



# Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 12:16 am BST

PDB ID : 5MIO  
Title : KIF2C-DARPIN FUSION PROTEIN BOUND TO TUBULIN  
Authors : Wang, W.; Gigant, B.  
Deposited on : 2016-11-28  
Resolution : 3.19 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](mailto: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.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

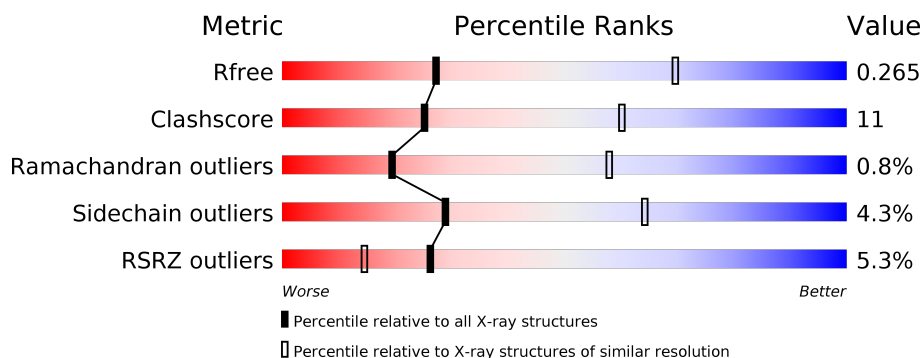
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.19 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))
$R_{free}$	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	<div> <div>3%</div> <div> <div></div> <div>84%</div> <div>10%</div> <div>5%</div> </div> </div>
2	B	445	<div> <div>4%</div> <div> <div></div> <div>85%</div> <div>10%</div> <div>5%</div> </div> </div>
3	C	573	<div> <div>6%</div> <div> <div></div> <div>58%</div> <div>21%</div> <div>• •</div> <div>17%</div> </div> </div>

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 10421 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	429	Total	C	N	O	S	0	0	0
			3364	2133	572	637	22			

- Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	423	Total	C	N	O	S	0	0	0
			3331	2095	568	641	27			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	203	CYS	SER	conflict	UNP D0VWY9
B	318	ILE	VAL	conflict	UNP D0VWY9

- Molecule 3 is a protein called Kinesin-like protein KIF2C,KIF2C FUSED TO A DARPIN,KIF2C FUSED TO A DARPIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	477	Total	C	N	O	S	0	0	0
			3604	2267	633	681	23			

There are 27 discrepancies between the modelled and reference sequences:

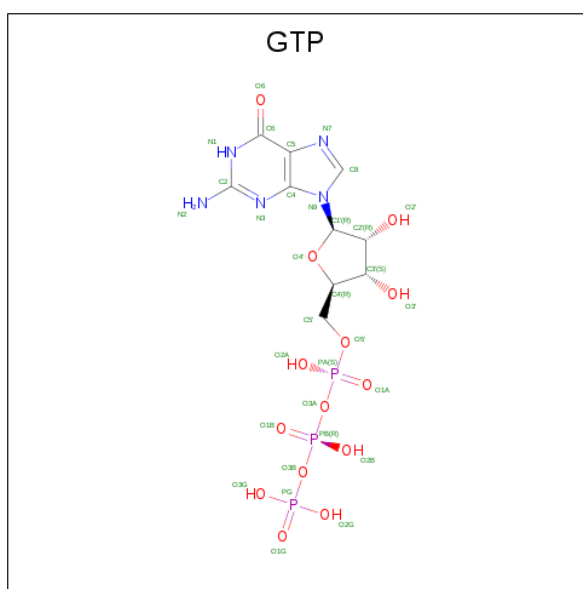
Chain	Residue	Modelled	Actual	Comment	Reference
C	214	MET	-	initiating methionine	UNP Q99661
C	215	GLY	-	expression tag	UNP Q99661
C	330	ALA	ARG	engineered mutation	UNP Q99661
C	379	ALA	ARG	engineered mutation	UNP Q99661
C	599	GLY	-	linker	UNP Q99661
C	600	GLY	-	linker	UNP Q99661
C	601	GLY	-	linker	UNP Q99661

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Chain	Residue	Modelled	Actual	Comment	Reference
C	602	GLY	-	linker	UNP Q99661
C	603	SER	-	linker	UNP Q99661
C	604	GLY	-	linker	UNP Q99661
C	605	GLY	-	linker	UNP Q99661
C	606	GLY	-	linker	UNP Q99661
C	607	GLY	-	linker	UNP Q99661
C	608	SER	-	linker	UNP Q99661
C	609	GLY	-	linker	UNP Q99661
C	610	GLY	-	linker	UNP Q99661
C	611	GLY	-	linker	UNP Q99661
C	612	GLY	-	linker	UNP Q99661
C	613	SER	-	linker	UNP Q99661
C	614	GLY	-	linker	UNP Q99661
C	615	GLY	-	linker	UNP Q99661
C	616	GLY	-	linker	UNP Q99661
C	617	GLY	-	linker	UNP Q99661
C	618	SER	-	linker	UNP Q99661
C	619	GLY	-	linker	UNP Q99661
C	620	GLY	-	linker	UNP Q99661
C	621	SER	-	linker	UNP Q99661

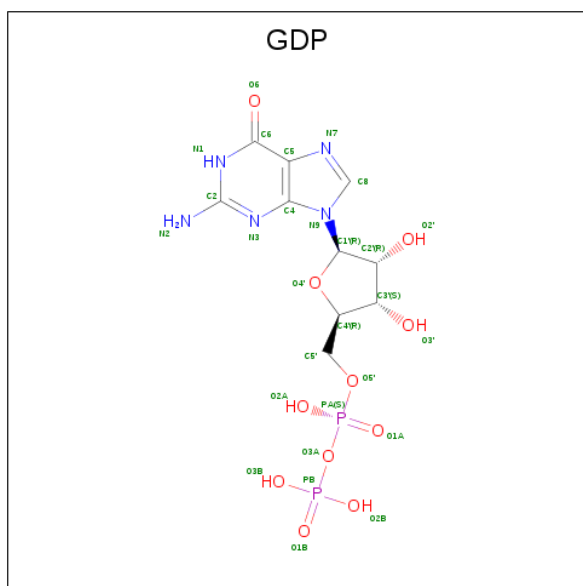
- Molecule 4 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula:  $C_{10}H_{16}N_5O_{14}P_3$ ).

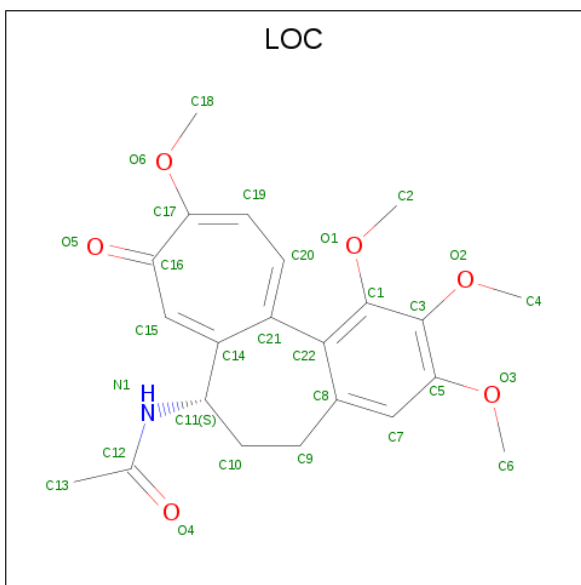


- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

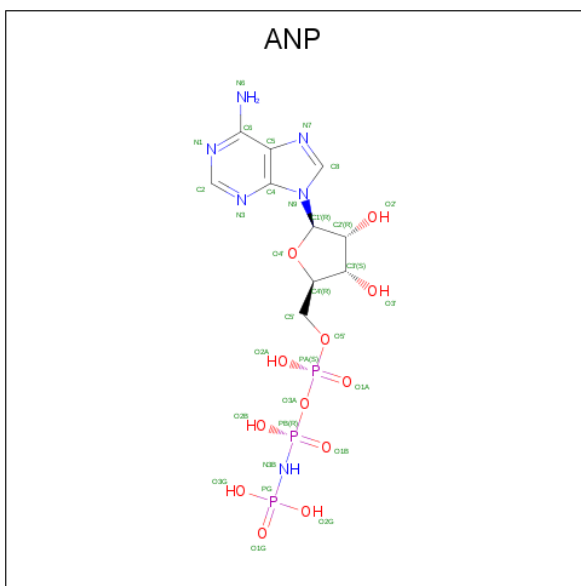
- Molecule 6 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>11</sub>P<sub>2</sub>).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	B	1	Total	C	N	O	0	0
			29	22	1	6		

- Molecule 8 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula:  $\text{C}_{10}\text{H}_{17}\text{N}_6\text{O}_{12}\text{P}_3$ ).

