



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:21 AM UTC

PDB ID : 6NNG / pdb_00006nng
Title : Tubulin-RB3_SLD-TTL in complex with compound DJ95
Authors : Kumar, G.; Wang, Y.; Li, W.; White, S.W.
Deposited on : 2019-01-15
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

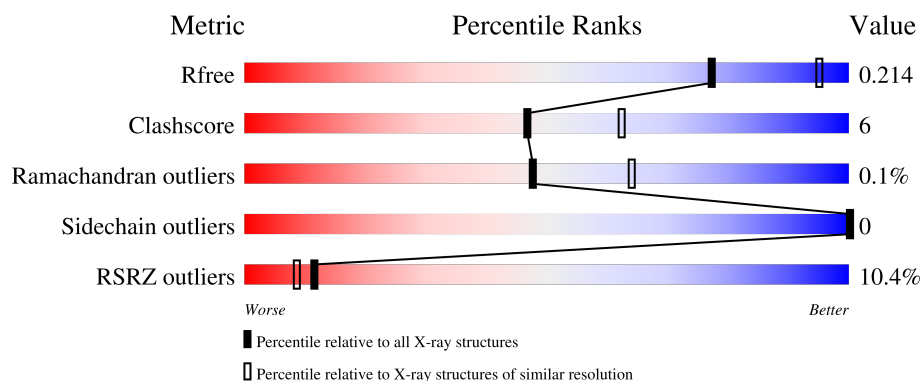
1 Overall quality at a glance

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	450	3% 85% 13% .
1	C	450	4% 89% 8% .
2	B	445	7% 82% 14% .
2	D	445	11% 78% 16% 5%
3	E	143	10% 77% 8% 15%

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Mol	Chain	Length	Quality of chain
4	F	384	26% 74% 14% 12%

2 Entry composition [i](#)

There are 12 unique types of molecules in this entry. The entry contains 17861 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	439	Total	C	N	O	S	0	0	0
			3412	2157	581	652	22			
1	C	440	Total	C	N	O	S	0	0	0
			3430	2171	583	655	21			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	427	Total	C	N	O	S	0	0	0
			3343	2101	571	645	26			
2	D	421	Total	C	N	O	S	0	0	0
			3264	2052	552	635	25			

- 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
			984	607	179	193	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	3	MET	-	expression tag	UNP Q9H169
E	4	ALA	-	expression tag	UNP Q9H169

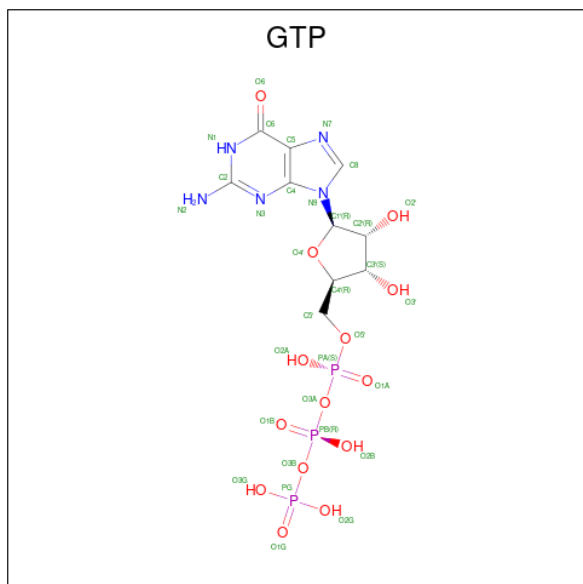
- Molecule 4 is a protein called Tubulin Tyrosine Ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	339	Total	C	N	O	S	0	0	0
			2643	1697	458	475	13			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	379	HIS	-	expression tag	UNP E1BQ43
F	380	HIS	-	expression tag	UNP E1BQ43
F	381	HIS	-	expression tag	UNP E1BQ43
F	382	HIS	-	expression tag	UNP E1BQ43
F	383	HIS	-	expression tag	UNP E1BQ43
F	384	HIS	-	expression tag	UNP E1BQ43

- Molecule 5 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
5	C	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
5	D	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

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

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

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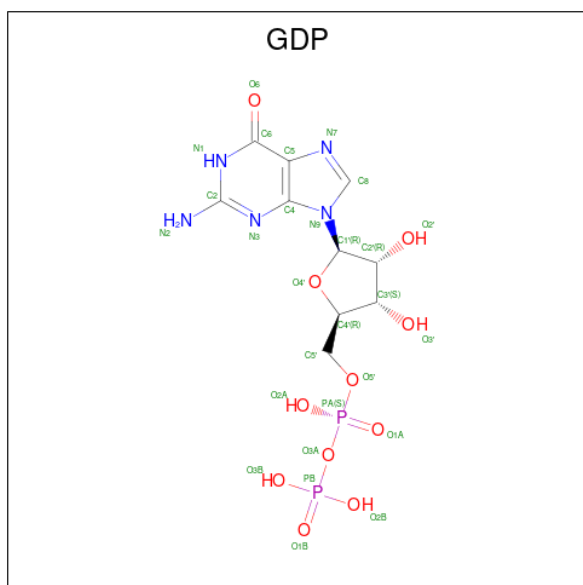
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	F	1	Total	Mg	0	0
			1	1		

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

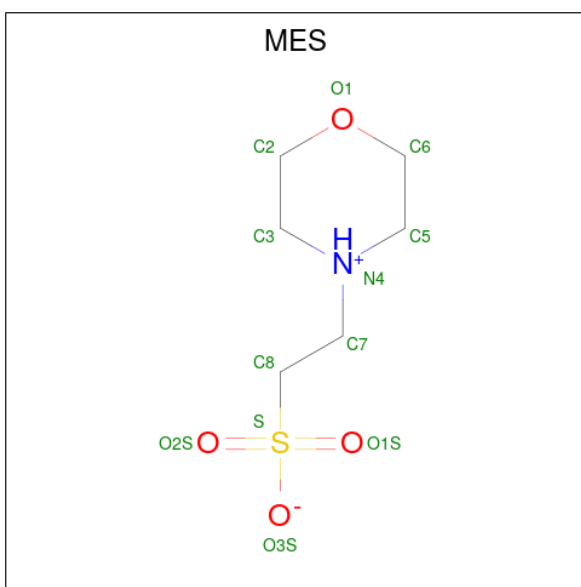
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Ca	0	0
			1	1		
7	C	1	Total	Ca	0	0
			1	1		

- Molecule 8 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



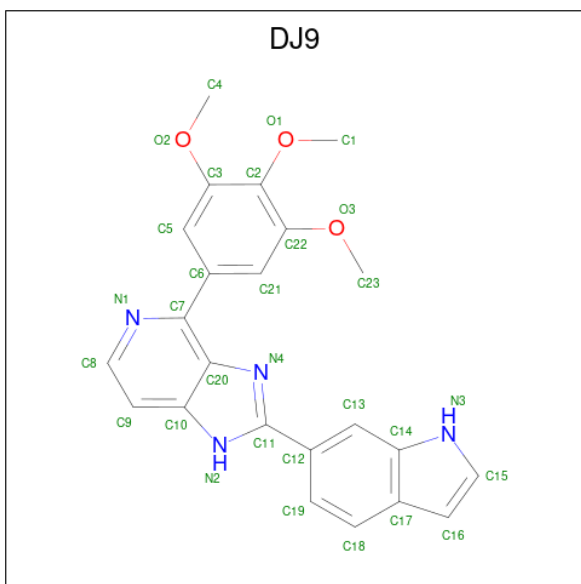
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	B	1	Total	C	N	O	P	
			28	10	5	11	2	0

- Molecule 9 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: C₆H₁₃NO₄S).



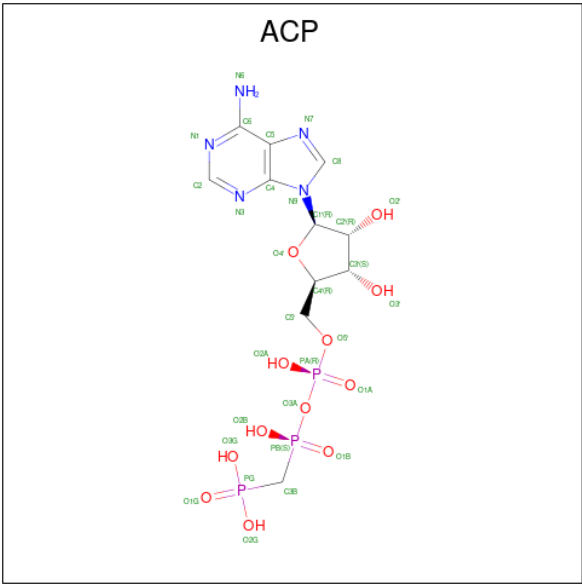
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
9	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 10 is 2-(1H-indol-6-yl)-4-(3,4,5-trimethoxyphenyl)-1H-imidazo[4,5-c]pyridine (CCD ID: DJ9) (formula: C₂₃H₂₀N₄O₃) (labeled as "Ligand of Interest" by depositor).



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

- 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	C	N	O	P	0	0
			31	11	5	12	3		

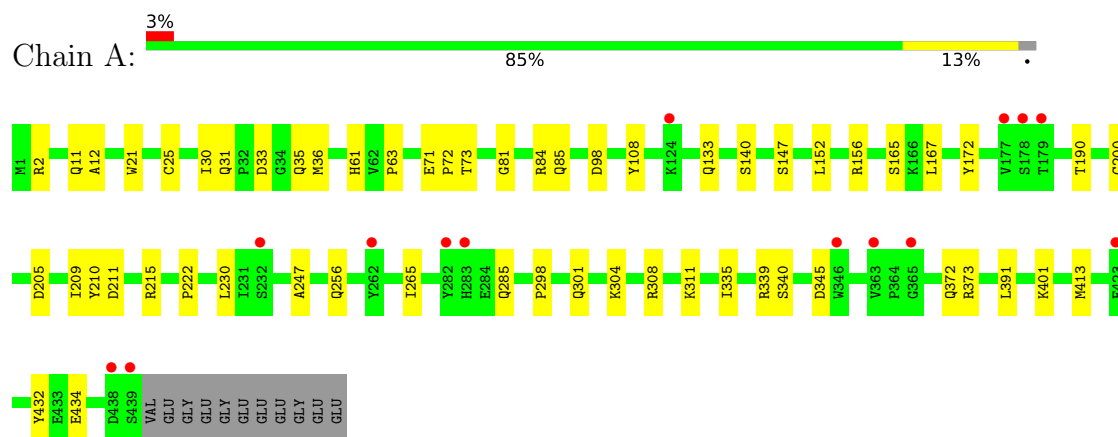
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	138	Total	O	0	0
			138	138		
12	B	119	Total	O	0	0
			119	119		
12	C	212	Total	O	0	0
			212	212		
12	D	41	Total	O	0	0
			41	41		
12	E	18	Total	O	0	0
			18	18		
12	F	42	Total	O	0	0
			42	42		

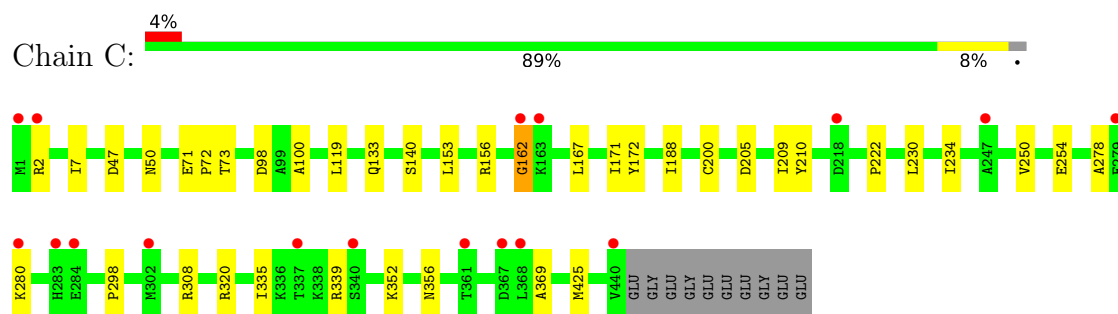
3 Residue-property plots

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.

