



Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 03:03 am BST

PDB ID : 5XI7
Title : Crystal structure of T2R-TTL bound with PO-7
Authors : Chu, Y.; Wang, Y.; Yang, J.; Li, W.
Deposited on : 2017-04-26
Resolution : 2.99 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 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

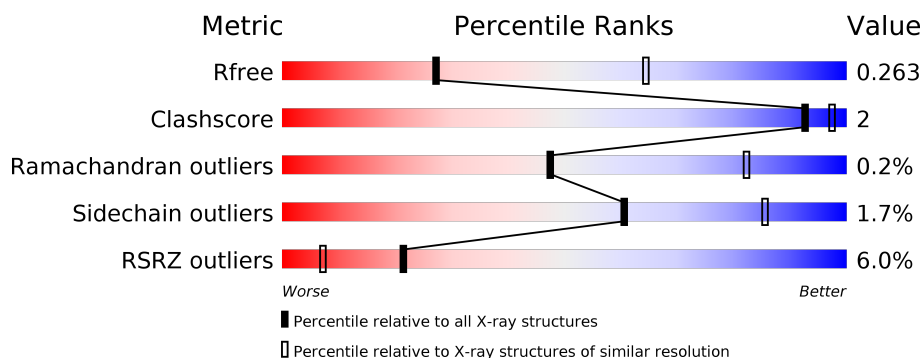
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.99 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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 ≥ 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	<div> <div>2%</div> <div>92%</div> <div>5%</div> <div>• •</div> </div>
1	C	450	<div> <div>93%</div> <div>5%</div> <div>•</div> </div>
2	B	445	<div> <div>3%</div> <div>89%</div> <div>6%</div> <div>5%</div> </div>
2	D	445	<div> <div>10%</div> <div>91%</div> <div>•</div> <div>5%</div> </div>
3	E	184	<div> <div>5%</div> <div>64%</div> <div>•</div> <div>35%</div> </div>
4	F	384	<div> <div>13%</div> <div>76%</div> <div>5%</div> <div>20%</div> </div>

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 17449 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 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	437	Total	C	N	O	S	0	4	0
			3441	2179	586	652	24			
1	C	440	Total	C	N	O	S	0	9	0
			3482	2200	589	668	25			

- Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	424	Total	C	N	O	S	0	2	0
			3353	2107	574	645	27			
2	D	421	Total	C	N	O	S	0	1	0
			3306	2079	562	638	27			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	120	Total	C	N	O	S	0	2	0
			1004	621	181	196	6			

- Molecule 4 is a protein called Tubulin tyrosine ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	309	Total	C	N	O	S	0	3	0
			2553	1645	438	455	15			

There are 6 discrepancies between the modelled and reference sequences:

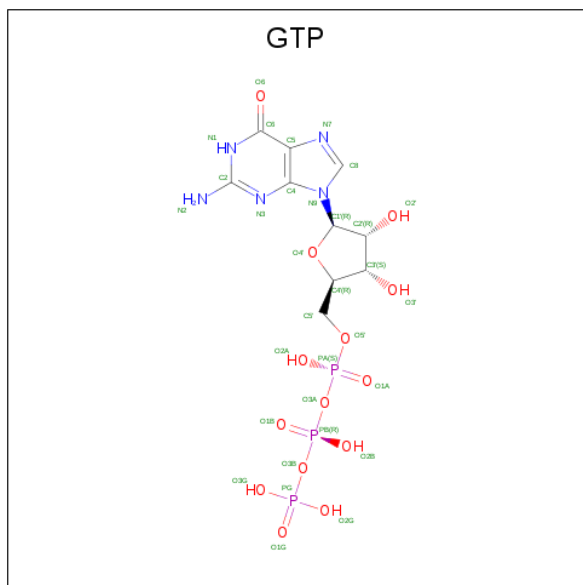
Chain	Residue	Modelled	Actual	Comment	Reference
F	379	HIS	-	expression tag	UNP E1BQ43
F	380	HIS	-	expression tag	UNP E1BQ43
F	381	HIS	-	expression tag	UNP E1BQ43
F	382	HIS	-	expression tag	UNP E1BQ43

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Chain	Residue	Modelled	Actual	Comment	Reference
F	383	HIS	-	expression tag	UNP E1BQ43
F	384	HIS	-	expression tag	UNP E1BQ43

- Molecule 5 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: 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		

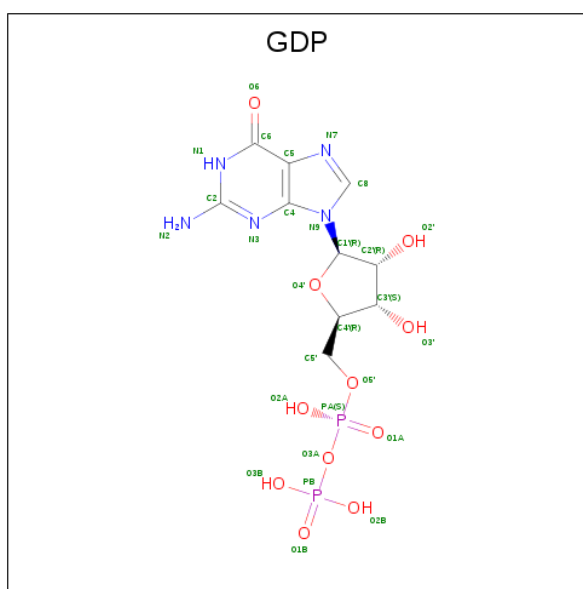
- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

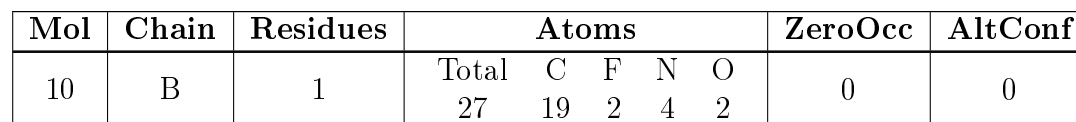
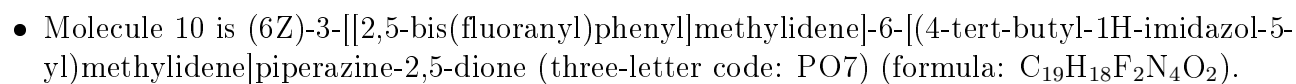
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1	Total	Ca	0	0
			1	1		
7	A	1	Total	Ca	0	0
			1	1		
7	C	1	Total	Ca	0	0
			1	1		

- Molecule 8 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



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

- Molecule 9 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).

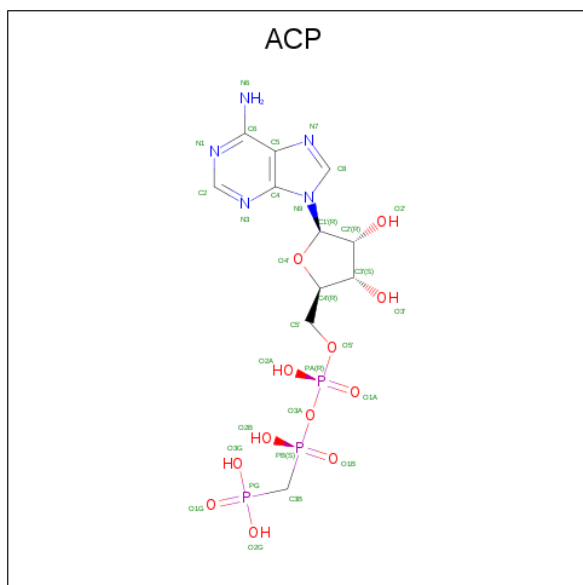


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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	D	1	Total	C	F	N	O	0	0
			27	19	2	4	2		

- Molecule 11 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (three-letter code: 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		

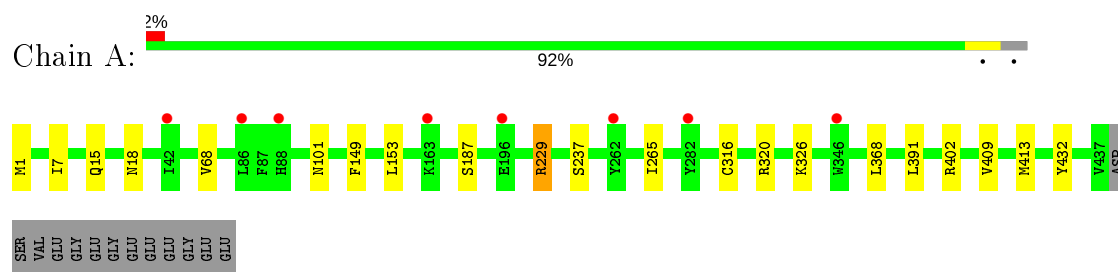
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	16	Total	O	0	0
			16	16		
12	B	15	Total	O	0	0
			15	15		
12	C	33	Total	O	0	0
			33	33		
12	E	2	Total	O	0	0
			2	2		
12	F	4	Total	O	0	0
			4	4		

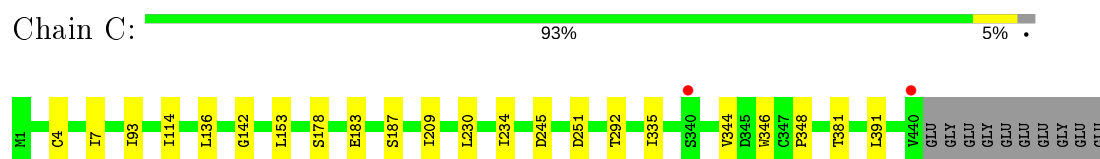
3 Residue-property plots [i](#)

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.

