



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2020 – 12:07 AM BST

PDB ID : 5XHC  
Title : Crystal structure of T2R-TTL-PO10 complex  
Authors : Chu, Y.; Wang, Y.; Yang, J.; Li, W.  
Deposited on : 2017-04-20  
Resolution : 2.75 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 : 2.13.1  
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) : 2.13.1

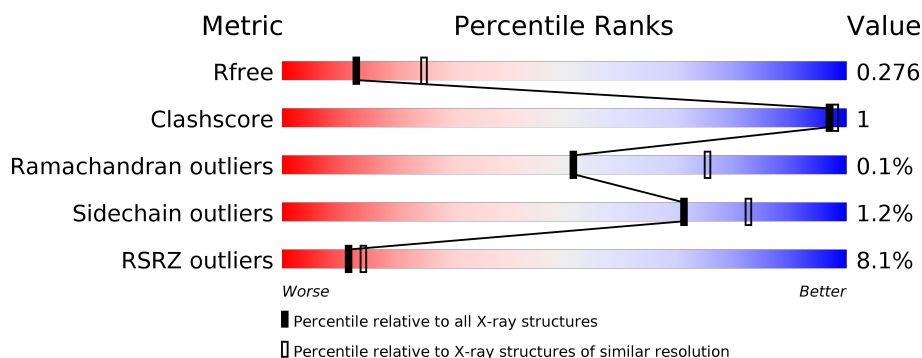
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.75 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	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

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	450	<div> <div>4%</div> <div>94%</div> <div>• •</div> </div>
1	C	450	<div> <div>95%</div> <div>• •</div> </div>
2	B	445	<div> <div>3%</div> <div>92%</div> <div>• 5%</div> </div>
2	D	445	<div> <div>13%</div> <div>92%</div> <div>• 5%</div> </div>
3	E	184	<div> <div>6%</div> <div>64%</div> <div>• 35%</div> </div>
4	F	384	<div> <div>18%</div> <div>79%</div> <div>• 20%</div> </div>

## 2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 17462 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:

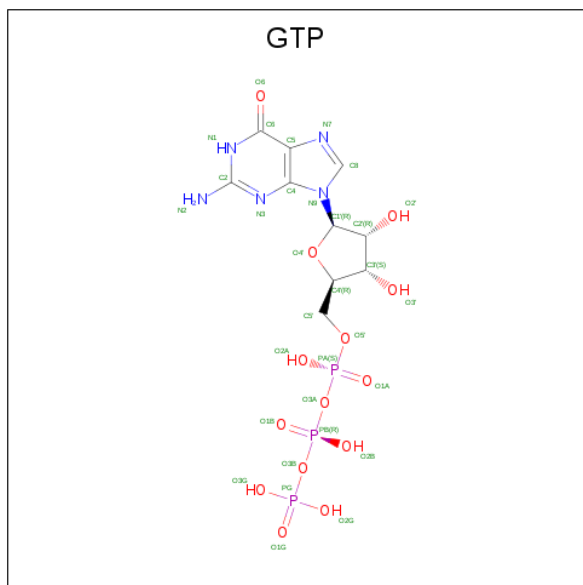
Chain	Residue	Modelled	Actual	Comment	Reference
F	379	HIS	-	expression tag	UNP E1BQ43
F	380	HIS	-	expression tag	UNP E1BQ43
F	381	HIS	-	expression tag	UNP E1BQ43
F	382	HIS	-	expression tag	UNP E1BQ43

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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		

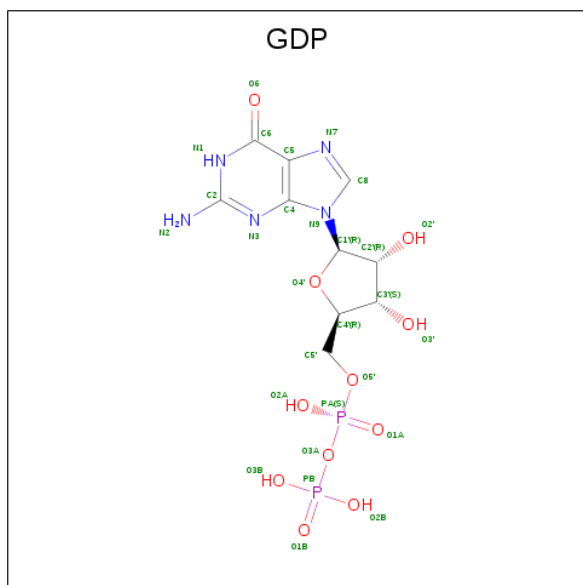
- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	2	Total	Mg	0	0
			2	2		
7	D	1	Total	Mg	0	0
			1	1		
7	C	1	Total	Mg	0	0
			1	1		

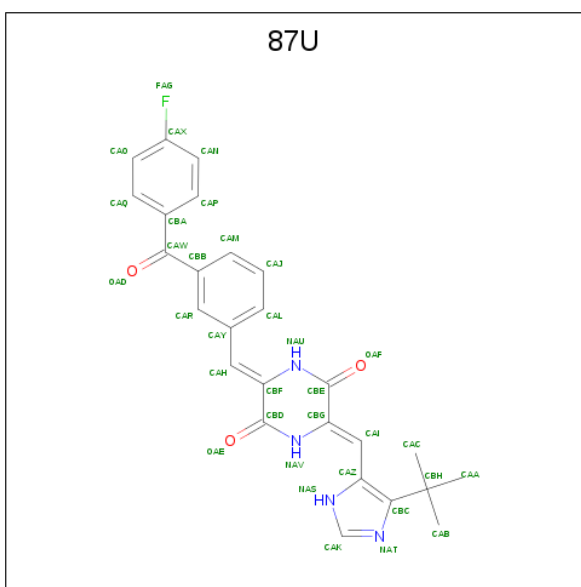
- Molecule 8 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula:  $C_{10}H_{15}N_5O_{11}P_2$ ).





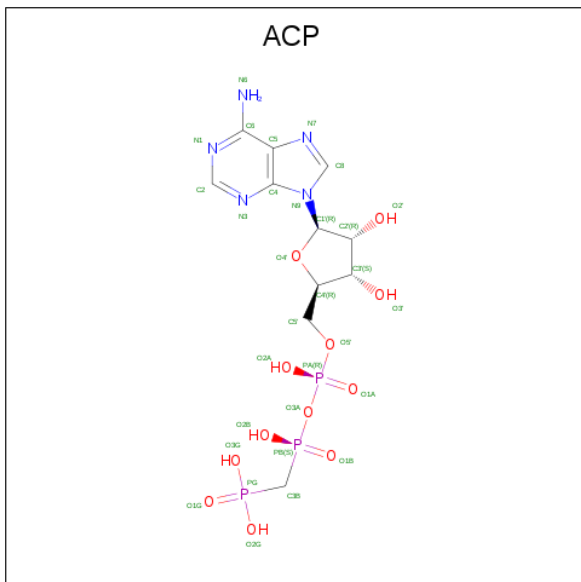
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
9	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 10 is (3Z,6Z)-3-[(4-tert-butyl-1H-imidazol-5-yl)methylidene]-6-[[3-(4-fluorophenyl)carbonylphenyl]methylidene]piperazine-2,5-dione (three-letter code: 87U) (formula: C<sub>26</sub>H<sub>23</sub>FN<sub>4</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	B	1	Total	C	F	N	O	0	0
			34	26	1	4	3		

- Molecule 11 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (three-letter code: ACP) (formula:  $\text{C}_{11}\text{H}_{18}\text{N}_5\text{O}_{12}\text{P}_3$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	F	1	Total 31	C 11	N 5	O 12	P 3	0	0