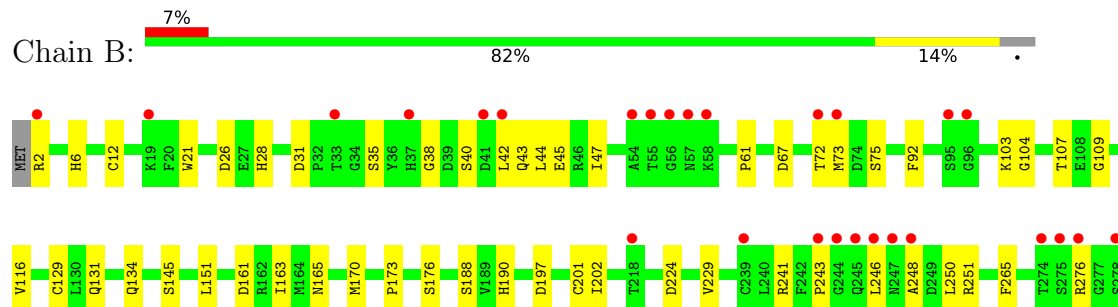
- Molecule 1: Tubulin alpha-1B chain



- Molecule 1: Tubulin alpha-1B chain

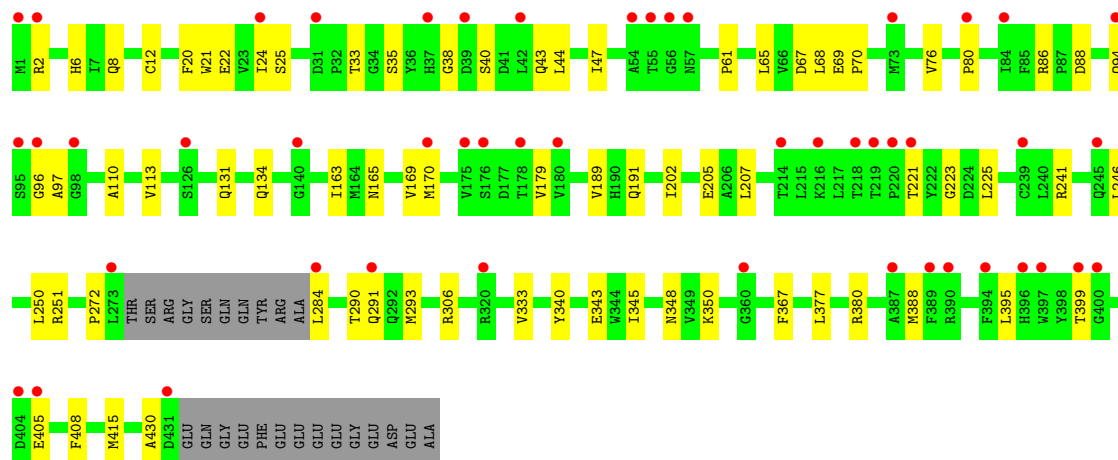
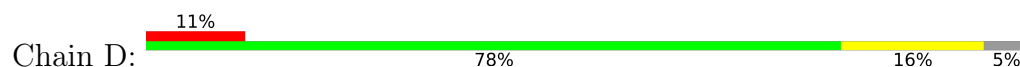


- Molecule 2: Tubulin beta-2B chain

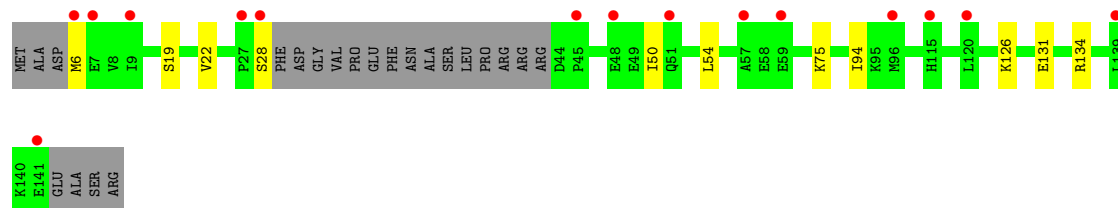




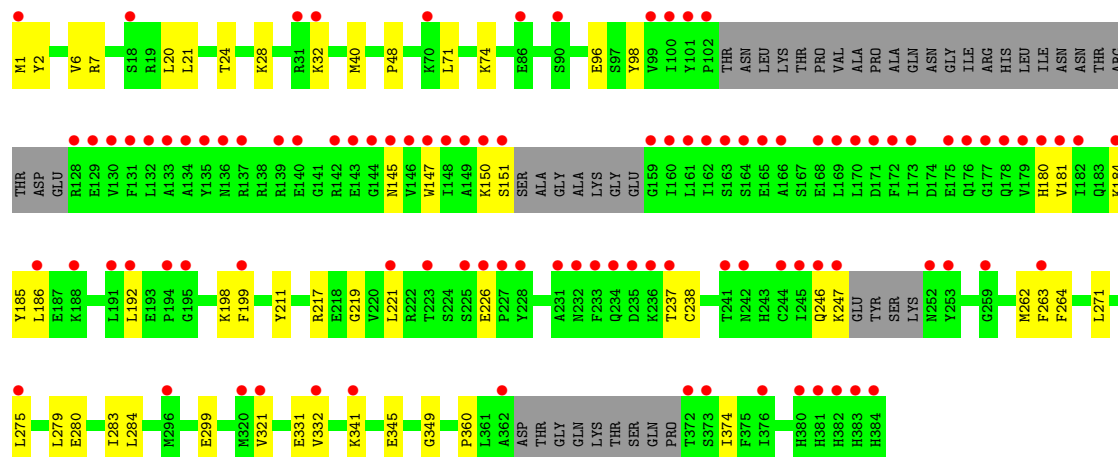
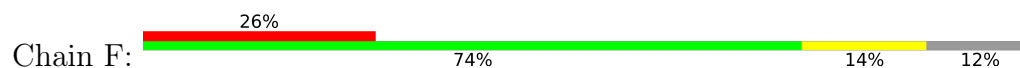
• Molecule 2: Tubulin beta-2B chain



• 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	105.42Å 157.98Å 182.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.25 – 2.40 48.25 – 2.40	Depositor EDS
% Data completeness (in resolution range)	98.1 (48.25-2.40) 98.2 (48.25-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.15 (at 2.39Å)	Xtriage
Refinement program	PHENIX 1.13_2998: ???	Depositor
R, R_{free}	0.192 , 0.227 (Not available) , 0.214	Depositor DCC
R_{free} test set	5845 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	35.6	Xtriage
Anisotropy	0.069	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 50.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	17861	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.40% 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: DJ9, MES, ACP, GTP, CA, GDP, MG

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	0.14	0/3489	0.39	1/4739 (0.0%)
1	C	0.17	0/3508	0.40	2/4764 (0.0%)
2	B	0.12	0/3417	0.31	0/4629
2	D	0.18	0/3336	0.37	0/4527
3	E	0.09	0/992	0.23	0/1319
4	F	0.15	0/2707	0.33	0/3671
All	All	0.15	0/17449	0.36	3/23649 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	280	LYS	CB-CG-CD	-8.87	90.91	111.30
1	C	280	LYS	CG-CD-CE	5.80	124.64	111.30
1	A	434	GLU	CA-CB-CG	5.69	125.47	114.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3412	0	3309	39	0
1	C	3430	0	3335	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	3343	0	3212	39	0
2	D	3264	0	3099	48	0
3	E	984	0	988	10	0
4	F	2643	0	2490	37	0
5	A	32	0	12	2	0
5	C	32	0	12	1	0
5	D	32	0	12	1	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	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	B	28	0	12	1	0
9	B	24	0	24	2	0
10	B	30	0	0	1	0
11	F	31	0	13	1	0
12	A	138	0	0	3	0
12	B	119	0	0	1	0
12	C	212	0	0	0	0
12	D	41	0	0	0	0
12	E	18	0	0	1	0
12	F	42	0	0	0	0
All	All	17861	0	16518	191	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 6.

