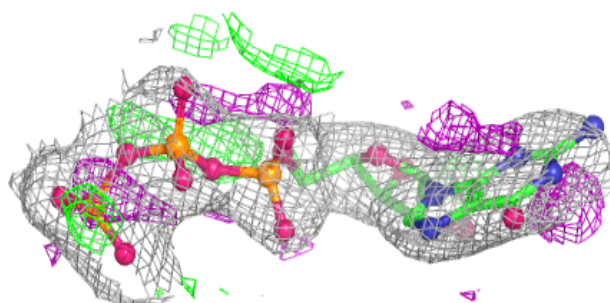
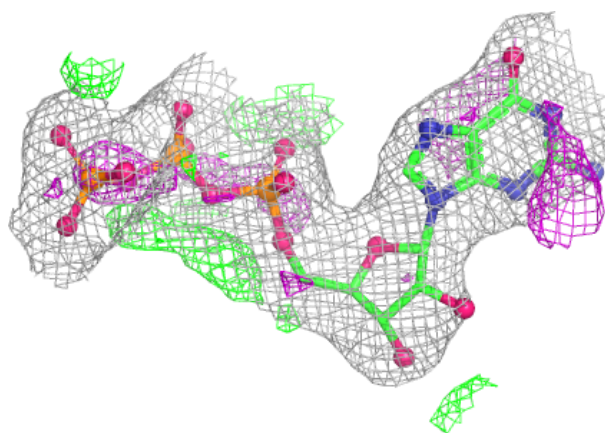
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	0.64	0.20	81,81,81,81	0
5	GTP	D	501	32/32	0.88	0.12	51,61,72,83	0
8	GOL	A	504	6/6	0.91	0.10	39,49,54,57	0
10	MES	B	503	12/12	0.94	0.10	43,48,55,56	0
11	890	B	504	22/22	0.96	0.07	26,32,33,35	0
11	890	D	503	22/22	0.97	0.07	30,40,43,43	0
7	CA	A	503	1/1	0.98	0.04	53,53,53,53	0
5	GTP	A	501	32/32	0.98	0.05	25,29,34,37	0
9	GDP	B	501	28/28	0.98	0.05	23,29,31,33	0
5	GTP	C	501	32/32	0.99	0.04	24,26,30,36	0
6	MG	A	502	1/1	0.99	0.02	33,33,33,33	0
7	CA	C	503	1/1	0.99	0.02	40,40,40,40	0
6	MG	B	502	1/1	0.99	0.02	27,27,27,27	0
6	MG	C	502	1/1	1.00	0.03	28,28,28,28	0

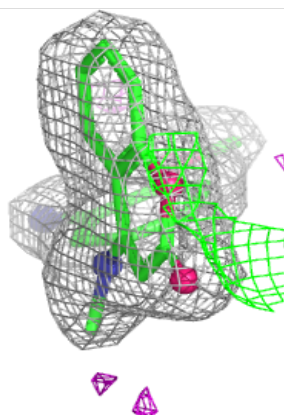
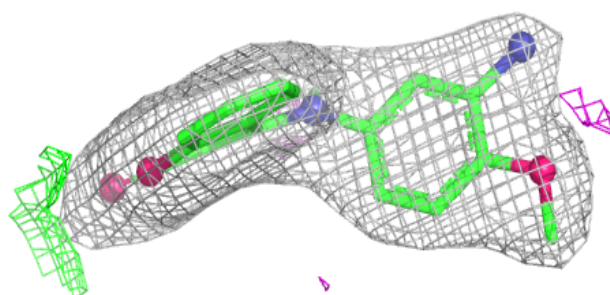
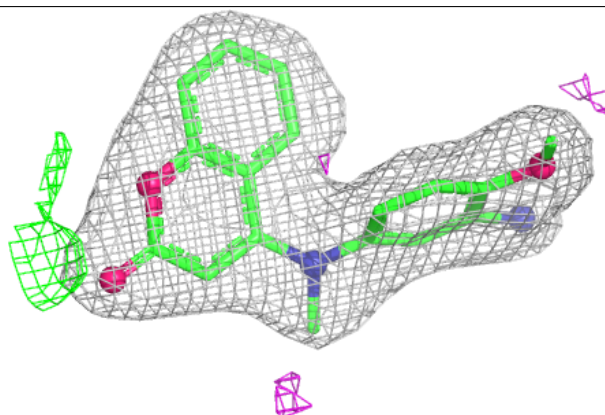
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 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)

