



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 27, 2025 – 12:14 PM EDT

PDB ID : 9YMG / pdb\_00009ymg  
Title : Human KIF18A-DARPin fusion protein bound to AMP-PNP and tubulin  
Authors : Lockbaum, G.J.; Lee, Y.-T.; Boriack-Sjodin, P.A.; Grigoriu, S.  
Deposited on : 2025-10-09  
Resolution : 2.41 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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 : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
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) : 2.46

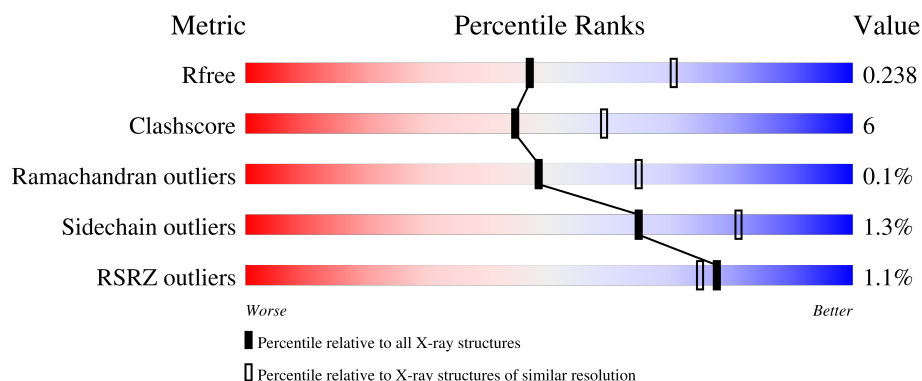
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.41 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))
$R_{free}$	164625	4642 (2.40-2.40)
Clashscore	180529	5218 (2.40-2.40)
Ramachandran outliers	177936	5158 (2.40-2.40)
Sidechain outliers	177891	5159 (2.40-2.40)
RSRZ outliers	164620	4642 (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  $\geq 3$ , 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>87%</div> <div>9%</div> <div>.</div> </div>
1	D	451	<div> <div>85%</div> <div>11%</div> <div>.</div> </div>
2	B	444	<div> <div>80%</div> <div>14%</div> <div>..</div> </div>
2	E	444	<div> <div>79%</div> <div>15%</div> <div>5%</div> </div>
3	C	555	<div> <div>76%</div> <div>11%</div> <div>12%</div> </div>

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Mol	Chain	Length	Quality of chain
3	F	555	<div><div><div>%</div><div><div></div></div><div>79%</div><div>8%</div><div>12%</div></div></div>

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 21620 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	436	Total	C	N	O	S	0	0	0
			3409	2158	580	649	22			
1	D	437	Total	C	N	O	S	0	0	0
			3416	2163	581	650	22			

- Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	425	Total	C	N	O	S	0	2	0
			3341	2099	569	647	26			
2	E	422	Total	C	N	O	S	0	1	0
			3314	2084	564	640	26			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	433	GLU	GLN	conflict	UNP P02554
B	434	GLU	GLY	conflict	UNP P02554
B	435	ASP	GLU	conflict	UNP P02554
B	437	GLY	GLU	conflict	UNP P02554
B	440	ALA	GLY	conflict	UNP P02554
B	443	GLU	ASP	conflict	UNP P02554
B	444	ALA	GLU	conflict	UNP P02554
E	433	GLU	GLN	conflict	UNP P02554
E	434	GLU	GLY	conflict	UNP P02554
E	435	ASP	GLU	conflict	UNP P02554
E	437	GLY	GLU	conflict	UNP P02554
E	440	ALA	GLY	conflict	UNP P02554
E	443	GLU	ASP	conflict	UNP P02554
E	444	ALA	GLU	conflict	UNP P02554

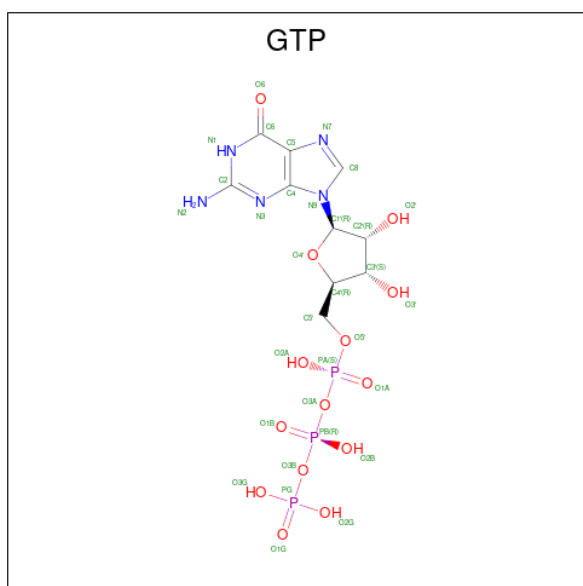
- Molecule 3 is a protein called Kinesin-like protein KIF18A, DARPin fusion protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	486	Total	C	N	O	S	0	1	0
			3737	2342	661	719	15			
3	F	488	Total	C	N	O	S	0	0	0
			3756	2354	665	722	15			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	SER	-	expression tag	UNP Q8NI77
C	-1	ASN	-	expression tag	UNP Q8NI77
C	0	ALA	-	expression tag	UNP Q8NI77
F	-2	SER	-	expression tag	UNP Q8NI77
F	-1	ASN	-	expression tag	UNP Q8NI77
F	0	ALA	-	expression tag	UNP Q8NI77

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

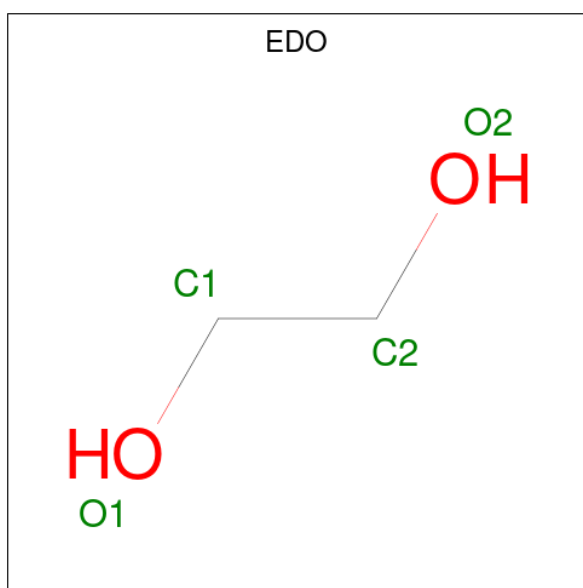


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
4	D	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

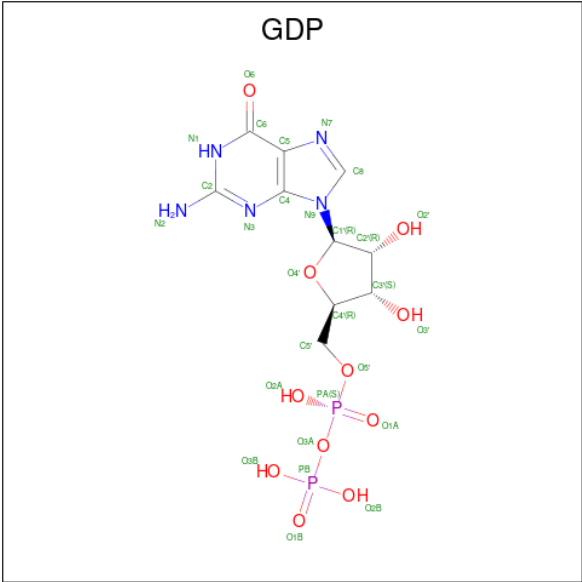
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	Mg	0	0
			2	2		
5	C	1	Total	Mg	0	0
			1	1		
5	D	2	Total	Mg	0	0
			2	2		
5	F	1	Total	Mg	0	0
			1	1		

- Molecule 6 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula:  $C_2H_6O_2$ ).



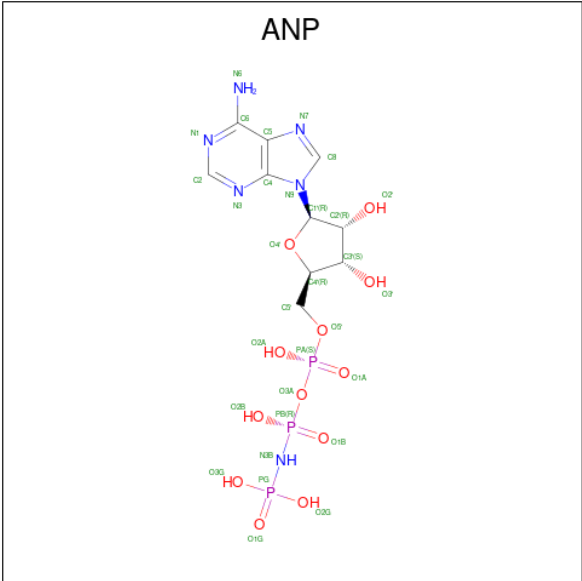
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 7 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula:  $C_{10}H_{15}N_5O_{11}P_2$ ).



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

- Molecule 8 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: C<sub>10</sub>H<sub>17</sub>N<sub>6</sub>O<sub>12</sub>P<sub>3</sub>).



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

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

- Molecule 9 is water.

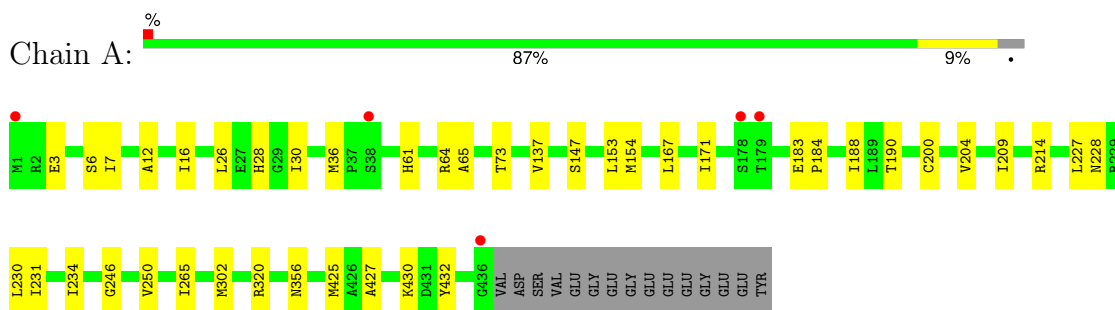
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	80	Total	O	0	0
			80	80		
9	B	79	Total	O	0	0
			79	79		
9	C	82	Total	O	0	0
			82	82		
9	D	88	Total	O	0	0
			88	88		
9	E	58	Total	O	0	0
			58	58		
9	F	68	Total	O	0	0
			68	68		



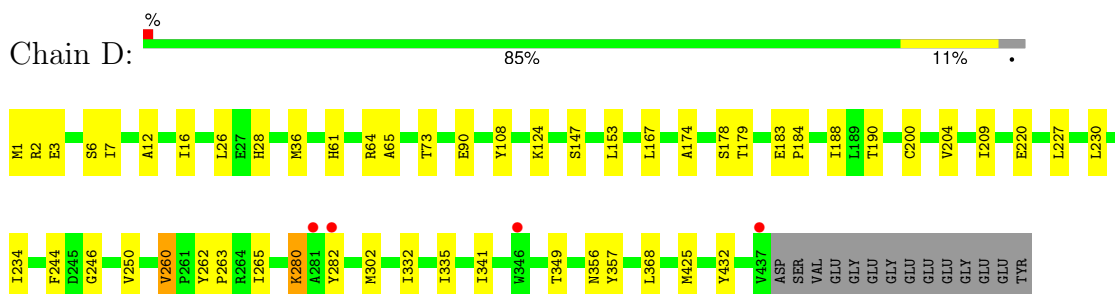
### 3 Residue-property plots

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.