All (191) 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:199:PHE:HB2	4:F:221:LEU:HD21	1.41	0.98
4:F:199:PHE:HB2	4:F:221:LEU:CD2	2.07	0.84
4:F:199:PHE:CB	4:F:221:LEU:HD21	2.20	0.72
1:A:372:GLN:HE21	1:A:373:ARG:HH12	1.38	0.70
4:F:271:LEU:HD23	4:F:275:LEU:HD12	1.79	0.64
2:B:173:PRO:HA	2:B:176:SER:HB2	1.82	0.61
1:C:71:GLU:HB2	1:C:98:ASP:HB3	1.81	0.61
1:C:278:ALA:HA	1:C:369:ALA:HB2	1.83	0.61
2:D:221:THR:HG22	2:D:223:GLY:H	1.65	0.61
1:C:209:ILE:HG23	1:C:230:LEU:HD23	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:GLU:OE1	1:A:73:THR:N	2.32	0.60
2:B:38:GLY:HA3	2:B:43:GLN:HE22	1.65	0.60
2:B:26:ASP:CG	2:B:359:ARG:HE	2.08	0.60
2:B:170:MET:HG2	2:B:377:LEU:HD21	1.85	0.58
1:C:71:GLU:OE2	1:C:73:THR:OG1	2.17	0.58
2:D:20:PHE:O	2:D:24:ILE:HG13	2.02	0.58
4:F:226:GLU:HB2	4:F:238:CYS:HB3	1.86	0.58
1:C:47:ASP:H	1:C:50:ASN:HD22	1.52	0.57
2:D:70:PRO:HG3	2:D:94:GLN:HA	1.86	0.57
2:D:65:LEU:HD22	2:D:76:VAL:HG11	1.86	0.57
2:B:246:LEU:HD22	2:B:350:LYS:HE2	1.86	0.56
4:F:199:PHE:CD2	4:F:221:LEU:HD21	2.41	0.56
2:B:161:ASP:O	2:B:251:ARG:NH2	2.39	0.56
2:D:21:TRP:CE3	2:D:24:ILE:HD11	2.41	0.56
2:D:246:LEU:HD21	2:D:350:LYS:HB3	1.88	0.56
3:E:75:LYS:NZ	12:E:201:HOH:O	2.25	0.56
2:B:163:ILE:HG21	2:B:250:LEU:HB3	1.87	0.55
1:A:211:ASP:OD1	1:A:304:LYS:NZ	2.30	0.55
4:F:263:PHE:CE1	4:F:341:LYS:HD3	2.42	0.54
1:A:335:ILE:HG23	1:A:339:ARG:HG3	1.89	0.54
2:D:38:GLY:HA3	2:D:43:GLN:HE22	1.72	0.54
4:F:280:GLU:HA	4:F:284:LEU:HB2	1.90	0.54
2:B:42:LEU:HD13	2:B:243:PRO:HG2	1.89	0.53
2:D:97:ALA:HB3	5:D:501:GTP:O3G	2.09	0.53
1:A:71:GLU:HG2	1:A:72:PRO:HD2	1.90	0.52
1:A:308:ARG:HG2	1:A:340:SER:HB2	1.90	0.52
1:C:250:VAL:HG11	1:C:352:LYS:HE3	1.89	0.52
2:B:282:ARG:NH2	2:B:288:GLU:OE2	2.37	0.52
4:F:40:MET:HE1	4:F:48:PRO:HD2	1.90	0.52
2:B:44:LEU:HA	2:B:47:ILE:HB	1.92	0.52
2:D:395:LEU:CD1	2:D:399:THR:HG23	2.40	0.52
2:D:170:MET:HE2	2:D:377:LEU:HD21	1.91	0.51
1:A:209:ILE:HG23	1:A:230:LEU:HD23	1.92	0.51
4:F:32:LYS:N	4:F:32:LYS:HD3	2.26	0.51
2:D:272:PRO:HB3	2:D:284:LEU:HD22	1.92	0.51
2:D:205:GLU:HB3	2:D:380:ARG:HH12	1.75	0.51
4:F:145:ASN:CG	4:F:147:TRP:HE1	2.19	0.51
4:F:221:LEU:HD13	4:F:262:MET:HE3	1.93	0.51
1:A:71:GLU:HB2	1:A:98:ASP:HB3	1.92	0.51
1:A:311:LYS:NZ	12:A:607:HOH:O	2.43	0.51
4:F:7:ARG:HD3	4:F:40:MET:HE3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:6:HIS:HE2	2:D:8:GLN:HE21	1.56	0.51
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.30	0.50
3:E:6:MET:HE3	3:E:22:VAL:HG21	1.91	0.50
4:F:71:LEU:HG	4:F:332:VAL:HG11	1.94	0.50
2:B:134:GLN:HA	2:B:165:ASN:O	2.11	0.50
4:F:96:GLU:OE1	4:F:98:TYR:OH	2.28	0.49
2:B:26:ASP:OD1	2:B:359:ARG:NE	2.44	0.49
1:A:33:ASP:HA	1:A:85:GLN:HG3	1.94	0.49
2:D:6:HIS:HE2	2:D:8:GLN:HG3	1.77	0.49
4:F:184:LYS:O	11:F:402:ACP:N6	2.45	0.49
2:B:116:VAL:HG11	2:B:151:LEU:HD11	1.94	0.49
2:B:224:ASP:OD2	2:B:276:ARG:NH2	2.42	0.49
1:C:71:GLU:HG2	1:C:72:PRO:HD2	1.94	0.49
2:D:6:HIS:CD2	2:D:21:TRP:HE1	2.31	0.49
2:D:163:ILE:HG21	2:D:250:LEU:HB3	1.94	0.49
2:B:145:SER:OG	2:B:188:SER:OG	2.29	0.48
1:C:320:ARG:HA	1:C:356:ASN:O	2.13	0.48
4:F:1:MET:HE3	4:F:28:LYS:HB2	1.95	0.48
4:F:199:PHE:CG	4:F:221:LEU:HD21	2.48	0.48
2:B:21:TRP:CZ3	2:B:61:PRO:HB3	2.48	0.48
4:F:2:TYR:OH	4:F:360:PRO:O	2.28	0.48
4:F:21:LEU:O	4:F:24:THR:OG1	2.27	0.48
1:C:162:GLY:HA2	3:E:94:ILE:HD11	1.96	0.48
4:F:6:VAL:O	4:F:32:LYS:HG3	2.14	0.47
4:F:192:LEU:HD22	4:F:262:MET:HE1	1.97	0.47
2:D:343:GLU:HG3	2:D:430:ALA:HB2	1.97	0.47
1:A:172:TYR:HB3	1:A:205:ASP:HA	1.96	0.47
1:C:335:ILE:HG23	1:C:339:ARG:HG3	1.97	0.47
2:D:24:ILE:HG22	2:D:241:ARG:CZ	2.44	0.47
2:B:12:CYS:HB2	8:B:501:GDP:C8	2.49	0.47
1:C:167:LEU:HG	1:C:200:CYS:HB3	1.97	0.47
1:C:188:ILE:HD12	1:C:425:MET:HG3	1.96	0.47
2:D:191:GLN:HE22	3:E:126:LYS:NZ	2.14	0.47
1:A:210:TYR:CZ	1:A:222:PRO:HD2	2.50	0.46
3:E:131:GLU:HG2	3:E:134:ARG:HH21	1.79	0.46
1:A:165:SER:OG	1:A:256:GLN:NE2	2.48	0.46
2:D:33:THR:HG23	2:D:35:SER:H	1.80	0.46
2:D:21:TRP:CZ3	2:D:61:PRO:HB3	2.50	0.46
1:C:47:ASP:N	1:C:50:ASN:HD22	2.12	0.46
2:D:134:GLN:HA	2:D:165:ASN:O	2.15	0.46
2:B:72:THR:O	2:B:75:SER:OG	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:40:SER:H	2:D:43:GLN:NE2	2.13	0.46
1:A:98:ASP:HB2	5:A:501:GTP:O3G	2.16	0.46
2:D:44:LEU:HA	2:D:47:ILE:HB	1.98	0.46
1:A:31:GLN:HG2	1:A:35:GLN:O	2.16	0.46
1:A:31:GLN:NE2	1:A:35:GLN:HB2	2.30	0.46
2:B:246:LEU:HG	2:B:248:ALA:HB2	1.98	0.46
2:B:317:PHE:HB2	2:B:353:VAL:HG22	1.98	0.46
4:F:279:LEU:HD12	4:F:283:ILE:HB	1.97	0.46
1:C:210:TYR:CZ	1:C:222:PRO:HD2	2.51	0.46
1:A:285:GLN:NE2	12:A:611:HOH:O	2.47	0.45
2:B:202:ILE:HD13	2:B:229:VAL:HG13	1.98	0.45
1:A:152:LEU:HD11	3:E:54:LEU:HD11	1.98	0.45
1:A:247:ALA:HB3	3:E:19:SER:OG	2.16	0.45
1:A:108:TYR:CE2	1:A:413:MET:HG3	2.51	0.45
2:B:201:CYS:SG	2:B:265:PHE:HB3	2.57	0.45
1:C:2:ARG:HB3	1:C:133:GLN:HB2	1.99	0.45
2:D:24:ILE:HD12	2:D:25:SER:N	2.31	0.45
1:A:12:ALA:HB3	1:A:140:SER:HB3	1.99	0.45
1:A:167:LEU:HG	1:A:200:CYS:HB3	1.99	0.45
4:F:217:ARG:NH2	4:F:345:GLU:OE1	2.50	0.45
2:B:2:ARG:HA	2:B:129:CYS:O	2.17	0.45
4:F:185:TYR:OH	4:F:198:LYS:NZ	2.44	0.45
4:F:247:LYS:HD3	4:F:247:LYS:H	1.82	0.45
2:B:190:HIS:HD2	2:B:411:ALA:HA	1.81	0.44
1:C:119:LEU:HD11	1:C:156:ARG:HB3	1.99	0.44
1:A:210:TYR:CE1	1:A:222:PRO:HD2	2.51	0.44
2:B:73:MET:SD	2:B:92:PHE:HB3	2.58	0.44
2:D:2:ARG:CZ	2:D:131:GLN:HB3	2.47	0.44
2:D:388:MET:HE2	2:D:388:MET:HB3	1.73	0.44
2:B:40:SER:OG	2:B:42:LEU:HB2	2.18	0.44
4:F:151:SER:HA	4:F:180:HIS:CD2	2.53	0.44
2:B:380:ARG:NH1	12:B:612:HOH:O	2.44	0.44
1:A:298:PRO:HA	1:A:301:GLN:CD	2.42	0.44
3:E:50:ILE:O	3:E:54:LEU:HG	2.18	0.44
4:F:211:TYR:CD2	4:F:299:GLU:HG3	2.53	0.44
2:D:69:GLU:HG2	2:D:96:GLY:HA2	1.99	0.44
2:D:86:ARG:HE	2:D:88:ASP:HB2	1.82	0.43
1:A:372:GLN:HE21	1:A:373:ARG:NH1	2.13	0.43
2:B:2:ARG:CZ	2:B:131:GLN:HB3	2.49	0.43
1:A:85:GLN:H	1:A:85:GLN:HG2	1.66	0.43
2:D:179:VAL:CG1	2:D:388:MET:HE1	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:211:TYR:CE2	4:F:299:GLU:HG3	2.53	0.43
1:A:11:GLN:HB3	5:A:501:GTP:O2A	2.18	0.43
2:B:31:ASP:OD2	2:B:35:SER:N	2.45	0.43
9:B:504:MES:H51	9:B:504:MES:H81	1.56	0.43
1:C:230:LEU:O	1:C:234:ILE:HD12	2.18	0.43
2:D:170:MET:HG3	2:D:377:LEU:HD11	2.00	0.43
2:D:293:MET:CG	2:D:367:PHE:HB2	2.48	0.43
2:D:6:HIS:NE2	2:D:8:GLN:HG3	2.34	0.43
2:B:197:ASP:OD2	9:B:503:MES:H31	2.19	0.42
1:C:254:GLU:HG2	1:C:352:LYS:HE2	2.01	0.42
1:A:81:GLY:O	1:A:84:ARG:HG2	2.19	0.42
1:A:265:ILE:HG23	1:A:432:TYR:CZ	2.54	0.42
2:B:350:LYS:HB2	10:B:505:DJ9:C17	2.50	0.42
2:B:28:HIS:NE2	2:B:241:ARG:HB3	2.34	0.42
2:B:45:GLU:HB3	2:B:243:PRO:HG3	2.02	0.42
1:C:140:SER:HA	1:C:171:ILE:HB	2.01	0.42
2:D:110:ALA:O	2:D:113:VAL:HG12	2.20	0.42
2:B:67:ASP:O	2:B:92:PHE:HA	2.20	0.42
2:D:345:ILE:HG22	2:D:348:ASN:HB3	2.02	0.42
1:A:2:ARG:O	1:A:133:GLN:NE2	2.50	0.42
1:A:156:ARG:HA	1:A:156:ARG:HD2	1.89	0.42
2:D:12:CYS:SG	2:D:169:VAL:HG21	2.59	0.42
4:F:20:LEU:O	4:F:24:THR:HG23	2.20	0.42
4:F:150:LYS:CB	4:F:181:VAL:H	2.33	0.42
2:D:293:MET:HG3	2:D:367:PHE:HB2	2.01	0.41
2:D:306:ARG:HG2	2:D:340:TYR:CZ	2.55	0.41
4:F:237:THR:O	4:F:246:GLN:NE2	2.53	0.41
2:B:276:ARG:HE	2:B:276:ARG:HB3	1.57	0.41
2:D:405:GLU:O	2:D:408:PHE:HB2	2.20	0.41
3:E:131:GLU:HG2	3:E:134:ARG:NH2	2.34	0.41
4:F:74:LYS:NZ	4:F:331:GLU:OE2	2.45	0.41
2:D:207:LEU:HB3	2:D:225:LEU:HD22	2.02	0.41
2:D:290:THR:HG22	2:D:333:VAL:HG21	2.02	0.41
1:A:36:MET:HB3	1:A:61:HIS:CE1	2.56	0.41
2:D:291:GLN:O	2:D:291:GLN:HG2	2.20	0.41
1:A:25:CYS:HB3	1:A:30:ILE:O	2.21	0.41
1:A:215:ARG:NH2	12:A:619:HOH:O	2.53	0.41
1:A:401:LYS:HE3	2:B:428:ALA:HB1	2.02	0.41
2:D:67:ASP:OD2	2:D:68:LEU:N	2.54	0.41
2:D:169:VAL:HA	2:D:202:ILE:O	2.21	0.41
1:C:98:ASP:HB2	5:C:501:GTP:O2G	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:172:TYR:HB3	1:C:205:ASP:HA	2.03	0.41
2:D:189:VAL:HG11	2:D:415:MET:HE3	2.03	0.41
4:F:184:LYS:HD2	4:F:185:TYR:N	2.36	0.41
4:F:219:GLY:HA3	4:F:264:PHE:CZ	2.55	0.41
1:A:147:SER:HB2	1:A:190:THR:HB	2.03	0.41
1:A:345:ASP:HB3	3:E:28:SER:HB2	2.02	0.40
1:C:7:ILE:HG21	1:C:153:LEU:HD21	2.03	0.40
2:D:395:LEU:HD13	2:D:399:THR:HG23	2.04	0.40
2:B:103:LYS:HA	2:B:107:THR:OG1	2.22	0.40
1:C:298:PRO:HG2	1:C:308:ARG:NH2	2.36	0.40
2:D:22:GLU:OE1	2:D:80:PRO:HG2	2.21	0.40
1:A:21:TRP:CZ3	1:A:63:PRO:HB3	2.56	0.40
4:F:349:GLY:HA3	4:F:374:ILE:HD11	2.03	0.40
1:A:172:TYR:CE2	1:A:391:LEU:HD22	2.56	0.40
2:B:104:GLY:O	2:B:109:GLY:HA3	2.21	0.40
1:C:100:ALA:HB1	2:D:251:ARG:HG2	2.03	0.40
4:F:199:PHE:CZ	4:F:321:VAL:HG22	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	437/450 (97%)	429 (98%)	8 (2%)	0	100	100
1	C	438/450 (97%)	431 (98%)	6 (1%)	1 (0%)	43	58
2	B	425/445 (96%)	418 (98%)	7 (2%)	0	100	100
2	D	417/445 (94%)	411 (99%)	6 (1%)	0	100	100
3	E	117/143 (82%)	116 (99%)	1 (1%)	0	100	100
4	F	329/384 (86%)	314 (95%)	14 (4%)	1 (0%)	36	50
All	All	2163/2317 (93%)	2119 (98%)	42 (2%)	2 (0%)	48	64

