



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 28, 2021 – 04:13 PM JST

PDB ID : 7CLD  
Title : Crystal structure of T2R-TTL-Cevipabulin complex  
Authors : Chen, L.J.; Chen, Q.; Yu, Y.; Yang, J.H.  
Deposited on : 2020-07-20  
Resolution : 2.61 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 : 2.20  
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) : 2.20

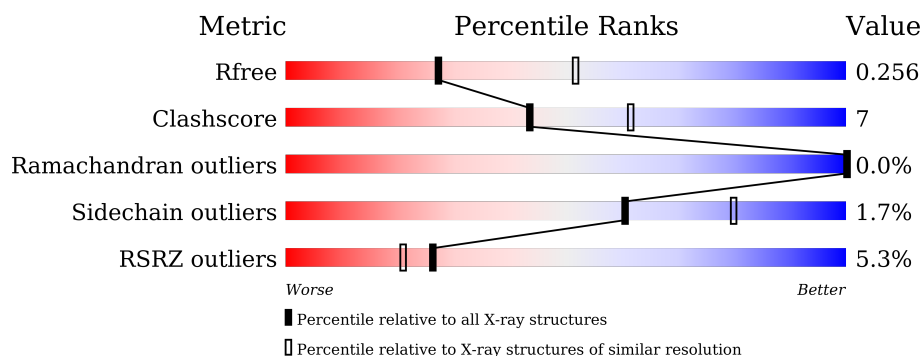
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.61 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	3797 (2.64-2.60)
Clashscore	141614	4168 (2.64-2.60)
Ramachandran outliers	138981	4093 (2.64-2.60)
Sidechain outliers	138945	4093 (2.64-2.60)
RSRZ outliers	127900	3731 (2.64-2.60)

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	450	<div> <div>2%</div> <div>85%</div> <div>12%</div> <div>.</div> </div>
1	C	450	<div> <div>85%</div> <div>12%</div> <div>.</div> </div>
2	B	445	<div> <div>3%</div> <div>80%</div> <div>14%</div> <div>6%</div> </div>
2	D	445	<div> <div>5%</div> <div>77%</div> <div>19%</div> <div>.</div> </div>
3	E	143	<div> <div>8%</div> <div>69%</div> <div>14%</div> <div>.</div> <div>14%</div> </div>
4	F	384	<div> <div>15%</div> <div>68%</div> <div>22%</div> <div>.</div> <div>9%</div> </div>

## 2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 35069 atoms, of which 17070 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	438	Total	C	H	N	O	S	0	4	0
			6802	2182	3351	588	657	24			
1	C	440	Total	C	H	N	O	S	0	7	0
			6827	2196	3361	587	660	23			

- Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	418	Total	C	H	N	O	S	0	3	0
			6491	2077	3184	566	636	28			
2	D	426	Total	C	H	N	O	S	0	1	0
			6563	2100	3217	570	649	27			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	E	123	Total	C	H	N	O	S	0	1	0
			2053	629	1031	185	203	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	3	MET	-	expression tag	UNP P63043
E	4	ALA	-	expression tag	UNP P63043

- Molecule 4 is a protein called Tubulin tyrosine ligase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	F	351	Total	C	H	N	O	S	0	1	0
			5696	1838	2824	491	528	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
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	H	N	O	P	0	0
			42	10	10	5	14	3		
5	C	1	Total	C	H	N	O	P	0	0
			42	10	10	5	14	3		
5	D	1	Total	C	H	N	O	P	0	0
			42	10	10	5	14	3		

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

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

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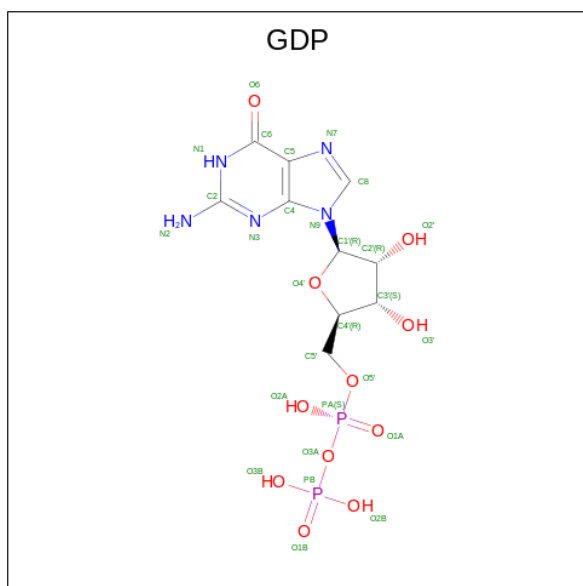
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	1	Total	Mg	0	0
			1	1		
6	F	1	Total	Mg	0	0
			1	1		

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

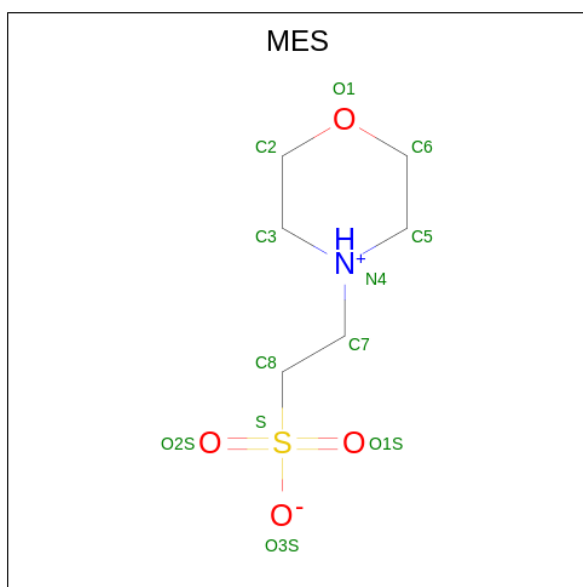
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	2	Total	Ca	0	0
			2	2		
7	B	2	Total	Ca	0	0
			2	2		
7	C	2	Total	Ca	0	0
			2	2		
7	D	1	Total	Ca	0	0
			1	1		

- Molecule 8 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>11</sub>P<sub>2</sub>).



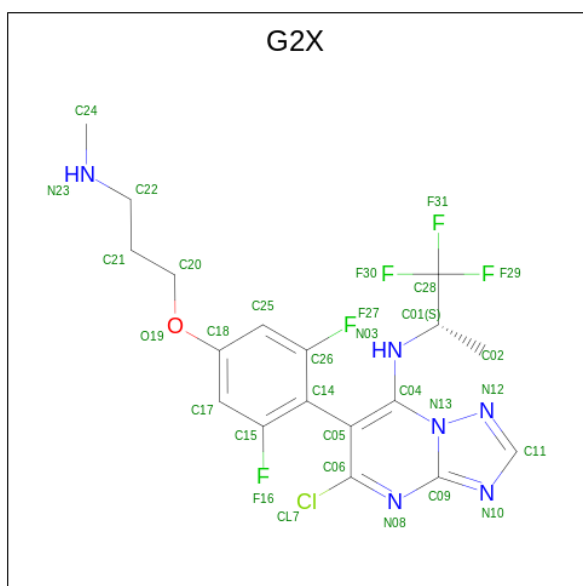
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	B	1	Total	C	H	N	O	P	
			38	10	10	5	11	2	0

- Molecule 9 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C<sub>6</sub>H<sub>13</sub>NO<sub>4</sub>S).



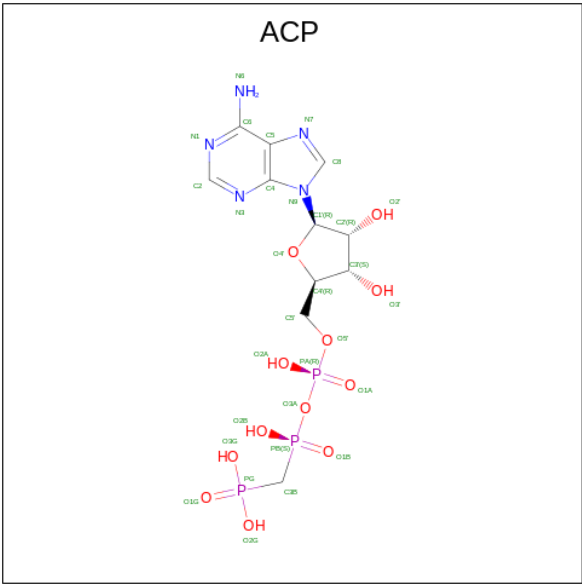
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
9	B	1	Total	C	H	N	O	S	0	0
			24	6	12	1	4	1		

- Molecule 10 is 6-[2,6-bis(fluoranyl)-4-[3-(methylamino)propoxy]phenyl]-5-chloranyl-N-[(2S)-1,1,1-tris(fluoranyl)propan-2-yl]-[1,2,4]triazolo[1,5-a]pyrimidin-7-amine (three-letter code: G2X) (formula:  $C_{18}H_{18}ClF_5N_6O$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
10	B	1	Total	C	Cl	F	H	N	O	0	0
			49	18	1	5	18	6	1		
10	C	1	Total	C	Cl	F	H	N	O	0	0
			49	18	1	5	18	6	1		

- Molecule 11 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (three-letter code: ACP) (formula: C<sub>11</sub>H<sub>18</sub>N<sub>5</sub>O<sub>12</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	F	1	Total	C	H	N	O	P	
			45	11	14	5	12	3	

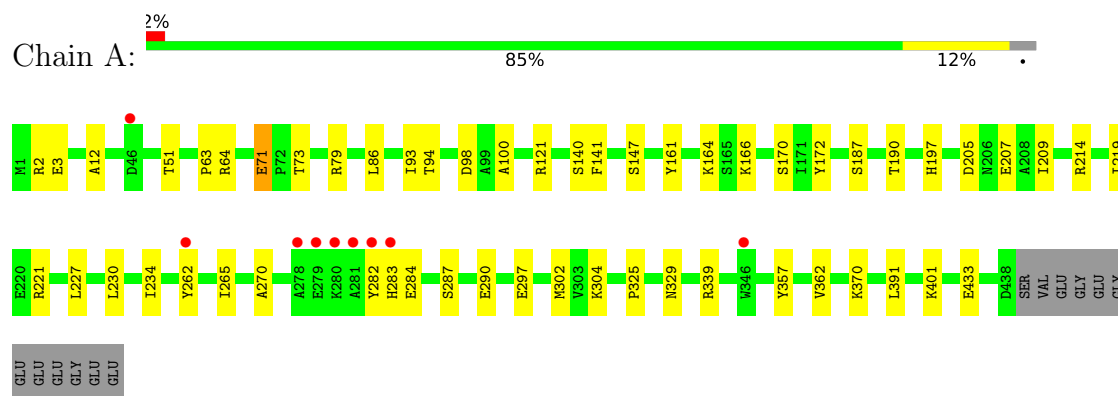
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	72	Total	O	0	0
			72	72		
12	B	53	Total	O	0	0
			53	53		
12	C	104	Total	O	0	0
			104	104		
12	D	32	Total	O	0	0
			32	32		
12	E	13	Total	O	0	0
			13	13		
12	F	20	Total	O	0	0
			20	20		

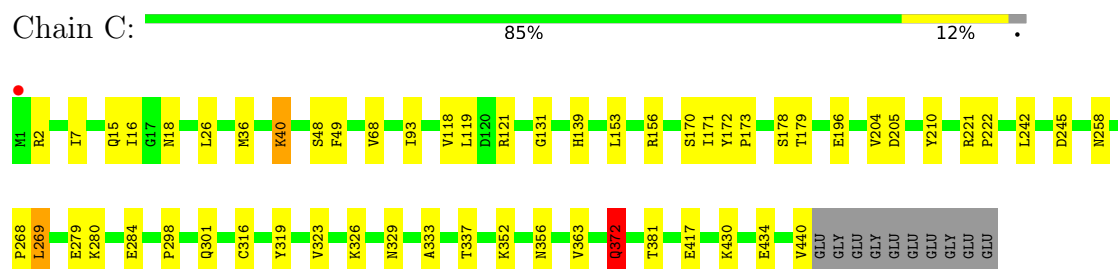
### 3 Residue-property plots

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.