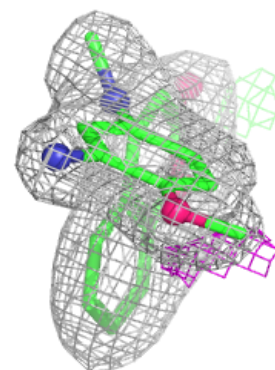
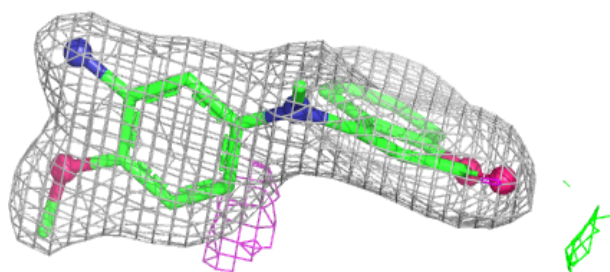
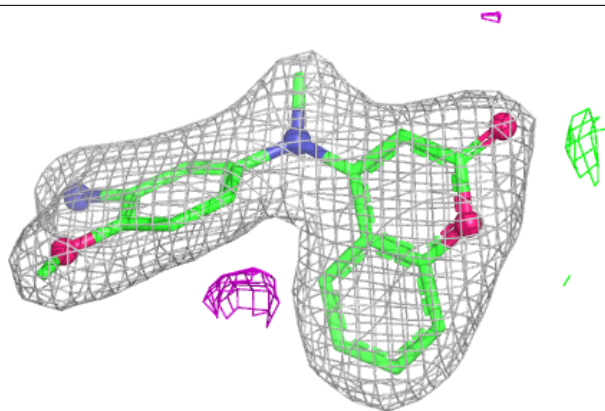
**Electron density around 890 B 504:**

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

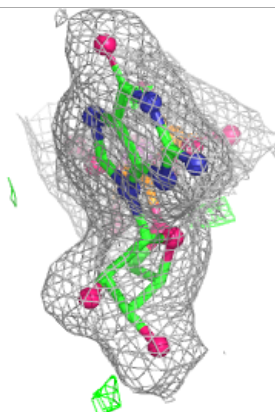
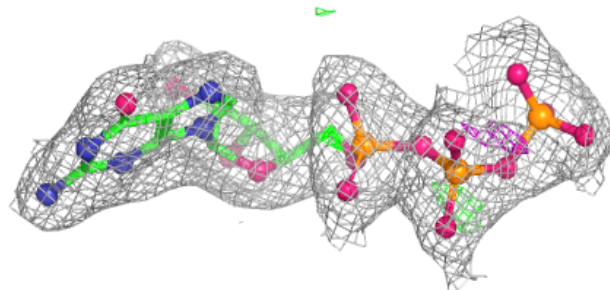
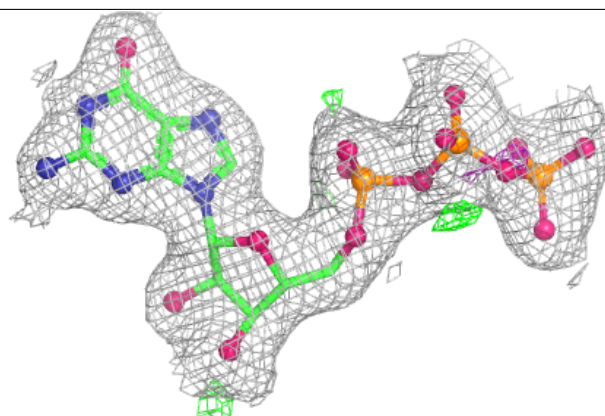


Electron density around 890 D 503:

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

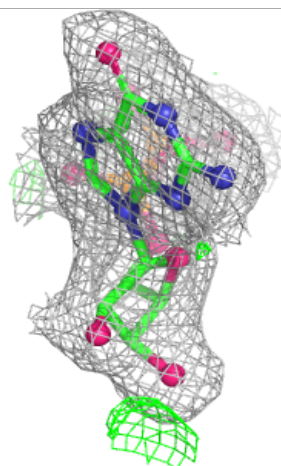
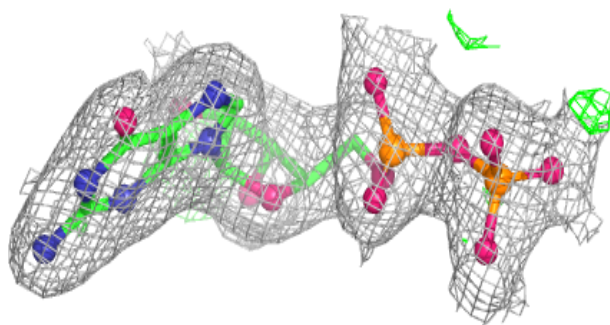
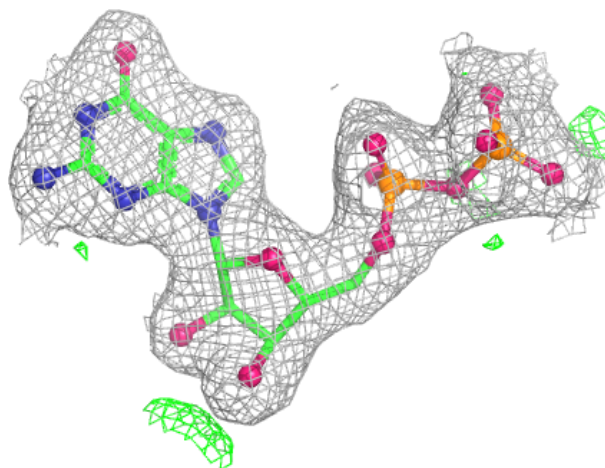
**Electron density around GTP A 501:**