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	162	GLY
4	F	186	LEU

5.3.2 Protein sidechains [i](#)

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	240/378 (64%)	240 (100%)	0	100	100
1	C	369/378 (98%)	369 (100%)	0	100	100
2	B	79/383 (21%)	79 (100%)	0	100	100
2	D	352/383 (92%)	352 (100%)	0	100	100
3	E	105/127 (83%)	105 (100%)	0	100	100
4	F	269/342 (79%)	269 (100%)	0	100	100
All	All	1414/1991 (71%)	1414 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	101	ASN
1	A	256	GLN
2	B	52	ASN
2	B	426	GLN
1	C	50	ASN
2	D	14	ASN
2	D	37	HIS
2	D	43	GLN
2	D	99	ASN
2	D	100	ASN
2	D	134	GLN
2	D	335	ASN
2	D	337	ASN

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Mol	Chain	Res	Type
2	D	424	GLN
3	E	90	ASN
3	E	92	ASN
3	E	136	ASN
4	F	180	HIS
4	F	260	ASN
4	F	269	GLN
4	F	310	GLN
4	F	340	GLN
4	F	382	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 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	DJ9	B	505	-	34,34,34	2.12	8 (23%)	48,49,49	2.07	12 (25%)
8	GDP	B	501	6	29,30,30	1.16	2 (6%)	45,47,47	1.74	7 (15%)
5	GTP	C	501	6	33,34,34	3.52	19 (57%)	50,54,54	1.61	9 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	MES	B	503	-	12,12,12	2.30	1 (8%)	15,16,16	2.18	6 (40%)
5	GTP	D	501	-	33,34,34	3.55	20 (60%)	50,54,54	1.61	10 (20%)
9	MES	B	504	-	12,12,12	2.32	1 (8%)	15,16,16	1.94	5 (33%)
5	GTP	A	501	6	33,34,34	3.60	20 (60%)	50,54,54	1.64	10 (20%)
11	ACP	F	402	6	31,33,33	3.20	11 (35%)	47,52,52	2.07	13 (27%)

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	DJ9	B	505	-	-	0/14/14/14	0/5/5/5
8	GDP	B	501	6	-	3/16/32/32	0/3/3/3
5	GTP	C	501	6	-	5/22/38/38	0/3/3/3
9	MES	B	503	-	-	2/6/14/14	0/1/1/1
5	GTP	D	501	-	-	6/22/38/38	0/3/3/3
9	MES	B	504	-	-	3/6/14/14	0/1/1/1
5	GTP	A	501	6	-	3/22/38/38	0/3/3/3
11	ACP	F	402	6	-	8/19/38/38	0/3/3/3

All (82) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	501	GTP	C2'-C3'	-10.80	1.24	1.53
5	C	501	GTP	C2'-C3'	-10.69	1.24	1.53
5	A	501	GTP	C2'-C3'	-10.55	1.24	1.53
11	F	402	ACP	O4'-C1'	8.83	1.62	1.42
10	B	505	DJ9	C6-C7	-8.51	1.39	1.49
9	B	504	MES	C8-S	-7.76	1.66	1.77
9	B	503	MES	C8-S	-7.66	1.66	1.77
11	F	402	ACP	C2'-C1'	-7.15	1.31	1.53
5	D	501	GTP	C4-N3	6.70	1.49	1.34
5	A	501	GTP	C4-N3	6.63	1.49	1.34
5	C	501	GTP	C4-N3	6.56	1.49	1.34
11	F	402	ACP	O4'-C4'	-6.32	1.30	1.45
11	F	402	ACP	PB-O3A	6.27	1.65	1.58
5	D	501	GTP	C2-N3	5.59	1.46	1.33
11	F	402	ACP	PA-O3A	5.56	1.65	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	501	GTP	C2-N3	5.52	1.46	1.33
5	C	501	GTP	C2-N3	5.52	1.46	1.33
5	A	501	GTP	PB-O3A	5.22	1.65	1.59
5	C	501	GTP	PB-O3B	5.01	1.64	1.59
5	A	501	GTP	PA-O3A	4.98	1.64	1.59
5	D	501	GTP	C2-N2	4.91	1.45	1.34
5	A	501	GTP	O4'-C1'	-4.89	1.30	1.42
5	A	501	GTP	PB-O3B	4.86	1.64	1.59
5	A	501	GTP	C2-N2	4.81	1.45	1.34
5	C	501	GTP	C2-N2	4.78	1.45	1.34
5	D	501	GTP	O4'-C1'	-4.65	1.31	1.42
10	B	505	DJ9	C12-C11	-4.62	1.38	1.47
5	C	501	GTP	O4'-C1'	-4.57	1.31	1.42
5	D	501	GTP	PB-O3B	4.52	1.64	1.59
5	D	501	GTP	PA-O3A	4.47	1.64	1.59
11	F	402	ACP	C6-N6	4.45	1.45	1.34
5	D	501	GTP	PB-O3A	4.37	1.64	1.59
5	C	501	GTP	PA-O3A	4.35	1.64	1.59
5	C	501	GTP	C2'-C1'	4.29	1.67	1.53
5	C	501	GTP	C5'-C4'	-4.28	1.38	1.51
5	D	501	GTP	C2'-C1'	4.26	1.66	1.53
5	D	501	GTP	C5'-C4'	-4.20	1.38	1.51
5	A	501	GTP	C2'-C1'	4.18	1.66	1.53
5	C	501	GTP	PB-O3A	4.11	1.63	1.59
5	A	501	GTP	C5'-C4'	-3.99	1.39	1.51
5	A	501	GTP	C3'-C4'	3.34	1.61	1.53
5	D	501	GTP	C3'-C4'	3.14	1.61	1.53
5	A	501	GTP	O3'-C3'	3.11	1.50	1.43
8	B	501	GDP	C5-C4	3.06	1.47	1.38
5	C	501	GTP	O3'-C3'	3.03	1.50	1.43
5	D	501	GTP	O3'-C3'	3.01	1.50	1.43
5	C	501	GTP	C3'-C4'	2.98	1.60	1.53
11	F	402	ACP	C5-C4	-2.87	1.34	1.39
10	B	505	DJ9	C15-N3	-2.83	1.32	1.38
11	F	402	ACP	O3'-C3'	-2.79	1.36	1.43
5	A	501	GTP	C2-N1	2.79	1.44	1.37
5	C	501	GTP	C2-N1	2.78	1.44	1.37
5	D	501	GTP	C2-N1	2.78	1.44	1.37
5	D	501	GTP	C5-N7	-2.76	1.33	1.39
5	C	501	GTP	O4'-C4'	2.76	1.51	1.45
5	A	501	GTP	C5-N7	-2.76	1.33	1.39
5	D	501	GTP	O4'-C4'	2.71	1.51	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	F	402	ACP	O2'-C2'	2.71	1.49	1.43
5	C	501	GTP	C5-N7	-2.68	1.33	1.39
10	B	505	DJ9	C10-C20	-2.61	1.37	1.40
5	A	501	GTP	O6-C6	-2.58	1.18	1.23
5	A	501	GTP	O4'-C4'	2.58	1.50	1.45
5	C	501	GTP	O6-C6	-2.56	1.18	1.23
5	D	501	GTP	C5-C6	2.52	1.53	1.44
5	C	501	GTP	C6-N1	2.52	1.43	1.38
11	F	402	ACP	C5-N7	-2.52	1.34	1.39
5	A	501	GTP	C6-N1	2.51	1.43	1.38
5	C	501	GTP	C5-C6	2.51	1.53	1.44
5	D	501	GTP	O6-C6	-2.51	1.18	1.23
5	D	501	GTP	C6-N1	2.48	1.43	1.38
5	A	501	GTP	C5-C6	2.46	1.53	1.44
10	B	505	DJ9	C7-C20	2.37	1.42	1.40
8	B	501	GDP	C6-N1	-2.37	1.34	1.38
10	B	505	DJ9	O2-C3	2.19	1.40	1.37
10	B	505	DJ9	C17-C14	-2.17	1.37	1.41
5	A	501	GTP	C1'-N9	-2.14	1.41	1.47
11	F	402	ACP	C8-N9	-2.12	1.33	1.37
10	B	505	DJ9	O3-C22	2.11	1.40	1.37
5	A	501	GTP	O2'-C2'	2.09	1.48	1.43
5	D	501	GTP	O2'-C2'	2.06	1.48	1.43
5	C	501	GTP	O2'-C2'	2.03	1.48	1.43
5	D	501	GTP	C1'-N9	-2.01	1.41	1.47