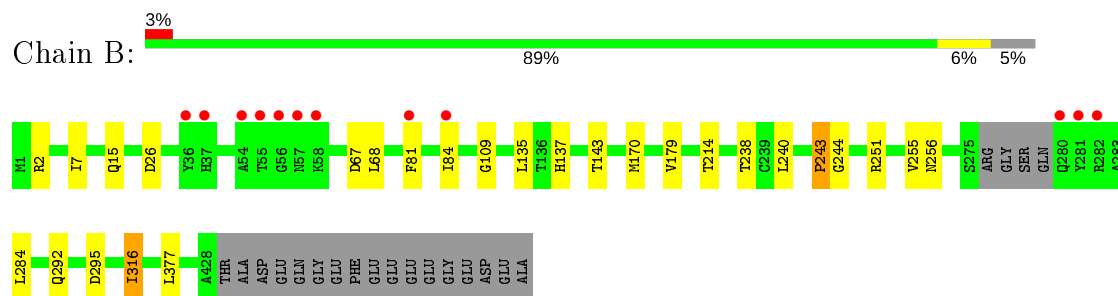
- Molecule 1: Tubulin alpha chain



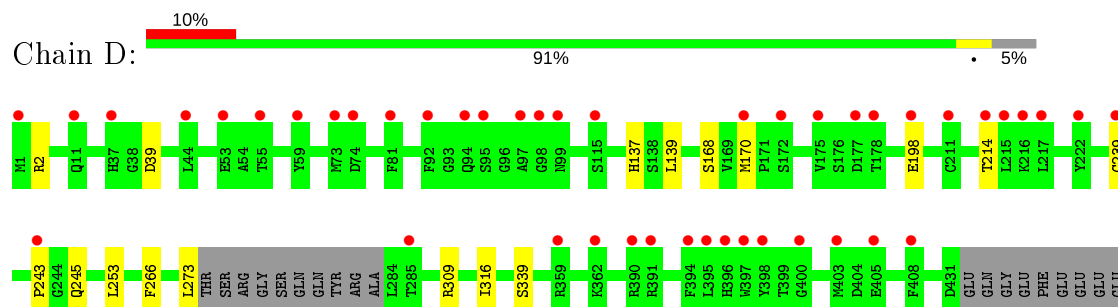
- Molecule 1: Tubulin alpha chain



- Molecule 2: Tubulin beta chain



- Molecule 2: Tubulin beta chain



GLY
GLU
ASP
GLU
ALA

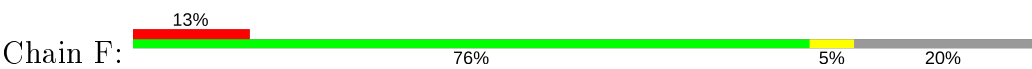
● Molecule 3: Stathmin-4



TYR
LYS
GLU
LYS
MET
LYS
GLU
LEU
PRO
LEU
VAL
SER
LEU
PHE
CYS
SER
CYS
PHE
LEU
SER
ASP
PRO
LEU
ASN
LYS
SER
SER
TYR
LYS
TYR
GLU
ALA
ASP
THR
VAL
ASP
LEU
ASN
TRP
CYS
ILE
SER
ASP
PHE
K25
P26
P27
SER
PHE
ASP
GLY
VAL
PRO
GLU
PHE
ASN
ALA
SER

LEU
PRO
ARG
ARG
ARG
D44
P45
S46
L47
E48
Q51
L54
Q103
E131
N136
K140
E141
GLU
ALA
SER
ARG

● Molecule 4: Tubulin tyrosine ligase



M1
E9
N10
S11
S12
L22
A23
T24
K32
L47
P48
F49
A75
I81
E86
L87
S88
E89
Y98
V99
I100
Y101
P102
THR
ASN
LEU
LYS
THR
PRO
VAL
ALA
PRO
ALA
GLN
ASN
ILE
GLY
ILE
ARG
HIS
LEU
ILE
ASN
ASN
THR
THR
ASP
GLU
ARG
VAL
PHE

LEU
ALA
TYR
ASN
ARG
ARG
GLU
GLY
ARG
GLU
G144
N145
V146
W147
I148
A149
K150
S151
SER
ALA
GLY
ALA
LYS
GLY
GLU
G159
I160
L161
I162
S163
S164
E165
A166
SER
GLU
LEU
LEU
PHE
ASP
ILE
ASP
GLU
GLN
GLN
VAL
H180
V181
I182
Q183
K184
I191
I192
E193
F194
R197

K198
F199
Y211
S224
P227
Y228
N229
S230
A231
N232
F233
Q234
C238
H239
L240
T241
C244
I245
Q246
K247
GLU
TYR
SER
LYS
N252
R255
I256
G259
N262
F263
F264
Y270
L275
I287
F319
K320
E323
G349
L361
A362
ASP
THR
GLY
GLN
LYS

THR
SER
GLN
PRO
THR
S373
I374
E384

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	105.25Å 157.38Å 182.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	119.17 – 2.99 48.12 – 2.99	Depositor EDS
% Data completeness (in resolution range)	97.3 (119.17-2.99) 97.3 (48.12-2.99)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.36 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.222 , 0.266 0.221 , 0.263	Depositor DCC
R_{free} test set	3119 reflections (5.19%)	wwPDB-VP
Wilson B-factor (Å ²)	53.7	Xtriage
Anisotropy	0.017	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 32.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	17449	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.82% 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: GDP, MG, PO7, CA, GTP, ACP, MES

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	0.38	0/3525	0.61	0/4784
1	C	0.38	0/3572	0.61	0/4850
2	B	0.39	0/3427	0.60	0/4640
2	D	0.41	0/3379	0.59	0/4577
3	E	0.40	0/1018	0.55	0/1350
4	F	0.40	0/2618	0.56	0/3537
All	All	0.39	0/17539	0.59	0/23738

There are no bond length outliers.

There are no bond angle outliers.

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	3441	0	3363	15	0
1	C	3482	0	3384	11	0
2	B	3353	0	3228	16	0
2	D	3306	0	3181	6	0
3	E	1004	0	1028	0	0
4	F	2553	0	2519	5	0
5	A	32	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	32	0	12	0	0
5	D	32	0	12	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
8	B	28	0	12	0	0
9	B	24	0	26	2	0
10	B	27	0	0	1	0
10	D	27	0	0	2	0
11	F	31	0	14	0	0
12	A	16	0	0	0	0
12	B	15	0	0	0	0
12	C	33	0	0	0	0
12	E	2	0	0	0	0
12	F	4	0	0	0	0
All	All	17449	0	16791	52	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 2.

All (52) 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:229[A]:ARG:HG2	1:A:229[A]:ARG:HH11	1.09	1.08
1:A:229[A]:ARG:CG	1:A:229[A]:ARG:HH11	1.67	1.07
1:A:229[A]:ARG:NH1	1:A:229[A]:ARG:HG2	1.85	0.81
1:C:178:SER:OG	1:C:183:GLU:OE2	2.02	0.75
2:B:243:PRO:CB	2:B:244:GLY:HA2	2.19	0.73
2:B:295:ASP:HA	9:B:505:MES:O2S	1.95	0.66
2:B:243:PRO:HB2	2:B:244:GLY:HA2	1.80	0.63
1:A:368[B]:LEU:N	1:A:368[B]:LEU:HD12	2.15	0.61
1:A:229[A]:ARG:NH1	1:A:229[A]:ARG:CG	2.40	0.61
1:A:368[B]:LEU:H	1:A:368[B]:LEU:HD12	1.66	0.59
1:A:101:ASN:HD22	2:B:256:ASN:HD21	1.52	0.56
1:A:187:SER:HB3	1:A:391:LEU:HD21	1.87	0.55
1:C:187:SER:HB3	1:C:391:LEU:HD21	1.88	0.54
2:B:251:ARG:NH1	9:B:503:MES:O2S	2.40	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:238:THR:HB	2:B:316:ILE:HD11	1.90	0.52
1:A:68:VAL:HG11	1:A:149:PHE:CE2	2.45	0.51
1:A:187:SER:CB	1:A:391:LEU:HD21	2.41	0.50
2:B:179:VAL:HG12	1:C:348:PRO:HG2	1.94	0.48
4:F:224:SER:HB2	4:F:241:THR:HG22	1.94	0.48
4:F:349:GLY:HA3	4:F:374:ILE:HD11	1.94	0.48
2:D:309:ARG:NH1	2:D:339:SER:O	2.48	0.46
4:F:81:ILE:O	4:F:87:LEU:O	2.33	0.46
2:B:7:ILE:HB	2:B:135:LEU:HD12	1.98	0.45
2:D:139:LEU:HD12	2:D:170:MET:SD	2.57	0.45
1:C:142:GLY:HA3	1:C:183:GLU:OE1	2.17	0.45
1:A:265:ILE:HG23	1:A:432:TYR:CE2	2.52	0.44
2:B:251:ARG:O	2:B:255:VAL:HG23	2.17	0.44
2:B:284:LEU:HD21	2:B:292:GLN:HE22	1.83	0.44
1:C:292:THR:HG22	1:C:335:ILE:CD1	2.48	0.44
10:D:503:PO7:NAN	10:D:503:PO7:NAQ	2.66	0.43
1:A:229[A]:ARG:HH11	1:A:229[A]:ARG:HG3	1.70	0.43
1:C:4[A]:CYS:SG	1:C:136:LEU:HG	2.59	0.43
2:D:139:LEU:HD11	2:D:168:SER:HB3	2.00	0.43
2:B:68:LEU:HD21	2:B:109:GLY:HA2	2.01	0.42
2:B:240:LEU:HD12	10:B:506:PO7:FAF	2.10	0.42
1:A:15:GLN:HA	1:A:18:ASN:HD22	1.84	0.42
4:F:47:LEU:HD22	4:F:49:PHE:CE1	2.54	0.42
2:B:170:MET:HG3	2:B:377:LEU:HD21	2.02	0.42
2:B:67:ASP:HA	2:B:143:THR:HG21	2.01	0.42
1:C:230:LEU:O	1:C:234:ILE:HD12	2.19	0.42
1:C:344:VAL:HG21	1:C:346:TRP:CE2	2.54	0.42
2:B:243:PRO:HB3	2:B:244:GLY:HA2	1.99	0.42
1:C:7:ILE:HG21	1:C:153:LEU:HD21	2.03	0.41
2:D:239:CYS:SG	10:D:503:PO7:OAE	2.77	0.41
4:F:287:ILE:HG23	4:F:319:PHE:CE2	2.56	0.41
2:D:214:THR:HG21	2:D:273:LEU:HD12	2.03	0.41
1:A:409:VAL:HA	1:A:413:MET:O	2.20	0.40
1:C:209:ILE:HG23	1:C:230:LEU:HD23	2.03	0.40
2:D:198:GLU:HB2	2:D:266:PHE:CE2	2.56	0.40
2:B:81:PHE:O	2:B:84:ILE:HG22	2.22	0.40
1:A:7:ILE:HG21	1:A:153:LEU:HD21	2.03	0.40
1:C:93:ILE:HG22	1:C:114:ILE:HD11	2.04	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	439/450 (98%)	427 (97%)	12 (3%)	0	100	100
1	C	446/450 (99%)	437 (98%)	9 (2%)	0	100	100
2	B	422/445 (95%)	404 (96%)	17 (4%)	1 (0%)	47	82
2	D	417/445 (94%)	396 (95%)	19 (5%)	2 (0%)	29	68
3	E	118/184 (64%)	114 (97%)	4 (3%)	0	100	100
4	F	300/384 (78%)	286 (95%)	13 (4%)	1 (0%)	41	76
All	All	2142/2358 (91%)	2064 (96%)	74 (4%)	4 (0%)	47	82