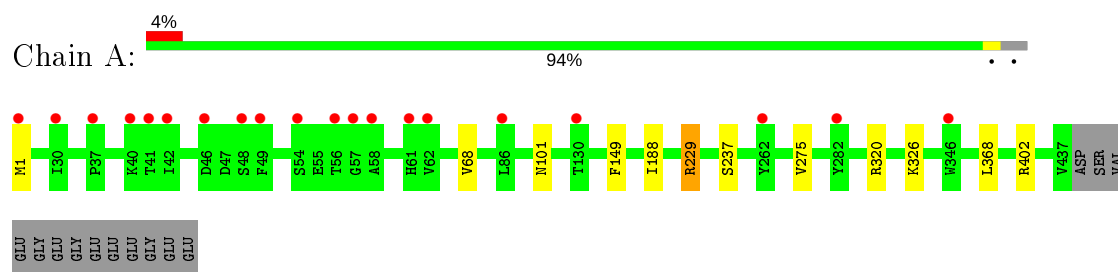
- Molecule 12 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	20	Total O 20 20	0	0
12	B	22	Total O 22 22	0	0
12	C	55	Total O 55 55	0	0
12	E	2	Total O 2 2	0	0
12	F	4	Total O 4 4	0	0

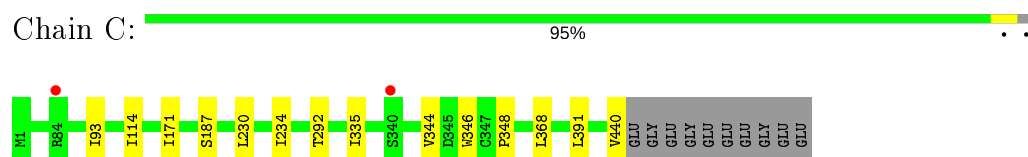
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

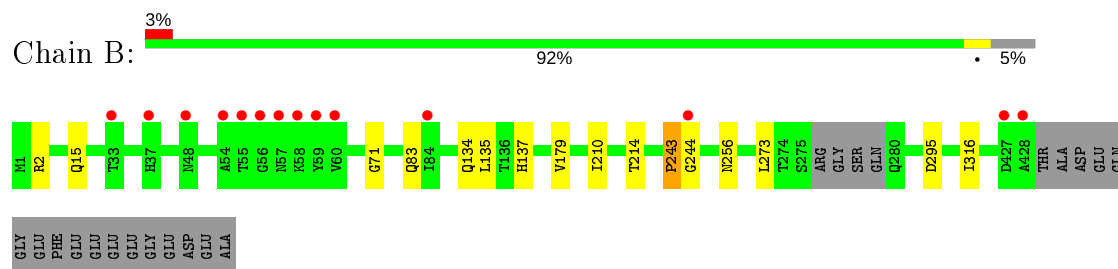
- Molecule 1: Tubulin alpha chain



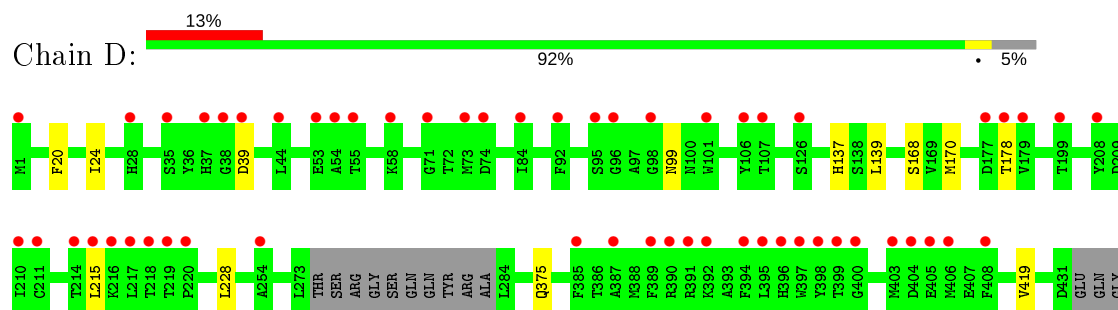
- Molecule 1: Tubulin alpha chain



- Molecule 2: Tubulin beta chain



- Molecule 2: Tubulin beta chain





GLU  
PHE  
GLU  
GLU  
GLU  
GLU  
GLY  
GLU  
ASP  
GLU  
ALA

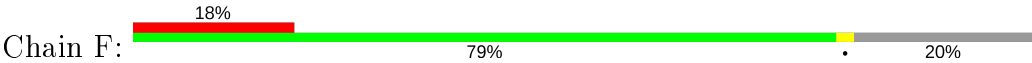
● Molecule 3: Stathmin-4



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  
VAL  
ILE  
SER  
ASP  
PHE  
P26  
P27  
SER  
PHE  
ASP  
GLY  
VAL  
PRO  
GLU  
PHE  
ASN  
ALA  
SER  
LEU

PRO  
ARG  
ARG  
ARG  
D44  
P45  
S46  
L47  
E48  
Q51  
E59  
K128  
E131  
E132  
V133  
N136  
K137  
E138  
L139  
K140  
E141  
GLU  
ALA  
SER  
ARG

● Molecule 4: TUBULIN TYROSINE LIGASE



M1  
V6  
E9  
N10  
Y14  
V17  
L20  
L21  
L22  
N27  
R31  
K32  
Y98  
V99  
I100  
Y101  
P102  
THR  
ASN  
LEU  
LYS  
THR  
LYS  
PRO  
VAL  
ALA  
PRO  
ALA  
GLN  
ASN  
GLY  
ILE  
ARG  
HIS  
LEU  
ILE  
ASN  
ASN  
THR  
ARG  
THR  
ASP  
GLU  
ARG  
GLU  
VAL  
PHE  
LEU  
ALA  
ALA  
TYR  
ASN  
ARG

ARG  
ARG  
GLU  
GLY  
ARG  
GLU  
G144  
N145  
V146  
I147  
I148  
A149  
K150  
S151  
SER  
ALA  
GLY  
ALA  
LYS  
GLY  
GLU  
G159  
I160  
L161  
I162  
S163  
S164  
E165  
A166  
SER  
GLU  
LEU  
LEU  
ASP  
PHE  
ILE  
ASP  
GLU  
GLN  
GLN  
VAL  
H180  
V181  
I182  
Q183  
K184  
L191  
L192  
E193  
P194  
G195  
H196  
R197  
K198  
F199  
Y211

T223  
S224  
E225  
E226  
Y227  
P228  
N229  
S230  
A231  
N232  
F233  
Q234  
D235  
K236  
T237  
C238  
E239  
L240  
T241  
N242  
H243  
C244  
I245  
Q246  
K247  
GLU  
TYR  
SER  
LYS  
N252  
Y253  
Q254  
R255  
Y256  
E257  
E258  
G259  
N260  
M320  
A335  
G349  
L361  
A362  
ASP  
THR  
GLY  
GLN  
LYS  
THR  
SER  
GLN  
PRO  
THR  
S373  
I374

H384

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	105.26 Å 157.88 Å 182.43 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	119.38 – 2.75 49.93 – 2.75	Depositor EDS
% Data completeness (in resolution range)	98.5 (119.38-2.75) 98.5 (49.93-2.75)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.11 (at 2.77 Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, $R_{free}$	0.227 , 0.277 0.228 , 0.276	Depositor DCC
$R_{free}$ test set	3932 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	46.9	Xtriage
Anisotropy	0.027	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 36.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	17462	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.62% 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: GDP, MG, CA, 87U, 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	0.37	0/3525	0.59	0/4784
1	C	0.37	0/3572	0.60	0/4850
2	B	0.39	0/3427	0.60	0/4640
2	D	0.38	0/3379	0.55	0/4577
3	E	0.38	0/1018	0.53	0/1350
4	F	0.38	0/2618	0.54	0/3537
All	All	0.38	0/17539	0.57	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	9	0
1	C	3482	0	3384	7	0
2	B	3353	0	3228	7	0
2	D	3306	0	3181	6	0
3	E	1004	0	1028	0	0
4	F	2553	0	2519	2	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
7	B	2	0	0	0	0
7	C	1	0	0	0	0
7	D	1	0	0	0	0
8	B	28	0	12	0	0
9	B	24	0	26	1	0
10	B	34	0	0	2	0
11	F	31	0	14	0	0
12	A	20	0	0	0	0
12	B	22	0	0	0	0
12	C	55	0	0	0	0
12	E	2	0	0	0	0
12	F	4	0	0	0	0
All	All	17462	0	16791	30	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 1.