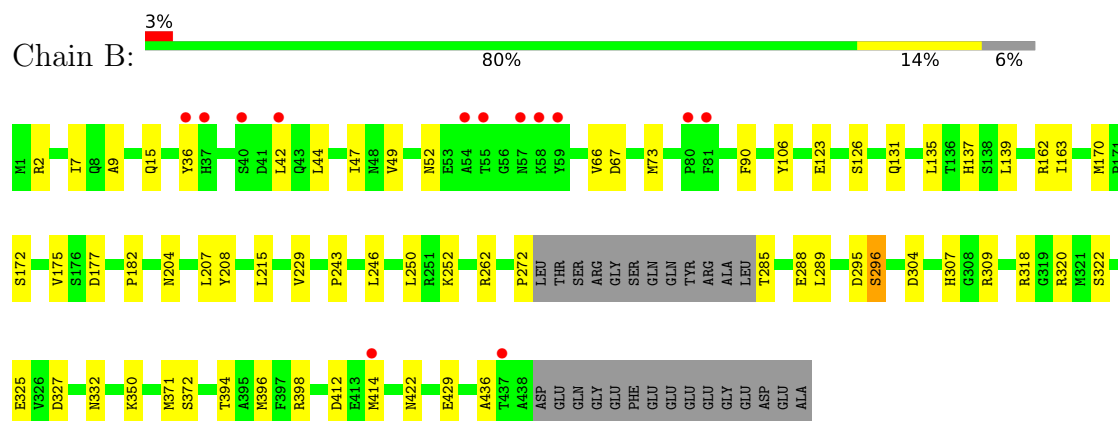
#### • Molecule 1: Tubulin alpha-1B chain



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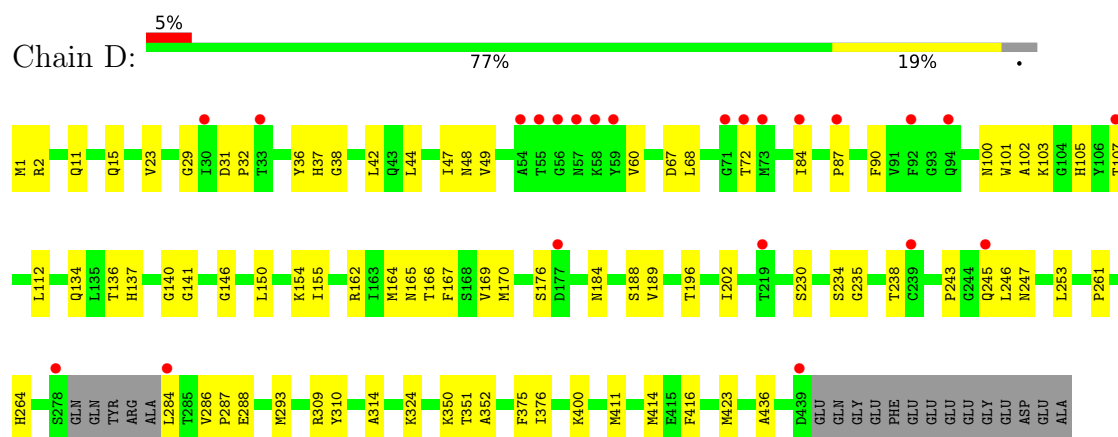


#### • Molecule 2: Tubulin beta chain

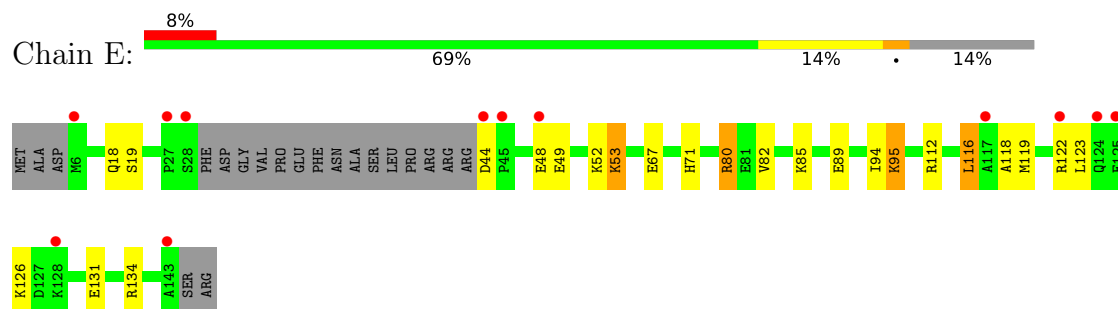


#### • Molecule 2: Tubulin beta chain

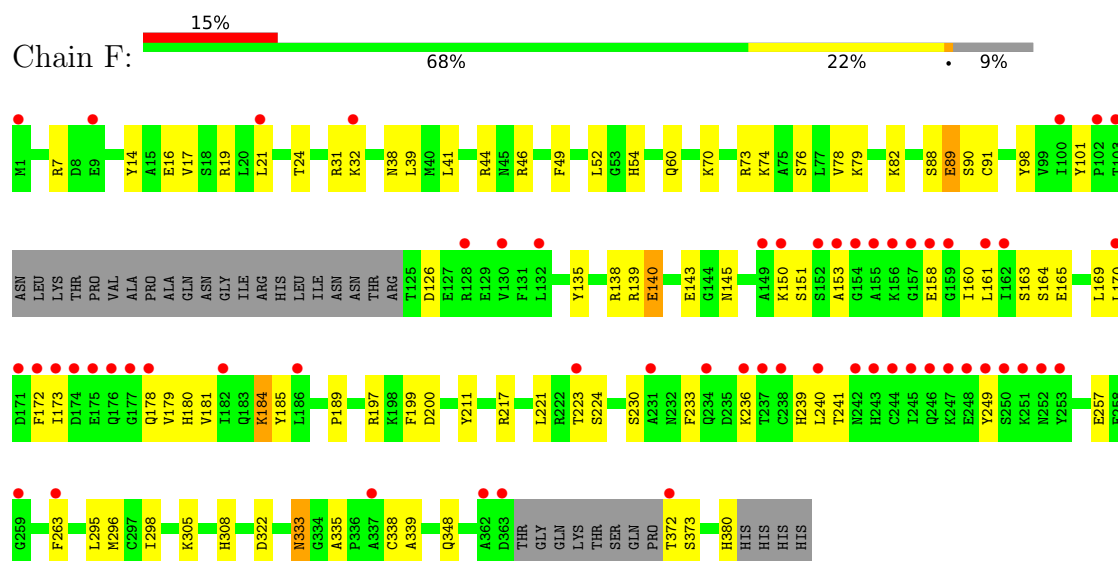




- Molecule 3: Stathmin-4



- Molecule 4: Tubulin tyrosine ligase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	104.42Å 160.78Å 174.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.03 – 2.61 50.03 – 2.61	Depositor EDS
% Data completeness (in resolution range)	93.4 (50.03-2.61) 93.5 (50.03-2.61)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.64 (at 2.61Å)	Xtriage
Refinement program	PHENIX 1.15.2_3472	Depositor
R, $R_{free}$	0.207 , 0.258 0.207 , 0.256	Depositor DCC
$R_{free}$ test set	1761 reflections (2.10%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	39.1	Xtriage
Anisotropy	0.052	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 54.0	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	0.92	EDS
Total number of atoms	35069	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 6.17% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, MES, CA, ACP, GTP, G2X, 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	0.36	0/3532	0.49	0/4794
1	C	0.50	3/3568 (0.1%)	0.56	2/4846 (0.0%)
2	B	0.35	0/3386	0.51	0/4584
2	D	0.34	0/3422	0.48	0/4634
3	E	0.58	3/1030 (0.3%)	0.65	3/1367 (0.2%)
4	F	0.34	0/2937	0.50	0/3967
All	All	0.40	6/17875 (0.0%)	0.52	5/24192 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	372	GLN	CD-NE2	-13.98	0.97	1.32
3	E	95	LYS	CE-NZ	-9.52	1.25	1.49
3	E	95	LYS	CG-CD	-8.74	1.22	1.52
1	C	279	GLU	CD-OE2	-7.32	1.17	1.25
1	C	372	GLN	CD-OE1	-5.45	1.11	1.24
3	E	95	LYS	CB-CG	-5.08	1.38	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	95	LYS	CD-CE-NZ	-12.69	82.52	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	372	GLN	CB-CG-CD	-9.65	86.50	111.60
3	E	80	ARG	NE-CZ-NH1	7.78	124.19	120.30
1	C	372	GLN	N-CA-CB	-6.54	98.82	110.60
3	E	95	LYS	CB-CG-CD	-5.92	96.21	111.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	372	GLN	Sidechain

## 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	3451	3351	3362	42	0
1	C	3466	3361	3376	35	0
2	B	3307	3184	3193	38	1
2	D	3346	3217	3227	49	0
3	E	1022	1031	1034	19	1
4	F	2872	2824	2835	63	0
5	A	32	10	12	0	0
5	C	32	10	12	1	0
5	D	32	10	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
6	F	1	0	0	0	0
7	A	2	0	0	0	0
7	B	2	0	0	0	0
7	C	2	0	0	0	0
7	D	1	0	0	0	0
8	B	28	10	12	1	0
9	B	12	12	12	0	0
10	B	31	18	0	0	0
10	C	31	18	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	F	31	14	14	2	0
12	A	72	0	0	2	0
12	B	53	0	0	2	0
12	C	104	0	0	5	0
12	D	32	0	0	6	0
12	E	13	0	0	2	0
12	F	20	0	0	0	0
All	All	17999	17070	17101	234	1

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 7.