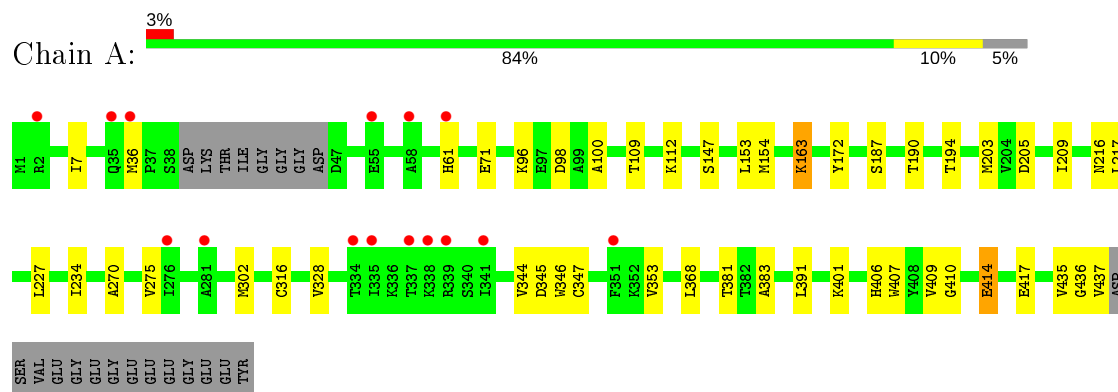


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	C	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

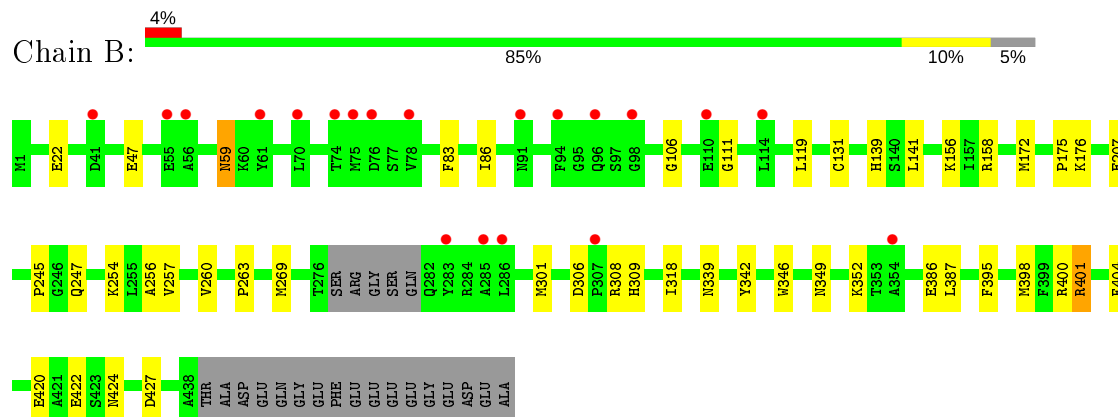
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

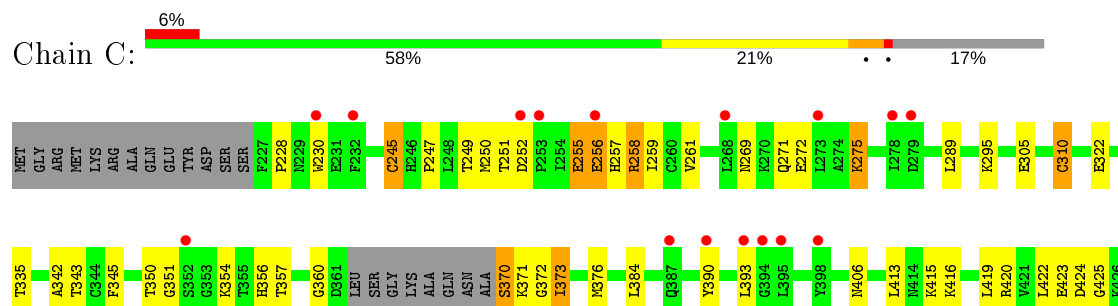
#### • Molecule 1: Tubulin alpha-1B chain

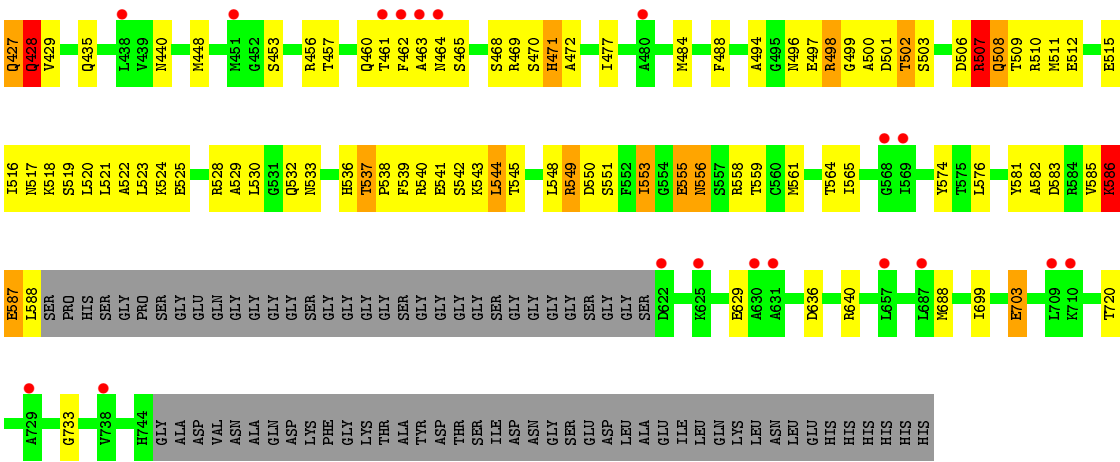


#### • Molecule 2: Tubulin beta chain



#### • Molecule 3: Kinesin-like protein KIF2C,KIF2C FUSED TO A DARPIN,KIF2C FUSED TO A DARPIN







## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	51.81Å 229.76Å 293.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.91 – 3.19 42.91 – 3.19	Depositor EDS
% Data completeness (in resolution range)	66.3 (42.91-3.19) 66.3 (42.91-3.19)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.49 (at 3.19Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, $R_{free}$	0.211 , 0.257 0.225 , 0.265	Depositor DCC
$R_{free}$ test set	1009 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	77.5	Xtriage
Anisotropy	0.500	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 71.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	10421	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	104.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.94% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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, LOC, MG, GDP, ANP

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	0.48	0/3441	0.58	0/4671
2	B	0.49	0/3405	0.57	0/4611
3	C	0.59	0/3661	0.81	3/4947 (0.1%)
All	All	0.52	0/10507	0.66	3/14229 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	498	ARG	N-CA-C	-6.03	94.71	111.00
3	C	275	LYS	N-CA-C	-5.89	95.09	111.00
3	C	373	ILE	CB-CG1-CD1	5.06	128.07	113.90

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	3364	0	3282	42	0
2	B	3331	0	3210	51	0
3	C	3604	0	3565	161	0
4	A	32	0	12	0	0
5	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	1	0	0	0	0
6	B	28	0	12	0	0
7	B	29	0	25	2	0
8	C	31	0	13	8	0
All	All	10421	0	10119	219	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 11.