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	505	DJ9	C6-C7-C20	-6.34	118.88	124.72
8	B	501	GDP	C5-C4-N3	-5.78	119.20	128.39
11	F	402	ACP	N3-C2-N1	-5.77	119.85	128.58
11	F	402	ACP	N6-C6-N1	-5.24	106.70	118.38
9	B	503	MES	C5-N4-C3	5.14	119.91	108.84
5	D	501	GTP	C5-C4-N3	-5.13	120.23	128.39
5	C	501	GTP	C5-C4-N3	-5.09	120.28	128.39
11	F	402	ACP	C5-C4-N3	-4.97	119.87	126.72
8	B	501	GDP	C2-N3-C4	4.97	120.86	112.30
5	A	501	GTP	C5-C4-N3	-4.94	120.53	128.39
10	B	505	DJ9	C20-C7-N1	4.90	120.74	118.02
5	C	501	GTP	C2-N3-C4	4.54	120.11	112.30
5	D	501	GTP	C2-N3-C4	4.50	120.06	112.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	501	GTP	C2-N3-C4	4.35	119.79	112.30
10	B	505	DJ9	C10-C20-N4	-4.25	106.63	110.31
8	B	501	GDP	N9-C4-N3	4.17	134.29	125.95
11	F	402	ACP	N9-C8-N7	-4.16	108.03	113.94
9	B	504	MES	C5-N4-C3	4.11	117.69	108.84
11	F	402	ACP	C5-C6-N6	4.09	133.41	123.29
10	B	505	DJ9	C9-C10-C20	-3.89	118.91	122.57
10	B	505	DJ9	C20-C10-N2	3.72	107.25	105.13
8	B	501	GDP	C6-C5-N7	3.57	136.78	130.29
11	F	402	ACP	C2-N3-C4	3.42	120.17	111.83
10	B	505	DJ9	C6-C7-N1	3.35	120.36	115.40
9	B	504	MES	C6-C5-N4	-3.28	105.13	110.12
5	A	501	GTP	N9-C8-N7	-3.14	107.58	113.40
5	D	501	GTP	N9-C8-N7	-3.09	107.68	113.40
10	B	505	DJ9	O3-C22-C2	3.06	120.38	115.14
5	D	501	GTP	N9-C4-N3	3.02	131.99	125.95
5	C	501	GTP	N9-C8-N7	-3.02	107.81	113.40
5	D	501	GTP	C2-N1-C6	-2.99	119.69	125.11
11	F	402	ACP	N3-C4-N9	2.98	132.23	127.17
5	C	501	GTP	C2-N1-C6	-2.97	119.73	125.11
5	A	501	GTP	C2-N1-C6	-2.96	119.74	125.11
11	F	402	ACP	C5-N7-C8	2.91	108.03	103.45
5	C	501	GTP	N9-C4-N3	2.89	131.73	125.95
11	F	402	ACP	C3'-C2'-C1'	2.88	106.92	101.46
5	A	501	GTP	N9-C4-N3	2.87	131.70	125.95
9	B	503	MES	C7-N4-C5	2.79	118.68	111.24
10	B	505	DJ9	O2-C3-C2	2.77	119.88	115.14
5	D	501	GTP	C5-C6-N1	2.64	119.98	113.25
8	B	501	GDP	C4-C5-N7	-2.64	106.49	110.67
5	A	501	GTP	C5-C6-N1	2.60	119.86	113.25
5	C	501	GTP	C5-C6-N1	2.59	119.86	113.25
9	B	503	MES	C7-N4-C3	2.58	118.12	111.24
10	B	505	DJ9	C13-C14-C17	-2.55	120.07	122.59
5	D	501	GTP	O6-C6-C5	-2.45	120.05	126.53
5	A	501	GTP	O6-C6-C5	-2.45	120.06	126.53
9	B	503	MES	C2-C3-N4	-2.44	106.41	110.12
5	C	501	GTP	O6-C6-C5	-2.38	120.24	126.53
11	F	402	ACP	PB-O3A-PA	-2.35	124.71	132.37
10	B	505	DJ9	O3-C22-C21	-2.31	120.09	124.08
5	A	501	GTP	C3'-C2'-C1'	2.29	105.79	101.46
11	F	402	ACP	C4-C5-N7	-2.27	107.98	110.58
5	D	501	GTP	C8-N7-C5	2.24	108.25	104.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	F	402	ACP	C4-N9-C8	2.21	108.06	105.74
5	A	501	GTP	C1'-N9-C4	-2.20	119.98	126.49
5	A	501	GTP	C8-N7-C5	2.20	108.18	104.26
5	C	501	GTP	C8-N7-C5	2.13	108.06	104.26
9	B	503	MES	C6-C5-N4	-2.13	106.88	110.12
5	C	501	GTP	C1'-N9-C4	-2.13	120.19	126.49
9	B	504	MES	C7-N4-C5	2.12	116.88	111.24
8	B	501	GDP	O2A-PA-O3A	2.07	112.88	107.27
9	B	504	MES	C7-N4-C3	2.07	116.74	111.24
10	B	505	DJ9	C20-N4-C11	2.05	108.45	105.09
10	B	505	DJ9	C23-O3-C22	-2.05	114.50	117.51
5	D	501	GTP	C1'-N9-C4	-2.04	120.45	126.49
8	B	501	GDP	O6-C6-C5	-2.03	121.17	126.53
9	B	503	MES	O1S-S-C8	2.01	109.77	106.73
5	D	501	GTP	C3'-C2'-C1'	2.01	105.26	101.46
11	F	402	ACP	C6-C5-C4	2.01	119.92	117.18
9	B	504	MES	O3S-S-C8	2.00	109.93	106.00

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	501	GTP	PB-O3B-PG-O2G
5	C	501	GTP	PB-O3B-PG-O3G
5	C	501	GTP	C5'-O5'-PA-O3A
5	C	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O2A
5	D	501	GTP	PB-O3B-PG-O2G
5	D	501	GTP	C5'-O5'-PA-O3A
5	D	501	GTP	C5'-O5'-PA-O1A
5	D	501	GTP	C5'-O5'-PA-O2A
8	B	501	GDP	C5'-O5'-PA-O3A
8	B	501	GDP	C5'-O5'-PA-O1A
8	B	501	GDP	C5'-O5'-PA-O2A
9	B	503	MES	N4-C7-C8-S
9	B	504	MES	C7-C8-S-O1S
11	F	402	ACP	PB-C3B-PG-O1G
11	F	402	ACP	PB-C3B-PG-O2G
11	F	402	ACP	PB-C3B-PG-O3G
11	F	402	ACP	C5'-O5'-PA-O1A
11	F	402	ACP	C5'-O5'-PA-O2A
9	B	504	MES	C7-C8-S-O3S

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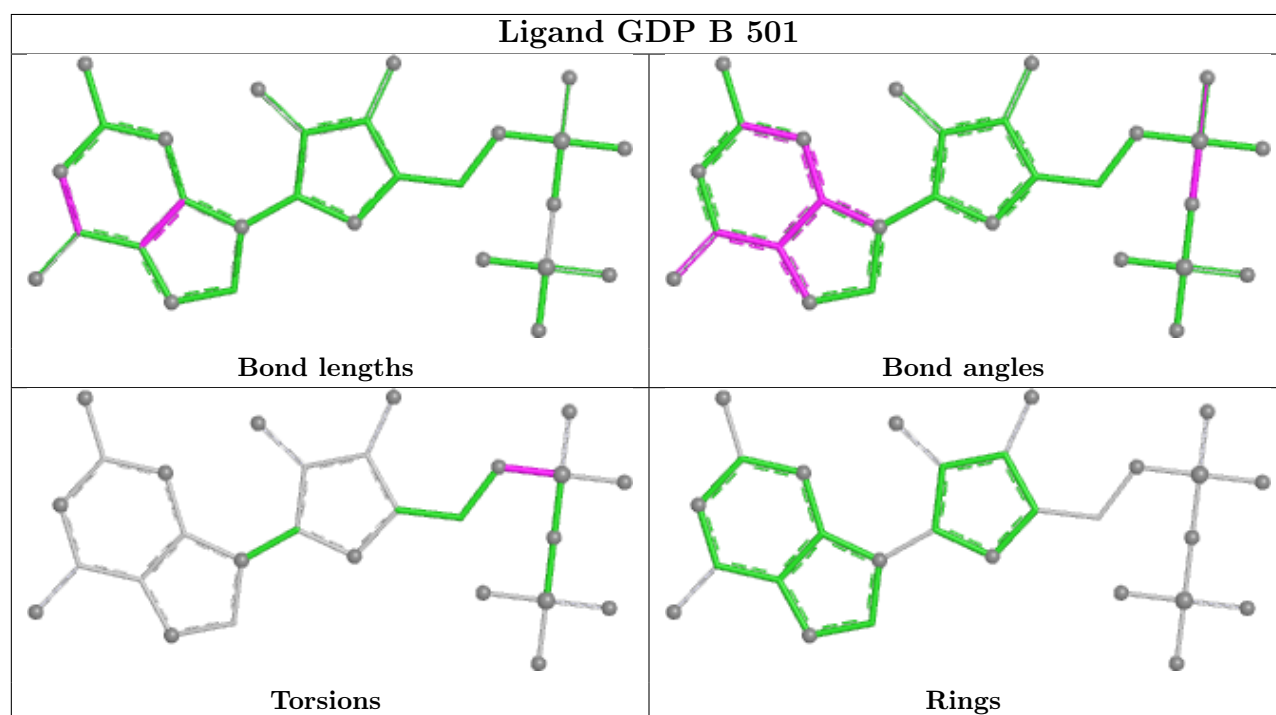
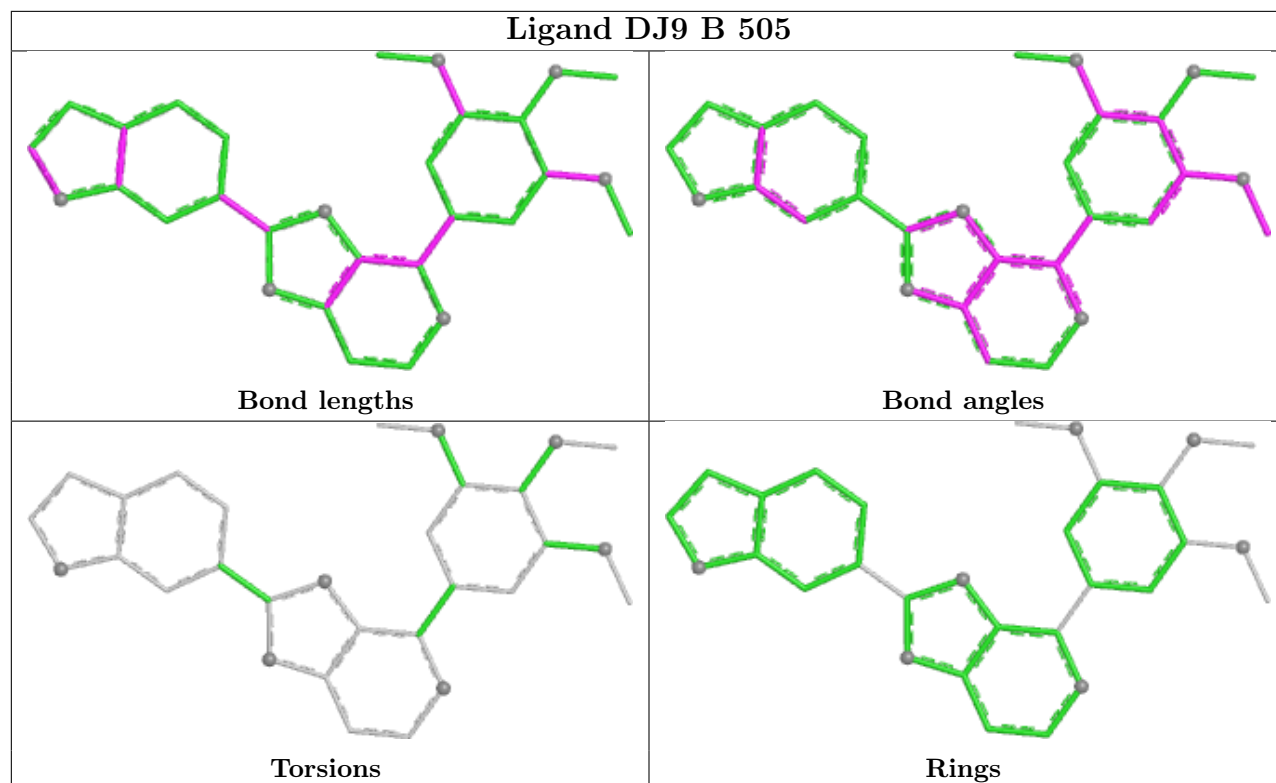
Mol	Chain	Res	Type	Atoms
9	B	503	MES	C8-C7-N4-C5
9	B	504	MES	C7-C8-S-O2S
11	F	402	ACP	C5'-O5'-PA-O3A
5	A	501	GTP	C4'-C5'-O5'-PA
11	F	402	ACP	PB-O3A-PA-O1A
5	A	501	GTP	PB-O3B-PG-O3G
5	C	501	GTP	PB-O3B-PG-O2G
5	D	501	GTP	PB-O3B-PG-O3G
11	F	402	ACP	PB-O3A-PA-O2A
5	D	501	GTP	PB-O3B-PG-O1G