All (234) 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:79:ARG:NH1	12:A:601:HOH:O	2.03	0.89
3:E:95:LYS:HD3	3:E:95:LYS:N	1.91	0.86
4:F:296[B]:MET:SD	4:F:380:HIS:ND1	2.51	0.83
4:F:140:GLU:O	4:F:140:GLU:OE1	2.04	0.76
2:B:285:THR:N	2:B:288:GLU:OE1	2.19	0.75
2:B:262:ARG:NH1	2:B:429:GLU:OE2	2.20	0.74
1:C:196:GLU:OE1	12:C:601:HOH:O	2.07	0.73
2:D:245:GLN:NE2	12:D:604:HOH:O	2.21	0.73
1:C:417:GLU:OE2	12:C:602:HOH:O	2.08	0.72
2:D:436:ALA:O	12:D:601:HOH:O	2.08	0.71
2:D:107:THR:OG1	12:D:602:HOH:O	2.12	0.66
1:A:287:SER:OG	1:A:290:GLU:N	2.27	0.66
4:F:160:ILE:HD11	4:F:240:LEU:HD13	1.79	0.65
4:F:78:VAL:HG21	4:F:181:VAL:HG21	1.78	0.64
1:A:282:TYR:CD1	1:A:283:HIS:N	2.65	0.64
4:F:101:TYR:N	4:F:126:ASP:OD2	2.20	0.64
4:F:233:PHE:O	4:F:236:LYS:HE3	1.99	0.63
4:F:101:TYR:HA	4:F:179:VAL:HG23	1.80	0.62
2:B:262:ARG:NH2	2:B:422:ASN:OD1	2.32	0.62
1:C:356:ASN:ND2	12:C:606:HOH:O	2.32	0.62
4:F:217:ARG:NH2	4:F:373:SER:O	2.33	0.62
2:D:324:LYS:HE2	2:D:324:LYS:HA	1.84	0.59
2:B:322:SER:OG	2:B:325:GLU:HB2	2.03	0.58
4:F:88:SER:O	4:F:91:CYS:N	2.34	0.58
1:A:304:LYS:HE3	4:F:308:HIS:HB3	1.86	0.58
2:B:44:LEU:HA	2:B:47:ILE:HB	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:138:ARG:HG3	4:F:145:ASN:ND2	2.19	0.57
4:F:197:ARG:NH2	4:F:257:GLU:OE2	2.36	0.57
2:B:36:TYR:CZ	2:B:44:LEU:HD11	2.39	0.57
2:D:67:ASP:OD2	12:D:603:HOH:O	2.18	0.57
3:E:94:ILE:HG22	3:E:95:LYS:NZ	2.20	0.57
4:F:21:LEU:O	4:F:24:THR:OG1	2.21	0.57
4:F:78:VAL:HG13	4:F:82:LYS:HE3	1.86	0.56
2:B:131:GLN:OE1	2:B:250:LEU:N	2.35	0.56
2:D:141:GLY:O	2:D:184:ASN:ND2	2.38	0.56
1:C:372:GLN:HE21	1:C:372:GLN:CA	2.17	0.55
4:F:14:TYR:HA	4:F:17:VAL:HG12	1.88	0.55
4:F:151:SER:HB2	4:F:180:HIS:HA	1.89	0.55
1:C:356:ASN:ND2	12:C:608:HOH:O	2.39	0.55
2:D:246:LEU:HB3	2:D:352:ALA:HB2	1.89	0.54
1:A:304:LYS:HE3	4:F:308:HIS:CB	2.37	0.54
1:A:209:ILE:HD11	1:A:302:MET:SD	2.47	0.54
3:E:49:GLU:O	3:E:53:LYS:HD2	2.08	0.54
2:D:155:ILE:HB	2:D:164:MET:HE1	1.90	0.53
1:C:2:ARG:HD2	1:C:131:GLY:O	2.09	0.53
1:A:187:SER:HB3	1:A:391:LEU:HD21	1.91	0.53
2:B:412:ASP:OD1	2:B:412:ASP:N	2.41	0.53
4:F:139:ARG:HG2	4:F:145:ASN:ND2	2.24	0.53
2:D:247:ASN:HB3	2:D:253:LEU:HB2	1.91	0.53
2:D:261:PRO:O	2:D:264:HIS:ND1	2.40	0.53
1:C:440:VAL:HG23	1:C:440:VAL:O	2.09	0.52
4:F:39:LEU:HD21	4:F:41:LEU:HD21	1.91	0.52
2:D:42:LEU:HD22	2:D:243:PRO:HG2	1.91	0.52
4:F:73:ARG:HG3	4:F:73:ARG:HH11	1.74	0.52
2:D:68:LEU:HD23	2:D:112:LEU:HD22	1.92	0.52
1:A:209:ILE:HG22	1:A:227:LEU:HD22	1.92	0.52
1:C:26:LEU:HD12	1:C:363:VAL:HG12	1.92	0.52
1:C:280:LYS:O	1:C:284:GLU:HB3	2.10	0.52
2:D:166:THR:HG21	2:D:196:THR:HG21	1.92	0.52
3:E:44:ASP:OD2	12:E:202:HOH:O	2.19	0.52
4:F:161:LEU:HD22	4:F:172:PHE:CG	2.45	0.52
1:A:221:ARG:NE	2:B:327:ASP:OD2	2.36	0.51
2:B:309:ARG:NH1	12:B:606:HOH:O	2.40	0.51
1:C:178:SER:OG	2:D:350:LYS:NZ	2.42	0.51
4:F:333:ASN:ND2	11:F:402:ACP:O3G	2.44	0.51
2:B:162[B]:ARG:NH1	12:B:608:HOH:O	2.44	0.51
2:B:42:LEU:HD23	2:B:243:PRO:HG2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:134:GLN:HA	2:D:165:ASN:O	2.11	0.51
1:A:79:ARG:NH2	1:A:94:THR:HG23	2.26	0.51
1:A:207:GLU:OE2	4:F:54:HIS:ND1	2.38	0.51
1:A:187:SER:CB	1:A:391:LEU:HD21	2.41	0.50
4:F:338:CYS:SG	4:F:339:ALA:N	2.85	0.50
2:B:73:MET:HG3	2:B:90:PHE:HD2	1.75	0.50
4:F:153:ALA:HB2	4:F:178:GLN:HG2	1.93	0.50
3:E:67:GLU:O	3:E:71:HIS:ND1	2.45	0.50
1:A:100:ALA:HA	2:B:252:LYS:HG3	1.94	0.49
2:D:72:THR:O	2:D:72:THR:HG22	2.12	0.49
4:F:158:GLU:OE2	4:F:158:GLU:HA	2.11	0.49
4:F:189:PRO:HA	4:F:322:ASP:HA	1.93	0.49
2:D:309:ARG:NH1	12:D:607:HOH:O	2.45	0.49
2:B:126:SER:O	2:B:126:SER:OG	2.25	0.49
4:F:233:PHE:HD1	4:F:239:HIS:NE2	2.11	0.49
4:F:197:ARG:NH2	4:F:223:THR:HG21	2.27	0.49
4:F:372:THR:OG1	4:F:373:SER:N	2.46	0.49
2:D:235:GLY:O	2:D:238:THR:HG22	2.13	0.49
2:D:246:LEU:HD21	2:D:350:LYS:HB3	1.94	0.48
4:F:161:LEU:HD23	4:F:169:LEU:HD23	1.95	0.48
2:B:67:ASP:HB2	2:B:73:MET:HE1	1.94	0.48
2:B:172:SER:HB2	2:B:175:VAL:HG22	1.95	0.48
1:C:204:VAL:HG12	1:C:205:ASP:N	2.28	0.48
2:B:295:ASP:OD1	2:B:296:SER:N	2.47	0.48
1:C:430:LYS:HD3	1:C:434:GLU:OE1	2.14	0.48
4:F:170:LEU:HA	4:F:173:ILE:HG22	1.95	0.48
2:D:36:TYR:CZ	2:D:38:GLY:HA3	2.49	0.48
1:A:2:ARG:O	1:A:51[B]:THR:HG23	2.13	0.48
2:D:169:VAL:HA	2:D:202:ILE:O	2.14	0.48
3:E:94:ILE:HG22	3:E:95:LYS:HZ3	1.79	0.47
1:A:172:TYR:HB3	1:A:205:ASP:HA	1.96	0.47
4:F:16:GLU:HG2	4:F:19:ARG:HE	1.79	0.47
2:B:394:THR:HG22	2:B:398:ARG:HG3	1.96	0.47
4:F:296[B]:MET:CE	4:F:380:HIS:HD1	2.27	0.47
1:C:372:GLN:HE21	1:C:372:GLN:HA	1.78	0.47
1:C:15:GLN:NE2	5:C:501:GTP:O6	2.45	0.47
1:C:298:PRO:HA	1:C:301:GLN:HG2	1.95	0.47
1:A:93:ILE:HD11	1:A:121:ARG:HG3	1.97	0.47
2:B:2:ARG:O	2:B:49:VAL:HG13	2.15	0.47
3:E:19:SER:OG	12:E:201:HOH:O	2.19	0.47
4:F:70:LYS:HA	4:F:76:SER:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:102:ALA:HB2	2:D:411:MET:SD	2.55	0.47
2:D:324:LYS:HA	2:D:324:LYS:CE	2.45	0.47
4:F:200:ASP:OD2	4:F:241:THR:OG1	2.26	0.47
4:F:78:VAL:CG1	4:F:82:LYS:HE3	2.45	0.47
2:B:318:ARG:O	2:B:371:MET:HA	2.15	0.46
2:D:1:MET:N	2:D:48:ASN:OD1	2.47	0.46
2:D:293:MET:HG2	2:D:375:PHE:HB2	1.96	0.46
4:F:160:ILE:CD1	4:F:240:LEU:HD13	2.44	0.46
1:A:161:TYR:HB3	1:A:164:LYS:HG3	1.97	0.46
4:F:73:ARG:HH11	4:F:73:ARG:CG	2.27	0.46
2:D:314:ALA:HB3	2:D:376:ILE:HB	1.98	0.46
1:A:433:GLU:OE1	4:F:46:ARG:NH2	2.49	0.46
2:D:101:TRP:HE1	2:D:188:SER:HG	1.62	0.46
2:D:162:ARG:NH2	12:D:608:HOH:O	2.49	0.46
1:C:48:SER:N	12:C:610:HOH:O	2.47	0.46
2:D:2:ARG:O	2:D:49:VAL:HG22	2.15	0.45
4:F:82:LYS:O	4:F:89:GLU:HG3	2.16	0.45
1:C:40:LYS:CA	1:C:40:LYS:HE2	2.46	0.45
1:A:230:LEU:O	1:A:234:ILE:HD12	2.16	0.45
1:A:79:ARG:HH21	1:A:94:THR:CG2	2.30	0.45
2:D:284:LEU:HD12	2:D:288:GLU:OE1	2.17	0.45
2:D:44:LEU:HA	2:D:47:ILE:HB	1.98	0.45
2:D:100:ASN:ND2	2:D:103:LYS:HE3	2.32	0.45
1:A:282:TYR:CG	1:A:283:HIS:N	2.84	0.45
2:B:272:PRO:HD3	2:B:289:LEU:HD21	1.99	0.45
2:D:150:LEU:O	2:D:154:LYS:HG2	2.17	0.45
4:F:38:ASN:O	4:F:60:GLN:HA	2.17	0.45
4:F:236:LYS:HB3	4:F:240:LEU:CD1	2.47	0.45
1:C:333:ALA:O	1:C:337:THR:HG23	2.17	0.45
3:E:48:GLU:O	3:E:52:LYS:HD3	2.17	0.45
4:F:236:LYS:HB3	4:F:240:LEU:HG	1.99	0.45
1:A:214:ARG:HG2	1:A:219:ILE:O	2.17	0.45
4:F:173:ILE:HD13	4:F:180:HIS:HB2	2.00	0.44
1:A:297:GLU:OE2	1:A:339:ARG:NH1	2.42	0.44
2:B:139:LEU:HD12	2:B:170:MET:SD	2.57	0.44
2:B:177:ASP:OD1	2:B:177:ASP:N	2.49	0.44
2:D:103:LYS:HA	2:D:107:THR:HB	1.99	0.44
4:F:199:PHE:CD2	4:F:221:LEU:HD23	2.52	0.44
2:B:207:LEU:HD11	2:B:229:VAL:CG2	2.47	0.44
2:D:136:THR:HG22	2:D:167:PHE:HB2	1.99	0.44
4:F:7:ARG:HA	4:F:32:LYS:HE2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:138:ARG:HB2	4:F:143:GLU:HB2	1.99	0.44
3:E:85:LYS:O	3:E:89:GLU:HG2	2.17	0.44
4:F:49:PHE:HA	4:F:52:LEU:HD12	2.00	0.44
1:A:265:ILE:HD12	1:A:265:ILE:N	2.32	0.44
1:A:63:PRO:HG2	1:A:86:LEU:HD23	2.00	0.44
1:C:172:TYR:CD1	1:C:173:PRO:HD2	2.52	0.44
1:C:269:LEU:HD21	1:C:381:THR:CG2	2.48	0.44
1:C:316:CYS:HA	1:C:352:LYS:O	2.18	0.44
4:F:98:TYR:O	4:F:181:VAL:HG23	2.18	0.44
1:A:79:ARG:HH21	1:A:94:THR:HG23	1.83	0.44
1:A:141:PHE:HB3	1:A:187:SER:OG	2.18	0.44
1:A:283:HIS:O	1:A:284:GLU:C	2.56	0.44
1:A:12:ALA:HB3	1:A:140:SER:HB3	2.00	0.43
1:A:270:ALA:HB3	1:A:302:MET:HG3	2.00	0.43
1:C:7:ILE:HG21	1:C:153:LEU:HD21	2.00	0.43
1:C:119:LEU:HD13	1:C:156:ARG:NH2	2.33	0.43
2:D:11:GLN:CG	2:D:15:GLN:OE1	2.67	0.43
3:E:95:LYS:HD3	3:E:95:LYS:H	1.78	0.43
1:C:68[A]:VAL:HG11	1:C:118:VAL:HG21	1.99	0.43
2:D:166:THR:CG2	2:D:196:THR:HG21	2.48	0.43
4:F:150:LYS:HE3	11:F:402:ACP:O2A	2.19	0.43
2:B:182:PRO:HG2	2:B:396:MET:SD	2.59	0.43
4:F:263:PHE:N	4:F:263:PHE:CD2	2.86	0.43
1:A:357:TYR:OH	3:E:18:GLN:OE1	2.37	0.43
1:A:357:TYR:OH	3:E:18:GLN:HG3	2.19	0.43
1:C:179:THR:HG23	10:C:504:G2X:F30	2.08	0.43
4:F:88:SER:C	4:F:90:SER:N	2.72	0.43
2:D:246:LEU:HD22	2:D:351:THR:C	2.39	0.43
3:E:112:ARG:O	3:E:116:LEU:HD23	2.19	0.43
4:F:184:LYS:HD2	4:F:185:TYR:N	2.34	0.43
1:A:401:LYS:HE3	2:B:436:ALA:HB1	2.00	0.43
4:F:88:SER:O	4:F:90:SER:N	2.52	0.43
2:D:23:VAL:HG21	2:D:230:SER:HB2	2.00	0.42
1:A:325:PRO:O	1:A:329:ASN:ND2	2.51	0.42
3:E:123:LEU:HD22	3:E:126:LYS:HD2	1.99	0.42
2:B:246:LEU:HD21	2:B:350:LYS:HB3	2.00	0.42
2:D:140:GLY:O	2:D:184:ASN:ND2	2.47	0.42
2:D:310:TYR:CE1	2:D:375:PHE:HZ	2.37	0.42
2:B:7:ILE:O	2:B:135:LEU:HA	2.18	0.42
2:D:31:ASP:HB2	2:D:32:PRO:CD	2.50	0.42
1:A:3:GLU:HG2	1:A:64:ARG:CZ	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:215:LEU:N	2:B:215:LEU:HD12	2.35	0.42
1:A:166:LYS:HE2	1:A:197:HIS:O	2.20	0.42
4:F:44:ARG:HD2	4:F:335:ALA:CB	2.50	0.42
2:D:29:GLY:O	2:D:37:HIS:N	2.46	0.42
3:E:134:ARG:HG3	3:E:134:ARG:HH11	1.83	0.42
1:C:319:TYR:HB3	1:C:323:VAL:HG21	2.00	0.42
2:D:60:VAL:HG23	2:D:84:ILE:O	2.19	0.42
2:D:411:MET:HE2	2:D:416:PHE:HE1	1.85	0.42
3:E:118:ALA:O	3:E:122:ARG:HB2	2.20	0.42
1:A:98:ASP:OD2	12:A:602:HOH:O	2.21	0.42
2:B:52:ASN:ND2	2:B:123:GLU:OE1	2.53	0.42
3:E:95:LYS:HA	3:E:95:LYS:HD2	1.64	0.42
3:E:116:LEU:HA	3:E:119:MET:H	1.84	0.42
4:F:101:TYR:CD1	4:F:179:VAL:CG2	3.02	0.42
1:C:242:LEU:N	1:C:242:LEU:HD12	2.34	0.41
4:F:135:TYR:OH	4:F:165:GLU:HA	2.20	0.41
1:A:147:SER:HB2	1:A:190:THR:HB	2.02	0.41
2:B:163:ILE:HG21	2:B:250:LEU:HB3	2.02	0.41
1:C:93:ILE:HD11	1:C:121:ARG:HG3	2.01	0.41
4:F:295:LEU:HD23	4:F:298:ILE:HD11	2.02	0.41
1:C:16:ILE:HD11	1:C:171:ILE:HD11	2.02	0.41
2:D:286:VAL:HB	2:D:287:PRO:HD3	2.01	0.41
4:F:163:SER:OG	4:F:164:SER:N	2.53	0.41
1:A:234:ILE:HD13	1:A:302:MET:SD	2.60	0.41
2:B:204:ASN:ND2	8:B:501:GDP:O2'	2.54	0.41
2:B:9:ALA:HA	2:B:66:VAL:O	2.20	0.41
2:D:189:VAL:HG11	2:D:423:MET:SD	2.60	0.41
2:B:304:ASP:HB3	2:B:307:HIS:ND1	2.36	0.41
4:F:74:LYS:HB3	4:F:181:VAL:HG11	2.02	0.41
1:C:139:HIS:O	1:C:170:SER:HA	2.21	0.41
1:C:280:LYS:O	1:C:284:GLU:CB	2.68	0.41
1:A:71:GLU:OE1	1:A:73:THR:OG1	2.38	0.41
1:A:362:VAL:HG21	1:A:370:LYS:HG3	2.03	0.41
2:B:318:ARG:HB2	2:B:372:SER:OG	2.21	0.41
2:B:208:TYR:OH	1:C:326:LYS:HG3	2.21	0.40
1:C:210:TYR:CZ	1:C:222:PRO:HD2	2.56	0.40
1:A:141:PHE:CE1	1:A:170:SER:HB3	2.57	0.40
2:B:106:TYR:CG	3:E:82:VAL:HG11	2.57	0.40
1:C:258:ASN:ND2	1:C:352:LYS:HD3	2.37	0.40
2:D:105:HIS:ND1	2:D:146:GLY:O	2.46	0.40
4:F:223:THR:HG22	4:F:224:SER:N	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:36:MET:HE2	1:C:49:PHE:CZ	2.57	0.40
2:D:87:PRO:HA	2:D:90:PHE:CE1	2.56	0.40
4:F:163:SER:HB3	4:F:169:LEU:HD21	2.02	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:320:ARG:HH21	3:E:131:GLU:OE1[4_455]	1.46	0.14

