



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 21, 2021 – 02:34 PM EDT

PDB ID : 5S65  
Title : Tubulin-Z1354416068-complex  
Authors : Muehlethaler, T.; Gioia, D.; Protá, A.E.; Sharpe, M.E.; Cavalli, A.; Steinmetz, M.O.  
Deposited on : 2020-11-08  
Resolution : 2.25 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

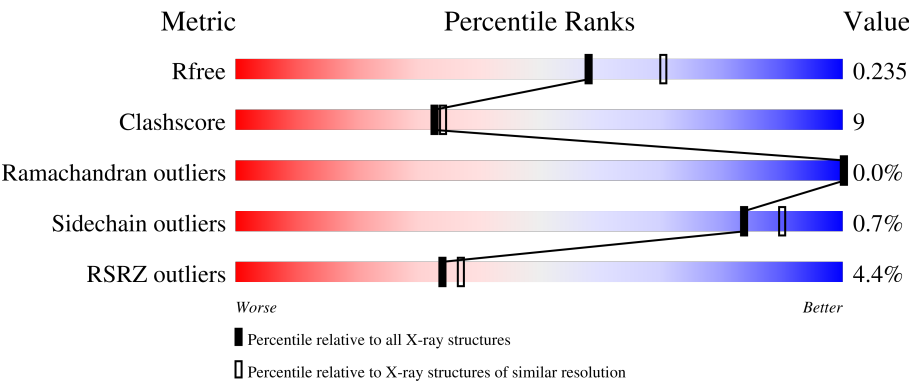
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.25 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 <sub>free</sub>	130704	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	451	<div><div>2%</div><div>77%</div><div>19%</div><div>..</div></div>
1	C	451	<div><div>2%</div><div>83%</div><div>14%</div><div>.</div></div>
2	B	445	<div><div>3%</div><div>71%</div><div>25%</div><div>.</div></div>
2	D	445	<div><div>3%</div><div>76%</div><div>20%</div><div>.</div></div>
3	E	143	<div><div>6%</div><div>73%</div><div>13%</div><div>14%</div></div>

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Mol	Chain	Length	Quality of chain
4	F	384	<div><div></div><div>11%</div><div>74%</div><div>18%</div><div>8%</div></div>

## 2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 18083 atoms, of which 12 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	N	O	S	0	0	0
			3424	2167	582	653	22			
1	C	440	Total	C	N	O	S	0	1	0
			3443	2178	585	657	23			

- Molecule 2 is a protein called Tubulin beta-2B chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	425	Total	C	N	O	S	1	1	0
			3359	2109	577	646	27			
2	D	427	Total	C	N	O	S	5	0	0
			3348	2101	571	649	27			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	123	Total	C	N	O	S	0	0	0
			1014	625	183	201	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	3	MET	-	initiating methionine	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	352	Total	C	N	O	S	0	0	0
			2877	1843	495	525	14			

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	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		

- 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		
6	D	1	Total	Mg	0	0
			1	1		

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

- | Mol | Chain | Residues | Atoms           | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 7   | A     | 2        | Total Ca<br>2 2 | 0       | 0       |
| 7   | B     | 1        | Total Ca<br>1 1 | 0       | 0       |
| 7   | C     | 1        | Total Ca<br>1 1 | 0       | 0       |

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- The image displays the chemical structure of GDP (Guanosine Diphosphate). It consists of a guanine base (a purine derivative) linked to a ribose sugar, which is in turn linked to two phosphate groups. The guanine base is shown with its characteristic fused ring system, including atoms N1, N2, N3, N7, C2, C4, C5, C6, and C8. The ribose sugar is a five-membered ring with carbons C1', C2', C3', C4', and C5'. The two phosphate groups are represented by phosphorus atoms (P) and their associated oxygen atoms (O). The structure is labeled with various atom names and numbers, indicating the specific atoms involved in the molecule.