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	243	PRO
2	D	243	PRO
4	F	11	SER
2	D	39	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	372/378 (98%)	363 (98%)	9 (2%)	49	79
1	C	379/378 (100%)	375 (99%)	4 (1%)	73	90
2	B	367/383 (96%)	361 (98%)	6 (2%)	62	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	362/383 (94%)	357 (99%)	5 (1%)	67	88
3	E	110/168 (66%)	108 (98%)	2 (2%)	59	85
4	F	281/342 (82%)	272 (97%)	9 (3%)	39	74
All	All	1871/2032 (92%)	1836 (98%)	35 (2%)	60	84

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	229[A]	ARG
1	A	229[B]	ARG
1	A	237	SER
1	A	316[A]	CYS
1	A	316[B]	CYS
1	A	320	ARG
1	A	326	LYS
1	A	402	ARG
2	B	2	ARG
2	B	15	GLN
2	B	26	ASP
2	B	137	HIS
2	B	214	THR
2	B	316	ILE
1	C	245	ASP
1	C	251[A]	ASP
1	C	251[B]	ASP
1	C	381	THR
2	D	2	ARG
2	D	137	HIS
2	D	245	GLN
2	D	253	LEU
2	D	316	ILE
3	E	131	GLU
3	E	136	ASN
4	F	1	MET
4	F	12	SER
4	F	24	THR
4	F	32	LYS
4	F	86	GLU
4	F	87	LEU
4	F	89	GLU

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Mol	Chain	Res	Type
4	F	211	TYR
4	F	238	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	GLN
1	A	101	ASN
2	B	292	GLN
1	C	249	ASN
1	C	356	ASN
3	E	136	ASN
4	F	242	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 16 ligands modelled in this entry, 7 are monoatomic - leaving 9 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	PO7	B	506	-	21,29,29	2.44	7 (33%)	24,43,43	1.91	6 (25%)
9	MES	B	505	-	12,12,12	2.04	2 (16%)	14,16,16	6.16	7 (50%)
5	GTP	A	501	6	26,34,34	1.18	2 (7%)	33,54,54	1.82	7 (21%)
8	GDP	B	501	6	24,30,30	1.31	2 (8%)	31,47,47	2.03	7 (22%)
5	GTP	C	501	6	26,34,34	1.09	2 (7%)	33,54,54	1.80	6 (18%)
11	ACP	F	401	-	27,33,33	2.00	8 (29%)	32,52,52	1.39	3 (9%)
5	GTP	D	501	6	26,34,34	1.26	2 (7%)	33,54,54	1.90	8 (24%)
10	PO7	D	503	-	21,29,29	2.63	6 (28%)	24,43,43	1.84	5 (20%)
9	MES	B	503	-	12,12,12	1.98	1 (8%)	14,16,16	7.23	9 (64%)

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	PO7	B	506	-	-	2/10/14/14	0/3/3/3
9	MES	B	505	-	-	2/6/14/14	0/1/1/1
5	GTP	A	501	6	-	3/18/38/38	0/3/3/3
8	GDP	B	501	6	-	3/12/32/32	0/3/3/3
5	GTP	C	501	6	-	6/18/38/38	0/3/3/3
11	ACP	F	401	-	-	6/15/38/38	0/3/3/3
5	GTP	D	501	6	-	5/18/38/38	0/3/3/3
10	PO7	D	503	-	-	2/10/14/14	0/3/3/3
9	MES	B	503	-	-	3/6/14/14	0/1/1/1

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	D	503	PO7	FAF-CAR	-6.30	1.21	1.36
9	B	503	MES	C8-S	-6.28	1.68	1.77
9	B	505	MES	C8-S	-6.28	1.68	1.77
11	F	401	ACP	PG-O1G	5.44	1.61	1.50
10	D	503	PO7	CAW-NAQ	4.98	1.41	1.33
10	B	506	PO7	CAW-NAQ	4.94	1.41	1.33
10	D	503	PO7	CAX-NAP	4.83	1.41	1.33
10	B	506	PO7	CAX-NAP	4.79	1.41	1.33
8	B	501	GDP	C6-C5	4.53	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	501	GTP	C6-C5	4.51	1.49	1.41
10	B	506	PO7	CAY-NAP	4.27	1.42	1.35
10	D	503	PO7	CAY-NAP	4.19	1.42	1.35
10	D	503	PO7	CAZ-NAQ	4.17	1.42	1.35
10	B	506	PO7	CAZ-NAQ	4.13	1.42	1.35
11	F	401	ACP	PB-O1B	4.04	1.61	1.51
5	A	501	GTP	C6-C5	3.99	1.48	1.41
10	B	506	PO7	CAT-CAH	-3.85	1.40	1.46
5	C	501	GTP	C6-C5	3.66	1.47	1.41
11	F	401	ACP	PB-O3A	3.48	1.62	1.58
10	B	506	PO7	FAF-CAR	-3.46	1.28	1.36
11	F	401	ACP	PB-O2B	-3.24	1.48	1.56
10	D	503	PO7	CAT-CAH	-3.18	1.41	1.46
11	F	401	ACP	PG-O2G	2.94	1.61	1.54
11	F	401	ACP	PG-O3G	-2.81	1.48	1.54
5	D	501	GTP	C5-C4	2.74	1.48	1.40
5	C	501	GTP	C5-C4	2.72	1.48	1.40
5	A	501	GTP	C5-C4	2.59	1.47	1.40
11	F	401	ACP	C5-C4	2.58	1.47	1.40
8	B	501	GDP	C5-C4	2.51	1.47	1.40
9	B	505	MES	O2S-S	2.19	1.51	1.45
10	B	506	PO7	CAT-CAS	2.03	1.42	1.39
11	F	401	ACP	C2-N3	2.01	1.35	1.32