## 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	440/450 (98%)	431 (98%)	9 (2%)	0	100	100
1	C	445/450 (99%)	432 (97%)	13 (3%)	0	100	100
2	B	417/445 (94%)	404 (97%)	13 (3%)	0	100	100
2	D	423/445 (95%)	408 (96%)	15 (4%)	0	100	100
3	E	120/143 (84%)	116 (97%)	4 (3%)	0	100	100
4	F	346/384 (90%)	337 (97%)	8 (2%)	1 (0%)	41	62
All	All	2191/2317 (95%)	2128 (97%)	62 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	F	89	GLU

### 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	373/378 (99%)	371 (100%)	2 (0%)	88	95
1	C	378/378 (100%)	371 (98%)	7 (2%)	57	78
2	B	364/383 (95%)	359 (99%)	5 (1%)	67	84
2	D	369/383 (96%)	363 (98%)	6 (2%)	62	81
3	E	111/127 (87%)	108 (97%)	3 (3%)	44	69
4	F	314/342 (92%)	304 (97%)	10 (3%)	39	63
All	All	1909/1991 (96%)	1876 (98%)	33 (2%)	60	80

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	GLU
1	A	262	TYR
2	B	15	GLN
2	B	137	HIS
2	B	296	SER
2	B	332	ASN
2	B	414	MET
1	C	18	ASN
1	C	40	LYS
1	C	221	ARG
1	C	245	ASP
1	C	268	PRO
1	C	269	LEU
1	C	329	ASN
2	D	137	HIS
2	D	170	MET
2	D	176	SER
2	D	234	SER
2	D	400	LYS
2	D	414	MET
3	E	53	LYS
3	E	80	ARG

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Mol	Chain	Res	Type
3	E	116	LEU
4	F	31	ARG
4	F	79	LYS
4	F	140	GLU
4	F	184	LYS
4	F	211	TYR
4	F	230	SER
4	F	249	TYR
4	F	305	LYS
4	F	333	ASN
4	F	348	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	128	GLN
2	B	15	GLN
2	B	204	ASN
1	C	356	ASN
1	C	372	GLN
2	D	37	HIS
2	D	422	ASN
3	E	18	GLN
4	F	60	GLN
4	F	180	HIS
4	F	183	GLN
4	F	252	ASN
4	F	310	GLN

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry

Of 20 ligands modelled in this entry, 12 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	503	-	12,12,12	2.11	1 (8%)	14,16,16	1.77	4 (28%)
5	GTP	C	501	6	26,34,34	1.00	2 (7%)	33,54,54	1.85	8 (24%)
10	G2X	C	504	-	28,33,33	2.80	10 (35%)	30,48,48	1.83	4 (13%)
5	GTP	A	501	6	26,34,34	0.95	1 (3%)	33,54,54	1.80	7 (21%)
8	GDP	B	501	-	24,30,30	1.24	3 (12%)	31,47,47	1.88	9 (29%)
5	GTP	D	503	6	26,34,34	1.04	2 (7%)	33,54,54	1.83	10 (30%)
10	G2X	B	506	-	28,33,33	2.66	9 (32%)	30,48,48	1.38	2 (6%)
11	ACP	F	402	6	27,33,33	2.54	8 (29%)	32,52,52	1.83	7 (21%)

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	503	-	-	0/6/14/14	0/1/1/1
5	GTP	C	501	6	-	7/18/38/38	0/3/3/3
10	G2X	C	504	-	-	3/20/20/20	0/3/3/3
5	GTP	A	501	6	-	6/18/38/38	0/3/3/3
8	GDP	B	501	-	-	3/12/32/32	0/3/3/3
5	GTP	D	503	6	-	5/18/38/38	0/3/3/3
10	G2X	B	506	-	-	3/20/20/20	0/3/3/3
11	ACP	F	402	6	-	2/15/38/38	0/3/3/3