All (30) 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	1.07	1.20
1:A:229[A]:ARG:HH11	1:A:229[A]:ARG:CG	1.75	0.98
1:A:229[A]:ARG:HG2	1:A:229[A]:ARG:NH1	1.87	0.84
2:B:243:PRO:HB2	2:B:244:GLY:HA2	1.67	0.75
2:B:243:PRO:CB	2:B:244:GLY:HA2	2.22	0.69
2:B:295:ASP:HA	9:B:507:MES:O2S	1.96	0.64
1:A:229[A]:ARG:NH1	1:A:229[A]:ARG:CG	2.46	0.63
1:A:368[B]:LEU:N	1:A:368[B]:LEU:HD12	2.13	0.63
1:A:368[B]:LEU:H	1:A:368[B]:LEU:HD12	1.62	0.62
1:C:187:SER:HB3	1:C:391:LEU:HD21	1.91	0.53
1:A:68:VAL:HG11	1:A:149:PHE:CE2	2.50	0.47
2:B:179:VAL:HG12	1:C:348:PRO:HG2	1.96	0.47
1:A:101:ASN:HD22	2:B:256:ASN:HD21	1.61	0.47
2:B:210:ILE:HG23	2:B:273:LEU:HD13	1.97	0.47
2:D:139:LEU:HD12	2:D:170:MET:SD	2.54	0.47
10:B:505:87U:NAV	10:B:505:87U:NAS	2.62	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:230:LEU:O	1:C:234:ILE:HD12	2.15	0.46
1:C:292:THR:HG22	1:C:335:ILE:CD1	2.46	0.45
2:D:139:LEU:HD11	2:D:168:SER:HB3	1.98	0.44
4:F:224:SER:HB2	4:F:241:THR:HG22	2.00	0.43
1:A:275:VAL:HG13	1:A:368[A]:LEU:HD21	2.01	0.43
1:C:344:VAL:HG21	1:C:346:TRP:CE2	2.53	0.43
4:F:349:GLY:HA3	4:F:374:ILE:HD11	2.00	0.42
2:D:375:GLN:HB2	2:D:419:VAL:HG13	2.01	0.42
1:C:171:ILE:HD12	1:C:171:ILE:N	2.35	0.41
2:D:20:PHE:CZ	2:D:24:ILE:HD13	2.55	0.41
1:C:93:ILE:HG22	1:C:114:ILE:HD11	2.02	0.41
2:D:99:ASN:HD22	2:D:178:THR:HG21	1.86	0.41
2:B:134:GLN:HB2	10:B:505:87U:CAP	2.51	0.41
2:D:215:LEU:HD11	2:D:228:LEU:HD21	2.03	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	439/450 (98%)	426 (97%)	13 (3%)	0	100	100
1	C	446/450 (99%)	435 (98%)	11 (2%)	0	100	100
2	B	422/445 (95%)	407 (96%)	13 (3%)	2 (0%)	29	47
2	D	417/445 (94%)	404 (97%)	12 (3%)	1 (0%)	47	69
3	E	118/184 (64%)	116 (98%)	2 (2%)	0	100	100
4	F	300/384 (78%)	286 (95%)	14 (5%)	0	100	100
All	All	2142/2358 (91%)	2074 (97%)	65 (3%)	3 (0%)	51	75

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	243	PRO
2	B	71	GLY
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%)	364 (98%)	8 (2%)	52	70
1	C	379/378 (100%)	377 (100%)	2 (0%)	88	92
2	B	367/383 (96%)	360 (98%)	7 (2%)	57	73
2	D	362/383 (94%)	361 (100%)	1 (0%)	92	95
3	E	110/168 (66%)	107 (97%)	3 (3%)	44	65
4	F	281/342 (82%)	278 (99%)	3 (1%)	73	84
All	All	1871/2032 (92%)	1847 (99%)	24 (1%)	71	81

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	188	ILE
1	A	229[A]	ARG
1	A	229[B]	ARG
1	A	237	SER
1	A	320	ARG
1	A	326	LYS
1	A	402	ARG
2	B	2	ARG
2	B	15	GLN
2	B	83	GLN
2	B	135	LEU
2	B	137	HIS
2	B	214	THR
2	B	316	ILE
1	C	368	LEU

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Mol	Chain	Res	Type
1	C	440	VAL
2	D	137	HIS
3	E	44	ASP
3	E	131	GLU
3	E	136	ASN
4	F	1	MET
4	F	32	LYS
4	F	211	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	101	ASN
2	B	83	GLN
1	C	249	ASN
3	E	136	ASN
4	F	252	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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 7 are monoatomic - leaving 8 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
9	MES	B	504	-	12,12,12	2.03	1 (8%)	14,16,16	7.44	10 (71%)
10	87U	B	505	-	29,37,37	2.45	8 (27%)	35,54,54	1.71	9 (25%)
9	MES	B	507	-	12,12,12	2.04	2 (16%)	14,16,16	6.14	6 (42%)
5	GTP	D	501	7	26,34,34	1.25	2 (7%)	33,54,54	1.94	8 (24%)
11	ACP	F	401	-	27,33,33	2.01	8 (29%)	32,52,52	1.34	3 (9%)
8	GDP	B	502	7	24,30,30	1.23	2 (8%)	31,47,47	1.98	6 (19%)
5	GTP	C	501	7	26,34,34	1.14	2 (7%)	33,54,54	1.96	10 (30%)
5	GTP	A	501	7	26,34,34	1.17	2 (7%)	33,54,54	1.93	9 (27%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	MES	B	504	-	-	3/6/14/14	0/1/1/1
10	87U	B	505	-	-	2/18/22/22	0/4/4/4
9	MES	B	507	-	-	2/6/14/14	0/1/1/1
5	GTP	D	501	7	-	4/18/38/38	0/3/3/3
11	ACP	F	401	-	-	4/15/38/38	0/3/3/3
8	GDP	B	502	7	-	3/12/32/32	0/3/3/3
5	GTP	C	501	7	-	6/18/38/38	0/3/3/3
5	GTP	A	501	7	-	3/18/38/38	0/3/3/3

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	504	MES	C8-S	-6.41	1.68	1.77
9	B	507	MES	C8-S	-6.36	1.68	1.77
10	B	505	87U	CBE-NAU	5.51	1.42	1.33
11	F	401	ACP	PG-O1G	5.46	1.61	1.50
10	B	505	87U	FAG-CAX	-5.44	1.23	1.36
10	B	505	87U	CBA-CAW	-4.93	1.41	1.49
5	D	501	GTP	C6-C5	4.49	1.49	1.41
10	B	505	87U	CBD-NAV	4.33	1.40	1.33
10	B	505	87U	CBB-CAW	-4.19	1.42	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	505	87U	CBG-NAV	4.16	1.42	1.35
11	F	401	ACP	PB-O1B	4.03	1.61	1.51
5	A	501	GTP	C6-C5	3.97	1.48	1.41
8	B	502	GDP	C6-C5	3.90	1.48	1.41
5	C	501	GTP	C6-C5	3.82	1.47	1.41
10	B	505	87U	CBF-NAU	3.60	1.41	1.35
11	F	401	ACP	PB-O3A	3.43	1.62	1.58
10	B	505	87U	CAY-CAH	-3.42	1.39	1.47
11	F	401	ACP	PB-O2B	-3.29	1.48	1.56
11	F	401	ACP	PG-O2G	2.95	1.61	1.54
11	F	401	ACP	PG-O3G	-2.72	1.48	1.54
5	D	501	GTP	C5-C4	2.68	1.48	1.40
11	F	401	ACP	C5-C4	2.62	1.47	1.40
5	C	501	GTP	C5-C4	2.60	1.47	1.40
8	B	502	GDP	C5-C4	2.53	1.47	1.40
5	A	501	GTP	C5-C4	2.48	1.47	1.40
11	F	401	ACP	C2-N3	2.17	1.35	1.32
9	B	507	MES	O2S-S	2.09	1.51	1.45