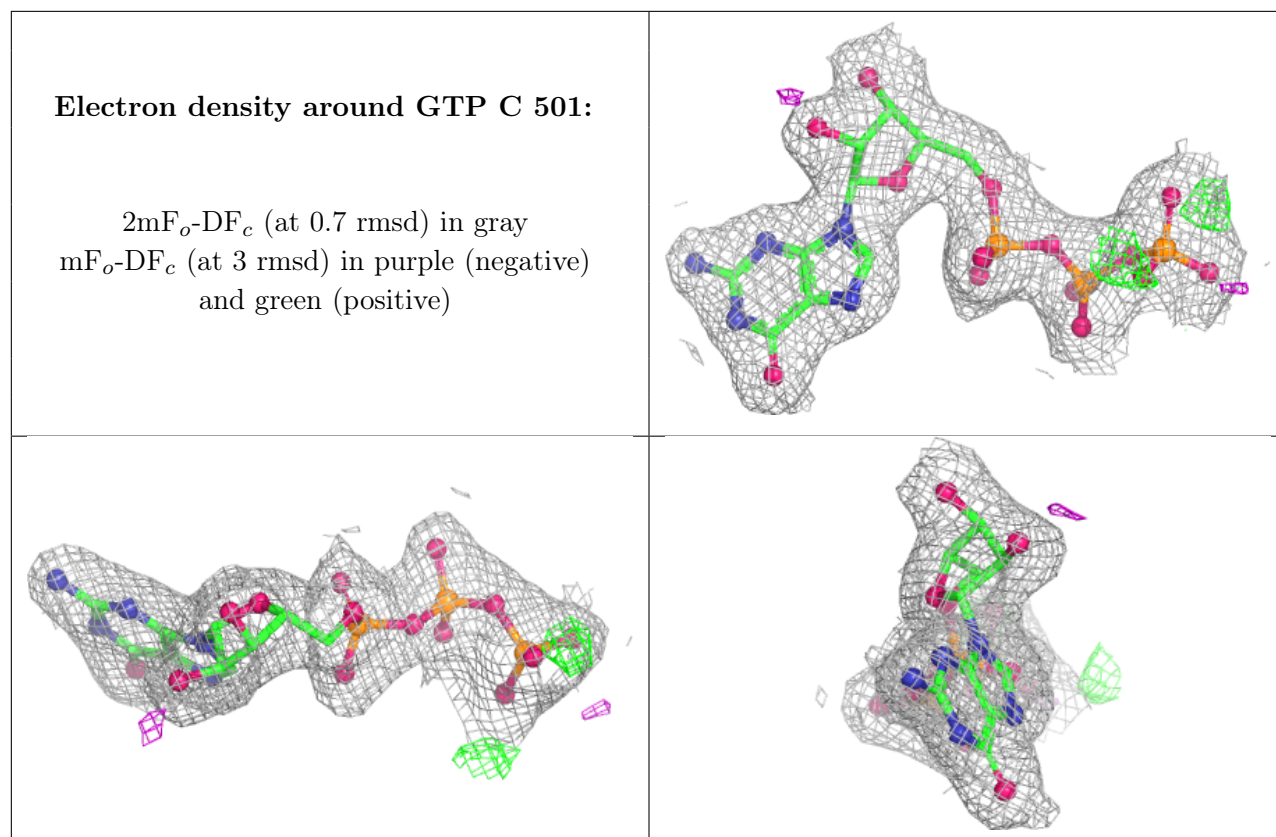
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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)





6.5 Other polymers [i](#)

There are no such residues in this entry.