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	F	402	ACP	O4'-C1'	7.73	1.51	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	C	504	G2X	C28-C01	7.45	1.60	1.51
10	C	504	G2X	C06-N08	7.24	1.37	1.30
9	B	503	MES	C8-S	-7.02	1.67	1.77
10	B	506	G2X	C28-C01	6.99	1.60	1.51
10	B	506	G2X	C06-N08	6.68	1.36	1.30
11	F	402	ACP	PB-O3A	5.48	1.64	1.58
10	C	504	G2X	C14-C15	4.37	1.45	1.39
8	B	501	GDP	C6-C5	4.35	1.48	1.41
10	B	506	G2X	C25-C26	3.96	1.44	1.37
10	B	506	G2X	C17-C15	3.77	1.44	1.37
10	C	504	G2X	C09-N10	3.72	1.41	1.35
10	C	504	G2X	C17-C15	3.72	1.44	1.37
11	F	402	ACP	C2'-C1'	-3.71	1.48	1.53
5	D	503	GTP	C6-N1	3.49	1.39	1.33
10	C	504	G2X	C25-C26	3.42	1.43	1.37
10	B	506	G2X	C14-C26	3.37	1.44	1.39
10	B	506	G2X	C14-C15	3.29	1.43	1.39
11	F	402	ACP	O4'-C4'	3.17	1.52	1.45
11	F	402	ACP	C6-N6	3.12	1.45	1.34
5	A	501	GTP	C6-N1	2.89	1.38	1.33
11	F	402	ACP	C2'-C3'	-2.88	1.45	1.53
10	C	504	G2X	C06-C05	2.88	1.42	1.39
10	B	506	G2X	C09-N10	2.87	1.39	1.35
11	F	402	ACP	C4-N3	-2.86	1.31	1.35
10	C	504	G2X	C11-N12	2.84	1.37	1.33
10	B	506	G2X	C06-C05	2.82	1.42	1.39
5	C	501	GTP	C6-N1	2.78	1.37	1.33
10	C	504	G2X	C21-C22	2.63	1.62	1.51
8	B	501	GDP	C5-C4	2.49	1.47	1.40
10	B	506	G2X	C11-N12	2.39	1.37	1.33
5	C	501	GTP	O4'-C1'	2.34	1.44	1.41
8	B	501	GDP	O4'-C1'	2.26	1.44	1.41
11	F	402	ACP	PB-O2B	-2.07	1.51	1.56
5	D	503	GTP	C2-N1	2.03	1.39	1.35
10	C	504	G2X	C25-C18	2.01	1.42	1.38

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	C	504	G2X	C05-C06-CL7	-5.99	115.29	119.27
5	C	501	GTP	N3-C2-N1	-5.50	119.89	127.22
5	A	501	GTP	N3-C2-N1	-5.35	120.09	127.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	F	402	ACP	C3'-C2'-C1'	5.02	108.54	100.98
5	D	503	GTP	N3-C2-N1	-4.92	120.67	127.22
10	C	504	G2X	C14-C05-C04	4.60	128.00	121.41
8	B	501	GDP	C6-C5-C4	-4.47	116.53	120.80
8	B	501	GDP	C2-N3-C4	4.24	120.20	115.36
5	A	501	GTP	C2-N3-C4	4.20	120.15	115.36
9	B	503	MES	C5-N4-C3	4.13	118.11	108.83
11	F	402	ACP	N3-C2-N1	-4.03	122.38	128.68
11	F	402	ACP	C4-C5-N7	-4.02	105.21	109.40
10	B	506	G2X	C05-C06-CL7	-3.93	116.66	119.27
5	D	503	GTP	C2-N3-C4	3.88	119.79	115.36
5	A	501	GTP	PB-O3B-PG	-3.72	120.05	132.83
5	C	501	GTP	PA-O3A-PB	-3.69	120.15	132.83
5	D	503	GTP	PB-O3B-PG	-3.60	120.48	132.83
5	C	501	GTP	C6-N1-C2	3.33	121.22	115.93
5	D	503	GTP	PA-O3A-PB	-3.33	121.40	132.83
10	C	504	G2X	C06-C05-C14	-3.28	117.54	123.88
5	C	501	GTP	PB-O3B-PG	-3.25	121.69	132.83
5	C	501	GTP	C5-C6-N1	-3.22	119.03	123.43
5	C	501	GTP	C2-N3-C4	3.22	119.03	115.36
8	B	501	GDP	C5-C6-N1	-3.21	119.05	123.43
8	B	501	GDP	C6-N1-C2	3.08	120.83	115.93
11	F	402	ACP	PA-O3A-PB	-3.06	122.85	132.56
10	B	506	G2X	C05-C04-N03	-3.06	117.82	121.93
11	F	402	ACP	C1'-N9-C4	-2.92	121.52	126.64
9	B	503	MES	O2S-S-C8	2.90	110.40	106.92
5	A	501	GTP	C5-C6-N1	-2.89	119.47	123.43
5	A	501	GTP	PA-O3A-PB	-2.89	122.89	132.83
8	B	501	GDP	PA-O3A-PB	-2.87	122.98	132.83
5	D	503	GTP	C5-C6-N1	-2.82	119.58	123.43
8	B	501	GDP	C4-C5-N7	-2.68	106.61	109.40
5	A	501	GTP	C6-N1-C2	2.64	120.12	115.93
11	F	402	ACP	C2'-C3'-C4'	2.60	107.69	102.64
8	B	501	GDP	N3-C2-N1	-2.41	124.00	127.22
10	C	504	G2X	C25-C18-C17	-2.39	117.18	120.98
5	D	503	GTP	C2'-C3'-C4'	2.33	107.18	102.64
11	F	402	ACP	O2A-PA-O1A	-2.33	100.72	112.24
8	B	501	GDP	C3'-C2'-C1'	2.29	104.42	100.98
5	A	501	GTP	O2G-PG-O3B	2.29	112.30	104.64
5	D	503	GTP	C6-N1-C2	2.22	119.45	115.93
8	B	501	GDP	C2'-C3'-C4'	2.21	106.94	102.64
5	C	501	GTP	C2'-C3'-C4'	2.17	106.87	102.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	503	GTP	C1'-N9-C4	-2.16	122.85	126.64
5	C	501	GTP	N2-C2-N3	2.14	121.28	117.79
9	B	503	MES	O1S-S-C8	2.10	109.45	106.92
9	B	503	MES	C7-N4-C5	2.10	116.61	111.23
5	D	503	GTP	C4-C5-N7	-2.10	107.21	109.40
5	D	503	GTP	N2-C2-N1	2.09	120.50	117.25

There are no chirality outliers.

All (29) torsion outliers are listed below:

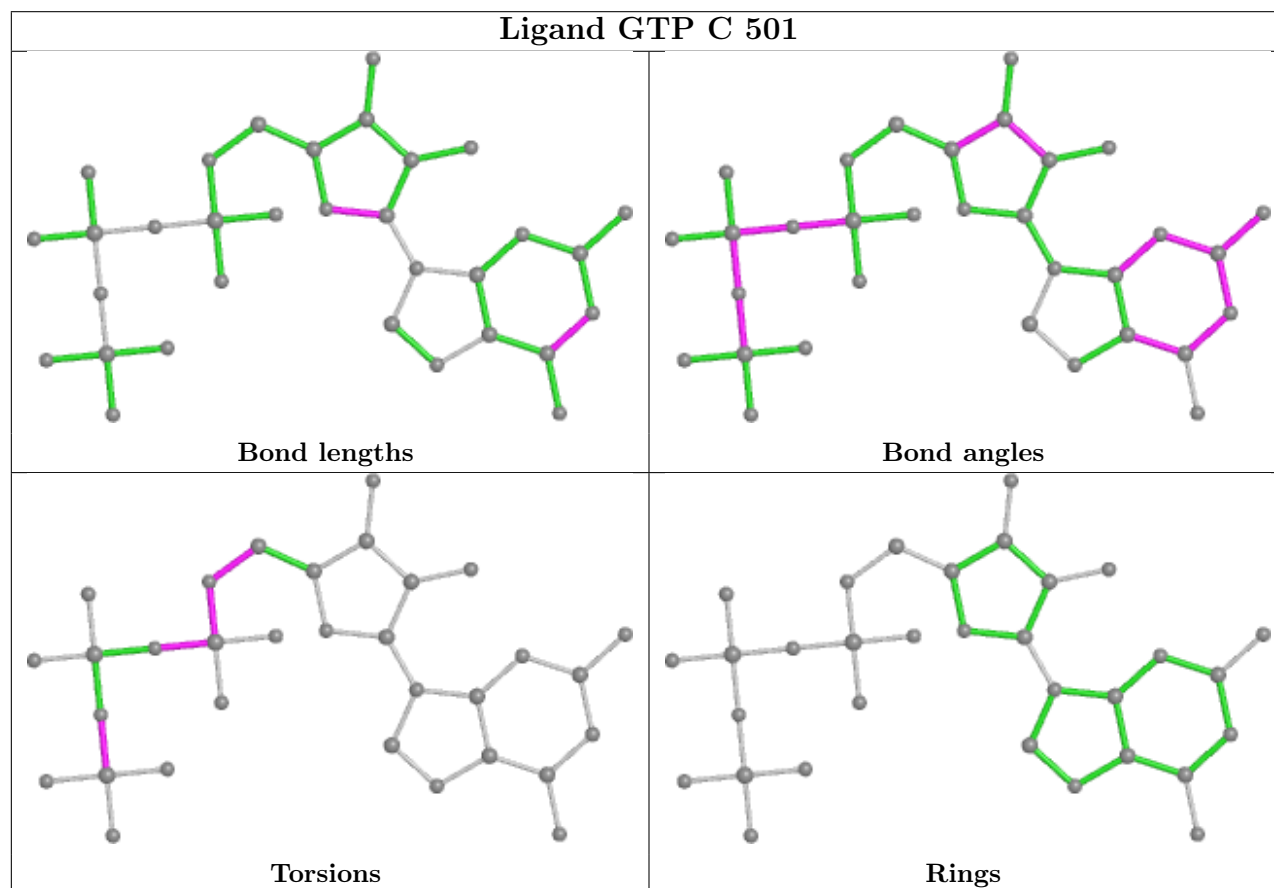
Mol	Chain	Res	Type	Atoms
5	A	501	GTP	PB-O3B-PG-O2G
5	A	501	GTP	C5'-O5'-PA-O1A
5	A	501	GTP	C5'-O5'-PA-O2A
5	C	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O2A
5	D	503	GTP	C5'-O5'-PA-O1A
5	D	503	GTP	C5'-O5'-PA-O2A
8	B	501	GDP	C5'-O5'-PA-O1A
8	B	501	GDP	C5'-O5'-PA-O2A
11	F	402	ACP	C5'-O5'-PA-O1A
10	C	504	G2X	N13-C04-N03-C01
5	D	503	GTP	PB-O3B-PG-O1G
10	C	504	G2X	C05-C04-N03-C01
10	B	506	G2X	C21-C22-N23-C24
5	C	501	GTP	PB-O3B-PG-O2G
5	C	501	GTP	C5'-O5'-PA-O3A
11	F	402	ACP	C5'-O5'-PA-O3A
5	C	501	GTP	PB-O3A-PA-O2A
10	B	506	G2X	O19-C20-C21-C22
5	C	501	GTP	C4'-C5'-O5'-PA
10	B	506	G2X	C02-C01-N03-C04
10	C	504	G2X	C02-C01-N03-C04
5	A	501	GTP	PB-O3B-PG-O3G
5	D	503	GTP	PB-O3B-PG-O2G
5	A	501	GTP	C5'-O5'-PA-O3A
5	D	503	GTP	C5'-O5'-PA-O3A
8	B	501	GDP	C5'-O5'-PA-O3A
5	A	501	GTP	PB-O3A-PA-O2A
5	C	501	GTP	PB-O3A-PA-O1A

There are no ring outliers.