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	504	MES	O1S-S-C8	-18.77	84.32	106.92
9	B	507	MES	O3S-S-O1S	-13.37	78.60	111.27
9	B	504	MES	O2S-S-C8	11.41	120.65	106.92
9	B	504	MES	O3S-S-O1S	-10.64	85.27	111.27
9	B	507	MES	O3S-S-C8	10.52	122.79	105.77
9	B	507	MES	O1S-S-C8	-10.18	94.65	106.92
9	B	504	MES	O2S-S-O1S	-8.81	83.47	113.95
9	B	507	MES	O2S-S-O1S	-8.78	83.57	113.95
9	B	504	MES	O3S-S-C8	7.64	118.12	105.77
9	B	507	MES	O3S-S-O2S	6.01	125.96	111.27
10	B	505	87U	CBG-CAI-CAZ	-4.91	121.88	128.66
8	B	502	GDP	C6-N1-C2	4.78	123.52	115.93
5	C	501	GTP	C6-C5-C4	-4.76	116.25	120.80
5	C	501	GTP	C6-N1-C2	4.72	123.44	115.93
5	D	501	GTP	C2-N3-C4	4.61	120.62	115.36
8	B	502	GDP	C6-C5-C4	-4.59	116.42	120.80
5	A	501	GTP	C6-C5-C4	-4.56	116.44	120.80
5	A	501	GTP	C6-N1-C2	4.46	123.01	115.93
8	B	502	GDP	C2-N3-C4	4.38	120.36	115.36
5	C	501	GTP	C5-C6-N1	-4.34	117.50	123.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	501	GTP	C6-N1-C2	4.34	122.82	115.93
5	A	501	GTP	C5-C6-N1	-4.25	117.62	123.43
9	B	504	MES	C2-C3-N4	4.22	116.50	110.10
5	D	501	GTP	C6-C5-C4	-4.12	116.87	120.80
5	D	501	GTP	C5-C6-N1	-4.11	117.81	123.43
5	C	501	GTP	C2-N3-C4	4.09	120.02	115.36
5	A	501	GTP	C2-N3-C4	4.07	120.01	115.36
8	B	502	GDP	C5-C6-N1	-4.03	117.93	123.43
8	B	502	GDP	N3-C2-N1	-3.92	122.00	127.22
11	F	401	ACP	N3-C2-N1	-3.75	122.82	128.68
10	B	505	87U	CAY-CAR-CBB	3.68	124.04	121.13
5	C	501	GTP	N3-C2-N1	-3.50	122.55	127.22
5	D	501	GTP	N3-C2-N1	-3.47	122.59	127.22
5	A	501	GTP	N3-C2-N1	-3.37	122.72	127.22
11	F	401	ACP	C3'-C2'-C1'	3.14	105.70	100.98
9	B	504	MES	O3S-S-O2S	2.90	118.35	111.27
10	B	505	87U	CAM-CBB-CAR	-2.76	115.97	119.24
11	F	401	ACP	C4-C5-N7	-2.72	106.57	109.40
10	B	505	87U	CBD-NAV-CBG	2.69	122.37	116.41
10	B	505	87U	CBH-CBC-NAT	2.63	123.77	120.50
9	B	504	MES	C5-N4-C3	2.53	114.53	108.83
5	A	501	GTP	C4-C5-N7	-2.47	106.83	109.40
5	D	501	GTP	C4-C5-N7	-2.44	106.85	109.40
5	D	501	GTP	PA-O3A-PB	-2.39	124.62	132.83
5	A	501	GTP	O3B-PG-O1G	-2.38	97.99	111.19
5	C	501	GTP	O3G-PG-O2G	2.38	116.73	107.64
8	B	502	GDP	C4-C5-N7	-2.34	106.96	109.40
9	B	504	MES	C6-C5-N4	2.32	113.61	110.10
10	B	505	87U	CBE-NAU-CBF	2.30	121.51	116.41
10	B	505	87U	CBF-CAH-CAY	-2.25	127.11	130.01
5	C	501	GTP	C4-C5-N7	-2.24	107.07	109.40
5	C	501	GTP	PA-O3A-PB	-2.19	125.31	132.83
5	A	501	GTP	PA-O3A-PB	-2.19	125.32	132.83
9	B	504	MES	O1-C6-C5	-2.16	107.03	111.80
10	B	505	87U	CAM-CBB-CAW	2.14	125.27	120.57
5	D	501	GTP	PB-O3B-PG	-2.13	125.51	132.83
5	C	501	GTP	PB-O3B-PG	-2.13	125.53	132.83
9	B	507	MES	C6-C5-N4	2.11	113.31	110.10
10	B	505	87U	CAJ-CAL-CAY	-2.09	118.12	120.65
5	C	501	GTP	C1'-N9-C4	-2.06	123.02	126.64
5	A	501	GTP	C1'-N9-C4	-2.06	123.03	126.64

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	B	504	MES	N4-C7-C8-S
9	B	504	MES	C7-C8-S-O2S
5	D	501	GTP	C5'-O5'-PA-O1A
5	D	501	GTP	C5'-O5'-PA-O2A
10	B	505	87U	CBG-CAI-CAZ-NAS
10	B	505	87U	CBG-CAI-CAZ-CBC
8	B	502	GDP	C5'-O5'-PA-O1A
8	B	502	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	A	501	GTP	C5'-O5'-PA-O1A
5	A	501	GTP	C5'-O5'-PA-O2A
11	F	401	ACP	O4'-C4'-C5'-O5'
9	B	504	MES	C7-C8-S-O3S
11	F	401	ACP	C3'-C4'-C5'-O5'
9	B	507	MES	C7-C8-S-O3S
9	B	507	MES	C7-C8-S-O1S
5	C	501	GTP	C4'-C5'-O5'-PA
11	F	401	ACP	PG-C3B-PB-O1B
5	D	501	GTP	C4'-C5'-O5'-PA
5	C	501	GTP	PB-O3B-PG-O1G
5	D	501	GTP	C5'-O5'-PA-O3A
8	B	502	GDP	C5'-O5'-PA-O3A
5	C	501	GTP	C5'-O5'-PA-O3A
5	A	501	GTP	C5'-O5'-PA-O3A
11	F	401	ACP	C4'-C5'-O5'-PA