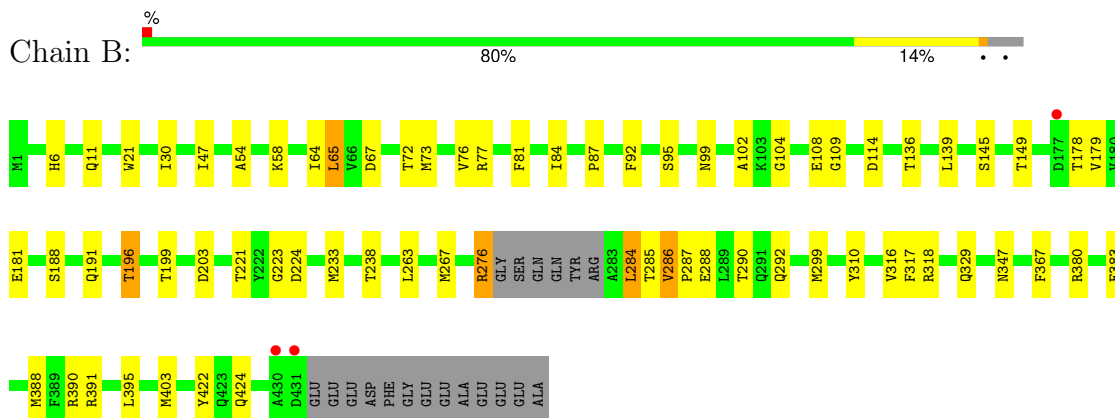
- Molecule 1: Tubulin alpha-1B chain



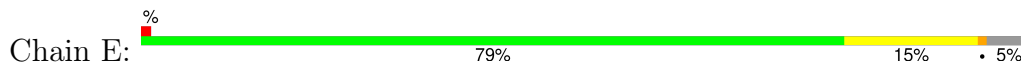
- Molecule 1: Tubulin alpha-1B chain



- Molecule 2: Tubulin beta chain

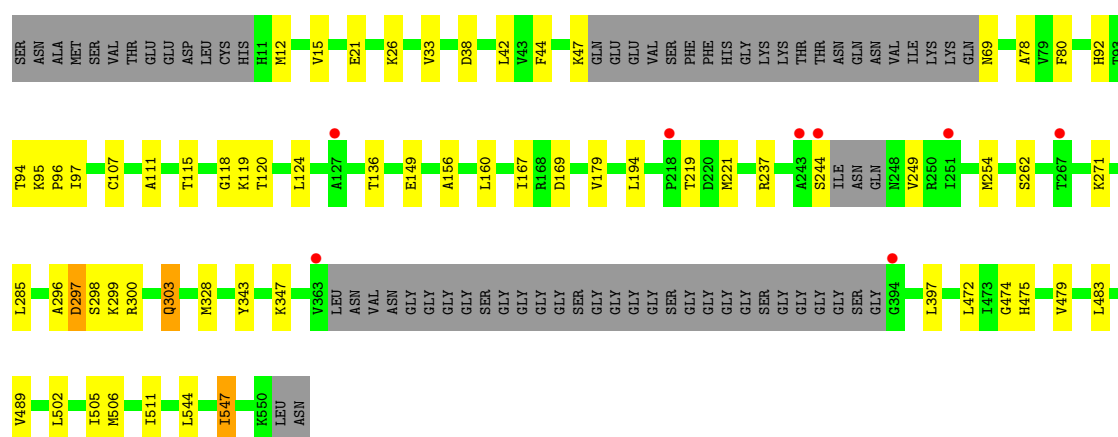
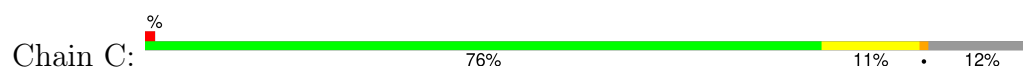


- Molecule 2: Tubulin beta chain

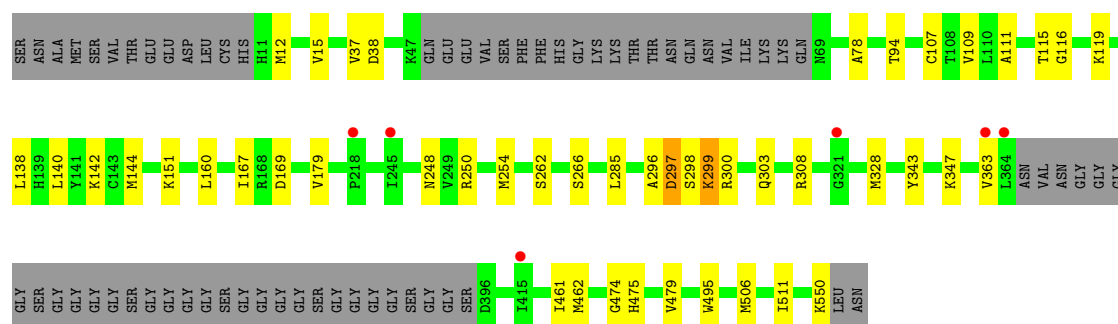
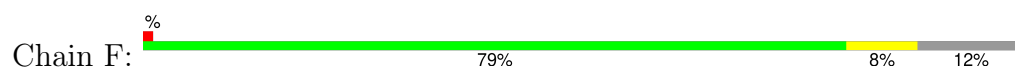




- Molecule 3: Kinesin-like protein KIF18A, DARPin fusion protein



- Molecule 3: Kinesin-like protein KIF18A, DARPin fusion protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	105.38Å 135.47Å 117.67Å 90.00° 107.67° 90.00°	Depositor
Resolution (Å)	48.67 – 2.41 48.67 – 2.41	Depositor EDS
% Data completeness (in resolution range)	99.3 (48.67-2.41) 99.3 (48.67-2.41)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.82 (at 2.39Å)	Xtrriage
Refinement program	REFMAC 5.8.0425	Depositor
R, $R_{free}$	0.191 , 0.238 0.193 , 0.238	Depositor DCC
$R_{free}$ test set	6162 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	48.8	Xtrriage
Anisotropy	0.183	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 52.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	21620	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	61.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 43.35 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.7873e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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 ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GTP, ANP, EDO, 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	0.45	0/3487	1.03	1/4733 (0.0%)
1	D	0.45	0/3494	1.03	2/4743 (0.0%)
2	B	0.45	0/3420	1.04	1/4634 (0.0%)
2	E	0.45	0/3390	1.03	1/4594 (0.0%)
3	C	0.46	0/3796	1.03	2/5132 (0.0%)
3	F	0.45	0/3813	1.03	1/5157 (0.0%)
All	All	0.45	0/21400	1.03	8/28993 (0.0%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	286	VAL	N-CA-CB	11.48	117.73	110.50
2	E	31	ASP	CA-CB-CG	6.14	118.75	112.60
1	D	244	PHE	N-CA-C	-5.76	101.65	109.95
1	D	73	THR	CA-CB-OG1	-5.66	101.11	109.60
1	A	73	THR	CA-CB-OG1	-5.33	101.61	109.60
3	C	38	ASP	CA-CB-CG	5.21	117.81	112.60
3	C	169	ASP	CA-CB-CG	5.18	117.78	112.60
3	F	169	ASP	CA-CB-CG	5.09	117.69	112.60