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	503	MES	O1S-S-C8	-17.46	85.89	106.92
9	B	505	MES	O3S-S-O1S	-13.78	77.59	111.27
9	B	503	MES	O2S-S-C8	11.46	120.71	106.92
9	B	505	MES	O3S-S-C8	11.05	123.64	105.77
9	B	503	MES	O3S-S-O1S	-10.92	84.60	111.27
9	B	505	MES	O1S-S-C8	-9.44	95.54	106.92
9	B	503	MES	O2S-S-O1S	-9.29	81.79	113.95
9	B	505	MES	O2S-S-O1S	-8.38	84.94	113.95
9	B	503	MES	O3S-S-C8	7.12	117.28	105.77
9	B	505	MES	O3S-S-O2S	6.14	126.28	111.27
8	B	501	GDP	C6-C5-C4	-4.82	116.20	120.80
5	C	501	GTP	C5-C6-N1	-4.73	116.97	123.43
8	B	501	GDP	C6-N1-C2	4.61	123.25	115.93
8	B	501	GDP	C2-N3-C4	4.61	120.62	115.36
5	A	501	GTP	C5-C6-N1	-4.58	117.16	123.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	501	GTP	C6-N1-C2	4.51	123.09	115.93
10	B	506	PO7	CAZ-CAI-CAU	-4.47	122.49	128.66
5	C	501	GTP	C6-N1-C2	4.40	122.92	115.93
10	D	503	PO7	CAZ-CAI-CAU	-4.38	122.62	128.66
5	D	501	GTP	C6-C5-C4	-4.35	116.64	120.80
5	D	501	GTP	C2-N3-C4	4.35	120.32	115.36
10	D	503	PO7	CAY-CAH-CAT	-4.23	122.61	130.81
8	B	501	GDP	C5-C6-N1	-3.99	117.97	123.43
5	A	501	GTP	C6-C5-C4	-3.94	117.04	120.80
5	D	501	GTP	C6-N1-C2	3.91	122.15	115.93
9	B	503	MES	C2-C3-N4	3.88	115.98	110.10
11	F	401	ACP	N3-C2-N1	-3.82	122.71	128.68
10	B	506	PO7	CAY-CAH-CAT	-3.77	123.50	130.81
5	D	501	GTP	C5-C6-N1	-3.76	118.29	123.43
8	B	501	GDP	N3-C2-N1	-3.74	122.23	127.22
5	C	501	GTP	C2-N3-C4	3.67	119.55	115.36
5	A	501	GTP	C2-N3-C4	3.49	119.35	115.36
10	B	506	PO7	FAG-CAS-CAT	3.48	122.97	118.10
11	F	401	ACP	C3'-C2'-C1'	3.29	105.94	100.98
5	C	501	GTP	C6-C5-C4	-3.28	117.67	120.80
5	D	501	GTP	N3-C2-N1	-3.13	123.05	127.22
9	B	503	MES	O3S-S-O2S	3.10	118.86	111.27
10	D	503	PO7	FAG-CAS-CAT	3.08	122.41	118.10
5	A	501	GTP	N3-C2-N1	-2.93	123.32	127.22
5	C	501	GTP	N3-C2-N1	-2.92	123.32	127.22
10	B	506	PO7	CAW-NAQ-CAZ	2.88	122.80	116.41
10	D	503	PO7	CAW-NAQ-CAZ	2.87	122.76	116.41
11	F	401	ACP	C4-C5-N7	-2.80	106.48	109.40
10	B	506	PO7	CBA-CAV-NAO	2.77	123.95	120.50
10	B	506	PO7	CAX-NAP-CAY	2.76	122.53	116.41
5	D	501	GTP	PA-O3A-PB	-2.75	123.41	132.83
8	B	501	GDP	PA-O3A-PB	-2.60	123.90	132.83
10	D	503	PO7	CAX-NAP-CAY	2.53	122.03	116.41
9	B	503	MES	C6-C5-N4	2.52	113.93	110.10
8	B	501	GDP	C4-C5-N7	-2.48	106.81	109.40
9	B	505	MES	C6-C5-N4	2.47	113.85	110.10
5	D	501	GTP	C4-C5-N7	-2.46	106.84	109.40
5	A	501	GTP	C4-C5-N7	-2.36	106.94	109.40
5	C	501	GTP	PA-O3A-PB	-2.23	125.16	132.83
9	B	503	MES	C5-N4-C3	2.16	113.69	108.83
5	A	501	GTP	PA-O3A-PB	-2.12	125.55	132.83
9	B	505	MES	C7-N4-C5	-2.10	105.88	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	501	GTP	PB-O3B-PG	-2.03	125.84	132.83

There are no chirality outliers.

All (32) torsion outliers are listed below:

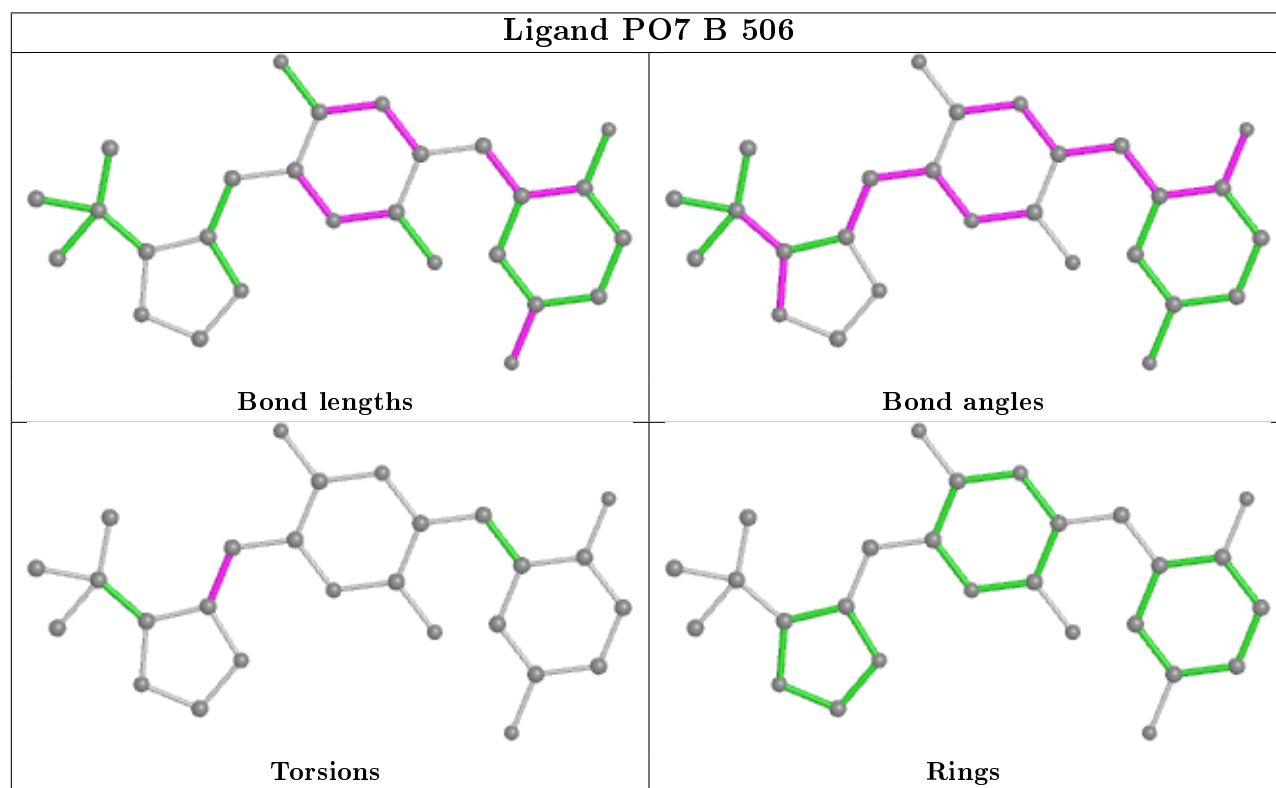
Mol	Chain	Res	Type	Atoms
10	B	506	PO7	CAZ-CAI-CAU-NAN
10	B	506	PO7	CAZ-CAI-CAU-CAV
5	A	501	GTP	C5'-O5'-PA-O1A
5	A	501	GTP	C5'-O5'-PA-O2A
8	B	501	GDP	C5'-O5'-PA-O1A
8	B	501	GDP	C5'-O5'-PA-O2A
5	C	501	GTP	PB-O3B-PG-O3G
5	C	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O2A
5	D	501	GTP	C5'-O5'-PA-O1A
5	D	501	GTP	C5'-O5'-PA-O2A
10	D	503	PO7	CAZ-CAI-CAU-NAN
10	D	503	PO7	CAZ-CAI-CAU-CAV
9	B	503	MES	N4-C7-C8-S
11	F	401	ACP	O4'-C4'-C5'-O5'
9	B	503	MES	C7-C8-S-O3S
11	F	401	ACP	C3'-C4'-C5'-O5'
9	B	505	MES	C7-C8-S-O3S
5	C	501	GTP	C4'-C5'-O5'-PA
9	B	505	MES	C7-C8-S-O1S
9	B	503	MES	C7-C8-S-O2S
11	F	401	ACP	PB-C3B-PG-O2G
11	F	401	ACP	PB-C3B-PG-O3G
5	D	501	GTP	C4'-C5'-O5'-PA
11	F	401	ACP	PG-C3B-PB-O1B
11	F	401	ACP	PB-C3B-PG-O1G
5	C	501	GTP	PB-O3B-PG-O2G
5	A	501	GTP	C5'-O5'-PA-O3A
8	B	501	GDP	C5'-O5'-PA-O3A
5	C	501	GTP	C5'-O5'-PA-O3A
5	D	501	GTP	C5'-O5'-PA-O3A
5	D	501	GTP	C3'-C4'-C5'-O5'