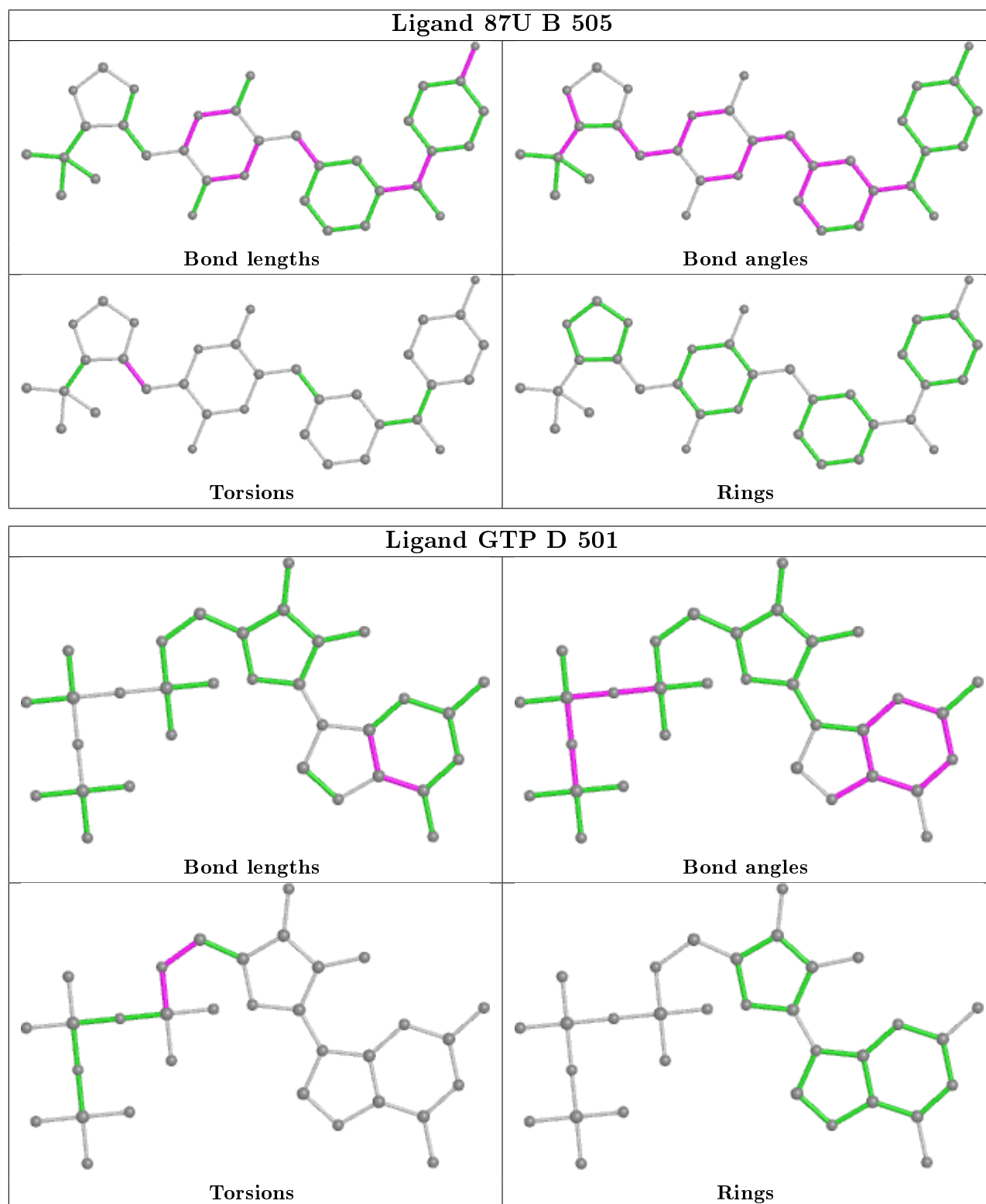
There are no ring outliers.

2 monomers are involved in 3 short contacts:

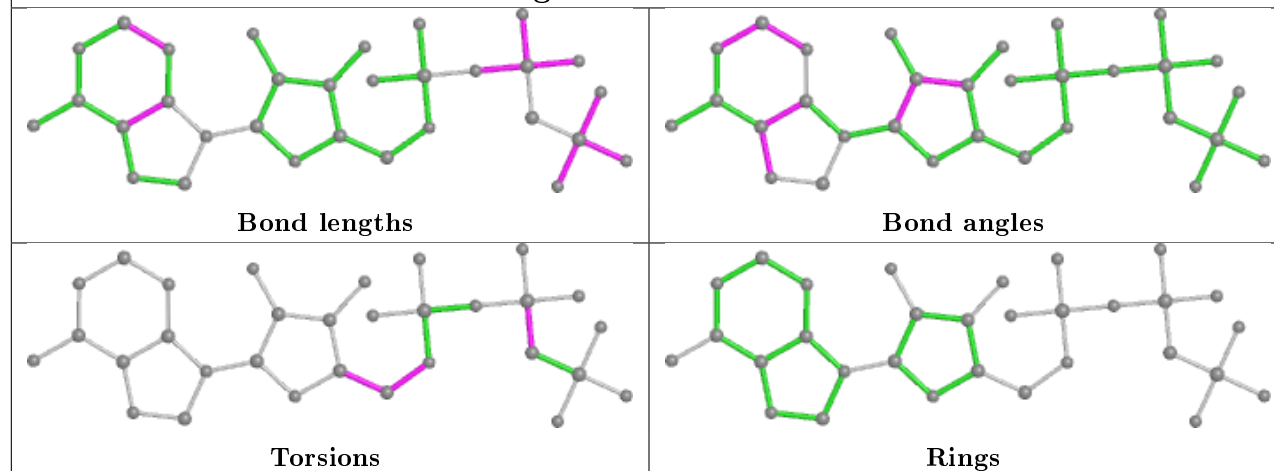
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	B	505	87U	2	0
9	B	507	MES	1	0

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

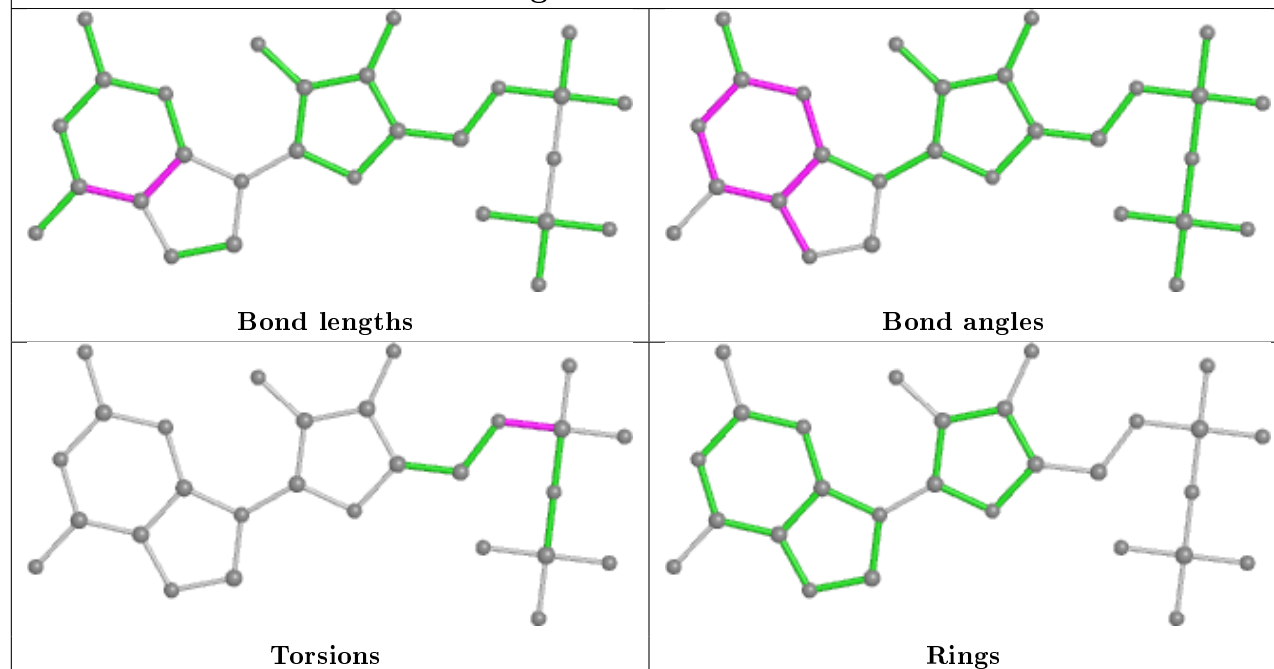
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified 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.