There are no ring outliers.

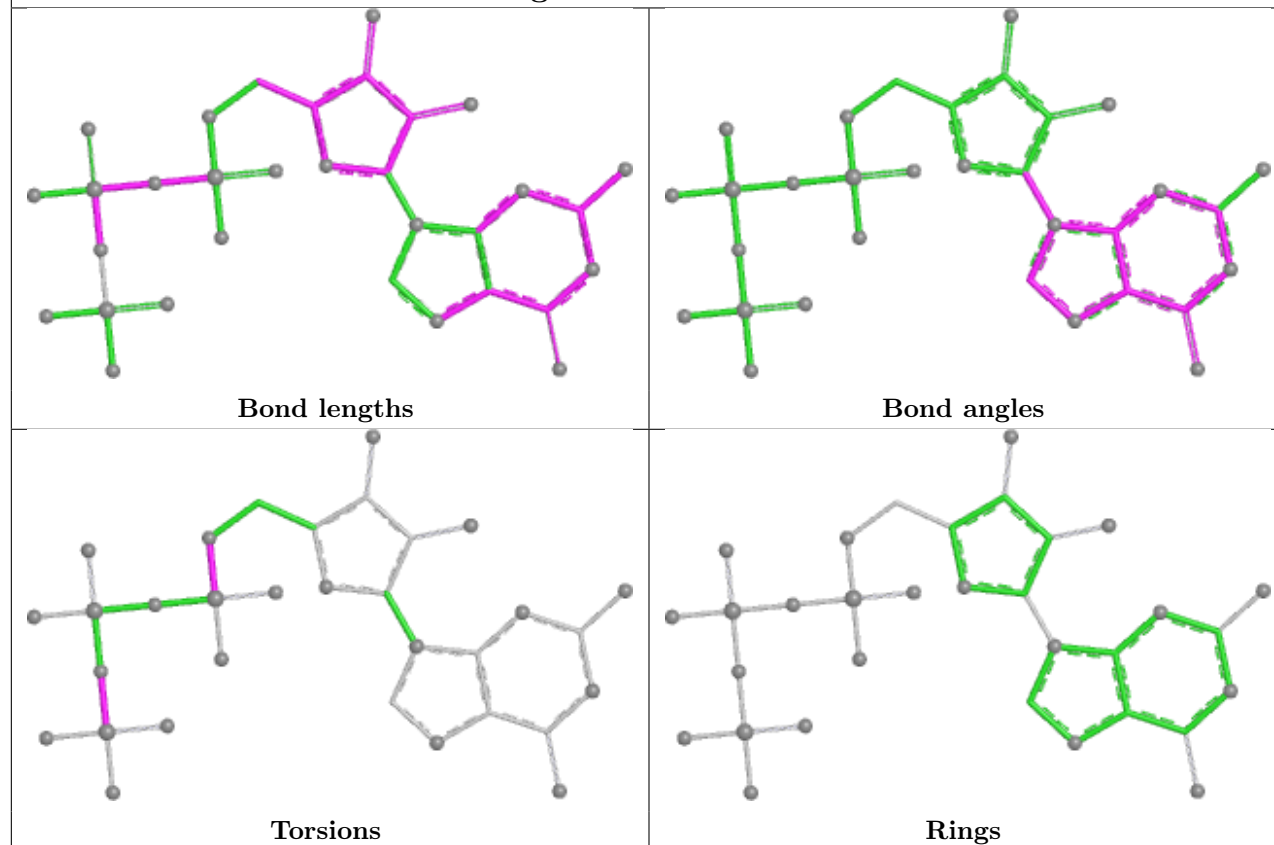
8 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	B	505	DJ9	1	0
8	B	501	GDP	1	0
5	C	501	GTP	1	0
9	B	503	MES	1	0
5	D	501	GTP	1	0
9	B	504	MES	1	0
5	A	501	GTP	2	0
11	F	402	ACP	1	0

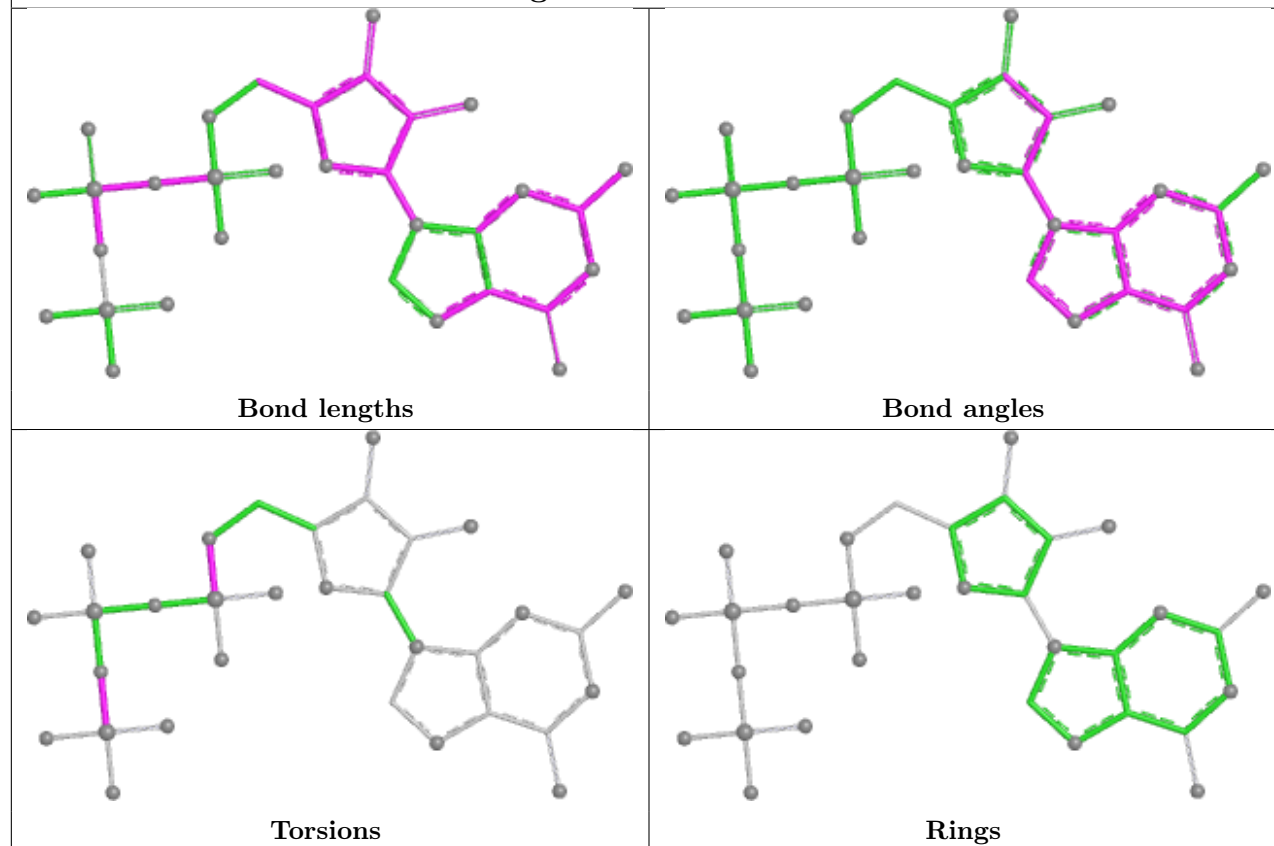
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