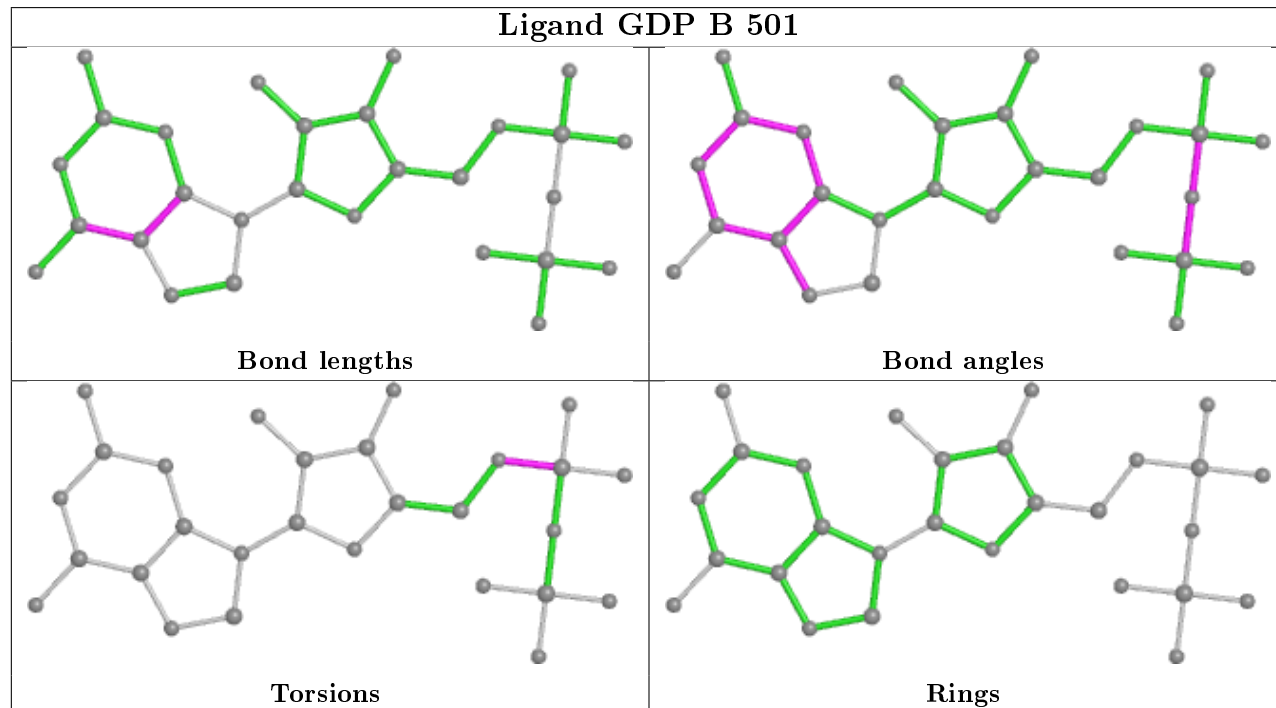
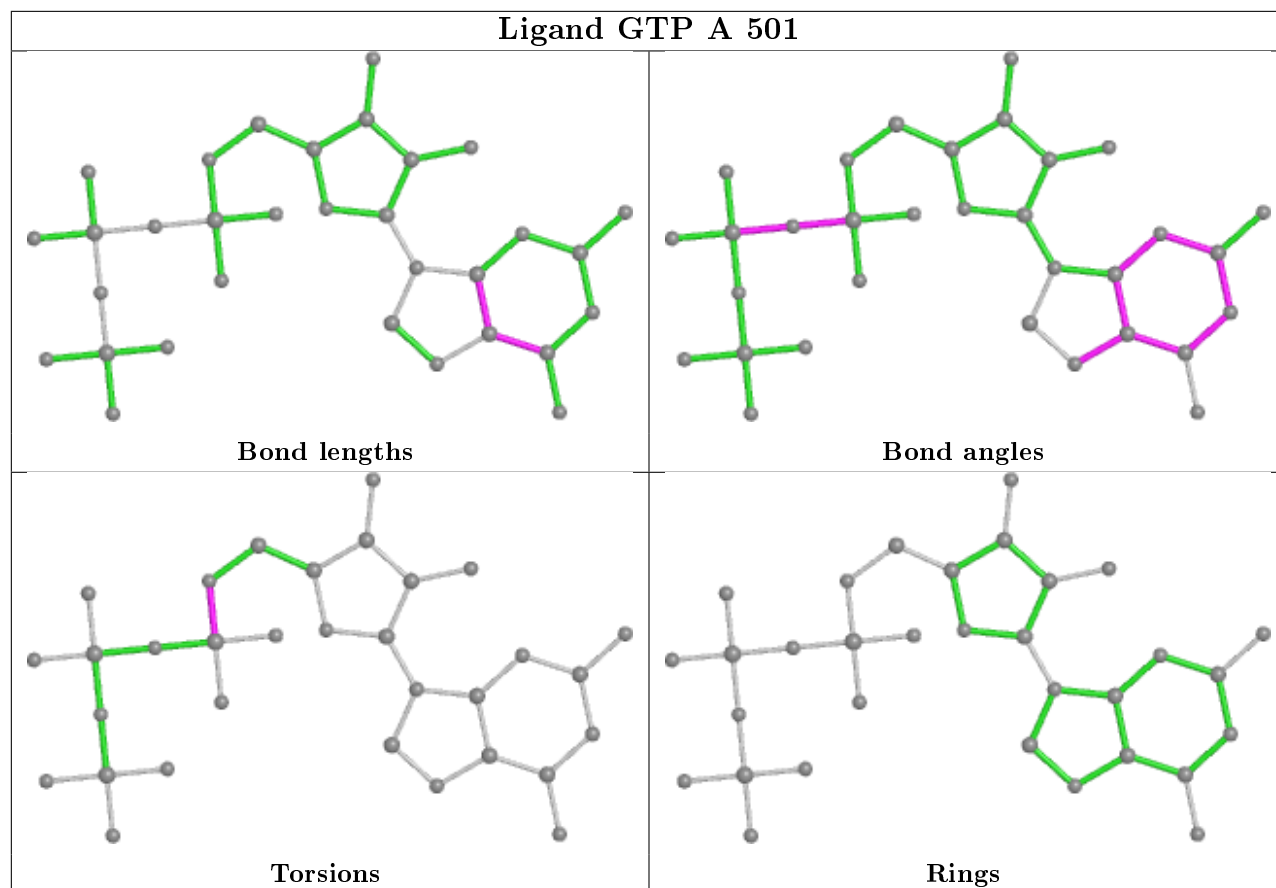
There are no ring outliers.

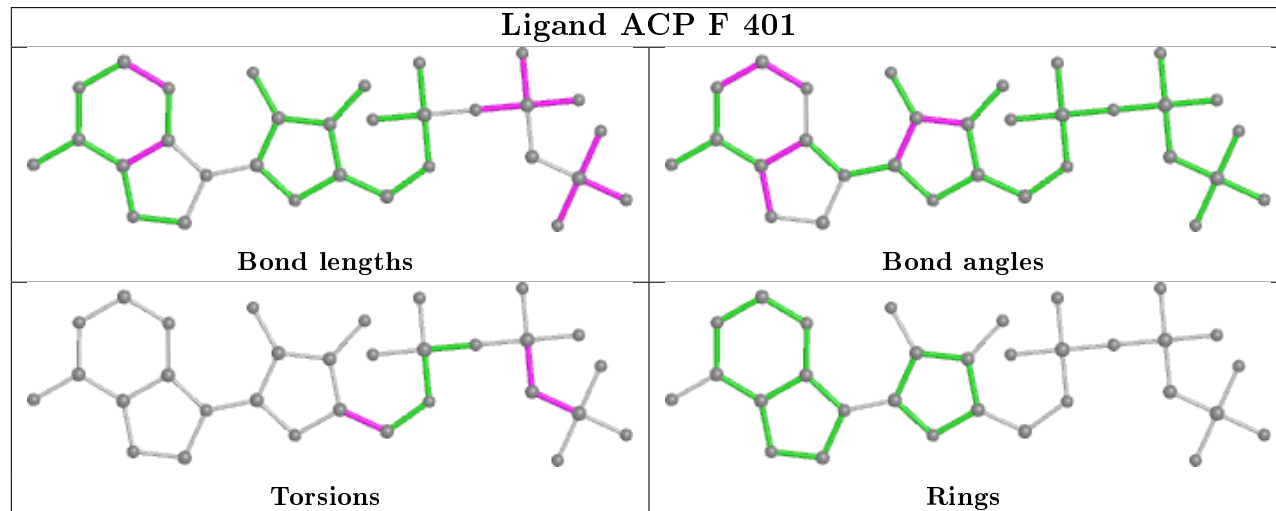
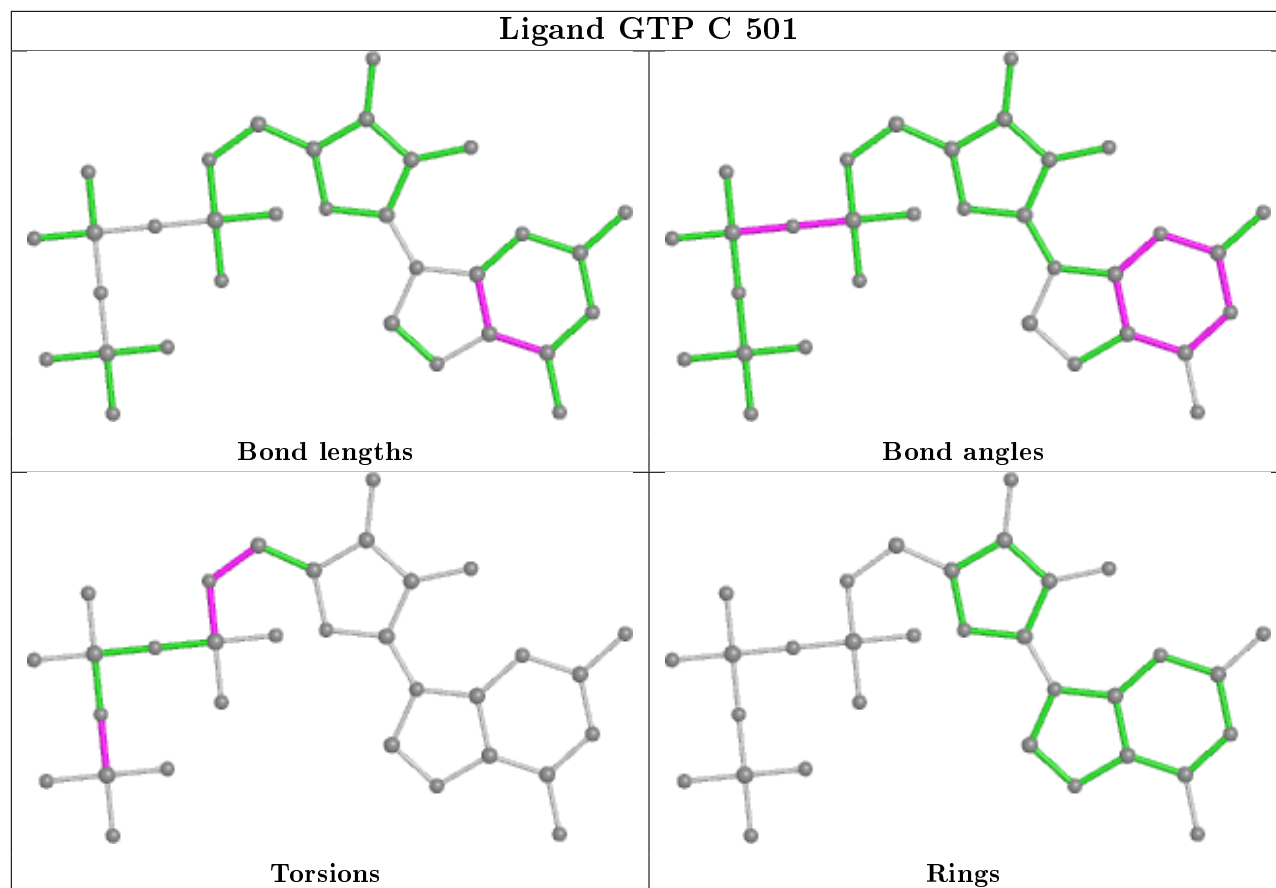
4 monomers are involved in 5 short contacts:

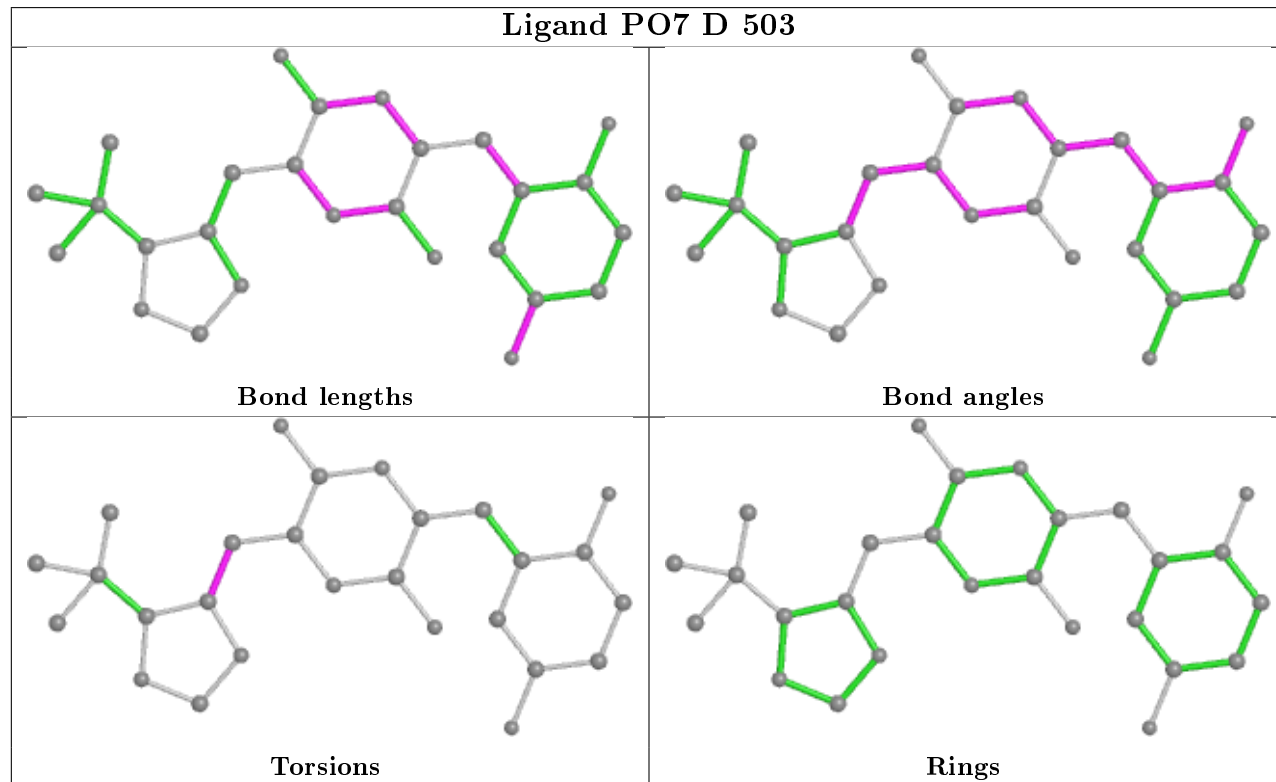
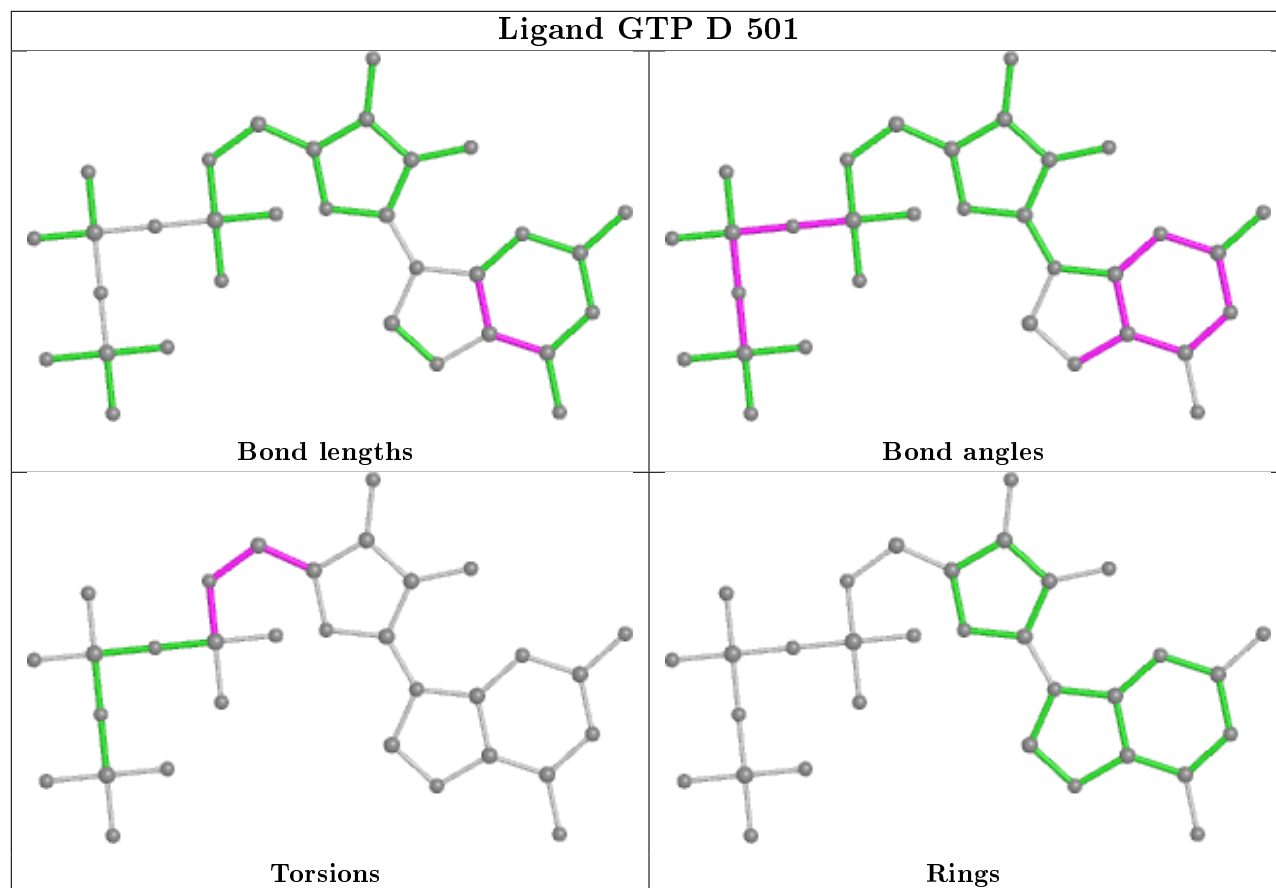
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	B	506	PO7	1	0
9	B	505	MES	1	0
10	D	503	PO7	2	0
9	B	503	MES	1	0

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









5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	437/450 (97%)	0.05	8 (1%) 68 40	31, 49, 78, 98	0
1	C	440/450 (97%)	-0.17	2 (0%) 91 75	23, 39, 66, 81	1 (0%)
2	B	424/445 (95%)	0.02	12 (2%) 53 25	27, 48, 78, 114	1 (0%)
2	D	421/445 (94%)	0.67	45 (10%) 6 2	37, 75, 111, 149	4 (0%)
3	E	120/184 (65%)	0.53	10 (8%) 11 3	39, 71, 104, 116	0
4	F	309/384 (80%)	0.78	51 (16%) 1 0	40, 77, 120, 147	0
All	All	2151/2358 (91%)	0.25	128 (5%) 21 7	23, 55, 104, 149	6 (0%)

All (128) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	161	LEU	8.4
4	F	182	ILE	7.6
2	D	55	THR	5.4
2	D	396	HIS	5.3
4	F	149	ALA	5.0
2	D	215	LEU	4.4
4	F	100	ILE	4.4
2	D	394	PHE	4.2
4	F	147	TRP	4.1
4	F	233	PHE	4.0
4	F	245	ILE	4.0
4	F	362	ALA	4.0
4	F	150	LYS	3.9
2	D	403	MET	3.8
4	F	101	TYR	3.8
4	F	192	LEU	3.8
4	F	180	HIS	3.6
4	F	228	TYR	3.6
2	B	280	GLN	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	86	LEU	3.5
4	F	184	LYS	3.5
1	A	346	TRP	3.5
2	B	56	GLY	3.5
2	B	55	THR	3.4
4	F	256	TYR	3.4
2	D	97	ALA	3.4
4	F	191	LEU	3.4
4	F	240	LEU	3.4
2	B	57	ASN	3.4
2	D	397	TRP	3.4
4	F	264	PHE	3.3
2	B	37	HIS	3.3
4	F	98	TYR	3.3
2	D	92	PHE	3.3
2	D	1	MET	3.2
2	D	37	HIS	3.2
2	B	281	TYR	3.2
2	D	391	ARG	3.2
4	F	262	MET	3.2
4	F	197	ARG	3.2
2	D	98	GLY	3.2
2	B	282	ARG	3.1
1	A	163	LYS	3.1
4	F	159	GLY	3.1
4	F	255	ARG	3.1
2	D	211	CYS	3.1
3	E	26	PRO	3.0
1	C	440	VAL	3.0
4	F	165	GLU	2.9
4	F	151	SER	2.9
4	F	199	PHE	2.9
2	D	405	GLU	2.9
2	D	44	LEU	2.9
2	D	214	THR	2.9
4	F	234	GLN	2.9
4	F	320	MET	2.9
2	D	285	THR	2.8
4	F	227	PRO	2.8
2	D	359	ARG	2.8
4	F	361	LEU	2.8
2	D	408	PHE	2.7