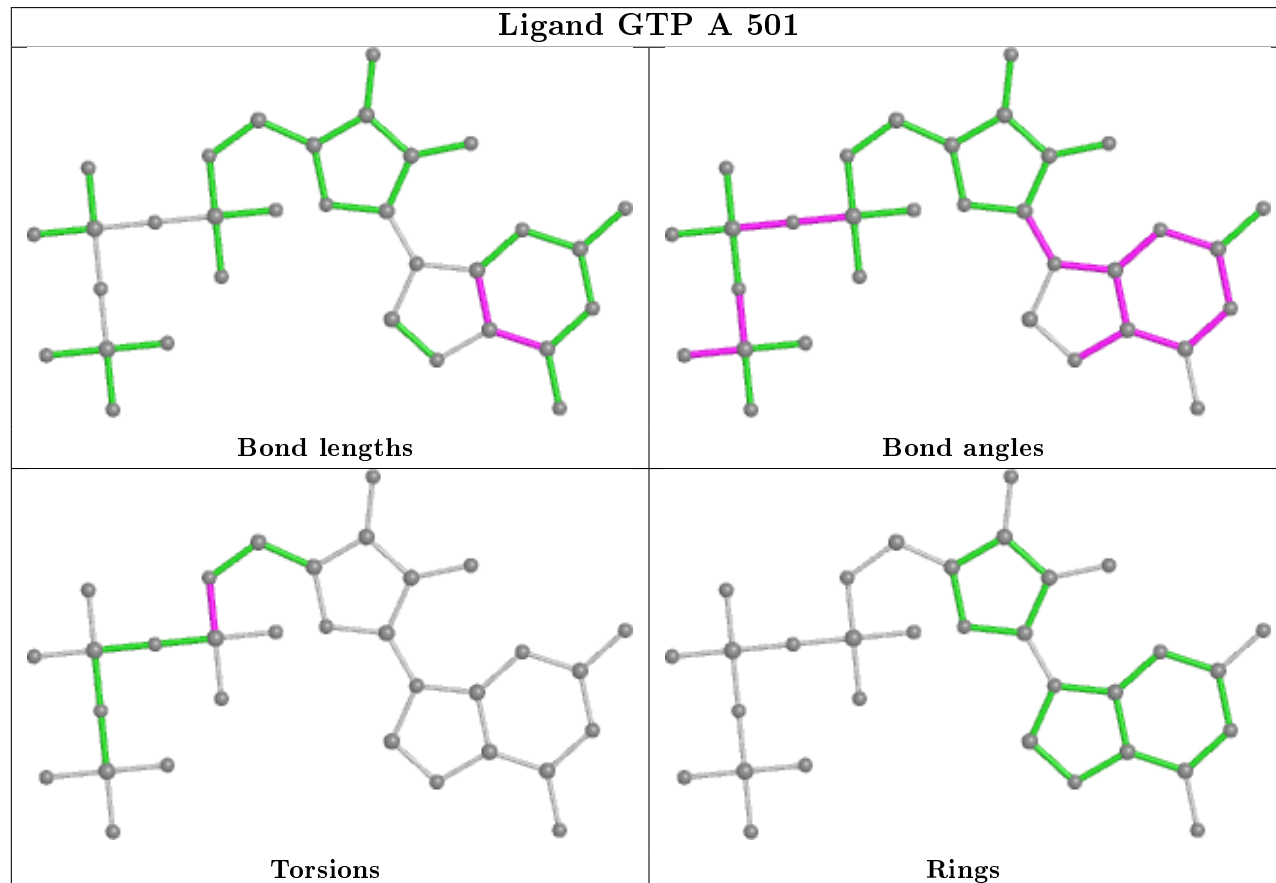
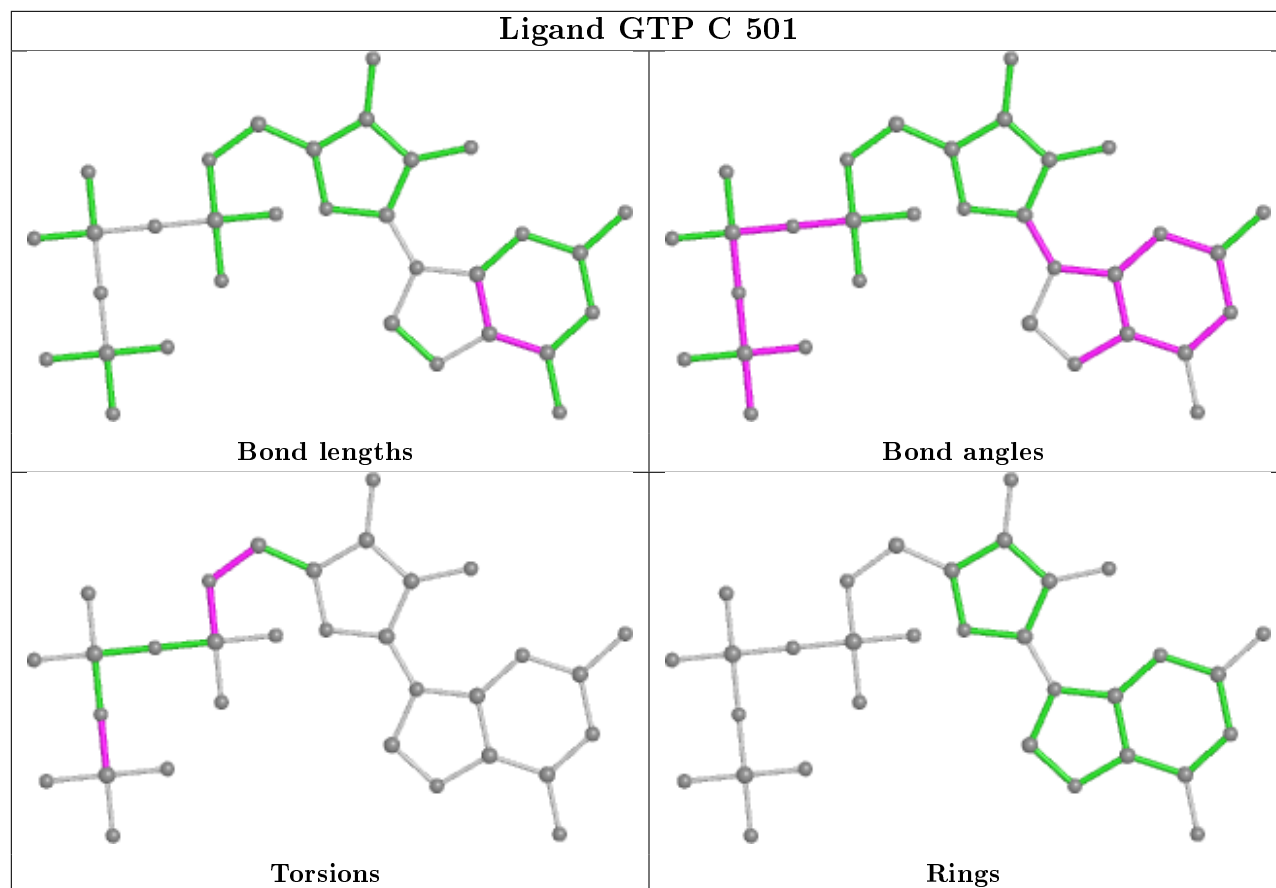


## Ligand ACP F 401



## Ligand GDP B 502





## 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	437/450 (97%)	0.20	20 (4%) 32 39	23, 45, 71, 91	0
1	C	440/450 (97%)	-0.08	2 (0%) 91 94	19, 36, 58, 80	1 (0%)
2	B	424/445 (95%)	0.21	14 (3%) 46 54	25, 45, 75, 102	1 (0%)
2	D	421/445 (94%)	0.79	56 (13%) 3 4	35, 64, 96, 126	4 (0%)
3	E	120/184 (65%)	0.64	11 (9%) 9 10	34, 64, 95, 106	0
4	F	309/384 (80%)	1.06	71 (22%) 0 0	35, 68, 107, 122	0
All	All	2151/2358 (91%)	0.41	174 (8%) 12 14	19, 51, 92, 126	6 (0%)

All (174) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	182	ILE	9.1
2	D	37	HIS	8.3
4	F	233	PHE	6.4
2	D	395	LEU	5.7
4	F	100	ILE	5.5
4	F	244	CYS	5.4
4	F	253	TYR	5.4
4	F	194	PRO	5.2
4	F	256	TYR	5.1
4	F	161	LEU	4.9
2	D	92	PHE	4.8
4	F	240	LEU	4.6
4	F	245	ILE	4.6
4	F	149	ALA	4.6
4	F	225	SER	4.6
2	D	403	MET	4.6
2	B	54	ALA	4.5
4	F	180	HIS	4.4
4	F	191	LEU	4.4