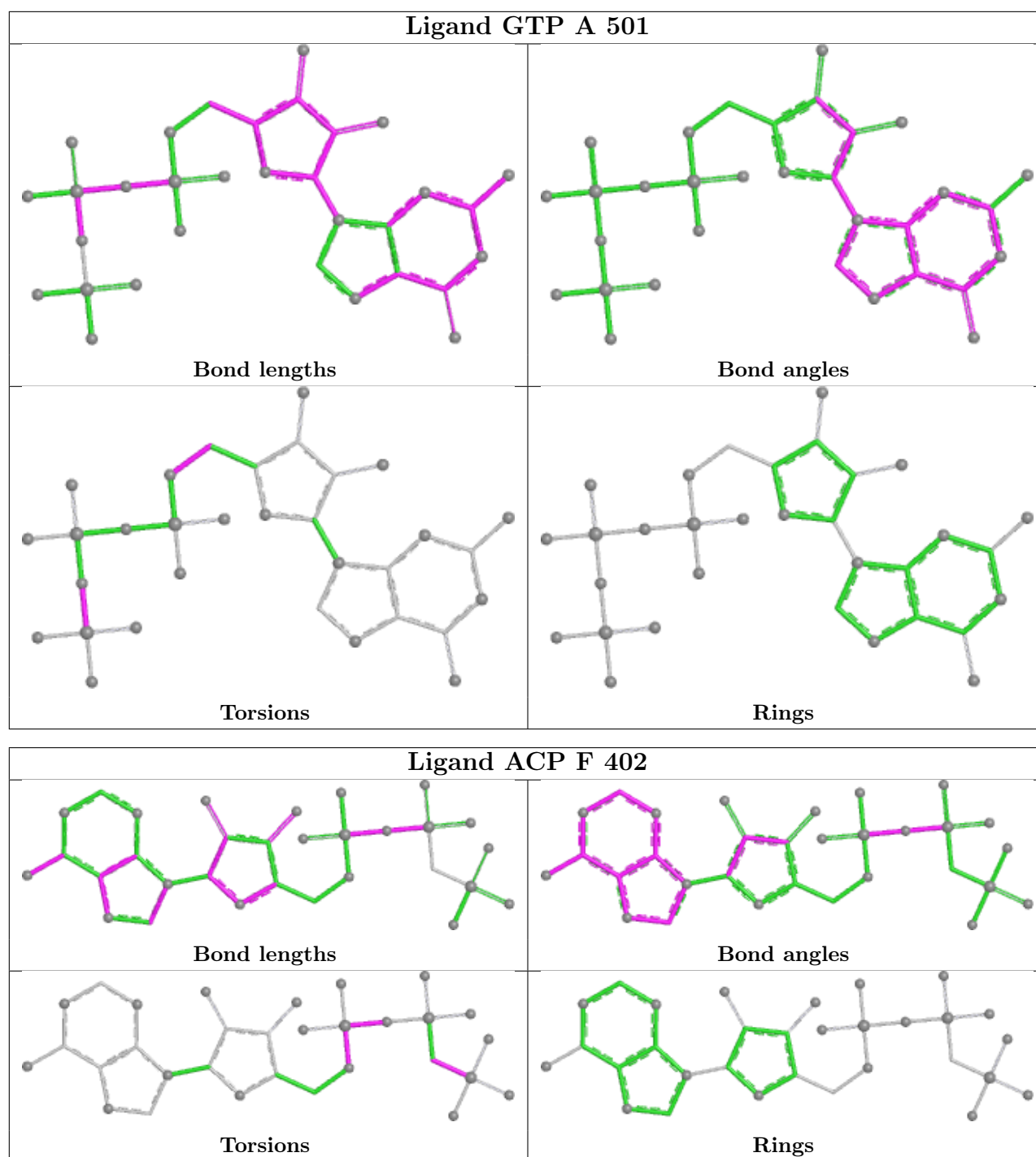


Ligand GTP C 501



Ligand GTP D 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	439/450 (97%)	0.21	14 (3%)	50	46	25, 43, 71, 95	0
1	C	440/450 (97%)	-0.03	17 (3%)	43	39	20, 33, 57, 79	0
2	B	427/445 (95%)	0.35	32 (7%)	20	17	20, 41, 78, 118	0
2	D	421/445 (94%)	0.87	49 (11%)	9	7	31, 58, 89, 112	0
3	E	121/143 (84%)	0.84	15 (12%)	8	6	30, 57, 88, 109	0
4	F	339/384 (88%)	1.39	101 (29%)	1	1	29, 66, 112, 133	0
All	All	2187/2317 (94%)	0.54	228 (10%)	11	9	20, 47, 91, 133	0

All (228) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	95	SER	6.0
2	D	397	TRP	6.0
4	F	199	PHE	5.8
4	F	132	LEU	5.5
1	A	179	THR	5.4
2	B	57	ASN	5.3
4	F	100	ILE	5.2
4	F	151	SER	5.2
2	B	245	GLN	5.1
4	F	101	TYR	5.1
4	F	235	ASP	5.1
4	F	177	GLY	5.1
2	D	1	MET	5.0
4	F	159	GLY	5.0
2	D	394	PHE	4.9
3	E	141	GLU	4.7
4	F	362	ALA	4.7
2	D	55	THR	4.6
4	F	252	ASN	4.5

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Mol	Chain	Res	Type	RSRZ
4	F	169	LEU	4.4
3	E	48	GLU	4.4
4	F	171	ASP	4.4
4	F	245	ILE	4.3
4	F	149	ALA	4.2
4	F	244	CYS	4.1
4	F	173	ILE	4.0
2	D	219	THR	4.0
4	F	172	PHE	4.0
4	F	135	TYR	4.0
4	F	160	ILE	3.9
4	F	131	PHE	3.8
4	F	144	GLY	3.8
4	F	161	LEU	3.8
4	F	128	ARG	3.8
3	E	139	LEU	3.7
2	D	178	THR	3.7
2	D	54	ALA	3.7
2	D	405	GLU	3.7
1	A	346	TRP	3.7
2	D	284	LEU	3.7
4	F	170	LEU	3.7
2	B	274	THR	3.7
4	F	231	ALA	3.7
2	D	96	GLY	3.6
1	A	262	TYR	3.6
4	F	247	LYS	3.6
1	C	1	MET	3.6
4	F	130	VAL	3.6
2	D	80	PRO	3.5
4	F	181	VAL	3.5
3	E	6	MET	3.5
1	A	438	ASP	3.5
4	F	232	ASN	3.5
4	F	237	THR	3.5
2	B	246	LEU	3.5
2	D	273	LEU	3.5
2	D	218	THR	3.4
2	D	239	CYS	3.4
4	F	383	HIS	3.4
4	F	221	LEU	3.4
4	F	99	VAL	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	439	SER	3.3
2	D	37	HIS	3.3
4	F	382	HIS	3.3
2	B	275	SER	3.3
2	D	390	ARG	3.3
2	B	72	THR	3.3
2	D	221	THR	3.3
1	C	280	LYS	3.2
2	B	55	THR	3.2
2	D	73	MET	3.2
4	F	373	SER	3.2
4	F	146	VAL	3.2
1	A	178	SER	3.2
2	B	278	SER	3.2
2	B	248	ALA	3.2
4	F	178	GLN	3.2
4	F	168	GLU	3.1
3	E	28	SER	3.1
4	F	142	ARG	3.1
1	C	247	ALA	3.1
2	D	389	PHE	3.1
4	F	143	GLU	3.0
4	F	381	HIS	3.0
1	C	340	SER	3.0
3	E	9	ILE	3.0
4	F	182	ILE	3.0
4	F	166	ALA	3.0
4	F	136	ASN	3.0
2	B	280	GLN	3.0
4	F	175	GLU	3.0
4	F	102	PRO	3.0
1	C	283	HIS	2.9
1	C	163	LYS	2.9
4	F	236	LYS	2.9
4	F	162	ILE	2.9
2	D	140	GLY	2.9
2	D	360	GLY	2.9
2	B	244	GLY	2.9
2	D	31	ASP	2.9
1	A	124	LYS	2.9
2	D	175	VAL	2.9
4	F	296	MET	2.9

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Mol	Chain	Res	Type	RSRZ
4	F	259	GLY	2.9
1	C	368	LEU	2.9
2	B	54	ALA	2.9
4	F	148	ILE	2.9
2	B	96	GLY	2.8
2	D	42	LEU	2.8
4	F	133	ALA	2.8
4	F	332	VAL	2.8
2	B	56	GLY	2.8
1	A	282	TYR	2.8
4	F	129	GLU	2.8
4	F	372	THR	2.8
4	F	165	GLU	2.8
4	F	137	ARG	2.8
4	F	380	HIS	2.8
4	F	227	PRO	2.8
4	F	150	LYS	2.8
2	D	98	GLY	2.7
4	F	188	LYS	2.7
4	F	139	ARG	2.7
4	F	176	GLN	2.7
2	D	24	ILE	2.7
2	B	239	CYS	2.7
2	D	170	MET	2.7
2	B	279	GLN	2.7
2	D	84	ILE	2.7
1	C	302	MET	2.7
2	B	42	LEU	2.6
2	D	216	LYS	2.6
2	D	57	ASN	2.6
4	F	191	LEU	2.6
4	F	234	GLN	2.6
2	B	37	HIS	2.6
4	F	145	ASN	2.6
4	F	263	PHE	2.6
4	F	246	GLN	2.5
2	B	323	MET	2.5
2	B	95	SER	2.5
4	F	147	TRP	2.5
2	D	176	SER	2.5
4	F	321	VAL	2.5
2	B	406	MET	2.5

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Mol	Chain	Res	Type	RSRZ
3	E	96	MET	2.5
2	D	56	GLY	2.5
4	F	134	ALA	2.5
1	A	232	SER	2.4
2	D	291	GLN	2.4
3	E	57	ALA	2.4
2	D	214	THR	2.4
1	C	440	VAL	2.4
1	C	218	ASP	2.4
2	D	2	ARG	2.4
4	F	242	ASN	2.4
4	F	86	GLU	2.4
2	D	387	ALA	2.4
1	A	177	VAL	2.4
4	F	228	TYR	2.4
4	F	384	HIS	2.4
2	B	243	PRO	2.4
2	D	245	GLN	2.3
2	B	281	TYR	2.3
4	F	70	LYS	2.3
4	F	194	PRO	2.3
1	C	337	THR	2.3
4	F	241	THR	2.3
4	F	164	SER	2.3
3	E	115	HIS	2.3
4	F	186	LEU	2.3
3	E	27	PRO	2.3
4	F	225	SER	2.3
3	E	7	GLU	2.3
4	F	32	LYS	2.3
3	E	120	LEU	2.2
1	A	365	GLY	2.2
4	F	320	MET	2.2
1	C	279	GLU	2.2
2	D	220	PRO	2.2
3	E	45	PRO	2.2
1	A	423	GLU	2.2
2	D	396	HIS	2.2
4	F	163	SER	2.2
2	B	276	ARG	2.2
2	D	400	GLY	2.2
4	F	226	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
2	D	94	GLN	2.2
4	F	31	ARG	2.2
1	C	361	THR	2.2
2	B	33	THR	2.2
2	D	126	SER	2.2
4	F	192	LEU	2.1
2	B	247	ASN	2.1
2	D	431	ASP	2.1
4	F	179	VAL	2.1
4	F	140	GLU	2.1
4	F	233	PHE	2.1
4	F	195	GLY	2.1
4	F	90	SER	2.1
1	C	2	ARG	2.1
2	B	41	ASP	2.1
2	D	39	ASP	2.1
2	B	218	THR	2.1
2	B	73	MET	2.1
1	C	284	GLU	2.1
3	E	59	GLU	2.1
2	D	404	ASP	2.1
2	B	2	ARG	2.1
2	D	399	THR	2.1
4	F	341	LYS	2.1
4	F	1	MET	2.1
1	C	367	ASP	2.1
3	E	51	GLN	2.1
4	F	180	HIS	2.1
4	F	253	TYR	2.1
1	A	363	VAL	2.1
2	D	180	VAL	2.1
2	D	320	ARG	2.1
4	F	184	LYS	2.0
4	F	18	SER	2.0
4	F	223	THR	2.0
4	F	376	ILE	2.0
1	C	162	GLY	2.0
2	B	19	LYS	2.0
1	A	283	HIS	2.0
4	F	275	LEU	2.0
2	B	58	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](#)