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	3409	0	3322	28	0
1	D	3416	0	3331	38	0
2	B	3341	0	3224	53	0
2	E	3314	0	3196	54	0
3	C	3737	0	3766	51	0
3	F	3756	0	3786	42	0
4	A	32	0	12	0	0
4	D	32	0	12	0	0
5	A	2	0	0	0	0
5	C	1	0	0	0	0
5	D	2	0	0	0	0
5	F	1	0	0	0	0
6	A	4	0	6	0	0
7	B	28	0	12	0	0
7	E	28	0	12	0	0
8	C	31	0	13	4	0
8	F	31	0	13	3	0
9	A	80	0	0	1	0
9	B	79	0	0	1	0
9	C	82	0	0	2	0
9	D	88	0	0	2	0
9	E	58	0	0	1	0
9	F	68	0	0	0	0
All	All	21620	0	20705	248	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 (248) 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)
1:A:12:ALA:HB1	1:A:171:ILE:HD12	1.54	0.90
2:B:102:ALA:HB2	2:B:403:MET:CE	2.04	0.88
1:D:108:TYR:HE1	3:F:266:SER:HB3	1.37	0.88
3:C:483:LEU:CD2	3:C:489[A]:VAL:HG12	2.05	0.87
2:E:73:MET:HA	2:E:76:VAL:HG12	1.53	0.87
2:E:102:ALA:HB2	2:E:403:MET:CE	2.06	0.84
1:A:427:ALA:HA	1:A:430:LYS:HE2	1.60	0.82
2:B:102:ALA:HB2	2:B:403:MET:HE1	1.63	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:108:TYR:CE1	3:F:266:SER:HB3	2.16	0.81
1:A:234:ILE:HD13	1:A:302:MET:SD	2.23	0.79
2:E:102:ALA:HB2	2:E:403:MET:HE1	1.65	0.76
1:D:368:LEU:HD12	9:D:657:HOH:O	1.85	0.76
3:C:483:LEU:CD2	3:C:489[B]:VAL:HG22	2.17	0.74
3:C:483:LEU:HD21	3:C:489[A]:VAL:HG12	1.72	0.71
2:B:73:MET:CE	2:B:92:PHE:HB3	2.20	0.71
2:B:347:ASN:HB3	9:B:623:HOH:O	1.91	0.70
3:F:111:ALA:HB1	3:F:119:LYS:HB2	1.74	0.70
2:E:73:MET:CE	2:E:92:PHE:HB3	2.23	0.69
3:C:111:ALA:HB1	3:C:119:LYS:HB2	1.76	0.68
1:D:209:ILE:HG22	1:D:227:LEU:HD22	1.75	0.67
1:A:12:ALA:O	1:A:16:ILE:HG12	1.94	0.67
1:D:12:ALA:O	1:D:16:ILE:HG12	1.95	0.67
3:C:483:LEU:HD22	3:C:489[A]:VAL:HG12	1.77	0.66
2:B:102:ALA:CB	2:B:403:MET:CE	2.75	0.65
3:C:33:VAL:O	3:C:44:PHE:O	2.14	0.65
3:C:94:THR:HG21	3:C:136:THR:HG23	1.77	0.65
2:E:196:THR:HG21	2:E:199:THR:OG1	1.96	0.65
2:B:73:MET:HE1	2:B:92:PHE:HB3	1.78	0.65
2:B:196:THR:HG21	2:B:199:THR:OG1	1.96	0.65
1:D:260:VAL:HG23	1:D:260:VAL:O	1.97	0.64
2:B:391:ARG:NH2	3:C:502:LEU:HD21	2.13	0.64
3:C:149:GLU:HB2	9:C:779:HOH:O	1.96	0.64
2:E:11:GLN:HG2	2:E:72:THR:HG21	1.78	0.64
1:D:108:TYR:HE1	3:F:266:SER:CB	2.09	0.64
2:B:388:MET:HE3	3:C:506:MET:HE2	1.80	0.64
3:C:483:LEU:HD22	3:C:489[B]:VAL:HG22	1.81	0.63
2:E:67:ASP:HB3	2:E:73:MET:HE2	1.79	0.63
2:E:390:ARG:HD2	3:F:495:TRP:CE2	2.33	0.63
3:F:250:ARG:HG2	3:F:363:VAL:HG22	1.79	0.63
2:B:67:ASP:HB3	2:B:73:MET:HE2	1.79	0.63
2:B:178:THR:HG23	2:B:181:GLU:HG3	1.80	0.62
2:E:102:ALA:CB	2:E:403:MET:CE	2.77	0.62
3:F:37:VAL:HG23	3:F:38:ASP:H	1.63	0.62
2:E:73:MET:HE1	2:E:92:PHE:HB3	1.82	0.62
2:B:145:SER:HB2	2:B:188:SER:OG	2.01	0.61
1:D:234:ILE:HD13	1:D:302:MET:HE3	1.81	0.61
2:E:304:ASP:HB3	2:E:307:HIS:ND1	2.15	0.61
2:B:238:THR:HG21	2:B:318:ARG:HD3	1.83	0.61
2:E:149:THR:HB	2:E:191:GLN:HG2	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:145:SER:HB2	2:E:188:SER:OG	2.01	0.60
1:A:209:ILE:HG22	1:A:227:LEU:HD22	1.82	0.60
2:B:149:THR:HB	2:B:191:GLN:HG2	1.84	0.59
1:A:154:MET:HE2	1:A:154:MET:HA	1.85	0.59
1:D:204:VAL:HG22	1:D:302:MET:SD	2.42	0.59
2:E:388:MET:HE3	3:F:506:MET:HE2	1.84	0.58
2:B:267:MET:HE2	2:B:299:MET:HE2	1.85	0.58
2:E:104:GLY:O	2:E:109:GLY:HA3	2.02	0.58
2:E:179:VAL:HB	2:E:388:MET:HE3	1.86	0.58
2:E:166:THR:HG23	2:E:168:SER:OG	2.04	0.58
3:C:298:SER:O	3:C:299:LYS:HG2	2.04	0.57
3:C:489[B]:VAL:HG23	9:C:742:HOH:O	2.03	0.57
3:F:15:VAL:HG22	3:F:78:ALA:HB3	1.86	0.57
2:B:179:VAL:HB	2:B:388:MET:HE3	1.85	0.57
2:B:104:GLY:O	2:B:109:GLY:HA3	2.04	0.57
3:F:119:LYS:HG2	8:F:601:ANP:O1B	2.05	0.56
3:C:15:VAL:HG22	3:C:78:ALA:HB3	1.87	0.56
1:D:265:ILE:HG23	1:D:432:TYR:CE1	2.40	0.56
2:E:156:ARG:HH12	2:E:197:ASP:CG	2.14	0.56
1:A:16:ILE:HG13	1:A:171:ILE:HD11	1.87	0.56
2:E:24:ILE:HD11	2:E:241:ARG:HD2	1.86	0.56
2:E:267:MET:HE2	2:E:299:MET:HE2	1.87	0.56
3:C:94:THR:HG21	3:C:136:THR:CG2	2.36	0.56
3:F:116:GLY:H	8:F:601:ANP:HNB1	1.51	0.55
1:A:265:ILE:HG23	1:A:432:TYR:CE1	2.42	0.55
2:B:390:ARG:HB2	2:B:391:ARG:HH11	1.71	0.54
3:F:94:THR:CG2	3:F:109:VAL:HG21	2.37	0.54
3:F:474:GLY:HA2	3:F:511:ILE:HD12	1.89	0.54
3:F:300:ARG:HD3	3:F:303:GLN:CB	2.37	0.54
3:C:474:GLY:HA2	3:C:511:ILE:HD12	1.90	0.54
3:F:167:ILE:HD12	3:F:179:VAL:CG2	2.37	0.53
2:B:285:THR:HG23	2:B:287:PRO:HD2	1.91	0.53
2:B:54:ALA:HB3	2:B:58:LYS:HB2	1.90	0.53
3:C:237:ARG:HG3	3:C:249:VAL:HG11	1.91	0.53
2:E:11:GLN:HG2	2:E:72:THR:CG2	2.38	0.53
2:E:221:THR:HG22	2:E:224:ASP:OD2	2.09	0.53
1:A:30:ILE:CG1	1:A:36:MET:HE3	2.39	0.53
2:E:102:ALA:HB2	2:E:403:MET:HE3	1.90	0.52
2:B:221:THR:HG22	2:B:224:ASP:OD2	2.09	0.52
1:A:137:VAL:HG21	1:A:154:MET:CE	2.40	0.52
2:E:21:TRP:HA	2:E:24:ILE:HG22	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:167:ILE:HD12	3:F:179:VAL:HG22	1.91	0.52
2:B:424:GLN:HG3	3:C:303:GLN:HG3	1.92	0.52
3:C:167:ILE:HD12	3:C:179:VAL:CG2	2.40	0.52
3:C:300:ARG:HB3	3:C:303:GLN:HB2	1.91	0.52
1:D:260:VAL:O	1:D:260:VAL:CG2	2.58	0.52
2:B:284:LEU:HD21	2:B:292:GLN:NE2	2.26	0.51
3:C:47:LYS:NZ	3:C:69:ASN:O	2.44	0.50
2:E:44:LEU:O	2:E:47:ILE:HG13	2.12	0.50
2:B:290:THR:HG22	2:B:317:PHE:HZ	1.77	0.50
1:D:1:MET:HG3	1:D:2:ARG:N	2.27	0.50
2:E:31:ASP:OD1	2:E:32:PRO:HD2	2.12	0.50
2:B:136:THR:HG21	2:B:233:MET:HE1	1.93	0.50
3:F:151:LYS:HE2	3:F:250:ARG:HH22	1.77	0.50
2:E:286:VAL:HB	2:E:287:PRO:HD3	1.94	0.50
2:B:102:ALA:HB2	2:B:403:MET:HE3	1.89	0.50
2:B:388:MET:CE	3:C:506:MET:HE2	2.41	0.50
2:B:299:MET:HE1	2:B:367:PHE:CE2	2.47	0.50
2:E:139:LEU:HA	2:E:145:SER:HB3	1.94	0.49
2:E:299:MET:HE1	2:E:367:PHE:CE2	2.47	0.49
2:E:48:ASN:HB2	9:E:636:HOH:O	2.11	0.49
3:F:12:MET:HE2	3:F:328:MET:HB2	1.94	0.49
1:A:28:HIS:O	1:A:36:MET:HE2	2.11	0.49
1:D:188:ILE:HG23	1:D:425:MET:HG3	1.94	0.49
3:F:115:THR:HG23	8:F:601:ANP:O1G	2.12	0.49
1:A:137:VAL:HG21	1:A:154:MET:HE1	1.94	0.49
2:E:410:GLU:OE2	3:F:308:ARG:NH2	2.46	0.49
2:E:430:ALA:O	2:E:431:ASP:C	2.56	0.48
2:B:11:GLN:HG2	2:B:72:THR:HG21	1.95	0.48
1:A:188:ILE:HG23	1:A:425:MET:HG3	1.96	0.48
2:B:139:LEU:HA	2:B:145:SER:HB3	1.94	0.48
1:A:7:ILE:HG21	1:A:153:LEU:HD21	1.96	0.47
1:D:7:ILE:HG21	1:D:153:LEU:HD21	1.96	0.47
2:B:64:ILE:C	2:B:65:LEU:HD23	2.39	0.47
2:B:310:TYR:CE1	2:B:367:PHE:HZ	2.32	0.47
2:E:388:MET:CE	3:F:506:MET:HE2	2.44	0.47
2:E:166:THR:CG2	2:E:199:THR:HG23	2.44	0.47
3:C:12:MET:HE2	3:C:328:MET:HB2	1.95	0.47
3:C:119:LYS:HG2	8:C:601:ANP:O1B	2.14	0.47
3:C:120:THR:HG23	3:C:124:LEU:HD11	1.96	0.47
3:C:483:LEU:HD22	3:C:489[A]:VAL:CG1	2.42	0.47
1:D:1:MET:HG3	1:D:2:ARG:H	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:37:VAL:HG23	3:F:38:ASP:N	2.30	0.47
2:B:285:THR:HG22	2:B:288:GLU:CG	2.45	0.47
1:D:28:HIS:O	1:D:36:MET:HE3	2.14	0.47
1:A:214:ARG:HH12	3:F:550:LYS:C	2.23	0.47
1:D:204:VAL:HA	1:D:302:MET:HG2	1.96	0.46
2:E:81:PHE:O	2:E:84:ILE:HG22	2.14	0.46
2:E:310:TYR:CE1	2:E:367:PHE:HZ	2.33	0.46
2:B:285:THR:HG22	2:B:288:GLU:HG3	1.97	0.46
2:E:126:SER:O	2:E:126:SER:OG	2.34	0.46
2:B:81:PHE:O	2:B:84:ILE:HG22	2.15	0.46
2:E:47:ILE:HD12	2:E:48:ASN:N	2.30	0.46
1:A:320:ARG:HG3	9:A:610:HOH:O	2.14	0.46
2:E:290:THR:HG22	2:E:317:PHE:HZ	1.81	0.46
3:F:298:SER:O	3:F:300:ARG:NE	2.40	0.46
1:D:179:THR:HG21	9:D:622:HOH:O	2.15	0.45
2:B:390:ARG:HB2	2:B:391:ARG:NH1	2.31	0.45
1:D:167:LEU:HG	1:D:200:CYS:HB3	1.97	0.45
3:F:300:ARG:HD3	3:F:303:GLN:HB2	1.97	0.45
2:E:263:LEU:HG	2:E:422:TYR:CE1	2.52	0.45
1:D:332:ILE:O	1:D:335:ILE:HG13	2.16	0.45
3:F:296:ALA:O	3:F:297:ASP:C	2.59	0.45
3:C:160:LEU:C	3:C:160:LEU:HD12	2.42	0.45
1:D:36:MET:HB3	1:D:61:HIS:CE1	2.52	0.45
1:A:167:LEU:HG	1:A:200:CYS:HB3	1.98	0.45
2:B:238:THR:OG1	2:B:316:VAL:HG11	2.18	0.44
2:B:263:LEU:HG	2:B:422:TYR:CE1	2.52	0.44
3:C:21:GLU:HB2	3:C:26:LYS:HE3	1.99	0.44
3:F:160:LEU:C	3:F:160:LEU:HD12	2.42	0.44
1:A:209:ILE:HG23	1:A:230:LEU:HD23	2.00	0.44
3:C:115:THR:HG23	8:C:601:ANP:O2G	2.18	0.44
3:C:296:ALA:O	3:C:297:ASP:C	2.60	0.44
3:C:544:LEU:O	3:C:547:ILE:HG13	2.18	0.44
3:C:219:THR:HG22	3:C:221:MET:H	1.82	0.44
2:B:30:ILE:HD11	2:B:47:ILE:HD11	2.00	0.43
1:D:209:ILE:HG23	1:D:230:LEU:HD23	2.00	0.43
2:B:77:ARG:HH12	2:B:87:PRO:HB3	1.83	0.43
3:C:237:ARG:HG3	3:C:249:VAL:CG1	2.48	0.43
3:C:118:GLY:HA2	8:C:601:ANP:O1A	2.18	0.43
2:E:65:LEU:HD12	2:E:65:LEU:N	2.34	0.43
3:F:107:CYS:O	3:F:254:MET:HA	2.19	0.43
1:D:341:ILE:N	1:D:341:ILE:HD12	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:349:THR:O	1:D:349:THR:HG22	2.19	0.43
2:E:54:ALA:HB3	2:E:58:LYS:HB3	1.99	0.43
3:C:156:ALA:HB1	3:C:194:LEU:HG	2.01	0.43
1:D:183:GLU:N	1:D:184:PRO:CD	2.82	0.43
2:E:286:VAL:HG22	2:E:321:MET:CE	2.49	0.43
1:A:183:GLU:N	1:A:184:PRO:CD	2.82	0.43
2:B:203:ASP:OD2	2:B:380:ARG:NH2	2.47	0.43
2:E:166:THR:CG2	2:E:168:SER:OG	2.66	0.43
3:F:461:ILE:HG23	3:F:462:MET:HE3	2.00	0.43
1:A:36:MET:HB3	1:A:61:HIS:CE1	2.53	0.43
3:C:80:PHE:HZ	3:C:92:HIS:HB2	1.84	0.43
3:C:119:LYS:NZ	8:C:601:ANP:O1G	2.52	0.43
3:C:120:THR:CG2	3:C:124:LEU:HD11	2.49	0.43
2:B:284:LEU:HD21	2:B:292:GLN:CD	2.44	0.43
3:C:475:HIS:O	3:C:479:VAL:HG23	2.19	0.43
1:D:220:GLU:HG2	2:E:324:LYS:HD2	2.00	0.43
1:D:204:VAL:HG13	1:D:302:MET:HE2	2.01	0.42
3:F:111:ALA:CB	3:F:119:LYS:HB2	2.47	0.42
3:C:299:LYS:CB	3:F:299:LYS:HE3	2.50	0.42
1:D:147:SER:HB2	1:D:190:THR:HB	2.01	0.42
2:E:410:GLU:CD	3:F:308:ARG:HH22	2.27	0.42
3:F:475:HIS:O	3:F:479:VAL:HG23	2.18	0.42
2:B:395:LEU:HD23	2:B:395:LEU:HA	1.90	0.42
1:D:282:TYR:O	1:D:282:TYR:CG	2.73	0.42
1:D:262:TYR:HA	1:D:263:PRO:HD3	1.96	0.42
3:C:107:CYS:O	3:C:254:MET:HA	2.20	0.42
2:E:175:VAL:HG11	2:E:204:ASN:HB3	2.01	0.42
2:E:390:ARG:HD2	3:F:495:TRP:NE1	2.35	0.42
1:A:6:SER:O	1:A:65:ALA:HA	2.20	0.42
1:A:246:GLY:O	1:A:250:VAL:HG12	2.19	0.42
3:C:111:ALA:CB	3:C:119:LYS:HB2	2.47	0.42
2:E:203:ASP:OD2	2:E:380:ARG:NH2	2.47	0.42
2:B:223:GLY:C	2:B:276:ARG:HH21	2.28	0.41
2:B:290:THR:HG22	2:B:317:PHE:CZ	2.54	0.41
1:A:3:GLU:HG2	1:A:64:ARG:CZ	2.51	0.41
2:B:11:GLN:HG2	2:B:72:THR:CG2	2.50	0.41
1:D:174:ALA:O	1:D:178:SER:HB3	2.20	0.41
3:C:298:SER:O	3:C:300:ARG:HG3	2.20	0.41
1:A:147:SER:HB2	1:A:190:THR:HB	2.02	0.41
1:D:280:LYS:HE2	1:D:280:LYS:HB3	1.97	0.41
3:F:262:SER:HB3	3:F:285:LEU:HD12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:ILE:HD13	1:A:228:ASN:CG	2.46	0.41
1:A:184:PRO:O	1:A:188:ILE:HG12	2.21	0.41
2:B:67:ASP:CB	2:B:73:MET:HE2	2.49	0.41
3:C:271:LYS:HD2	3:C:271:LYS:HA	1.94	0.41
2:E:324:LYS:HE2	2:E:328:GLU:OE2	2.20	0.41
3:F:343:TYR:CZ	3:F:347:LYS:HD3	2.55	0.41
2:B:149:THR:HB	2:B:191:GLN:CG	2.49	0.41
3:C:42:LEU:HD12	3:C:42:LEU:C	2.46	0.41
2:E:189:VAL:O	2:E:193:VAL:HG23	2.21	0.41
1:D:6:SER:O	1:D:65:ALA:HA	2.20	0.41
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.39	0.41
2:B:391:ARG:HG3	3:C:472:LEU:HD22	2.02	0.41
3:C:474:GLY:HA2	3:C:511:ILE:CD1	2.51	0.41
1:D:184:PRO:O	1:D:188:ILE:HG12	2.20	0.41
1:D:246:GLY:O	1:D:250:VAL:HG12	2.21	0.41
2:E:246:LEU:HD21	2:E:350:LYS:HB3	2.03	0.41
3:F:474:GLY:HA2	3:F:511:ILE:CD1	2.50	0.41
1:A:234:ILE:CD1	1:A:302:MET:SD	3.03	0.41
3:F:297:ASP:C	3:F:299:LYS:N	2.77	0.41
2:B:67:ASP:HB3	2:B:73:MET:CE	2.50	0.40
3:C:262:SER:HB3	3:C:285:LEU:HD12	2.02	0.40
1:D:3:GLU:HG2	1:D:64:ARG:CZ	2.51	0.40
3:F:138:LEU:O	3:F:142:LYS:HG2	2.21	0.40
3:F:140:LEU:HG	3:F:144:MET:HE2	2.01	0.40
3:C:95:LYS:HB3	3:C:96:PRO:HD3	2.04	0.40
3:C:343:TYR:CE2	3:C:347:LYS:HD2	2.56	0.40
1:D:356:ASN:C	1:D:356:ASN:OD1	2.65	0.40
2:B:383:GLU:HG3	3:C:505:ILE:HG23	2.04	0.40
1:D:356:ASN:OD1	1:D:357:TYR:N	2.55	0.40
2:E:6:HIS:CD2	2:E:21:TRP:HE1	2.39	0.40
2:E:73:MET:HE1	2:E:92:PHE:CB	2.50	0.40
1:A:204:VAL:HG11	1:A:231:ILE:HG12	2.03	0.40
2:B:95:SER:OG	2:B:108:GLU:HG2	2.21	0.40
3:F:12:MET:CE	3:F:328:MET:HB2	2.52	0.40
3:F:297:ASP:C	3:F:299:LYS:H	2.30	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	434/451 (96%)	427 (98%)	7 (2%)	0	100	100
1	D	435/451 (96%)	429 (99%)	6 (1%)	0	100	100
2	B	423/444 (95%)	414 (98%)	9 (2%)	0	100	100
2	E	419/444 (94%)	410 (98%)	9 (2%)	0	100	100
3	C	479/555 (86%)	465 (97%)	13 (3%)	1 (0%)	44	59
3	F	482/555 (87%)	467 (97%)	14 (3%)	1 (0%)	44	59
All	All	2672/2900 (92%)	2612 (98%)	58 (2%)	2 (0%)	48	65