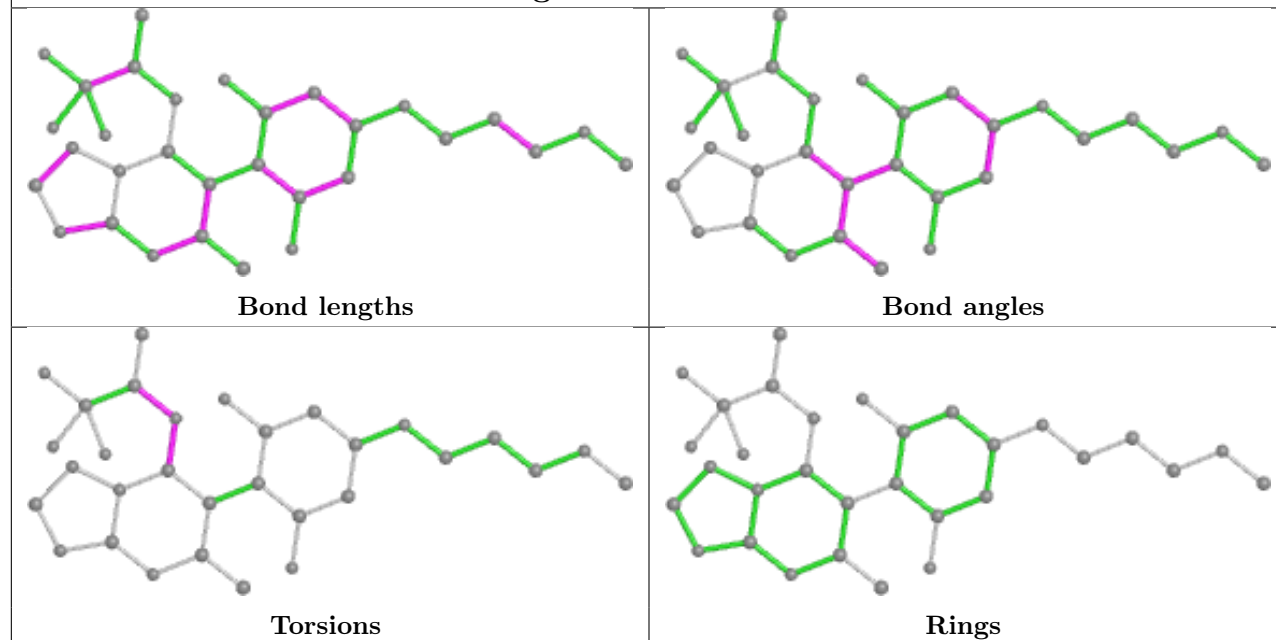
4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	501	GTP	1	0
10	C	504	G2X	1	0
8	B	501	GDP	1	0
11	F	402	ACP	2	0

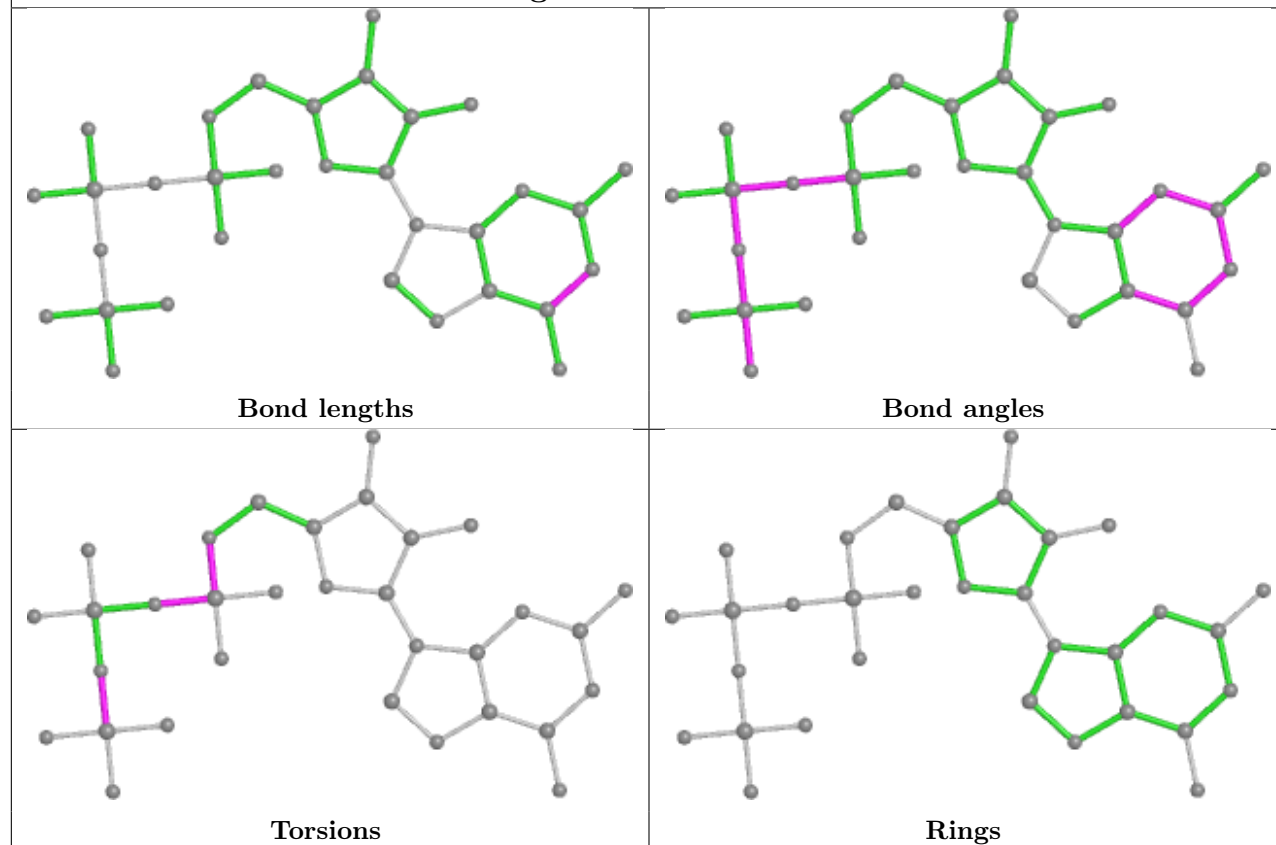
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

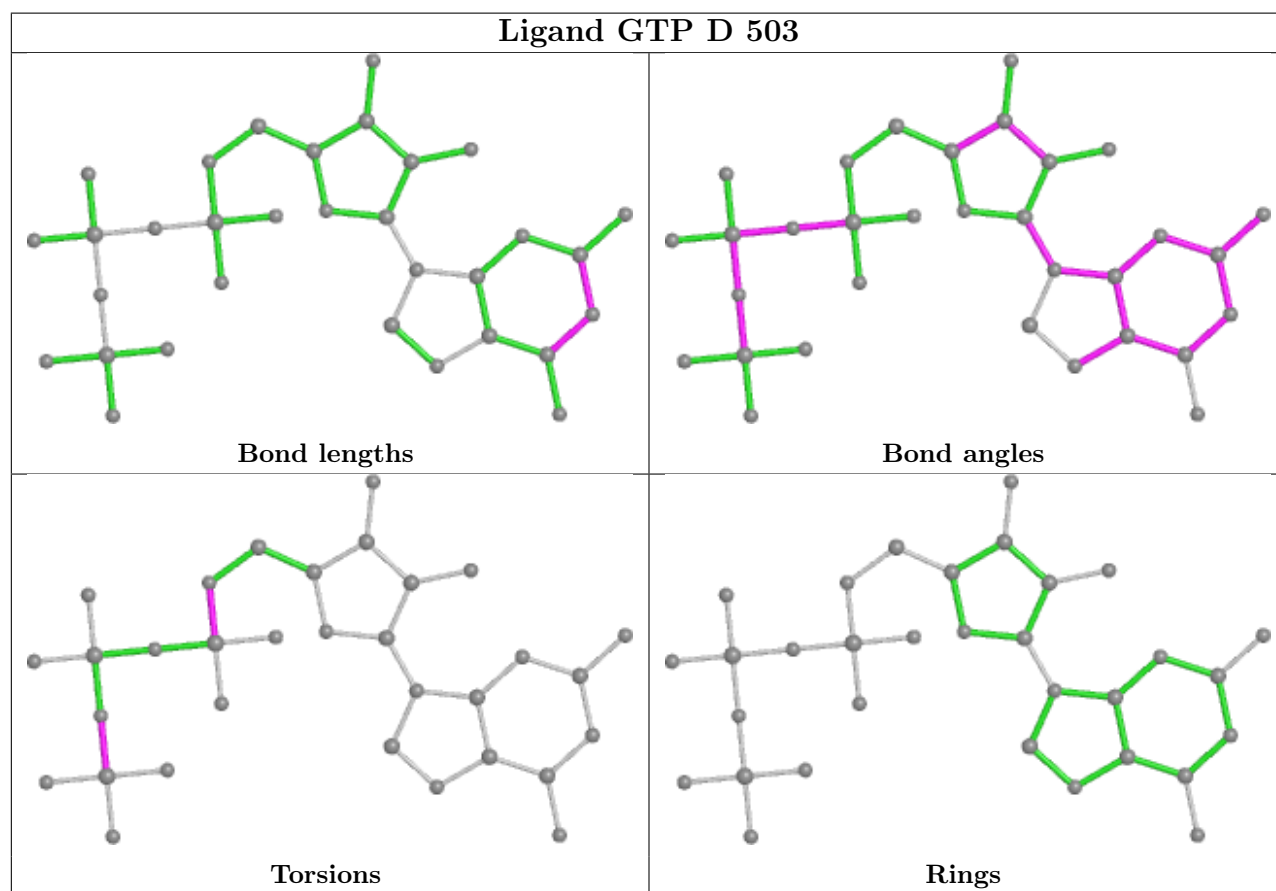
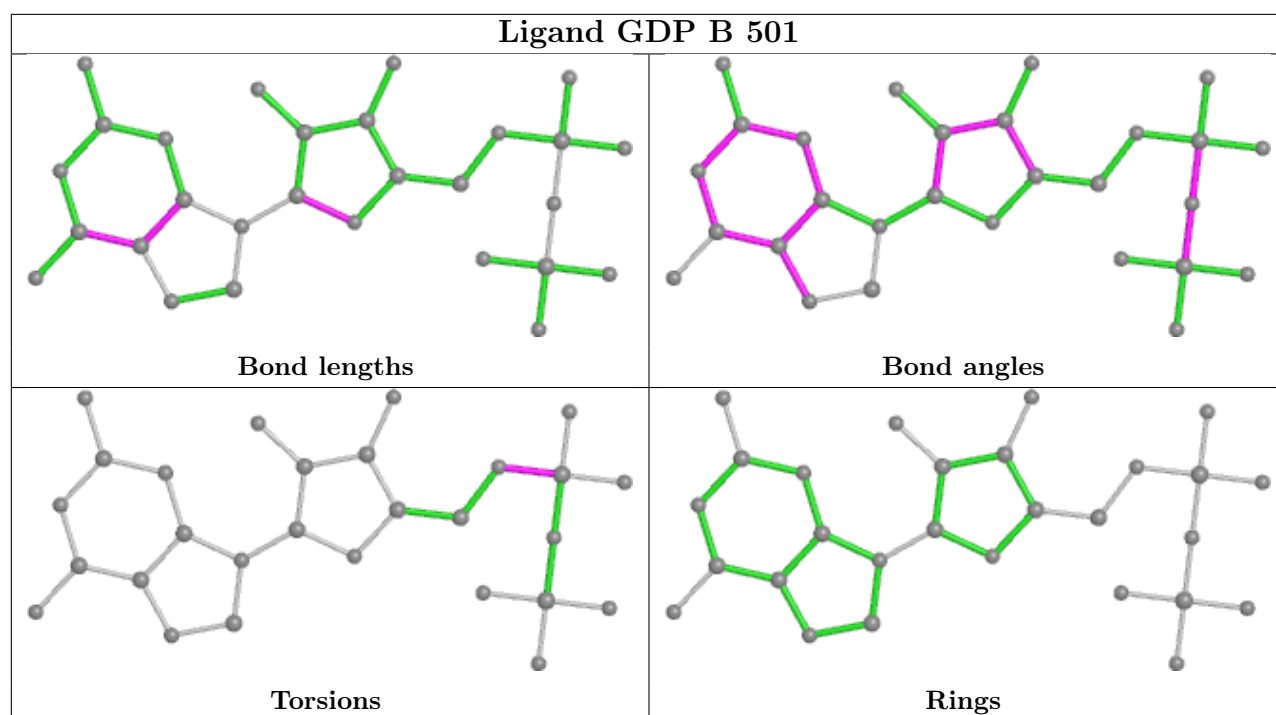