All (219) 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:398:MET:SD	2:B:398:MET:CE	2.01	1.48
3:C:549:ARG:HD3	3:C:553:ILE:HD11	1.20	1.10
1:A:414:GLU:HG2	3:C:517:ASN:HD22	1.17	1.10
3:C:529:ALA:HA	3:C:532:GLN:HB2	1.38	1.03
2:B:404:PHE:HE2	3:C:699:ILE:HD12	1.22	1.02
3:C:530:LEU:HD23	3:C:537:THR:HG22	1.51	0.92
3:C:343:THR:HG21	3:C:551:SER:OG	1.69	0.92
1:A:414:GLU:HG2	3:C:517:ASN:ND2	1.86	0.90
3:C:528:ARG:O	3:C:532:GLN:HG2	1.72	0.90
2:B:404:PHE:CE2	3:C:699:ILE:HD12	2.07	0.89
3:C:462:PHE:HB2	3:C:502:THR:HG22	1.57	0.87
1:A:209:ILE:HG22	1:A:227:LEU:HD22	1.55	0.87
3:C:413:LEU:HD13	3:C:448:MET:CE	2.05	0.86
3:C:350:THR:HG23	8:C:802:ANP:O1G	1.76	0.86
2:B:395:PHE:HE2	2:B:422:GLU:HB2	1.41	0.86
3:C:500:ALA:H	3:C:503:SER:H	1.22	0.84
1:A:346:TRP:HZ2	1:A:435:VAL:HG13	1.42	0.84
3:C:496:ASN:HB3	3:C:520:LEU:HD13	1.61	0.83
3:C:427:GLN:HG2	3:C:428:GLN:H	1.45	0.80
3:C:549:ARG:HD3	3:C:553:ILE:CD1	2.09	0.80
3:C:499:GLY:CA	3:C:503:SER:HB2	2.12	0.79
2:B:395:PHE:CE2	2:B:422:GLU:HB2	2.19	0.77
3:C:259:ILE:HG23	3:C:559:THR:HG23	1.66	0.77
3:C:549:ARG:CD	3:C:553:ILE:HD11	2.08	0.76
1:A:163:LYS:HD2	1:A:163:LYS:H	1.51	0.76
3:C:529:ALA:CA	3:C:532:GLN:HB2	2.14	0.76
1:A:406:HIS:CG	2:B:263:PRO:HD3	2.20	0.75
2:B:404:PHE:HZ	3:C:699:ILE:CG2	2.01	0.74
1:A:409:VAL:HG21	3:C:521:LEU:HD22	1.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:272:GLU:O	3:C:275:LYS:O	2.07	0.72
2:B:404:PHE:HZ	3:C:699:ILE:HG23	1.56	0.71
3:C:506:ASP:OD1	3:C:510:ARG:HB2	1.91	0.71
3:C:522:ALA:CB	3:C:542:SER:HB3	2.21	0.71
1:A:112:LYS:HE3	3:C:506:ASP:OD2	1.90	0.71
3:C:509:THR:HA	3:C:512:GLU:HB3	1.73	0.71
1:A:96:LYS:HD2	2:B:131:CYS:HB2	1.73	0.71
3:C:549:ARG:O	3:C:553:ILE:HG13	1.91	0.70
3:C:335:THR:HG23	3:C:558:ARG:HH11	1.57	0.70
1:A:344:VAL:HG23	1:A:347:CYS:HB2	1.74	0.69
3:C:370:SER:HA	3:C:372:GLY:H	1.58	0.69
3:C:461:THR:HG22	3:C:469:ARG:HH21	1.58	0.68
3:C:703:GLU:CD	3:C:703:GLU:H	1.95	0.68
3:C:500:ALA:H	3:C:503:SER:N	1.91	0.68
3:C:456:ARG:NH2	3:C:470:SER:O	2.27	0.67
3:C:530:LEU:HD23	3:C:537:THR:CG2	2.22	0.67
3:C:456:ARG:NH1	3:C:472:ALA:CB	2.58	0.67
3:C:456:ARG:HH12	3:C:472:ALA:HB3	1.58	0.66
2:B:404:PHE:CZ	3:C:699:ILE:HG23	2.32	0.65
3:C:494:ALA:HB1	3:C:516:ILE:HD13	1.77	0.65
3:C:456:ARG:NH1	3:C:472:ALA:HB3	2.12	0.65
1:A:346:TRP:CZ2	1:A:435:VAL:HG13	2.30	0.64
3:C:544:LEU:HG	3:C:545:THR:N	2.12	0.64
3:C:496:ASN:HB3	3:C:520:LEU:CD1	2.28	0.63
2:B:306:ASP:HB3	2:B:309:HIS:CE1	2.34	0.62
3:C:582:ALA:HA	3:C:585:VAL:HG13	1.81	0.62
1:A:328:VAL:HG11	1:A:353:VAL:HG11	1.82	0.62
3:C:424:ASP:OD1	3:C:427:GLN:O	2.18	0.62
3:C:528:ARG:O	3:C:532:GLN:CG	2.47	0.62
3:C:351:GLY:N	3:C:464:ASN:HD21	1.98	0.62
3:C:463:ALA:HB2	3:C:502:THR:HG21	1.82	0.61
3:C:255:GLU:O	3:C:256:GLU:HB2	2.00	0.59
3:C:259:ILE:HD12	3:C:259:ILE:N	2.17	0.59
3:C:350:THR:HA	8:C:802:ANP:O1G	2.03	0.59
2:B:306:ASP:HB3	2:B:309:HIS:ND1	2.18	0.59
3:C:469:ARG:HG3	3:C:469:ARG:HH11	1.68	0.59
3:C:343:THR:HG21	3:C:551:SER:HG	1.67	0.59
2:B:309:HIS:HE1	2:B:386:GLU:OE2	1.86	0.59
1:A:234:ILE:HG21	1:A:302:MET:SD	2.43	0.59
3:C:350:THR:HA	8:C:802:ANP:HNB1	1.67	0.59
3:C:524:LYS:HD3	3:C:581:TYR:CZ	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:420:GLU:HG2	3:C:422:LEU:HA	1.85	0.57
2:B:400:ARG:HB2	2:B:401:ARG:NH2	2.18	0.57
3:C:537:THR:O	3:C:539:PHE:CE2	2.57	0.57
3:C:537:THR:O	3:C:539:PHE:CD2	2.58	0.57
3:C:259:ILE:HG13	3:C:559:THR:CG2	2.36	0.56
1:A:209:ILE:CG2	1:A:227:LEU:HD22	2.30	0.55
3:C:587:GLU:HG2	3:C:588:LEU:N	2.21	0.55
3:C:550:ASP:O	3:C:553:ILE:O	2.24	0.55
3:C:556:ASN:N	3:C:556:ASN:HD22	2.04	0.55
3:C:350:THR:HA	8:C:802:ANP:PG	2.47	0.54
3:C:529:ALA:O	3:C:533:ASN:N	2.41	0.54
3:C:497:GLU:HA	3:C:574:TYR:HE1	1.72	0.54
3:C:373:ILE:HD12	3:C:376:MET:CE	2.38	0.53
2:B:398:MET:CG	2:B:398:MET:CE	2.84	0.53
1:A:163:LYS:H	1:A:163:LYS:CD	2.15	0.53
3:C:469:ARG:NH1	3:C:469:ARG:HG3	2.24	0.53
3:C:413:LEU:HD13	3:C:448:MET:HE3	1.86	0.53
3:C:499:GLY:HA3	3:C:503:SER:HB2	1.89	0.53
3:C:429:VAL:HG23	3:C:549:ARG:NH1	2.25	0.52
3:C:583:ASP:O	3:C:586:LYS:HD2	2.09	0.52
1:A:401:LYS:HG3	2:B:346:TRP:CD2	2.45	0.52
3:C:512:GLU:O	3:C:515:GLU:HB2	2.09	0.52
1:A:406:HIS:HE1	2:B:260:VAL:O	1.92	0.52
3:C:390:TYR:HA	3:C:393:LEU:HD12	1.92	0.52
3:C:453:SER:HA	3:C:456:ARG:HB2	1.92	0.52
3:C:429:VAL:HG23	3:C:549:ARG:HH12	1.73	0.52
3:C:245:CYS:SG	3:C:310:CYS:HB3	2.50	0.52
3:C:530:LEU:CD2	3:C:537:THR:CG2	2.88	0.52
3:C:456:ARG:NH1	3:C:472:ALA:HB2	2.25	0.51
1:A:409:VAL:CG1	3:C:518:LYS:HA	2.40	0.51
2:B:404:PHE:HZ	3:C:699:ILE:HG21	1.75	0.51
2:B:22:GLU:HG3	2:B:83:PHE:CD1	2.46	0.51
3:C:538:PRO:HB2	3:C:541:GLU:HG3	1.92	0.51
3:C:519:SER:O	3:C:522:ALA:HB3	2.10	0.51
3:C:249:THR:C	3:C:251:THR:H	2.14	0.51
3:C:350:THR:HA	8:C:802:ANP:N3B	2.25	0.51
3:C:335:THR:CG2	3:C:558:ARG:HD2	2.41	0.50
1:A:410:GLY:HA2	3:C:518:LYS:HD2	1.92	0.50
2:B:119:LEU:HD11	2:B:156:LYS:HB3	1.94	0.50
3:C:468:SER:HB2	8:C:802:ANP:O2G	2.12	0.50
1:A:407:TRP:CE2	2:B:257:VAL:HA	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:424:ASN:HD22	3:C:540:ARG:HH11	1.60	0.49