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	F	297	ASP
3	C	297	ASP

### 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	367/379 (97%)	365 (100%)	2 (0%)	86	94
1	D	368/379 (97%)	363 (99%)	5 (1%)	62	79
2	B	367/380 (97%)	358 (98%)	9 (2%)	42	63
2	E	363/380 (96%)	357 (98%)	6 (2%)	56	75
3	C	410/455 (90%)	405 (99%)	5 (1%)	67	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	F	412/455 (90%)	410 (100%)	2 (0%)	86	94
All	All	2287/2428 (94%)	2258 (99%)	29 (1%)	65	81

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	LEU
1	A	356	ASN
2	B	65	LEU
2	B	76	VAL
2	B	99	ASN
2	B	114	ASP
2	B	196	THR
2	B	276	ARG
2	B	284	LEU
2	B	286	VAL
2	B	329	GLN
3	C	97	ILE
3	C	244	SER
3	C	303	GLN
3	C	397	LEU
3	C	547	ILE
1	D	26	LEU
1	D	90	GLU
1	D	124	LYS
1	D	260	VAL
1	D	280	LYS
2	E	99	ASN
2	E	126	SER
2	E	166	THR
2	E	196	THR
2	E	329	GLN
2	E	342	VAL
3	F	248	ASN
3	F	299	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	99	ASN
3	C	121	HIS