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Mol	Chain	Res	Type	RSRZ
1	A	1	MET	4.4
2	D	405	GLU	4.4
4	F	362	ALA	4.4
2	D	215	LEU	4.3
2	D	398	TYR	4.1
4	F	20	LEU	4.1
4	F	227	PRO	4.1
3	E	139	LEU	4.1
4	F	21	LEU	4.1
2	D	95	SER	4.0
2	B	57	ASN	4.0
2	B	60	VAL	4.0
2	B	55	THR	3.9
4	F	232	ASN	3.9
4	F	163	SER	3.9
4	F	255	ARG	3.9
1	A	42	ILE	3.9
4	F	22	LEU	3.8
2	D	98	GLY	3.8
2	D	73	MET	3.8
2	D	106	TYR	3.8
2	D	390	ARG	3.8
4	F	162	ILE	3.8
4	F	234	GLN	3.7
2	D	38	GLY	3.7
4	F	242	ASN	3.7
2	D	55	THR	3.7
4	F	147	TRP	3.6
2	D	406	MET	3.5
2	D	218	THR	3.5
2	D	391	ARG	3.5
4	F	226	GLU	3.5
4	F	192	LEU	3.4
4	F	102	PRO	3.4
2	D	400	GLY	3.4
3	E	140	LYS	3.3
2	B	428	ALA	3.3
4	F	98	TYR	3.3
4	F	145	ASN	3.2
4	F	259	GLY	3.2
4	F	199	PHE	3.2
4	F	27	TRP	3.2

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Mol	Chain	Res	Type	RSRZ
4	F	181	VAL	3.2
2	B	59	TYR	3.2
4	F	235	ASP	3.1
4	F	252	ASN	3.1
1	A	61	HIS	3.1
2	B	58	LYS	3.1
1	A	282	TYR	3.0
2	D	396	HIS	3.0
4	F	237	THR	3.0
3	E	26	PRO	3.0
2	D	216	LYS	3.0
3	E	138	GLU	3.0
1	C	340	SER	3.0
4	F	196	HIS	2.9
1	A	86	LEU	2.9
4	F	101	TYR	2.9
3	E	132	GLU	2.9
2	D	217	LEU	2.8
1	A	41	THR	2.8
1	A	37	PRO	2.8
2	D	219	THR	2.8
4	F	246	GLN	2.8
2	D	74	ASP	2.8
2	B	56	GLY	2.8
2	D	177	ASP	2.8
4	F	335	ALA	2.8
2	D	1	MET	2.8
4	F	223	THR	2.8
1	A	54	SER	2.7
1	A	49	PHE	2.7
4	F	31	ARG	2.7
4	F	243	HIS	2.7
2	D	179	VAL	2.7
2	D	44	LEU	2.7
4	F	236	LYS	2.7
4	F	10	ASN	2.6
2	D	392	LYS	2.6
1	A	57	GLY	2.6
2	D	399	THR	2.6
2	D	210	ILE	2.6
2	D	214	THR	2.6
3	E	128	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	58	ALA	2.6
1	A	30	ILE	2.6
2	D	211	CYS	2.6
4	F	228	TYR	2.5
4	F	258	GLU	2.5
4	F	229	ASN	2.5
1	A	46	ASP	2.5
4	F	260	ASN	2.5
2	D	220	PRO	2.5
2	D	101	TRP	2.5
2	D	96	GLY	2.5
4	F	148	ILE	2.5
4	F	150	LYS	2.5
4	F	165	GLU	2.4
4	F	361	LEU	2.4
3	E	48	GLU	2.4
2	D	28	HIS	2.4
2	D	394	PHE	2.4
2	D	404	ASP	2.4
4	F	14	TYR	2.4
4	F	231	ALA	2.4
2	B	84	ILE	2.4
3	E	59	GLU	2.4
4	F	164	SER	2.4
1	A	56	THR	2.4
2	B	48	ASN	2.4
4	F	151	SER	2.3
2	B	427	ASP	2.3
1	A	48	SER	2.3
1	C	84	ARG	2.3
2	B	37	HIS	2.3
4	F	254	GLY	2.3
4	F	320	MET	2.3
4	F	6	VAL	2.3
4	F	146	VAL	2.3
1	A	130	THR	2.3
2	D	54	ALA	2.3
4	F	184	LYS	2.3
2	B	244	GLY	2.3
2	D	254	ALA	2.3
2	D	84	ILE	2.3
2	D	408	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
3	E	51	GLN	2.2
2	B	33	THR	2.2
2	D	53	GLU	2.2
2	D	387	ALA	2.2
2	D	397	TRP	2.2
4	F	239	HIS	2.2
2	D	389	PHE	2.2
3	E	133	VAL	2.2
2	D	385	PHE	2.2
2	D	35	SER	2.2
1	A	262	TYR	2.2
4	F	9	GLU	2.2
2	D	199	THR	2.2
2	D	58	LYS	2.1
4	F	195	GLY	2.1
4	F	197	ARG	2.1
3	E	46	SER	2.1
1	A	40	LYS	2.1
2	D	107	THR	2.1
4	F	198	LYS	2.1
2	D	39	ASP	2.1
4	F	17	VAL	2.1
2	D	208	TYR	2.1
1	A	346	TRP	2.1
2	D	126	SER	2.0
4	F	224	SER	2.0
1	A	62	VAL	2.0
2	D	71	GLY	2.0
2	D	178	THR	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 monosaccharides in this entry.

## 6.4 Ligands

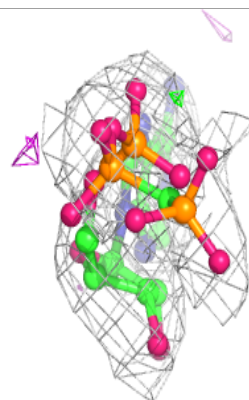
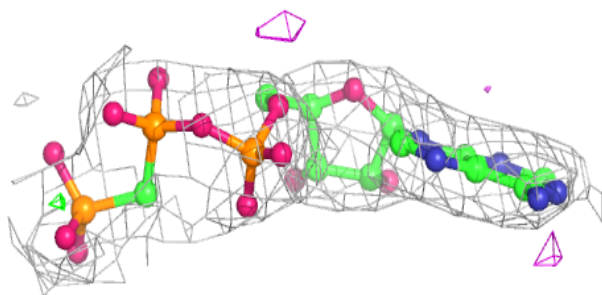
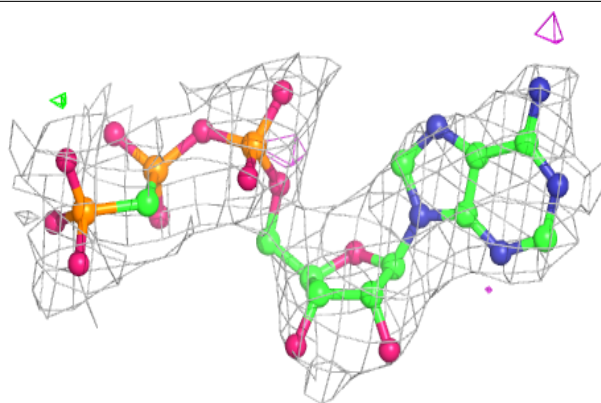
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
7	MG	D	502	1/1	0.85	0.13	52,52,52,52	0
11	ACP	F	401	31/31	0.85	0.29	79,83,112,115	0
9	MES	B	507	12/12	0.88	0.44	95,97,101,104	0
6	CA	B	506	1/1	0.88	0.15	78,78,78,78	0
6	CA	C	503	1/1	0.89	0.10	56,56,56,56	0
9	MES	B	504	12/12	0.89	0.21	70,74,76,78	0
5	GTP	D	501	32/32	0.93	0.17	45,49,67,70	0
10	87U	B	505	34/34	0.94	0.20	48,54,55,55	0
6	CA	A	502	1/1	0.96	0.13	67,67,67,67	0
7	MG	B	503	1/1	0.97	0.11	24,24,24,24	0
8	GDP	B	502	28/28	0.98	0.15	22,25,26,28	0
7	MG	C	502	1/1	0.98	0.11	24,24,24,24	0
5	GTP	C	501	32/32	0.98	0.14	24,26,28,30	0
7	MG	B	501	1/1	0.98	0.18	22,22,22,22	0
5	GTP	A	501	32/32	0.98	0.15	26,28,30,30	0