3:C:522:ALA:HB3	3:C:542:SER:HB3	1.94	0.49
3:C:523:LEU:HD12	3:C:523:LEU:O	2.12	0.49
3:C:529:ALA:HA	3:C:532:GLN:CB	2.28	0.49
1:A:100:ALA:HA	2:B:254:LYS:CG	2.42	0.49
2:B:47:GLU:HB3	2:B:245:PRO:HG3	1.95	0.49
3:C:499:GLY:C	3:C:503:SER:HB2	2.33	0.49
1:A:71:GLU:HG2	1:A:98:ASP:HB3	1.95	0.49
2:B:424:ASN:HD22	3:C:540:ARG:NH1	2.11	0.49
3:C:500:ALA:N	3:C:503:SER:HB2	2.28	0.49
3:C:351:GLY:H	3:C:464:ASN:HD21	1.60	0.49
2:B:176:LYS:HG3	2:B:207:GLU:HG3	1.95	0.49
3:C:247:PRO:HG3	3:C:310:CYS:SG	2.53	0.48
3:C:460:GLN:HA	3:C:465:SER:O	2.12	0.48
3:C:508:GLN:O	3:C:512:GLU:N	2.42	0.48
1:A:187:SER:HB3	1:A:391:LEU:HD21	1.94	0.48
2:B:401:ARG:HH21	2:B:401:ARG:HG2	1.78	0.48
3:C:427:GLN:HG2	3:C:428:GLN:N	2.23	0.47
3:C:555:GLU:HB3	3:C:556:ASN:HD22	1.79	0.47
2:B:318:ILE:HD11	7:B:502:LOC:H4	1.96	0.47
2:B:427:ASP:CG	3:C:540:ARG:HG3	2.34	0.47
2:B:172:MET:HG3	2:B:387:LEU:HD11	1.96	0.47
1:A:406:HIS:CE1	2:B:260:VAL:O	2.67	0.47
2:B:352:LYS:HG3	7:B:502:LOC:C16	2.44	0.47
1:A:172:TYR:HB3	1:A:205:ASP:HA	1.95	0.47
1:A:36:MET:HB3	1:A:61:HIS:CE1	2.50	0.47
3:C:456:ARG:NH2	3:C:468:SER:HB3	2.30	0.47
1:A:154:MET:HG3	1:A:194:THR:HG23	1.96	0.47
3:C:636:ASP:O	3:C:640:ARG:HG3	2.15	0.46
3:C:506:ASP:O	3:C:507:ARG:HG2	2.15	0.46
3:C:555:GLU:C	3:C:556:ASN:HD22	2.18	0.46
1:A:346:TRP:HH2	1:A:435:VAL:HA	1.81	0.46
3:C:427:GLN:CG	3:C:428:GLN:H	2.24	0.46
2:B:59:ASN:CG	2:B:59:ASN:O	2.54	0.46
3:C:269:ASN:HD21	3:C:271:GLN:HB2	1.80	0.46
3:C:582:ALA:HA	3:C:585:VAL:CG1	2.44	0.46
3:C:688:MET:HE2	3:C:720:THR:HG21	1.97	0.46
3:C:477:ILE:HG23	3:C:484:MET:CE	2.46	0.46
3:C:507:ARG:HB2	3:C:508:GLN:H	1.46	0.45
1:A:203:MET:O	1:A:302:MET:HE2	2.16	0.45
2:B:309:HIS:CE1	2:B:386:GLU:OE2	2.67	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:500:ALA:N	3:C:503:SER:H	2.02	0.45
1:A:216:ASN:HD22	1:A:275:VAL:HB	1.81	0.45
3:C:448:MET:HB3	3:C:448:MET:HE3	1.88	0.45
3:C:354:LYS:CG	3:C:564:THR:HG21	2.47	0.45
1:A:414:GLU:CG	3:C:517:ASN:HD22	2.06	0.45
3:C:350:THR:CG2	8:C:802:ANP:O1G	2.57	0.45
3:C:373:ILE:HD12	3:C:376:MET:HE1	1.97	0.45
3:C:469:ARG:HD2	3:C:512:GLU:OE1	2.17	0.44
2:B:420:GLU:HG2	3:C:423:GLU:H	1.82	0.44
3:C:524:LYS:HD3	3:C:581:TYR:CE2	2.52	0.44
2:B:339:ASN:HB3	2:B:342:TYR:HD2	1.82	0.44
3:C:345:PHE:CE2	3:C:561:MET:HG3	2.52	0.44
1:A:109:THR:HG23	3:C:510:ARG:HH11	1.83	0.44
1:A:409:VAL:HG11	3:C:518:LYS:HA	1.98	0.44
1:A:407:TRP:NE1	2:B:260:VAL:O	2.49	0.44
3:C:258:ARG:C	3:C:259:ILE:HD12	2.39	0.44
3:C:406:ASN:HA	3:C:515:GLU:HG3	1.99	0.44
1:A:7:ILE:HG21	1:A:153:LEU:HD21	2.00	0.44
1:A:100:ALA:HA	2:B:254:LYS:HG3	2.00	0.44
3:C:523:LEU:HA	3:C:545:THR:CG2	2.47	0.43
2:B:106:GLY:O	2:B:111:GLY:HA3	2.18	0.43
3:C:259:ILE:N	3:C:259:ILE:CD1	2.81	0.43
3:C:269:ASN:HD22	3:C:271:GLN:H	1.66	0.43
3:C:456:ARG:HH21	3:C:468:SER:HB3	1.83	0.43
3:C:506:ASP:C	3:C:507:ARG:HG2	2.39	0.43
3:C:543:LYS:HD3	3:C:543:LYS:HA	1.81	0.43
3:C:343:THR:CG2	3:C:551:SER:OG	2.54	0.43
3:C:471:HIS:NE2	3:C:544:LEU:HD22	2.34	0.43
3:C:456:ARG:HH12	3:C:472:ALA:CB	2.22	0.43
3:C:342:ALA:HA	3:C:558:ARG:O	2.19	0.43
2:B:420:GLU:CG	3:C:422:LEU:HA	2.49	0.43
3:C:460:GLN:O	3:C:461:THR:CG2	2.65	0.43
1:A:217:LEU:HD21	1:A:368:LEU:HD23	2.00	0.43
3:C:356:HIS:O	3:C:360:GLY:HA2	2.18	0.43
3:C:688:MET:HA	3:C:688:MET:HE2	2.01	0.43
2:B:308:ARG:HA	2:B:342:TYR:CE1	2.53	0.42
2:B:83:PHE:O	2:B:86:ILE:HG22	2.19	0.42
1:A:381:THR:HG22	1:A:383:ALA:H	1.85	0.42
2:B:141:LEU:HD12	2:B:172:MET:SD	2.60	0.42
3:C:289:LEU:HD11	3:C:565:ILE:HD11	2.01	0.42
1:A:270:ALA:HB3	1:A:302:MET:HE1	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:349:ASN:O	2:B:352:LYS:HE2	2.19	0.42
3:C:357:THR:O	3:C:373:ILE:HD13	2.19	0.42
3:C:508:GLN:HG3	3:C:512:GLU:HB2	2.02	0.42
2:B:306:ASP:O	2:B:309:HIS:CE1	2.74	0.41
3:C:413:LEU:HD13	3:C:448:MET:HE1	1.97	0.41
2:B:269:MET:HE2	2:B:301:MET:SD	2.60	0.41
3:C:523:LEU:HA	3:C:545:THR:HG21	2.03	0.41
3:C:528:ARG:O	3:C:532:GLN:N	2.53	0.41
1:A:407:TRP:CH2	2:B:256:ALA:HB1	2.55	0.41
3:C:351:GLY:N	3:C:464:ASN:ND2	2.68	0.41
1:A:414:GLU:HB2	3:C:498:ARG:HA	2.02	0.41
3:C:529:ALA:C	3:C:532:GLN:HB2	2.40	0.41
2:B:404:PHE:CZ	3:C:699:ILE:CG2	2.91	0.41
2:B:175:PRO:CB	3:C:733:GLY:HA3	2.51	0.41
3:C:295:LYS:CD	3:C:305:GLU:HB2	2.51	0.41
3:C:521:LEU:HD12	3:C:521:LEU:O	2.21	0.41
3:C:506:ASP:HB2	3:C:510:ARG:H	1.86	0.41
3:C:525:GLU:OE1	3:C:528:ARG:NE	2.53	0.41
3:C:582:ALA:CA	3:C:585:VAL:HG13	2.50	0.40
2:B:175:PRO:HB2	3:C:733:GLY:HA3	2.02	0.40
3:C:295:LYS:HD2	3:C:305:GLU:HB2	2.02	0.40
3:C:464:ASN:OD1	8:C:802:ANP:H5'1	2.22	0.40
1:A:147:SER:HB2	1:A:190:THR:HB	2.03	0.40
3:C:506:ASP:HB2	3:C:510:ARG:N	2.36	0.40
3:C:528:ARG:C	3:C:532:GLN:HG2	2.38	0.40
3:C:536:HIS:C	3:C:537:THR:OG1	2.59	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	425/451 (94%)	409 (96%)	15 (4%)	1 (0%)	47 79
2	B	419/445 (94%)	408 (97%)	11 (3%)	0	100 100
3	C	471/573 (82%)	446 (95%)	15 (3%)	10 (2%)	7 37
All	All	1315/1469 (90%)	1263 (96%)	41 (3%)	11 (1%)	19 58