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Mol	Chain	Res	Type	RSRZ
2	D	398	TYR	2.7
1	A	88	HIS	2.7
4	F	164	SER	2.7
2	D	177	ASP	2.7
2	B	81	PHE	2.7
4	F	102	PRO	2.7
3	E	48	GLU	2.6
2	B	36	TYR	2.6
4	F	231	ALA	2.6
2	B	54	ALA	2.6
2	D	395	LEU	2.6
4	F	239	HIS	2.6
4	F	270	TYR	2.6
4	F	194	PRO	2.6
2	D	73	MET	2.5
2	D	53	GLU	2.5
4	F	22	LEU	2.5
2	D	59	TYR	2.5
1	A	42	ILE	2.5
3	E	45	PRO	2.5
4	F	259	GLY	2.5
2	D	400	GLY	2.5
4	F	275	LEU	2.5
2	D	175	VAL	2.5
2	D	390	ARG	2.4
4	F	230	SER	2.4
2	D	170	MET	2.4
2	D	216	LYS	2.4
3	E	25	LYS	2.4
3	E	46	SER	2.4
2	D	81	PHE	2.4
3	E	51	GLN	2.4
2	D	95	SER	2.4
2	D	74	ASP	2.3
4	F	75	ALA	2.3
4	F	163	SER	2.3
2	D	99	ASN	2.3
2	D	115	SER	2.3
1	C	340	SER	2.3
4	F	145	ASN	2.3
4	F	252	ASN	2.3
2	D	11	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
2	D	178	THR	2.2
2	D	94	GLN	2.2
2	D	172	SER	2.2
4	F	384	HIS	2.2
2	B	58	LYS	2.2
4	F	244	CYS	2.2
4	F	9	GLU	2.1
4	F	181	VAL	2.1
1	A	262	TYR	2.1
2	B	84	ILE	2.1
2	D	243	PRO	2.1
1	A	282	TYR	2.1
1	A	196	GLU	2.1
3	E	44	ASP	2.1
2	D	222	TYR	2.1
4	F	323	GLU	2.1
2	D	362	LYS	2.1
2	D	198	GLU	2.0
3	E	140	LYS	2.0
2	D	217	LEU	2.0
3	E	103	GLN	2.0
4	F	99	VAL	2.0
2	D	239	CYS	2.0
3	E	54	LEU	2.0
4	F	148	ILE	2.0

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

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

6.3 Carbohydrates ⓘ

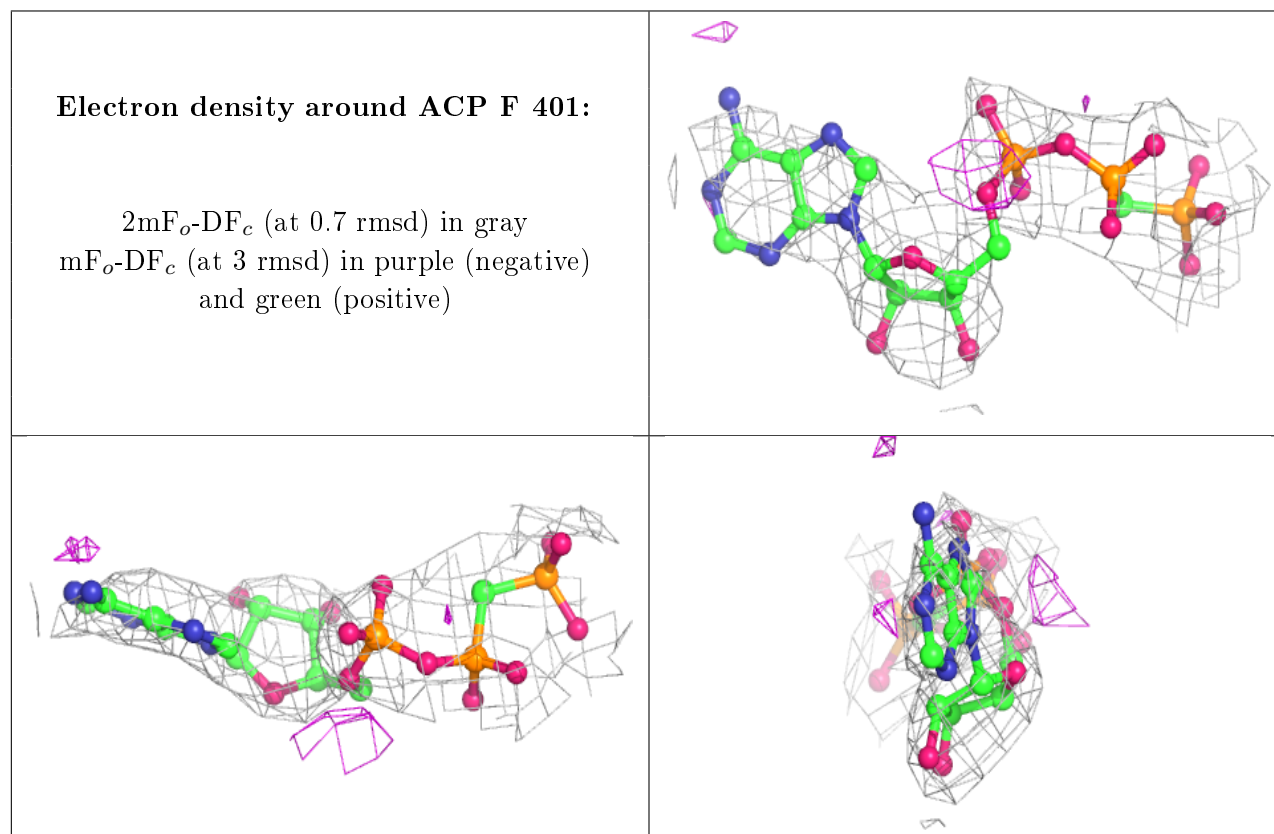
There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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

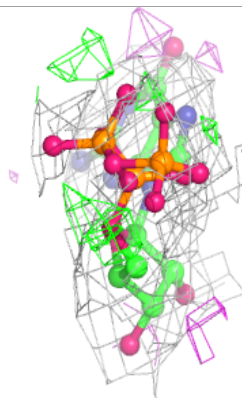
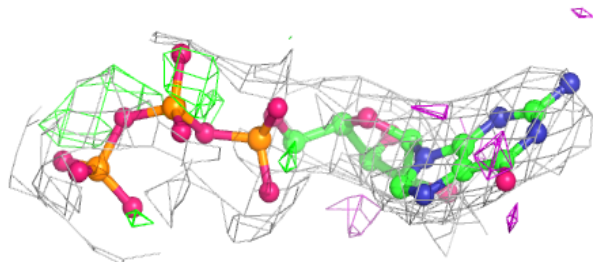
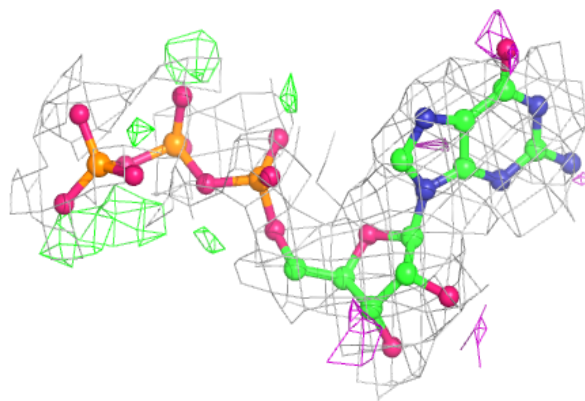
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
11	ACP	F	401	31/31	0.79	0.36	91,103,119,121	0
6	MG	D	502	1/1	0.85	0.19	60,60,60,60	0
9	MES	B	505	12/12	0.89	0.35	91,93,97,97	0
9	MES	B	503	12/12	0.89	0.23	77,83,87,90	0
7	CA	A	503	1/1	0.90	0.07	76,76,76,76	0
5	GTP	D	501	32/32	0.91	0.17	55,62,76,82	0
7	CA	B	504	1/1	0.91	0.11	65,65,65,65	0
10	PO7	D	503	27/27	0.94	0.21	48,57,67,68	0
10	PO7	B	506	27/27	0.94	0.22	33,41,59,66	0
7	CA	C	503	1/1	0.94	0.12	56,56,56,56	0
6	MG	B	502	1/1	0.96	0.11	40,40,40,40	0
5	GTP	C	501	32/32	0.97	0.17	26,30,31,32	0
5	GTP	A	501	32/32	0.98	0.20	29,32,35,36	0
8	GDP	B	501	28/28	0.98	0.19	28,30,32,33	0
6	MG	C	502	1/1	0.98	0.16	31,31,31,31	0
6	MG	A	502	1/1	0.99	0.23	25,25,25,25	0