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Mol	Chain	Res	Type
3	C	280	ASN
3	C	323	ASN
3	C	362	ASN
1	D	15	GLN
1	D	85	GLN
1	D	88	HIS
1	D	101	ASN
1	D	256	GLN
1	D	266	HIS
2	E	396	HIS
3	F	205	HIS
3	F	238	GLN
3	F	280	ASN
3	F	323	ASN
3	F	362	ASN
3	F	442	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 6 are monoatomic - leaving 7 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	ANP	C	601	5	29,33,33	1.22	5 (17%)	31,52,52	1.17	4 (12%)
8	ANP	F	601	5	29,33,33	1.28	5 (17%)	31,52,52	1.20	4 (12%)
7	GDP	E	501	-	25,30,30	1.01	2 (8%)	30,47,47	0.70	0
6	EDO	A	504	-	3,3,3	0.14	0	2,2,2	0.41	0
7	GDP	B	501	-	25,30,30	0.98	2 (8%)	30,47,47	0.71	1 (3%)
4	GTP	A	501	5	29,34,34	1.04	2 (6%)	35,54,54	0.77	0
4	GTP	D	501	5	29,34,34	1.03	2 (6%)	35,54,54	0.80	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	ANP	C	601	5	-	3/14/38/38	0/3/3/3
8	ANP	F	601	5	-	2/14/38/38	0/3/3/3
7	GDP	E	501	-	-	5/12/32/32	0/3/3/3
6	EDO	A	504	-	-	1/1/1/1	-
7	GDP	B	501	-	-	4/12/32/32	0/3/3/3
4	GTP	A	501	5	-	4/18/38/38	0/3/3/3
4	GTP	D	501	5	-	5/18/38/38	0/3/3/3

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	F	601	ANP	PG-O1G	3.45	1.51	1.46
8	C	601	ANP	PB-O1B	3.04	1.50	1.46
8	F	601	ANP	PB-O1B	2.97	1.50	1.46
4	D	501	GTP	C5-C6	-2.69	1.42	1.47
8	C	601	ANP	PG-O1G	2.68	1.50	1.46
7	E	501	GDP	C5-C6	-2.66	1.42	1.47
4	A	501	GTP	C5-C6	-2.58	1.42	1.47
8	F	601	ANP	PG-O3G	-2.45	1.50	1.56
7	B	501	GDP	C5-C6	-2.45	1.42	1.47
8	F	601	ANP	PG-O2G	-2.38	1.50	1.56
8	F	601	ANP	PB-O2B	-2.28	1.50	1.56
8	C	601	ANP	PG-O3G	-2.24	1.50	1.56
8	C	601	ANP	PG-O2G	-2.23	1.50	1.56
4	A	501	GTP	C8-N7	-2.14	1.31	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	C	601	ANP	PB-O2B	-2.12	1.51	1.56
4	D	501	GTP	C8-N7	-2.09	1.31	1.34
7	B	501	GDP	C8-N7	-2.03	1.31	1.34
7	E	501	GDP	C8-N7	-2.03	1.31	1.34

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	F	601	ANP	O2B-PB-O1B	4.09	118.64	109.87
8	C	601	ANP	O2B-PB-O1B	4.07	118.61	109.87
8	F	601	ANP	C5-C6-N6	2.38	123.93	120.31
8	F	601	ANP	O3G-PG-O1G	-2.27	107.75	113.45
8	F	601	ANP	O2G-PG-O1G	-2.27	107.76	113.45
8	C	601	ANP	C5-C6-N6	2.20	123.67	120.31
7	B	501	GDP	O6-C6-C5	2.10	128.48	124.32
8	C	601	ANP	O1G-PG-N3B	-2.06	108.74	111.77
8	C	601	ANP	O3G-PG-O1G	-2.05	108.31	113.45

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	501	GTP	PB-O3B-PG-O3G
4	A	501	GTP	C5'-O5'-PA-O3A
4	A	501	GTP	C5'-O5'-PA-O1A
4	A	501	GTP	C5'-O5'-PA-O2A
4	D	501	GTP	PB-O3B-PG-O2G
4	D	501	GTP	C5'-O5'-PA-O3A
4	D	501	GTP	C5'-O5'-PA-O1A
4	D	501	GTP	C5'-O5'-PA-O2A
7	B	501	GDP	C5'-O5'-PA-O3A
7	B	501	GDP	C5'-O5'-PA-O1A
7	B	501	GDP	C5'-O5'-PA-O2A
7	E	501	GDP	C5'-O5'-PA-O3A
7	E	501	GDP	C5'-O5'-PA-O1A
7	E	501	GDP	C5'-O5'-PA-O2A
8	C	601	ANP	PB-N3B-PG-O1G
8	C	601	ANP	PG-N3B-PB-O1B
8	C	601	ANP	PA-O3A-PB-O2B
8	F	601	ANP	PG-N3B-PB-O1B
8	F	601	ANP	PA-O3A-PB-O2B
4	D	501	GTP	PB-O3B-PG-O1G

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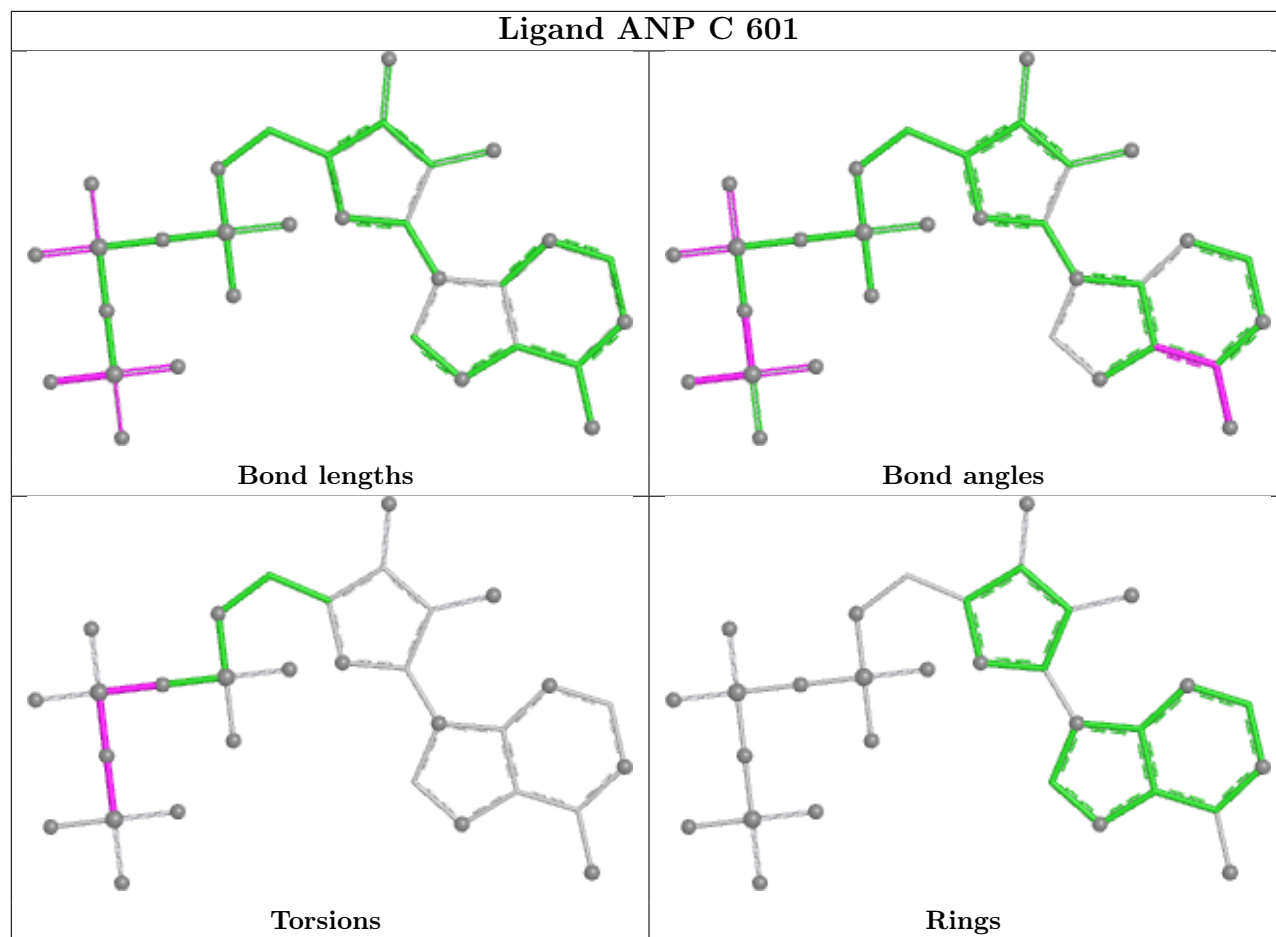
Mol	Chain	Res	Type	Atoms
7	E	501	GDP	PB-O3A-PA-O1A
6	A	504	EDO	O1-C1-C2-O2
7	B	501	GDP	PB-O3A-PA-O2A
7	E	501	GDP	PB-O3A-PA-O2A

There are no ring outliers.