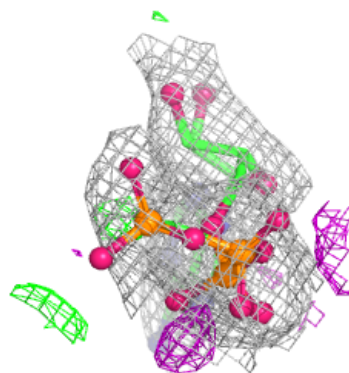
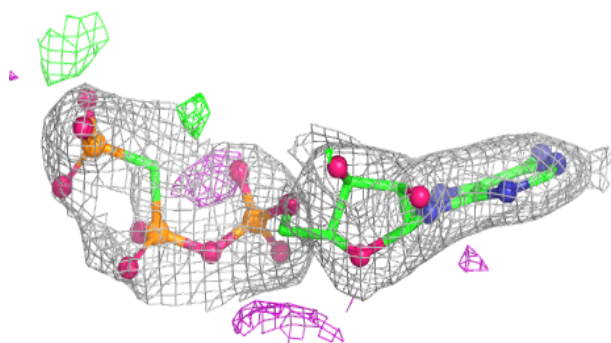
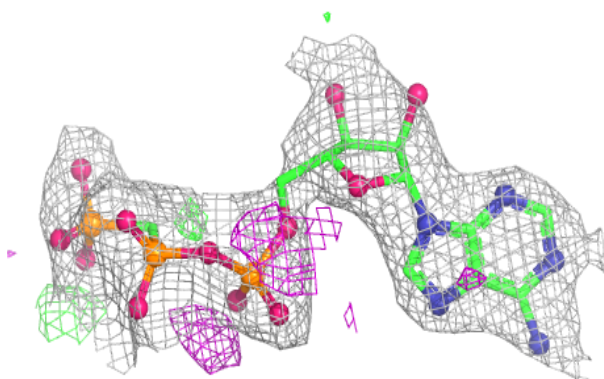
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
9	MES	B	503	12/12	0.83	0.22	64,85,106,110	0
11	ACP	F	402	31/31	0.83	0.14	63,86,116,117	0
9	MES	B	504	12/12	0.87	0.14	61,67,89,92	0
10	DJ9	B	505	30/30	0.88	0.16	51,61,68,74	0
6	MG	F	401	1/1	0.92	0.09	68,68,68,68	0
5	GTP	D	501	32/32	0.94	0.10	49,58,64,68	0
5	GTP	A	501	32/32	0.97	0.08	25,32,37,41	0
6	MG	A	502	1/1	0.98	0.04	26,26,26,26	0
5	GTP	C	501	32/32	0.98	0.05	25,27,31,32	0
7	CA	A	503	1/1	0.98	0.04	61,61,61,61	0
8	GDP	B	501	28/28	0.98	0.07	21,30,35,41	0
7	CA	C	503	1/1	0.99	0.03	46,46,46,46	0
6	MG	B	502	1/1	0.99	0.03	33,33,33,33	0
6	MG	C	502	1/1	0.99	0.02	26,26,26,26	0

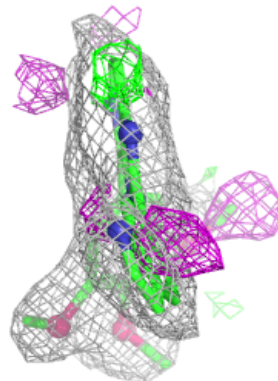
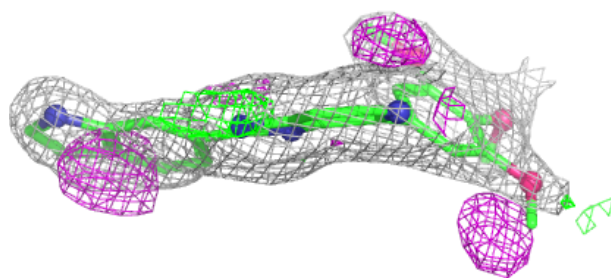
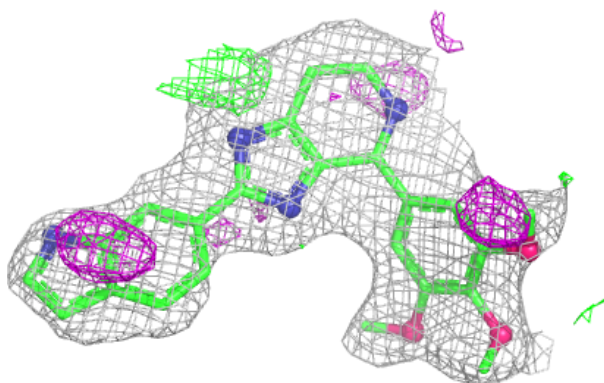
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ACP F 402:

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

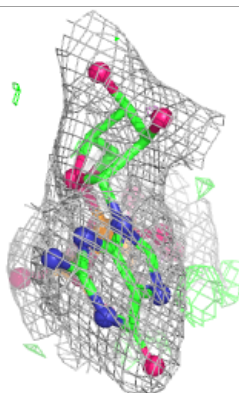
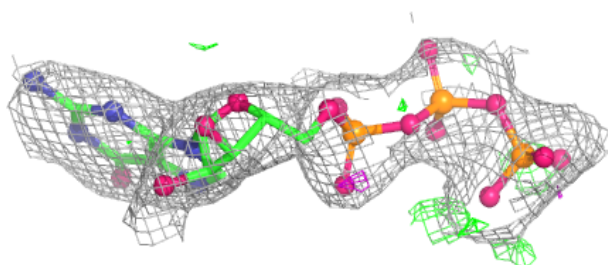
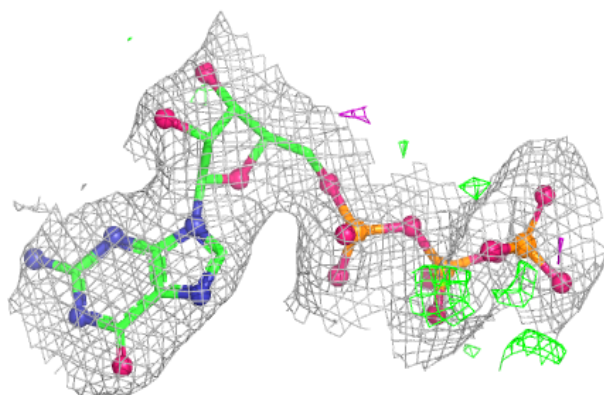
**Electron density around DJ9 B 505:**

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

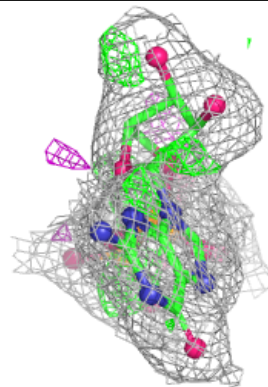
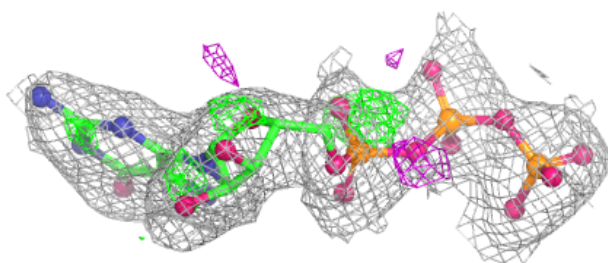
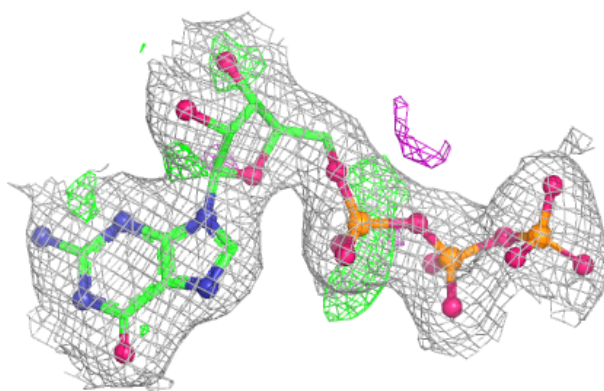


Electron density around GTP D 501:

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

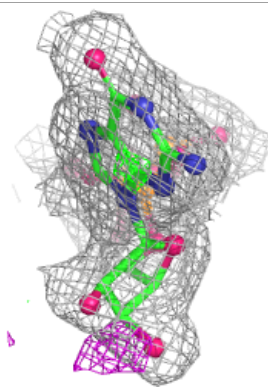
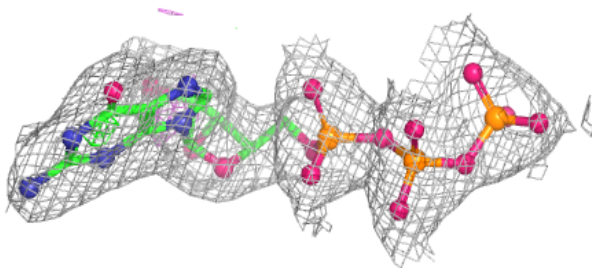
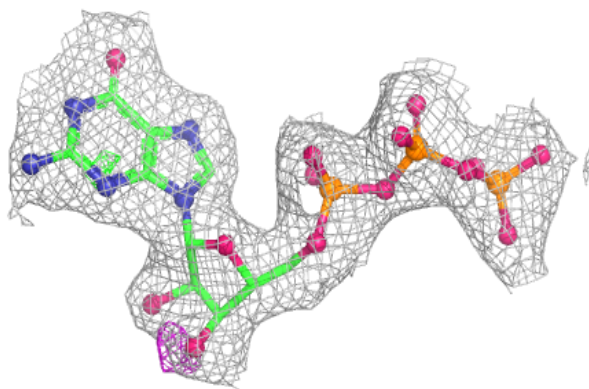
**Electron density around GTP A 501:**

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



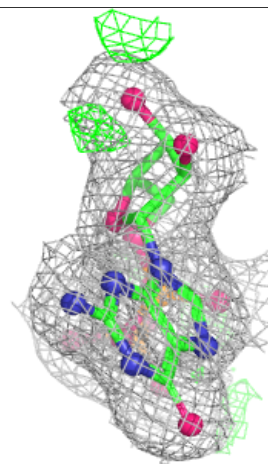
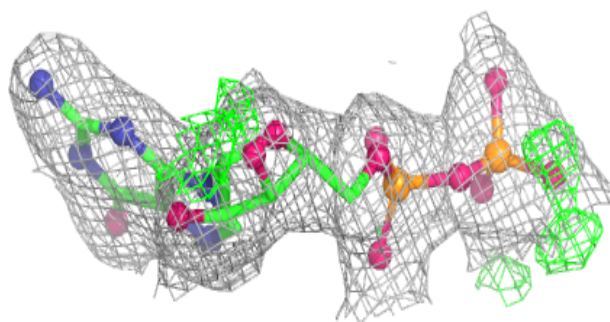
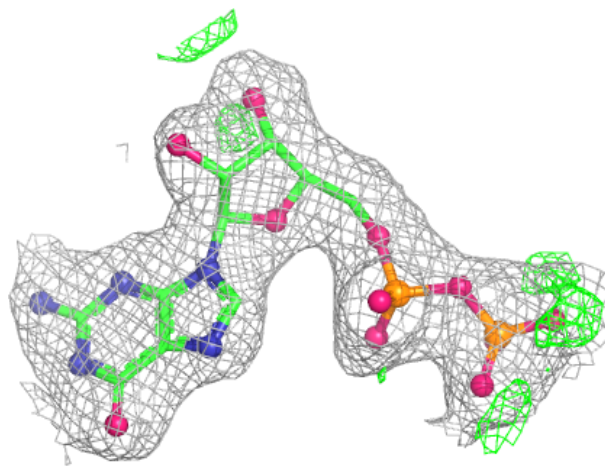
Electron density around GTP C 501:

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



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.