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	252	ASP
3	C	257	HIS
3	C	425	GLY
3	C	586	LYS
1	A	436	GLY
3	C	228	PRO
3	C	250	MET
3	C	427	GLN
3	C	507	ARG
3	C	256	GLU
3	C	428	GLN

### 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	363/379 (96%)	357 (98%)	6 (2%)	60 83
2	B	365/383 (95%)	360 (99%)	5 (1%)	67 86
3	C	377/462 (82%)	340 (90%)	37 (10%)	8 31
All	All	1105/1224 (90%)	1057 (96%)	48 (4%)	29 64

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	163	LYS
1	A	316	CYS

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Mol	Chain	Res	Type
1	A	345	ASP
1	A	414	GLU
1	A	417	GLU
1	A	437	VAL
2	B	59	ASN
2	B	139	HIS
2	B	158	ARG
2	B	247	GLN
2	B	401	ARG
3	C	230	TRP
3	C	245	CYS
3	C	255	GLU
3	C	258	ARG
3	C	261	VAL
3	C	310	CYS
3	C	322	GLU
3	C	370	SER
3	C	371	LYS
3	C	384	LEU
3	C	415	LYS
3	C	416	LYS
3	C	419	LEU
3	C	420	ARG
3	C	428	GLN
3	C	435	GLN
3	C	440	ASN
3	C	457	THR
3	C	471	HIS
3	C	488	PHE
3	C	501	ASP
3	C	502	THR
3	C	507	ARG
3	C	508	GLN
3	C	511	MET
3	C	537	THR
3	C	544	LEU
3	C	548	LEU
3	C	549	ARG
3	C	553	ILE
3	C	555	GLU
3	C	556	ASN
3	C	576	LEU

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Mol	Chain	Res	Type
3	C	586	LYS
3	C	587	GLU
3	C	629	GLU
3	C	703	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	50	ASN
1	A	61	HIS
1	A	406	HIS
2	B	197	ASN
2	B	247	GLN
2	B	309	HIS
2	B	339	ASN
2	B	424	ASN
3	C	269	ASN
3	C	307	GLN
3	C	460	GLN
3	C	517	ASN
3	C	532	GLN
3	C	546	GLN
3	C	556	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 carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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$
6	GDP	B	501	-	24,30,30	0.96	2 (8%)	31,47,47	2.05	4 (12%)
8	ANP	C	802	5	29,33,33	1.44	2 (6%)	31,52,52	1.26	3 (9%)
7	LOC	B	502	-	28,31,31	0.87	1 (3%)	28,44,44	0.64	0
4	GTP	A	501	5	26,34,34	1.09	2 (7%)	33,54,54	1.88	4 (12%)

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
6	GDP	B	501	-	-	5/12/32/32	0/3/3/3
8	ANP	C	802	5	-	0/14/38/38	0/3/3/3
7	LOC	B	502	-	-	0/10/25/25	0/3/3/3
4	GTP	A	501	5	-	6/18/38/38	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	C	802	ANP	PG-O1G	5.34	1.54	1.46
8	C	802	ANP	PG-O3G	-4.27	1.45	1.56
4	A	501	GTP	C6-N1	3.29	1.38	1.33
6	B	501	GDP	C6-N1	3.09	1.38	1.33
7	B	502	LOC	C15-C16	2.50	1.44	1.39
4	A	501	GTP	PG-O1G	2.45	1.58	1.50
6	B	501	GDP	C6-C5	2.37	1.45	1.41

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	501	GDP	C5-C6-N1	-7.87	112.66	123.43
4	A	501	GTP	C5-C6-N1	-7.21	113.56	123.43
6	B	501	GDP	C6-N1-C2	5.78	125.12	115.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	501	GTP	C6-N1-C2	5.24	124.26	115.93
8	C	802	ANP	O1G-PG-N3B	3.80	117.37	111.77
6	B	501	GDP	C6-C5-C4	-3.07	117.87	120.80
4	A	501	GTP	N3-C2-N1	-3.01	123.21	127.22
6	B	501	GDP	N3-C2-N1	-2.91	123.34	127.22
4	A	501	GTP	C6-C5-C4	-2.86	118.07	120.80
8	C	802	ANP	O3G-PG-O1G	-2.84	106.31	113.45
8	C	802	ANP	O2G-PG-O1G	-2.38	107.47	113.45

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	501	GDP	C5'-O5'-PA-O1A
4	A	501	GTP	PB-O3B-PG-O2G
4	A	501	GTP	C5'-O5'-PA-O1A
4	A	501	GTP	C5'-O5'-PA-O2A
6	B	501	GDP	C5'-O5'-PA-O2A
6	B	501	GDP	PB-O3A-PA-O2A
4	A	501	GTP	PB-O3A-PA-O2A
4	A	501	GTP	C4'-C5'-O5'-PA
6	B	501	GDP	C5'-O5'-PA-O3A
4	A	501	GTP	C5'-O5'-PA-O3A
6	B	501	GDP	PB-O3A-PA-O1A