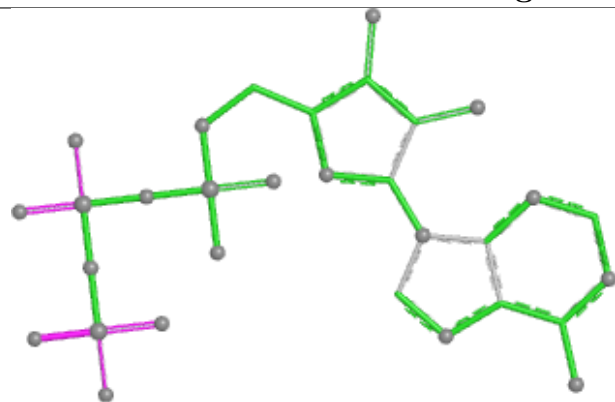
2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	C	601	ANP	4	0
8	F	601	ANP	3	0

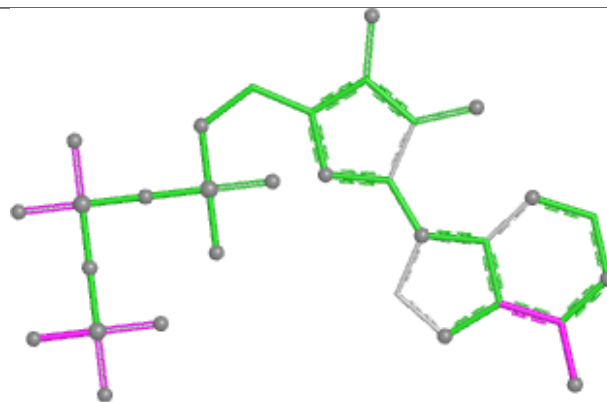
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



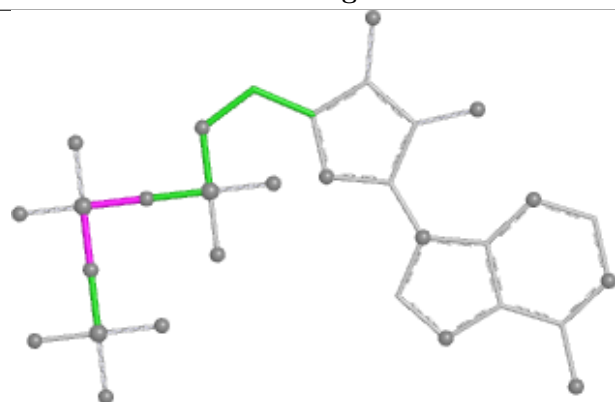
## Ligand ANP F 601



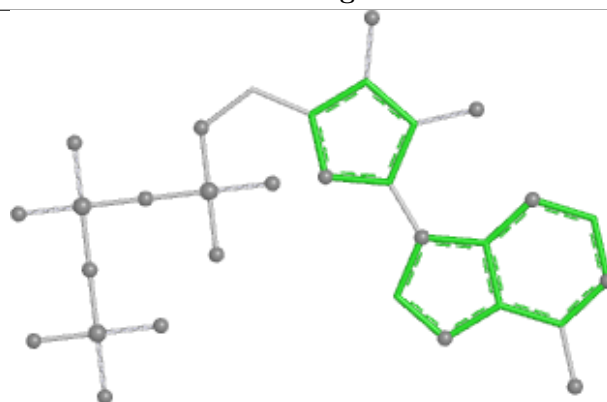
Bond lengths



Bond angles

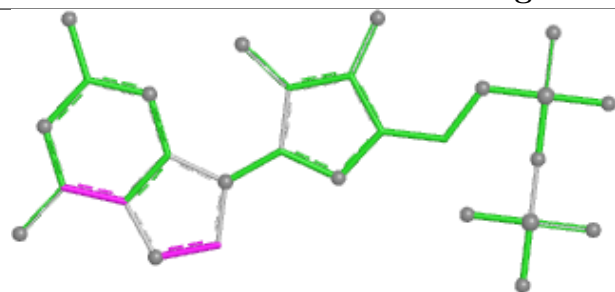


Torsions

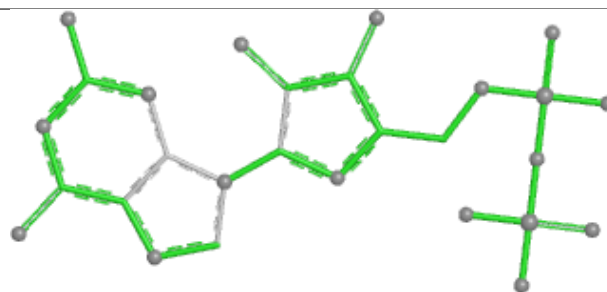


Rings

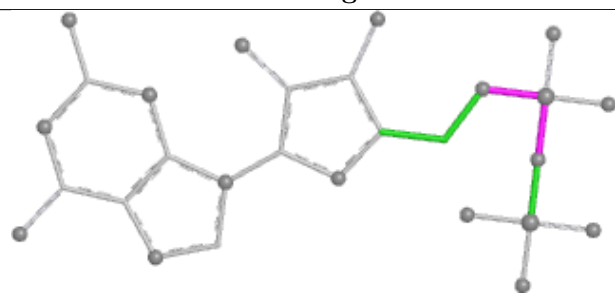
## Ligand GDP E 501



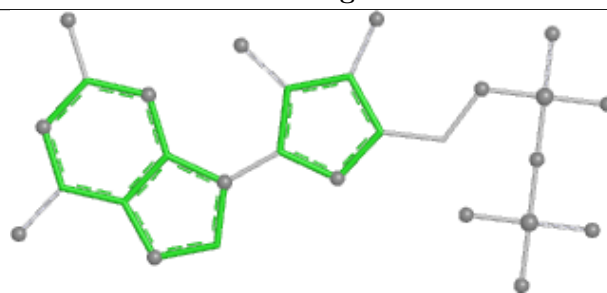
Bond lengths



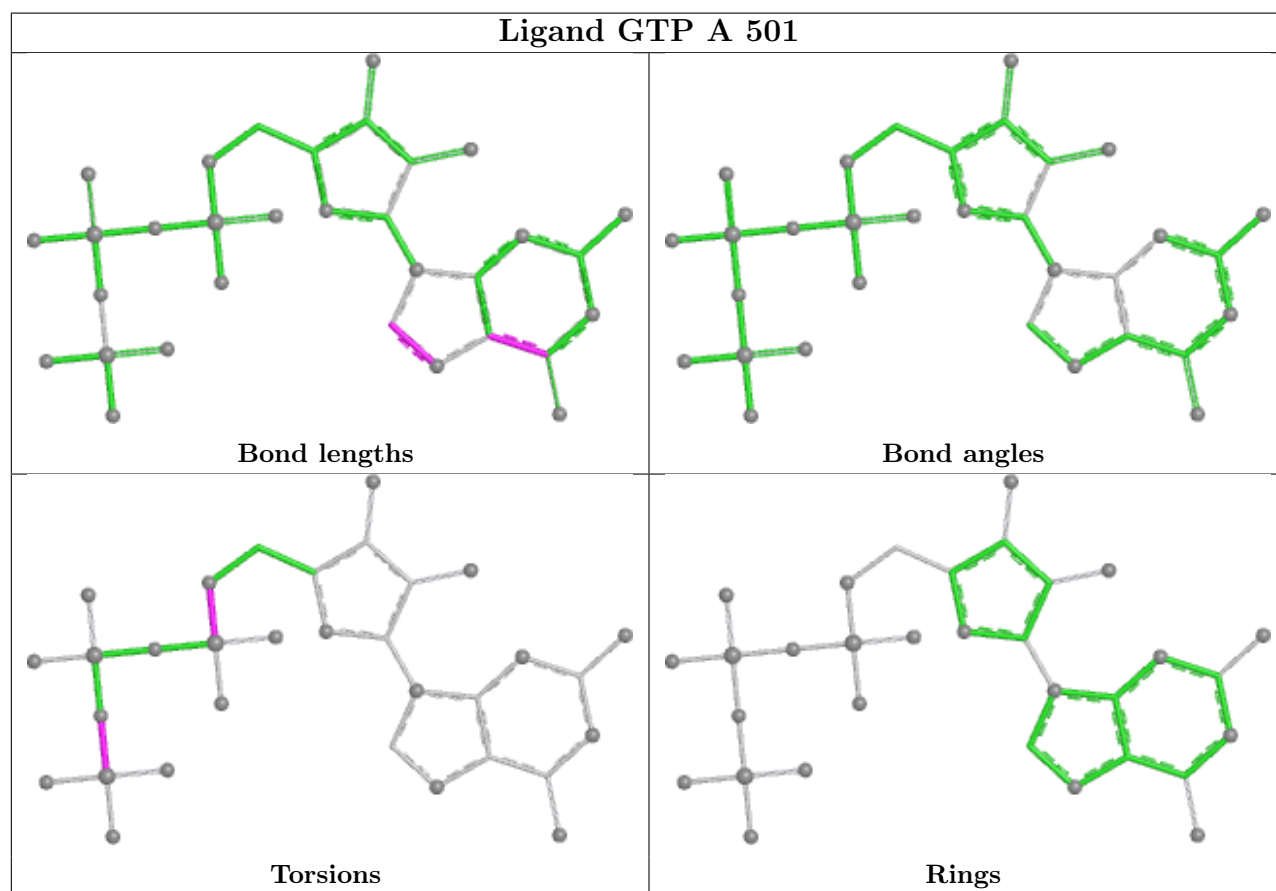
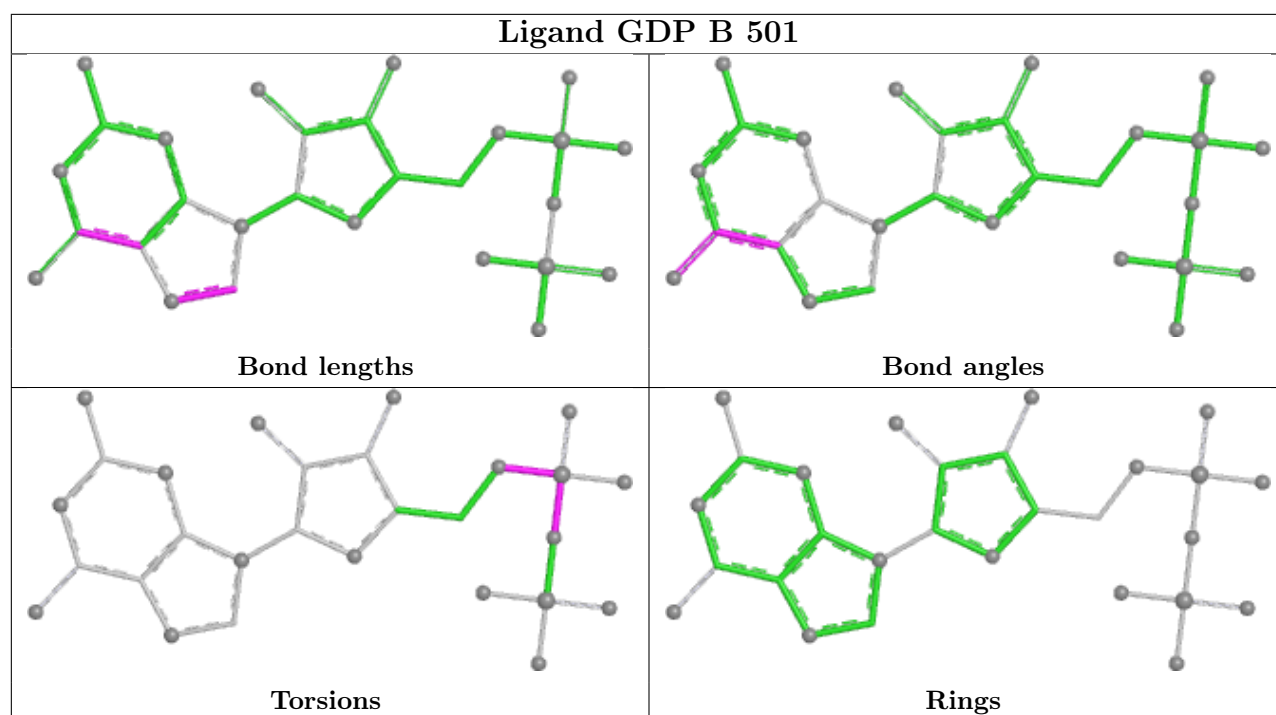
Bond angles