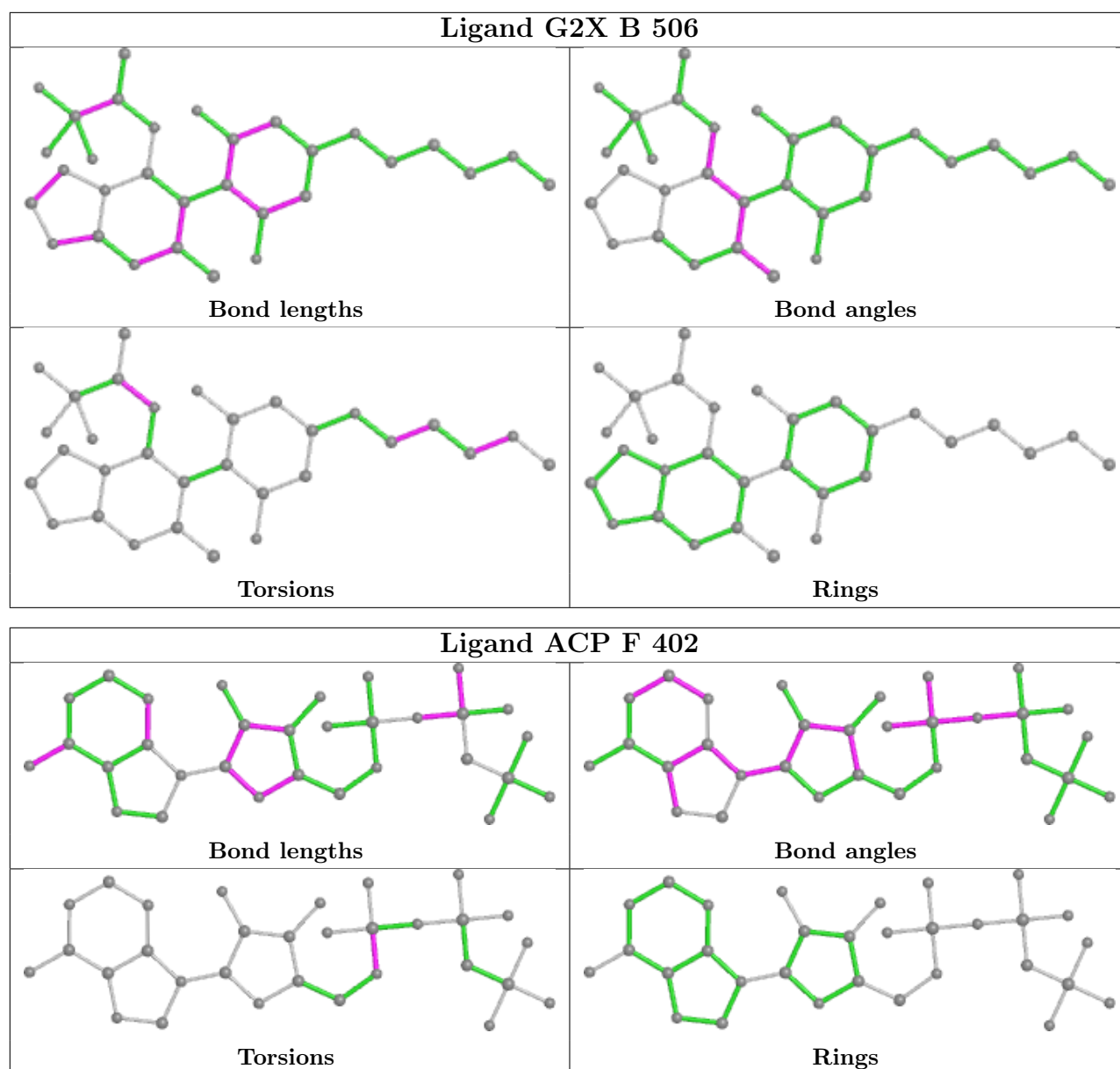
## Ligand G2X C 504



## Ligand GTP A 501







## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	438/450 (97%)	0.10	9 (2%) 63 58	14, 42, 77, 126	0
1	C	440/450 (97%)	-0.31	1 (0%) 95 95	9, 27, 53, 82	0
2	B	418/445 (93%)	-0.01	13 (3%) 49 42	8, 37, 76, 110	0
2	D	426/445 (95%)	0.38	23 (5%) 25 20	16, 52, 90, 116	0
3	E	123/143 (86%)	0.41	12 (9%) 7 5	19, 55, 96, 103	0
4	F	351/384 (91%)	0.76	58 (16%) 1 1	24, 68, 116, 130	0
All	All	2196/2317 (94%)	0.18	116 (5%) 26 21	8, 44, 93, 130	0

All (116) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	281	ALA	10.3
4	F	245	ILE	8.4
4	F	159	GLY	8.1
2	D	72	THR	7.4
1	A	282	TYR	6.5
4	F	157	GLY	6.0
4	F	249	TYR	5.9
4	F	177	GLY	5.9
4	F	236	LYS	5.8
2	B	55	THR	5.7
1	A	283	HIS	5.5
2	D	55	THR	5.2
4	F	251	LYS	5.2
2	D	56	GLY	5.1
4	F	172	PHE	4.6
1	A	279	GLU	4.6
4	F	246	GLN	4.3
4	F	153	ALA	4.2
4	F	244	CYS	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	262	TYR	4.2
3	E	28	SER	4.2
4	F	156	LYS	4.1
3	E	128	LYS	4.0
2	D	92	PHE	4.0
3	E	27	PRO	3.9
2	D	239	CYS	3.7
4	F	247	LYS	3.7
4	F	170	LEU	3.6
4	F	250	SER	3.6
1	C	1	MET	3.6
4	F	173	ILE	3.6
4	F	161	LEU	3.6
4	F	155	ALA	3.6
4	F	176	GLN	3.5
4	F	248	GLU	3.5
2	B	57	ASN	3.5
4	F	149	ALA	3.4
2	D	71	GLY	3.4
4	F	175	GLU	3.3
4	F	128	ARG	3.3
4	F	178	GLN	3.3
4	F	162	ILE	3.2
3	E	143	ALA	3.2
2	D	284	LEU	3.2
2	D	58	LYS	3.2
2	D	33	THR	3.2
4	F	362	ALA	3.2
2	D	219	THR	3.2
3	E	45	PRO	3.2
4	F	150	LYS	3.2
2	D	439	ASP	3.1
4	F	372	THR	3.1
4	F	240	LEU	3.1
4	F	102	PRO	3.0
4	F	158	GLU	2.9
1	A	346	TRP	2.9
1	A	278	ALA	2.9
4	F	9	GLU	2.8
2	D	57	ASN	2.8
4	F	103	THR	2.8
4	F	182	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
4	F	259	GLY	2.7
1	A	280	LYS	2.7
2	B	36	TYR	2.7
4	F	234	GLN	2.6
4	F	100	ILE	2.6
2	B	37	HIS	2.6
4	F	242	ASN	2.6
2	B	437	THR	2.6
2	B	414	MET	2.6
4	F	337	ALA	2.5
4	F	252	ASN	2.5
2	D	87	PRO	2.5
2	B	42	LEU	2.5
4	F	154	GLY	2.5
2	B	54	ALA	2.5
4	F	231	ALA	2.4
4	F	130	VAL	2.4
2	B	81	PHE	2.4
2	D	54	ALA	2.4
2	D	30	ILE	2.4
2	D	84	ILE	2.4
4	F	32	LYS	2.4
4	F	171	ASP	2.4
4	F	1	MET	2.4
4	F	174	ASP	2.3
2	D	177	ASP	2.3
4	F	132	LEU	2.3
4	F	152	SER	2.3
3	E	124	GLN	2.3
2	D	94	GLN	2.3
4	F	238	CYS	2.3
4	F	21	LEU	2.3
4	F	263	PHE	2.3
2	B	80	PRO	2.3
2	D	73	MET	2.3
4	F	186	LEU	2.3
3	E	44	ASP	2.3
2	B	58	LYS	2.2
2	B	59	TYR	2.2
2	D	245	GLN	2.2
4	F	253	TYR	2.2
3	E	122	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	40	SER	2.1
2	D	107	THR	2.1
3	E	125	GLU	2.1
4	F	237	THR	2.1
1	A	46	ASP	2.1
3	E	117	ALA	2.1
3	E	6	MET	2.1
4	F	363	ASP	2.1
2	D	59	TYR	2.1
2	D	278	SER	2.1
4	F	223	THR	2.1
4	F	243	HIS	2.0
3	E	48	GLU	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 monosaccharides 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	MG	D	501	1/1	0.74	0.19	59,59,59,59	0
7	CA	B	504	1/1	0.76	0.26	119,119,119,119	0
6	MG	F	401	1/1	0.85	0.17	89,89,89,89	0
7	CA	C	503	1/1	0.86	0.28	98,98,98,98	0
11	ACP	F	402	31/31	0.88	0.18	69,89,110,122	0
6	MG	B	502	1/1	0.89	0.48	44,44,44,44	0
7	CA	B	505	1/1	0.92	0.17	72,72,72,72	0
7	CA	A	504	1/1	0.93	0.14	98,98,98,98	0
5	GTP	D	503	32/32	0.94	0.15	38,48,61,69	0
7	CA	D	502	1/1	0.96	0.07	78,78,78,78	0

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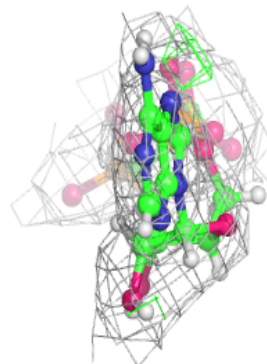
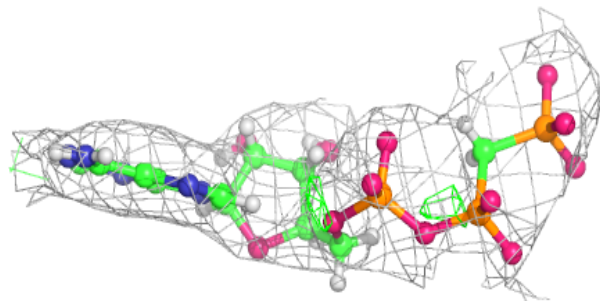
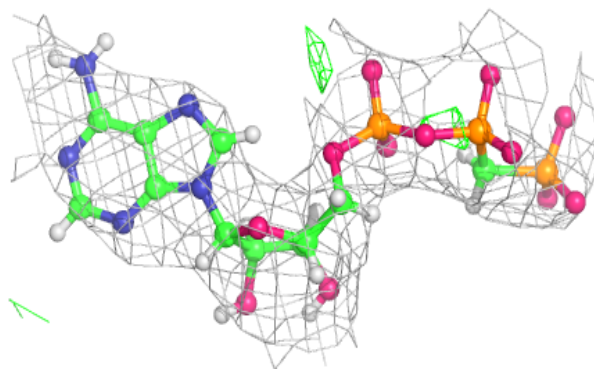
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
10	G2X	B	506	31/31	0.96	0.19	24,37,57,58	0
10	G2X	C	504	31/31	0.96	0.16	18,32,59,62	0
5	GTP	C	501	32/32	0.96	0.17	15,27,49,59	0
9	MES	B	503	12/12	0.97	0.17	36,43,51,54	0
6	MG	A	502	1/1	0.97	0.20	23,23,23,23	0
5	GTP	A	501	32/32	0.98	0.25	10,28,40,49	0
8	GDP	B	501	28/28	0.98	0.19	15,28,51,64	0
7	CA	A	503	1/1	0.98	0.06	75,75,75,75	0
6	MG	C	502	1/1	0.99	0.09	19,19,19,19	0
7	CA	C	505	1/1	0.99	0.09	30,30,30,30	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.