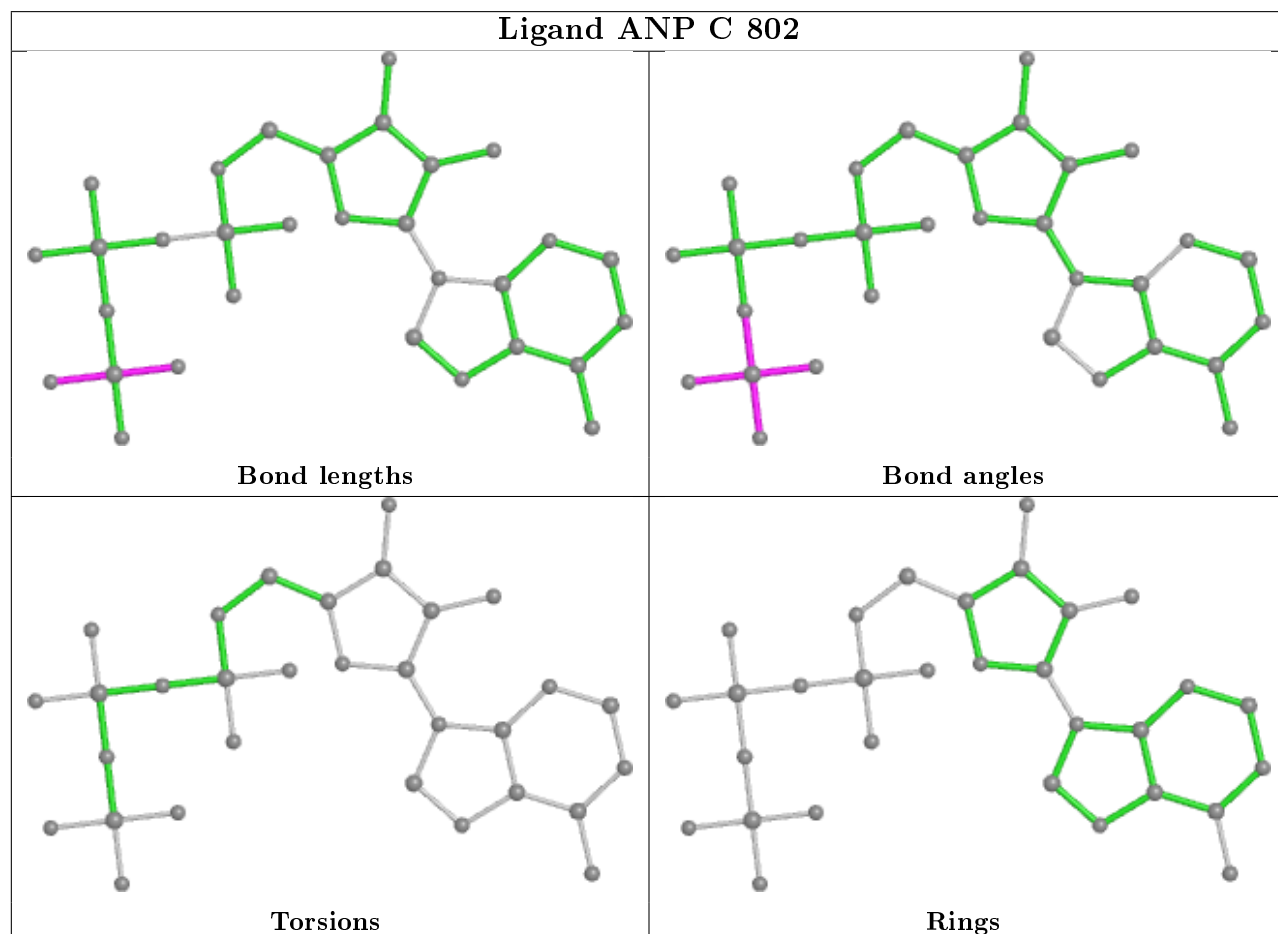
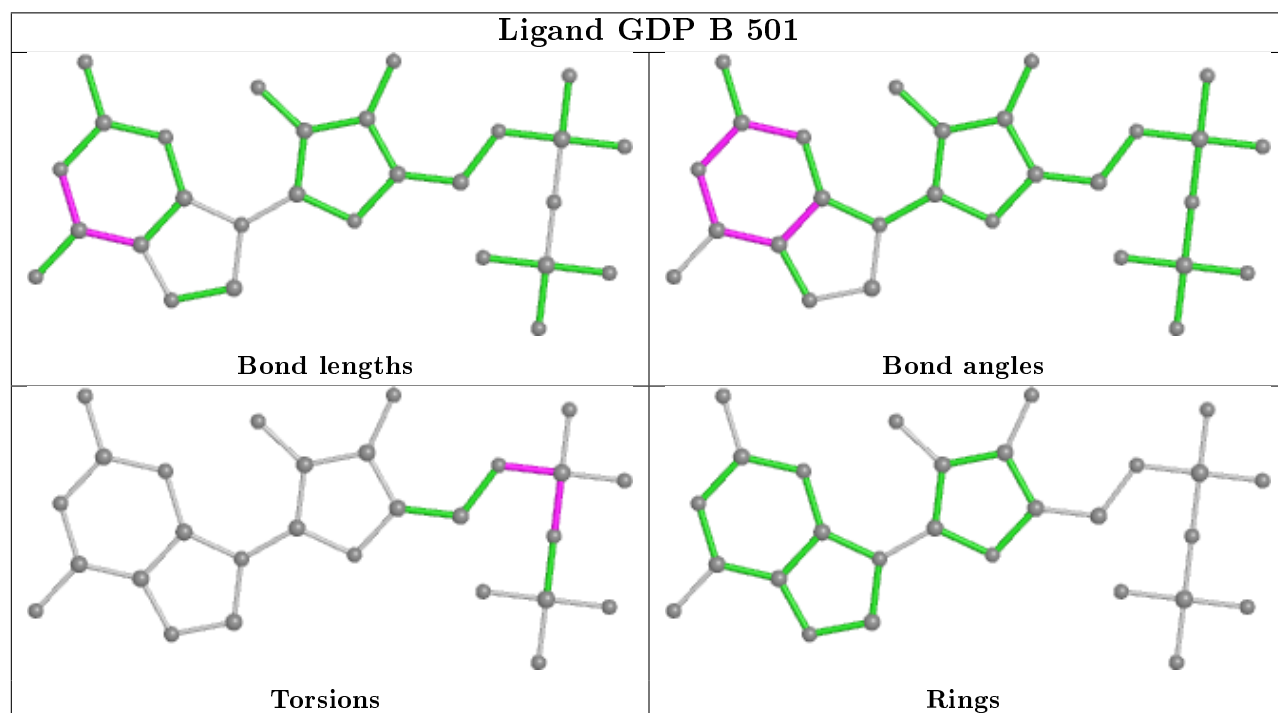
There are no ring outliers.

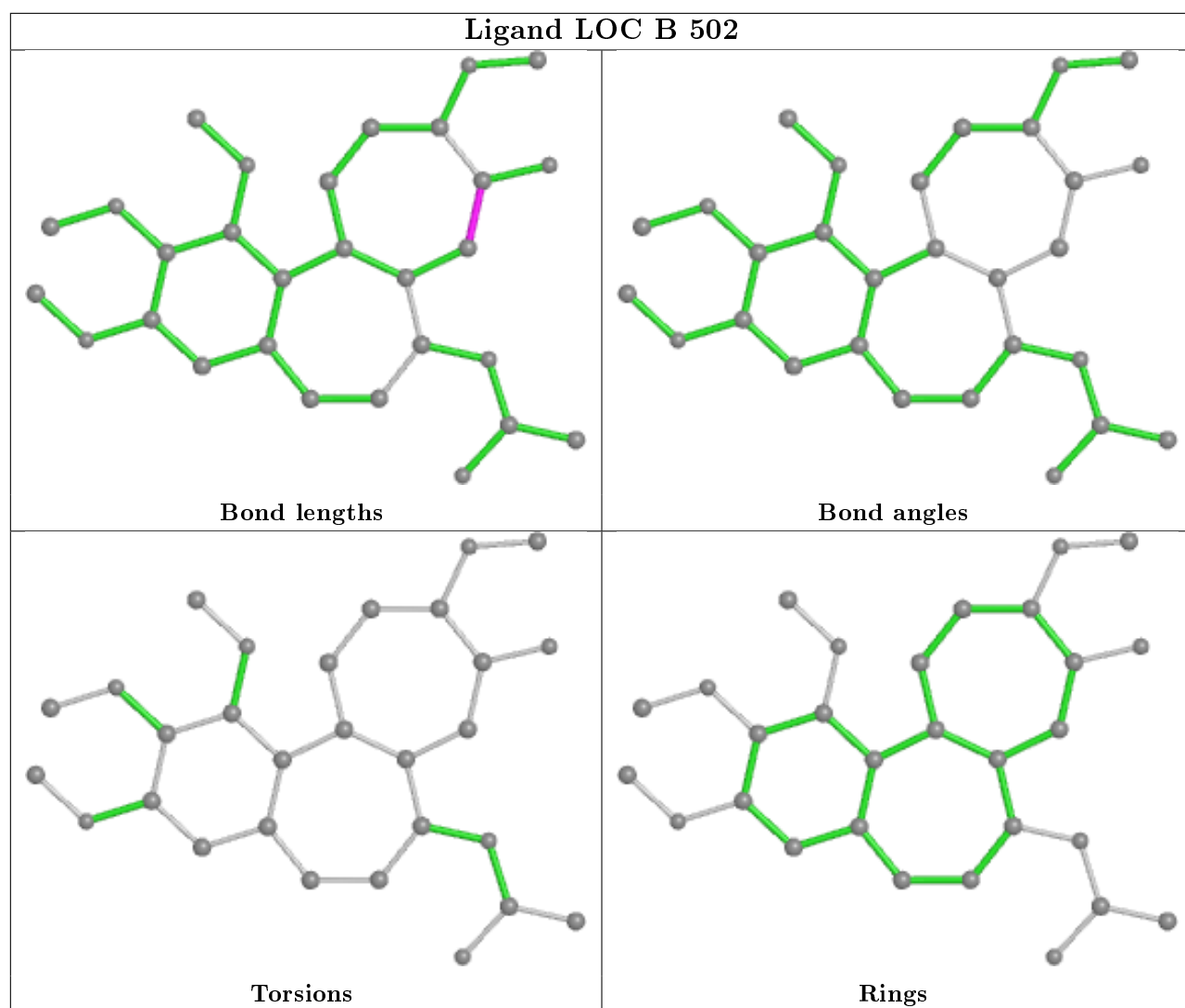
2 monomers are involved in 10 short contacts:

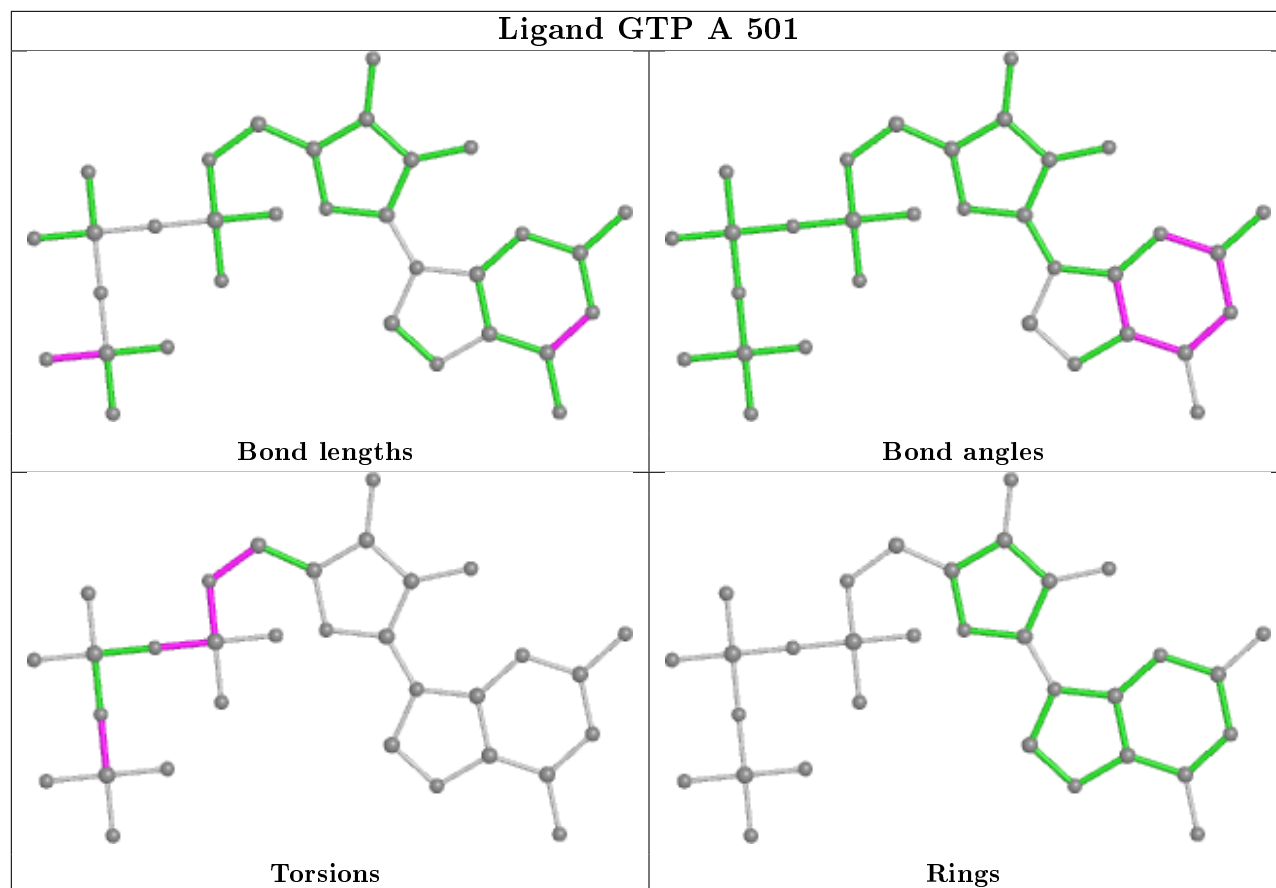
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	C	802	ANP	8	0
7	B	502	LOC	2	0

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	429/451 (95%)	0.02	15 (3%) 44 28	62, 94, 140, 161	0
2	B	423/445 (95%)	0.27	20 (4%) 31 19	66, 103, 136, 166	2 (0%)
3	C	477/573 (83%)	0.36	35 (7%) 15 9	68, 107, 145, 174	0
All	All	1329/1469 (90%)	0.22	70 (5%) 26 14	62, 102, 140, 174	2 (0%)

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	61	TYR	5.5
2	B	74	THR	5.1
3	C	462	PHE	4.5
2	B	96	GLN	4.3
2	B	75	MET	4.2
3	C	395	LEU	4.2
2	B	283	TYR	4.1
2	B	56	ALA	4.0
2	B	354	ALA	3.9
2	B	110	GLU	3.9
3	C	438	LEU	3.9
1	A	58	ALA	3.7
3	C	393	LEU	3.6
3	C	569	ILE	3.6
3	C	394	GLY	3.5
3	C	278	ILE	3.4
3	C	253	PRO	3.4
1	A	335	ILE	3.4
3	C	230	TRP	3.3
1	A	61	HIS	3.2
1	A	55	GLU	3.1
2	B	41	ASP	3.0
3	C	463	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
2	B	78	VAL	2.9
2	B	91	ASN	2.8
2	B	307	PRO	2.8
3	C	461	THR	2.8
3	C	657	LEU	2.8
2	B	94	PHE	2.7
3	C	398	TYR	2.7
2	B	114	LEU	2.7
2	B	286	LEU	2.7
1	A	36	MET	2.7
3	C	256	GLU	2.6
3	C	738	VAL	2.6
3	C	625	LYS	2.6
3	C	252	ASP	2.6
3	C	568	GLY	2.5
2	B	285	ALA	2.5
3	C	687	LEU	2.5
3	C	631	ALA	2.5
3	C	451	MET	2.5
3	C	268	LEU	2.4
2	B	98	GLY	2.4
2	B	55	GLU	2.4
3	C	273	LEU	2.4
3	C	630	ALA	2.4
1	A	339	ARG	2.3
3	C	387	GLN	2.3
3	C	709	LEU	2.3
3	C	232	PHE	2.3
3	C	279	ASP	2.3
1	A	281	ALA	2.3
1	A	334	THR	2.2
1	A	337	THR	2.2
3	C	622	ASP	2.2
3	C	464	ASN	2.2
1	A	2	ARG	2.2
3	C	480	ALA	2.2
3	C	352	SER	2.1
1	A	276	ILE	2.1
2	B	70	LEU	2.1
1	A	338	LYS	2.1
1	A	351	PHE	2.1
1	A	341	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
3	C	729	ALA	2.1
1	A	35	GLN	2.1
3	C	390	TYR	2.0
2	B	76	ASP	2.0
3	C	710	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 carbohydrates in this entry.