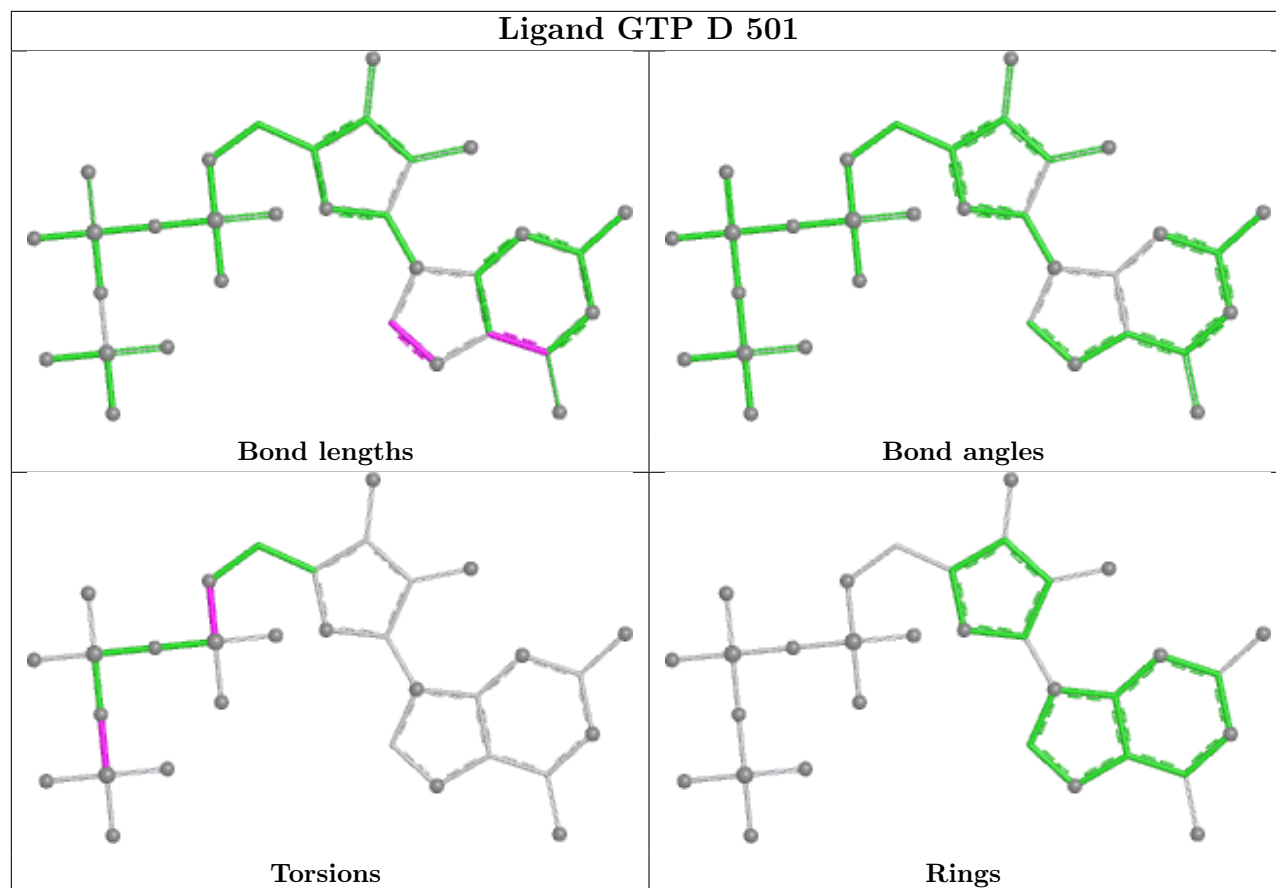


Torsions



Rings





## 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	436/451 (96%)	-0.52	5 (1%) 77 75	33, 51, 91, 127	0
1	D	437/451 (96%)	-0.56	4 (0%) 81 78	30, 49, 94, 141	0
2	B	425/444 (95%)	-0.47	3 (0%) 84 81	32, 50, 89, 125	2 (0%)
2	E	422/444 (95%)	-0.41	3 (0%) 84 81	27, 56, 96, 125	1 (0%)
3	C	486/555 (87%)	-0.12	8 (1%) 70 67	32, 69, 125, 155	1 (0%)
3	F	488/555 (87%)	-0.32	6 (1%) 76 73	39, 64, 113, 152	0
All	All	2694/2900 (92%)	-0.39	29 (1%) 77 75	27, 56, 104, 155	4 (0%)

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	281	ALA	4.3
2	B	431	ASP	3.3
2	E	430	ALA	3.3
3	C	243	ALA	3.0
2	B	430	ALA	2.9
3	F	245	ILE	2.9
1	A	1	MET	2.8
3	C	363	VAL	2.7
3	C	394	GLY	2.6
1	A	38	SER	2.5
3	C	218	PRO	2.5
3	C	127	ALA	2.5
2	B	177	ASP	2.4
3	C	244	SER	2.4
1	D	346	TRP	2.4
1	A	178	SER	2.4
3	F	218	PRO	2.3
1	A	436	GLY	2.3
1	A	179	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	282	TYR	2.2
1	D	437	VAL	2.2
3	F	363	VAL	2.2
2	E	177	ASP	2.2
2	E	429	THR	2.2
3	C	267	THR	2.2
3	F	364	LEU	2.1
3	F	415	ILE	2.1
3	F	321	GLY	2.0
3	C	251	ILE	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](#)

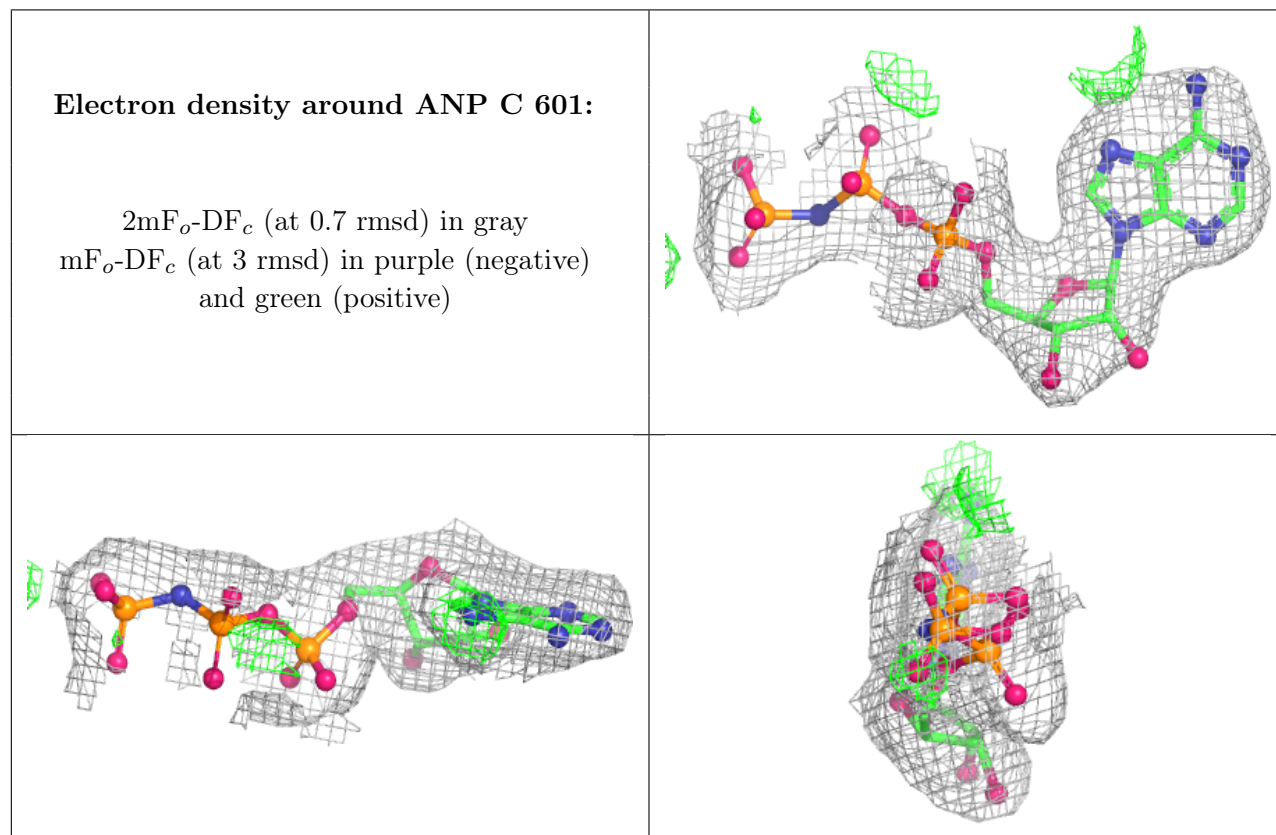
There are no oligosaccharides in this entry.