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

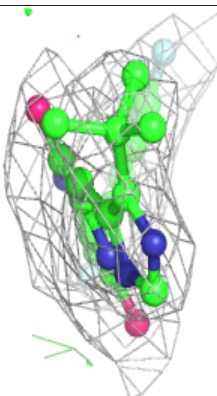
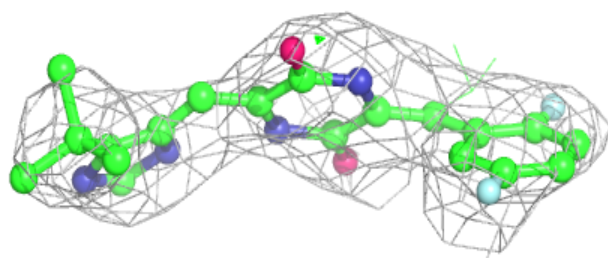
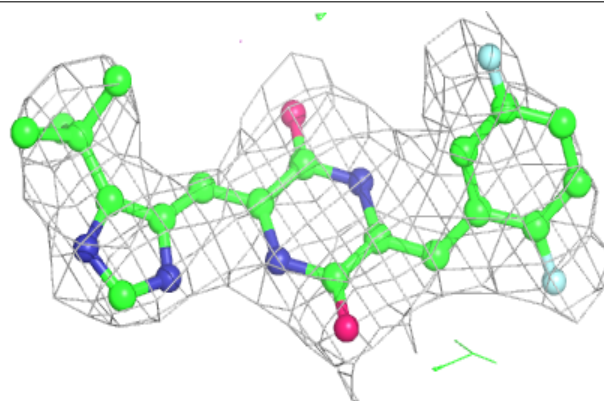


Electron density around GTP D 501:

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

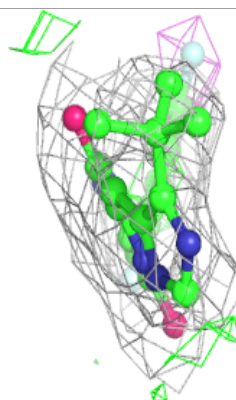
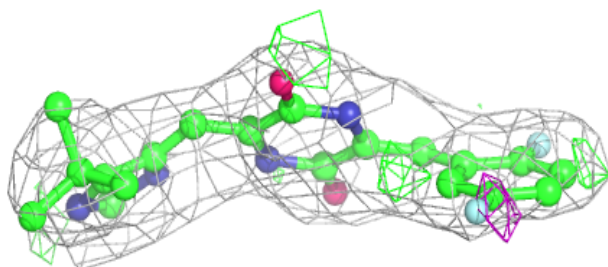
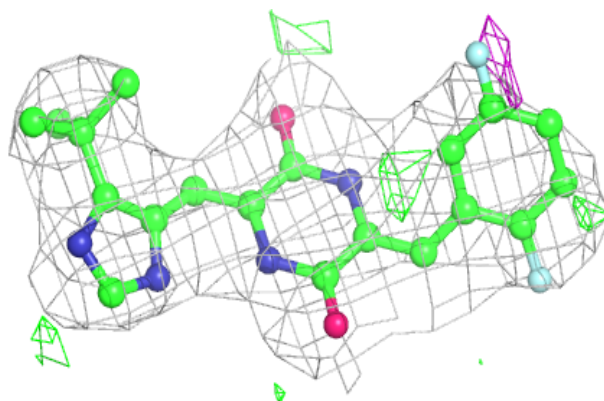
**Electron density around PO7 D 503:**

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

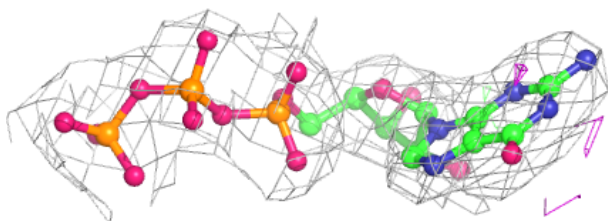
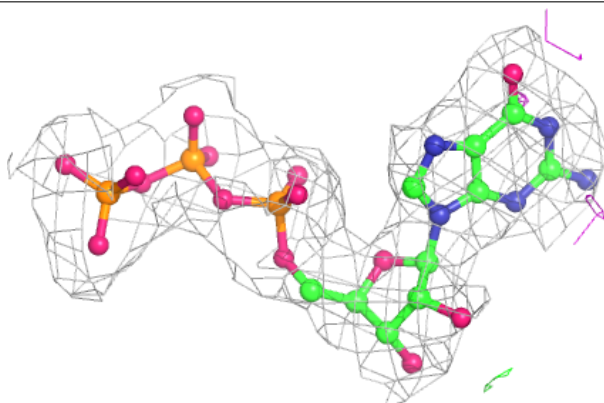


Electron density around PO7 B 506:

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

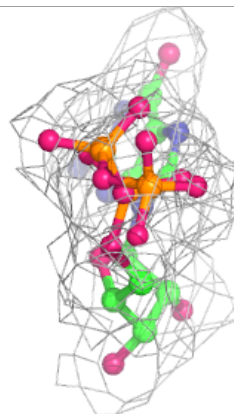
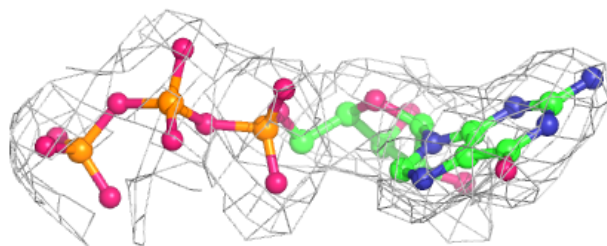
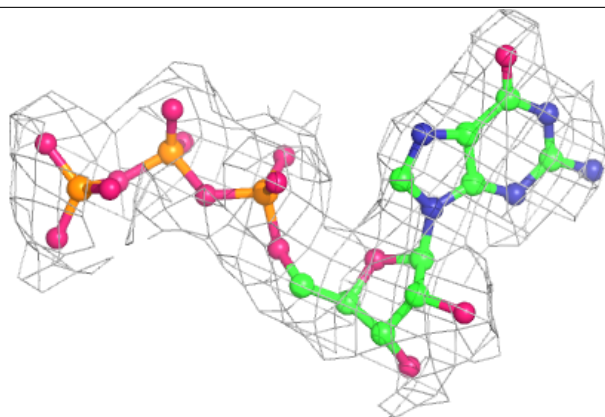
**Electron density around GTP C 501:**

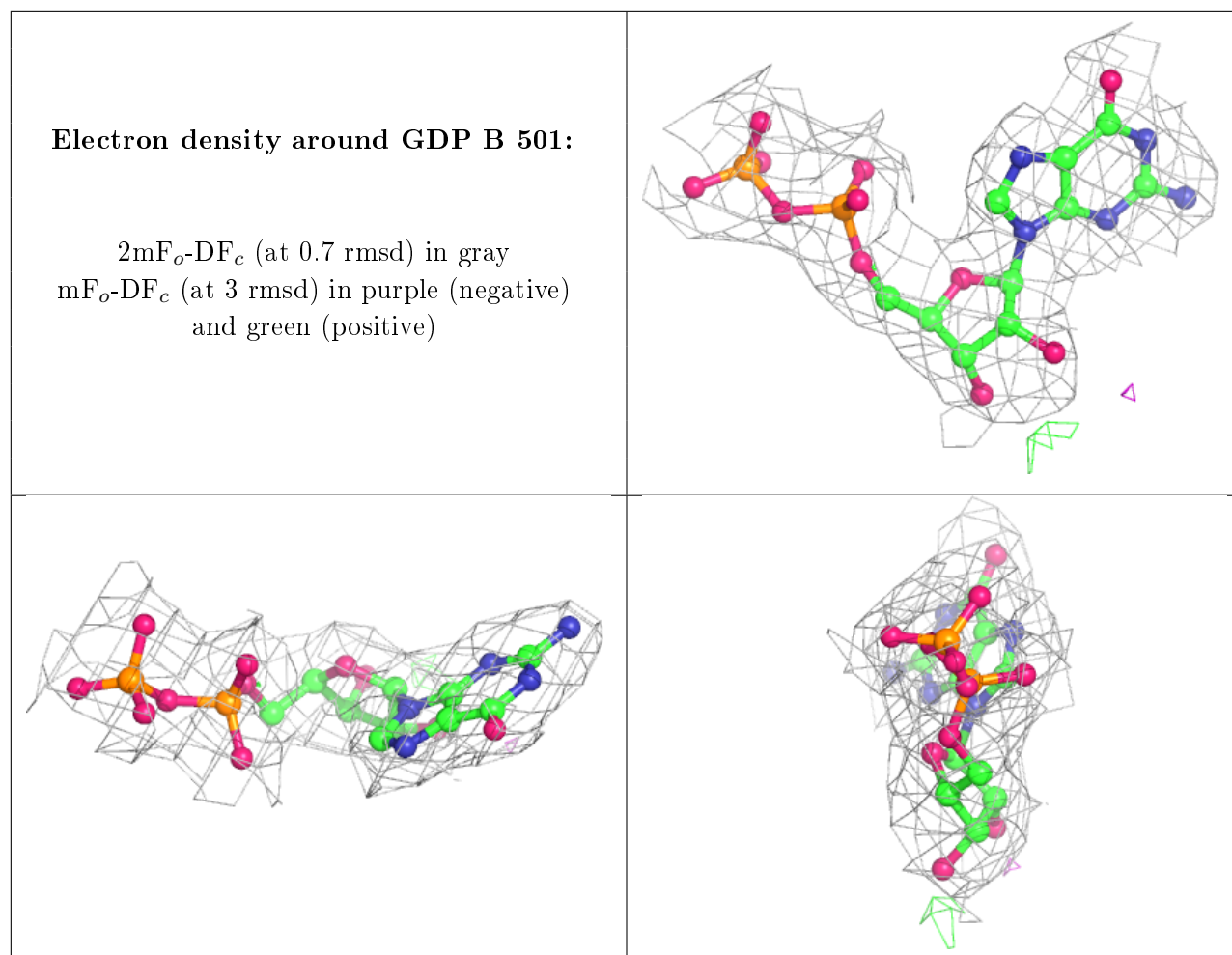
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around GTP A 501:

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





6.5 Other polymers [i](#)

There are no such residues in this entry.