## 6.4 Ligands [i](#)

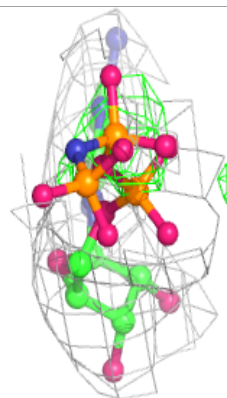
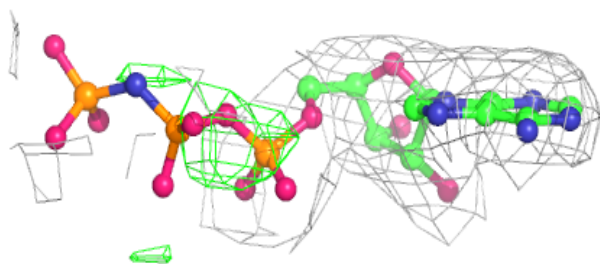
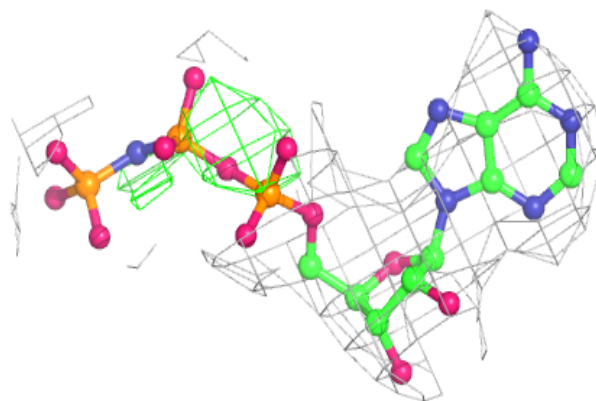
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
8	ANP	C	802	31/31	0.93	0.19	88,103,113,117	0
5	MG	A	502	1/1	0.94	0.32	54,54,54,54	0
7	LOC	B	502	29/29	0.95	0.22	75,84,90,92	0
4	GTP	A	501	32/32	0.95	0.26	72,82,89,93	0
6	GDP	B	501	28/28	0.96	0.20	103,108,119,122	0
5	MG	C	801	1/1	0.97	0.07	70,70,70,70	0

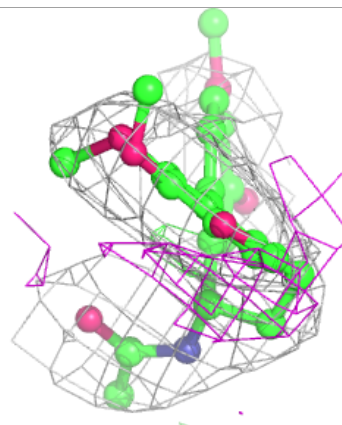
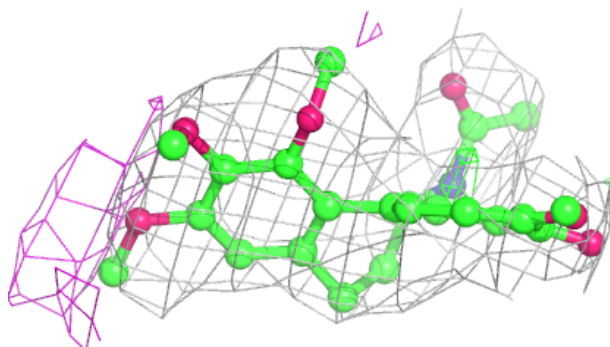
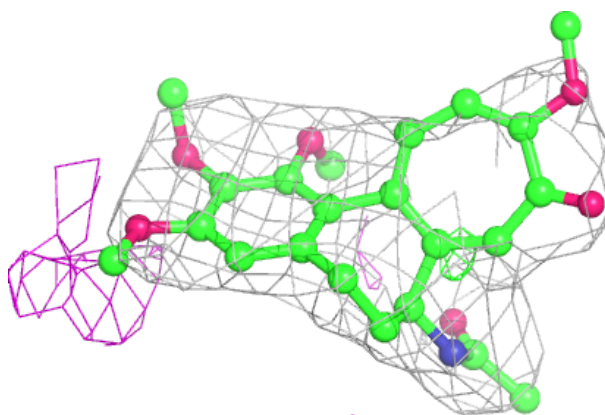
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around ANP C 802:**

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

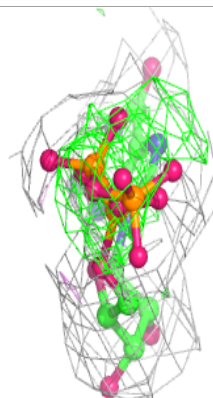
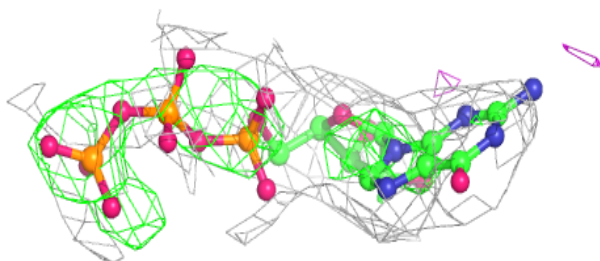
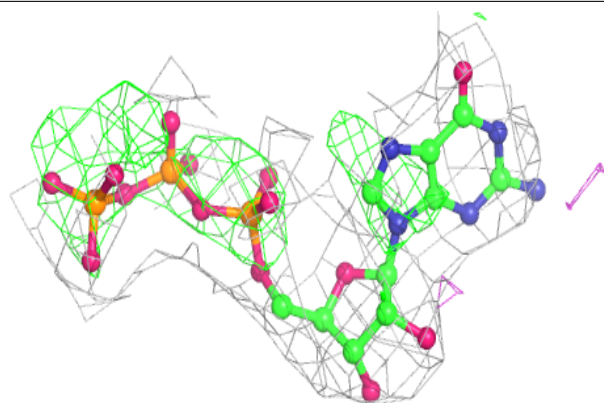
**Electron density around LOC B 502:**

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

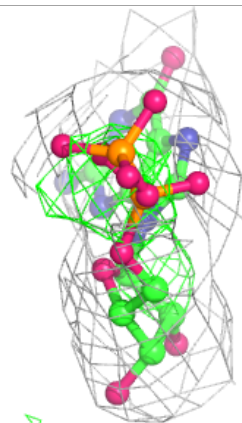
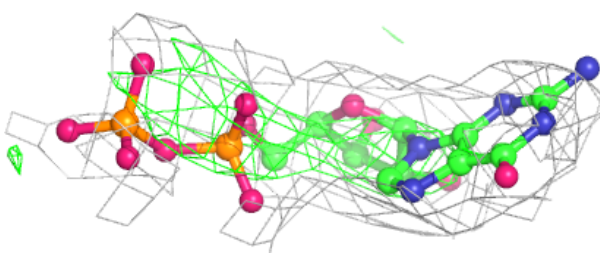
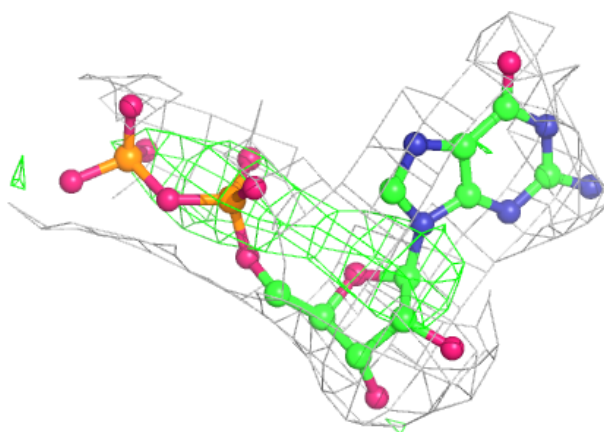


**Electron density around GTP A 501:**

$2mF_o-DF_c$  (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.