## 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, 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
6	EDO	A	504	4/4	0.86	0.14	54,55,56,58	0
8	ANP	C	601	31/31	0.94	0.07	64,72,75,82	0
7	GDP	E	501	28/28	0.97	0.05	41,45,48,50	0
8	ANP	F	601	31/31	0.97	0.06	55,71,76,83	0
5	MG	A	503	1/1	0.98	0.04	96,96,96,96	0
5	MG	F	602	1/1	0.99	0.02	57,57,57,57	0
4	GTP	D	501	32/32	0.99	0.04	31,34,37,38	0
7	GDP	B	501	28/28	0.99	0.03	37,38,41,42	0
4	GTP	A	501	32/32	0.99	0.04	33,35,36,37	0
5	MG	C	602	1/1	0.99	0.03	68,68,68,68	0
5	MG	D	503	1/1	0.99	0.04	80,80,80,80	0
5	MG	D	502	1/1	1.00	0.04	35,35,35,35	0
5	MG	A	502	1/1	1.00	0.04	33,33,33,33	0

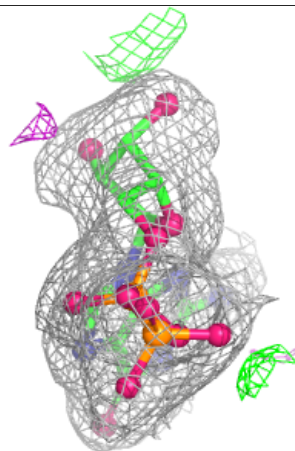
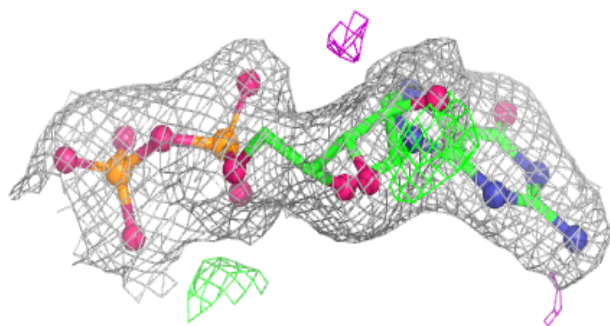
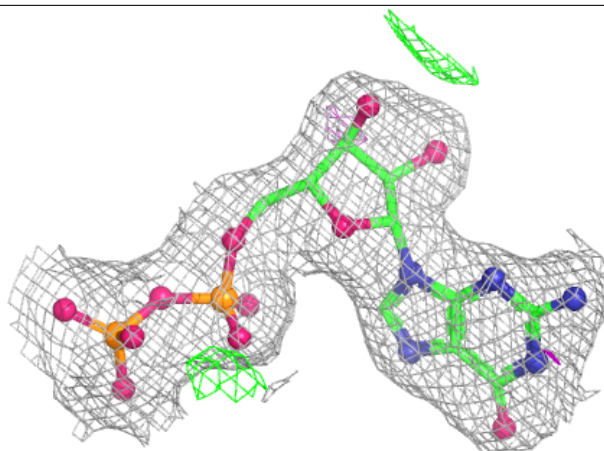
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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



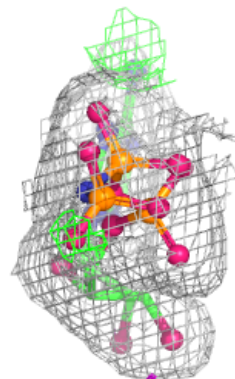
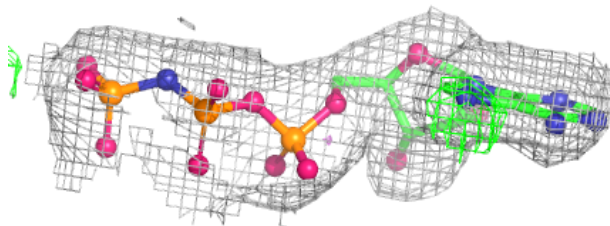
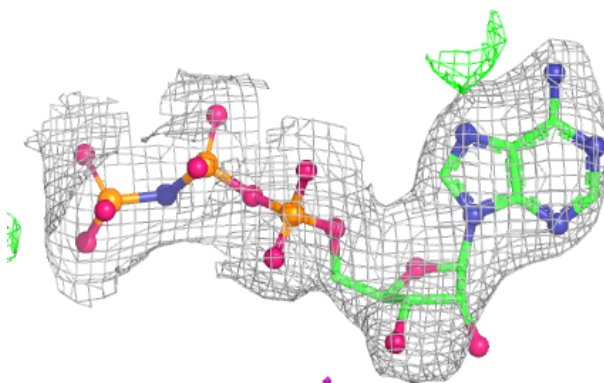


**Electron density around GDP E 501:**

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

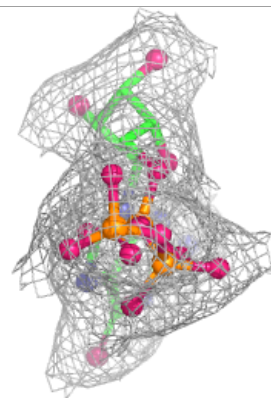
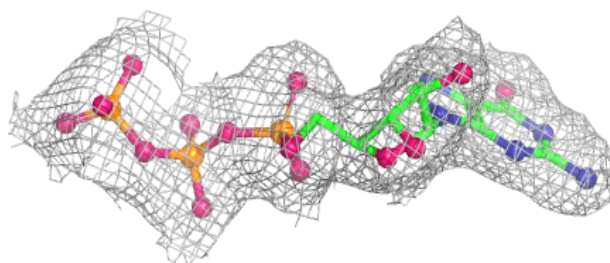
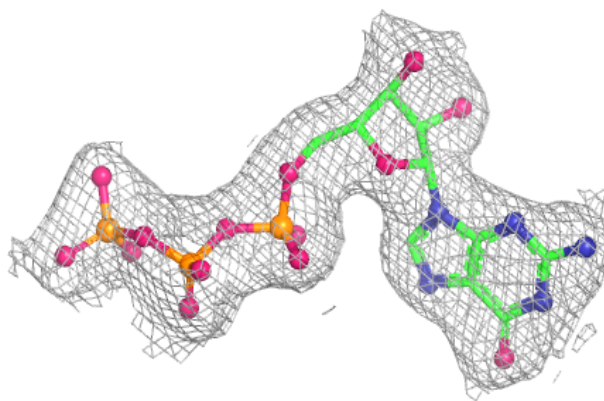
**Electron density around ANP F 601:**

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

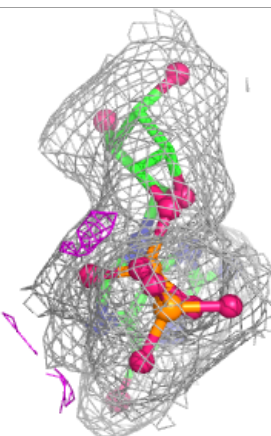
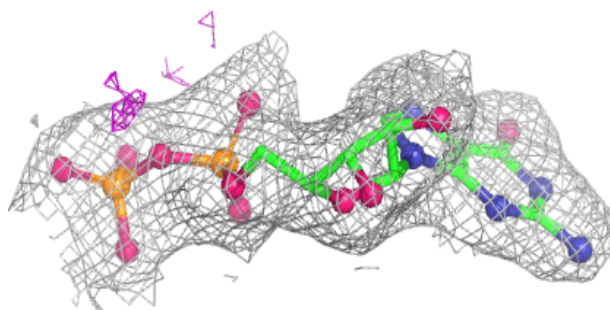
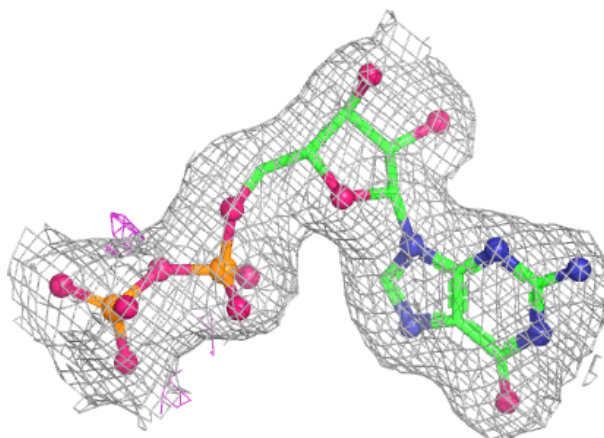


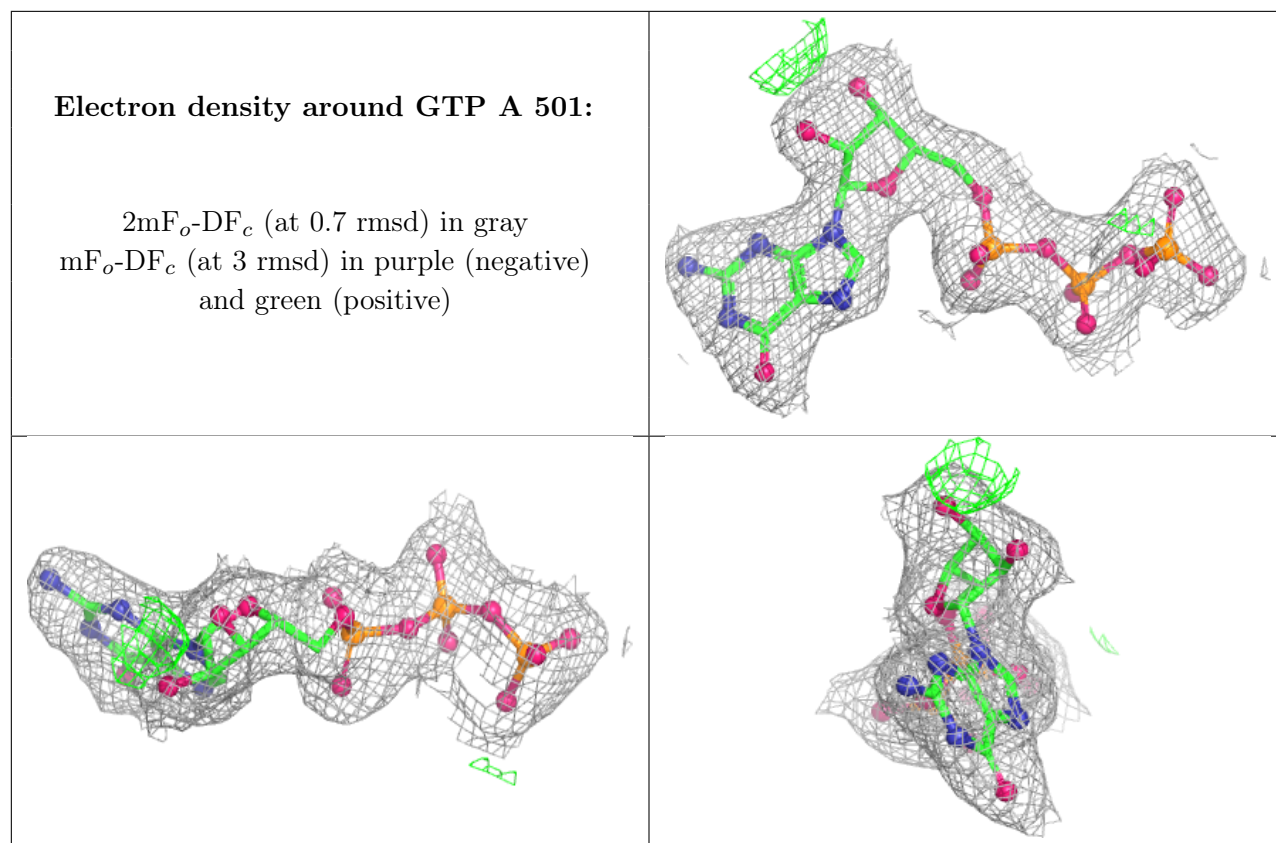
**Electron density around GTP D 501:**

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

**Electron density around GDP B 501:**

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





## 6.5 Other polymers [i](#)

There are no such residues in this entry.