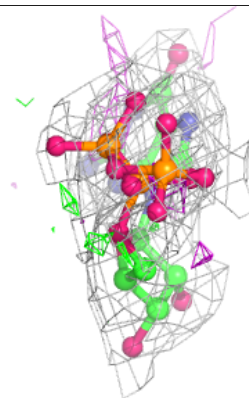
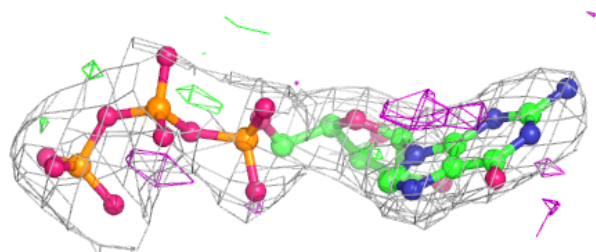
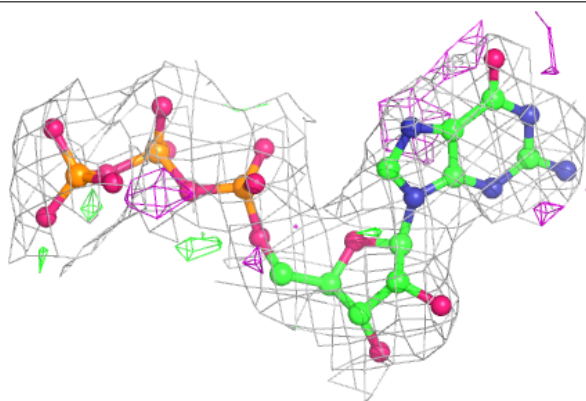
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around ACP F 401:**

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

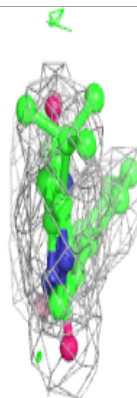
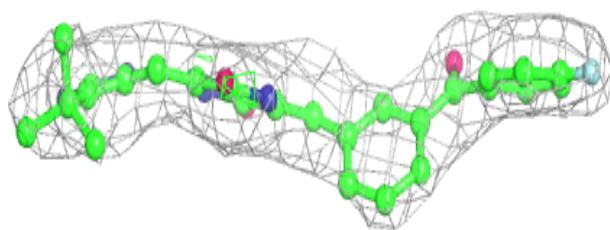
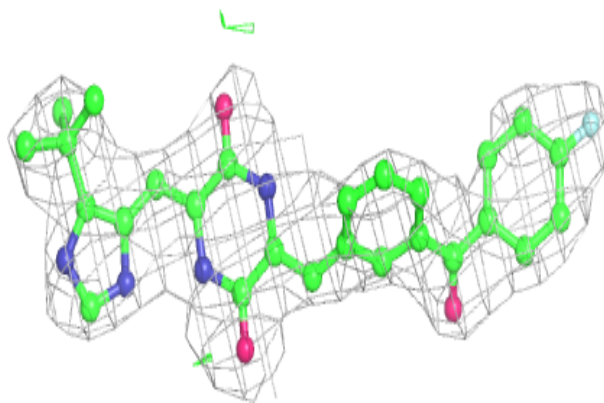
**Electron density around GTP D 501:**

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

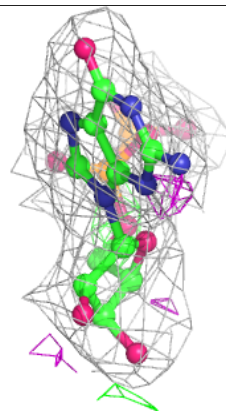
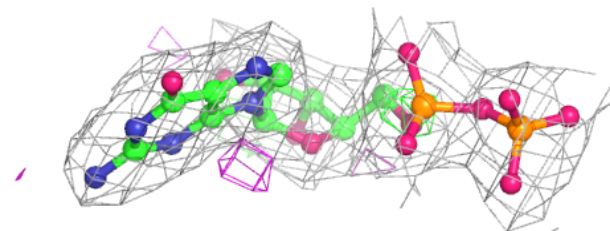
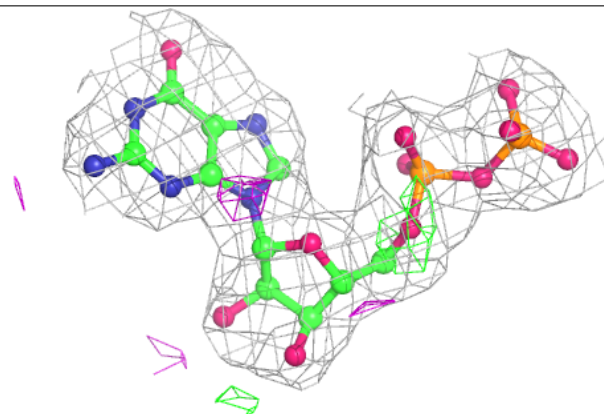


**Electron density around 87U B 505:**

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

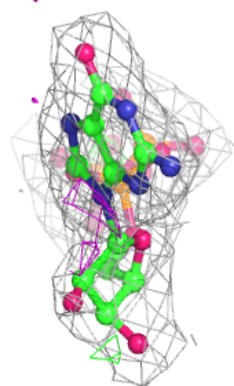
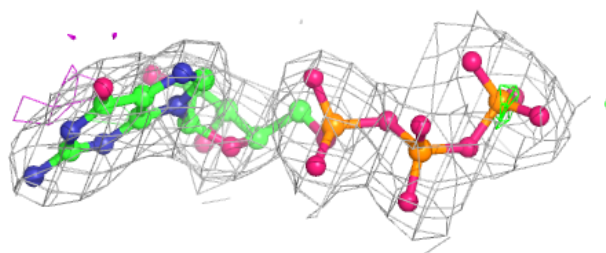
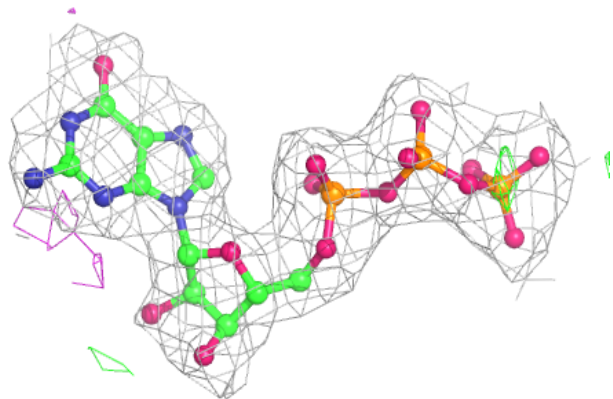
**Electron density around GDP B 502:**

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

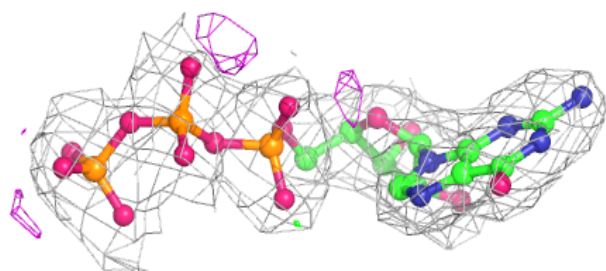
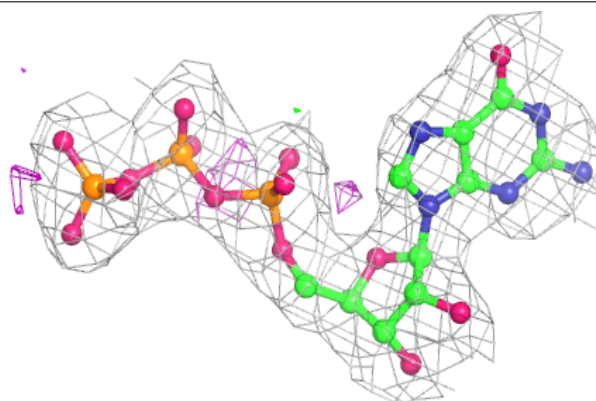


**Electron density around GTP C 501:**

$2mF_o-DF_c$  (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.