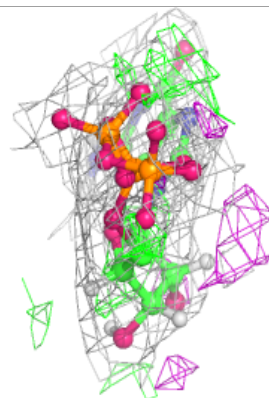
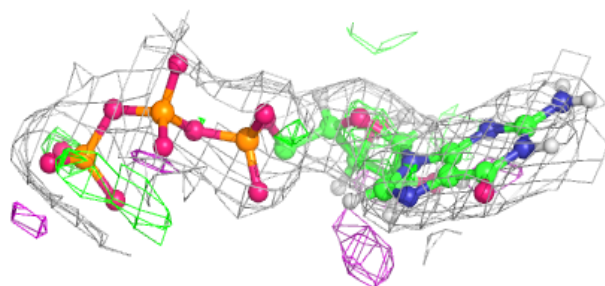
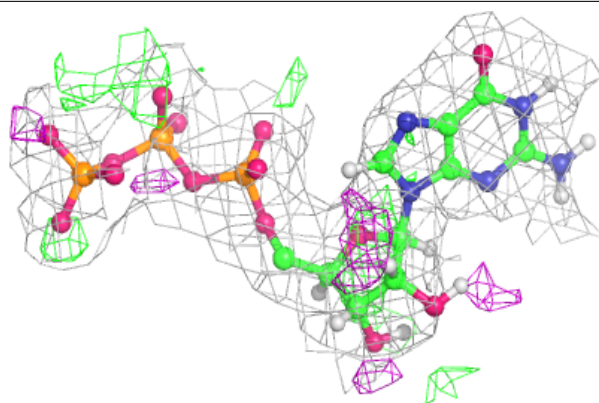
#### Electron density around ACP F 402:

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)

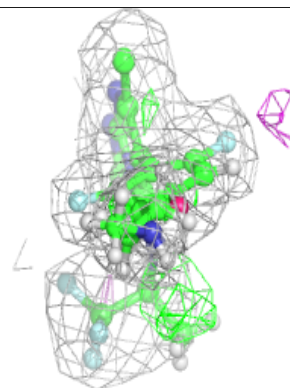
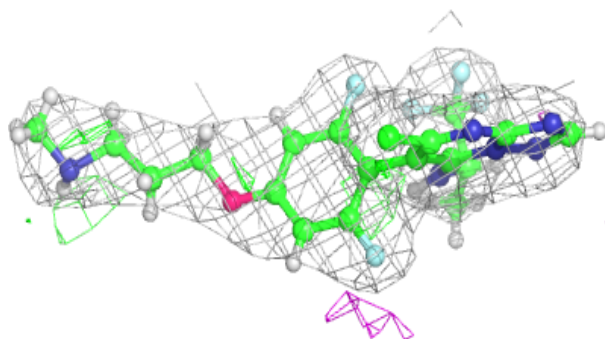
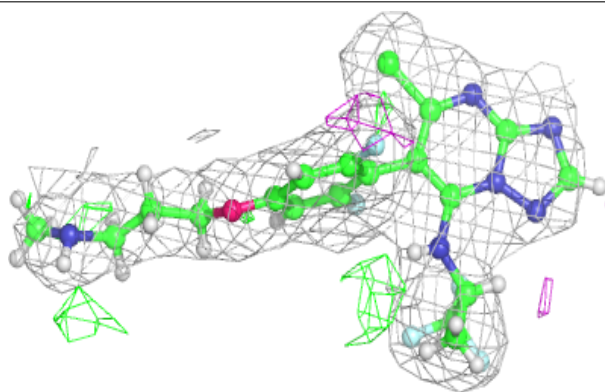


**Electron density around GTP D 503:**

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

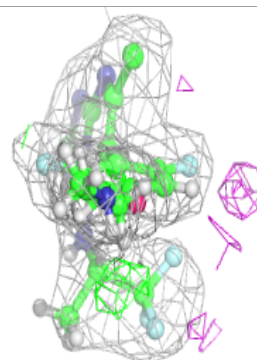
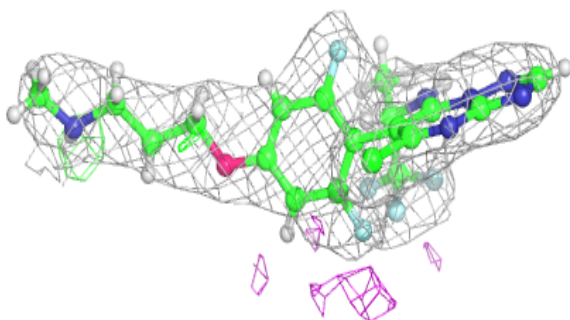
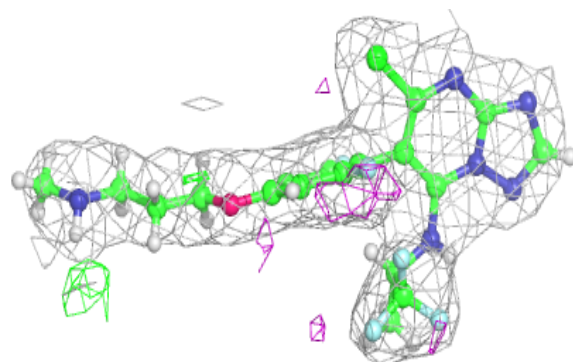
**Electron density around G2X B 506:**

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

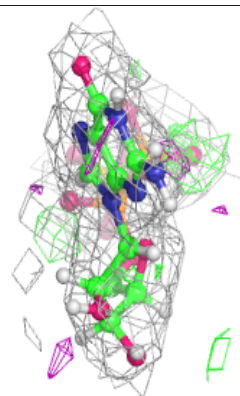
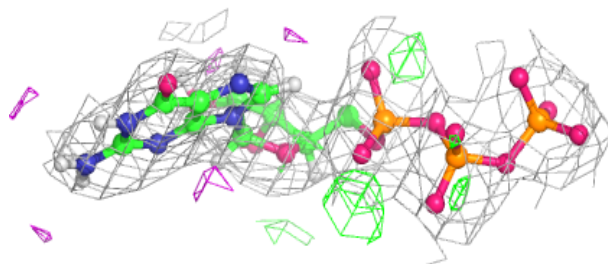
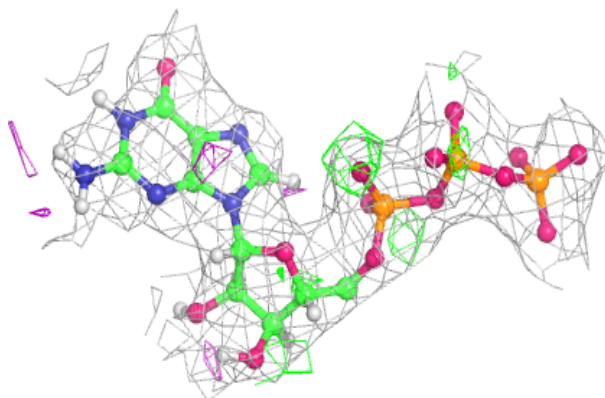


**Electron density around G2X C 504:**

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

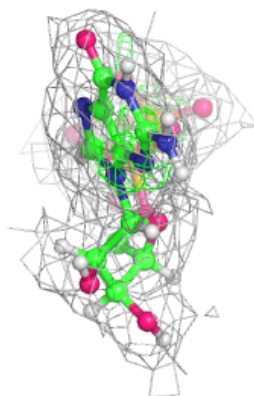
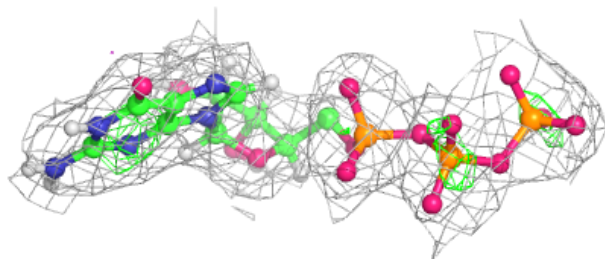
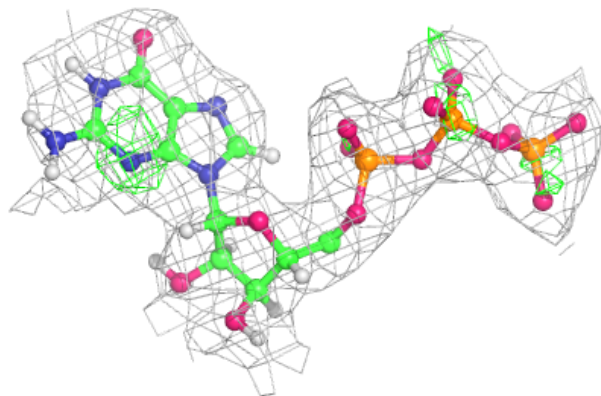
**Electron density around GTP C 501:**

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

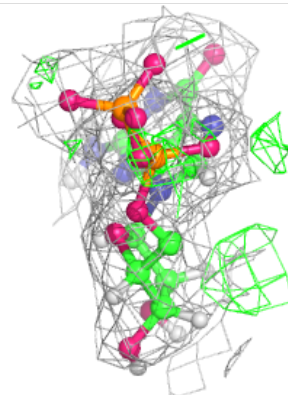
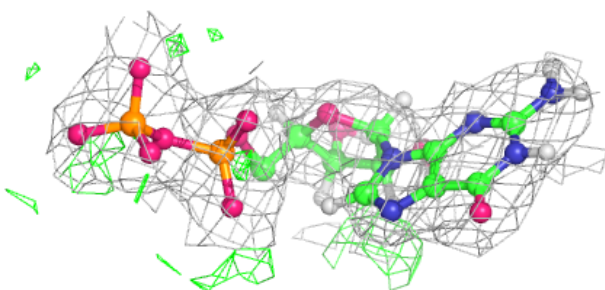
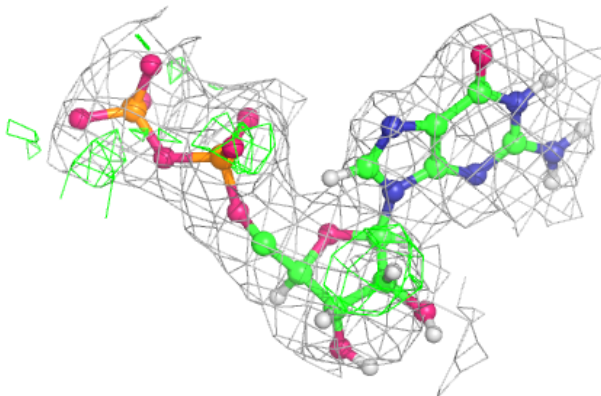


**Electron density around GTP A 501:**

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

**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.