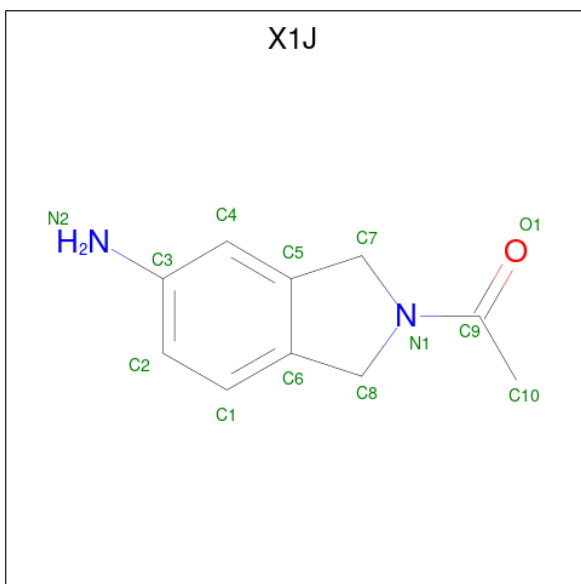
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	B	1	Total 28	C 10	N 5	O 11	P 2	0	0
8	D	1	Total 28	C 10	N 5	O 11	P 2	0	0

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- WORLD WIDE  
PDB  
PROTEIN DATA BANK



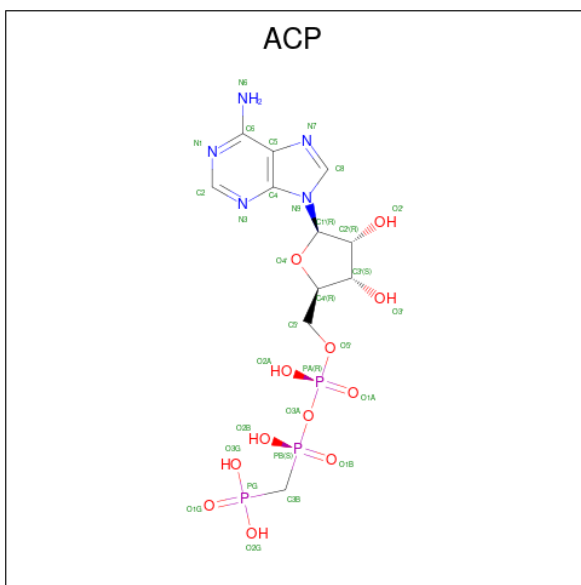
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 10 is 1-(5-amino-1,3-dihydro-2H-isoindol-2-yl)ethan-1-one (three-letter code: X1J) (formula:  $C_{10}H_{12}N_2O$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	C	1	Total	C	H	N	O	0	0
			25	10	12	2	1		

- 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 31	C 11	N 5	O 12	P 3	0	0

- Molecule 12 is water.

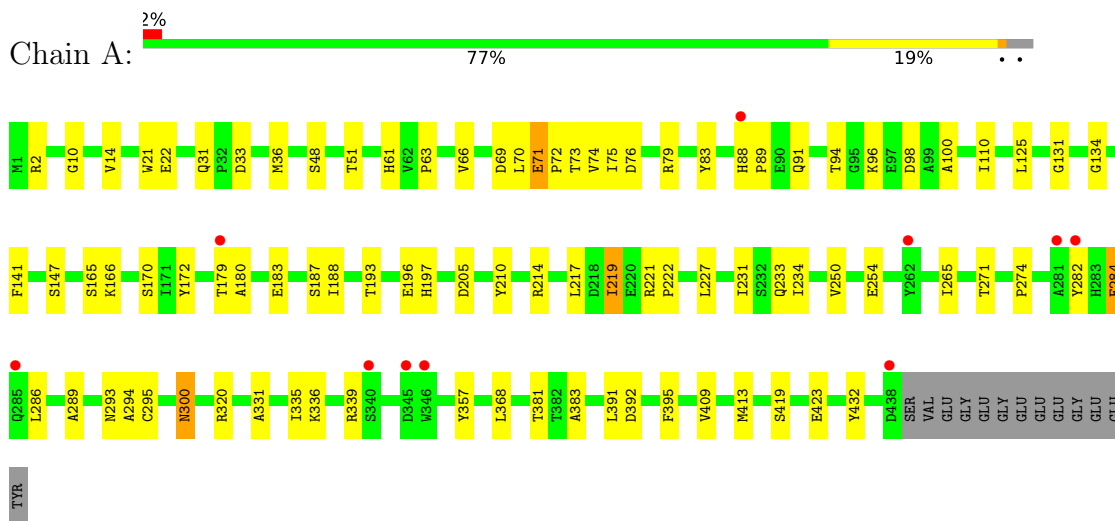
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	69	Total O 69 69	0	0
12	B	89	Total O 89 89	0	0
12	C	199	Total O 199 199	0	0
12	D	35	Total O 35 35	0	0
12	E	12	Total O 12 12	0	0
12	F	17	Total O 17 17	0	0



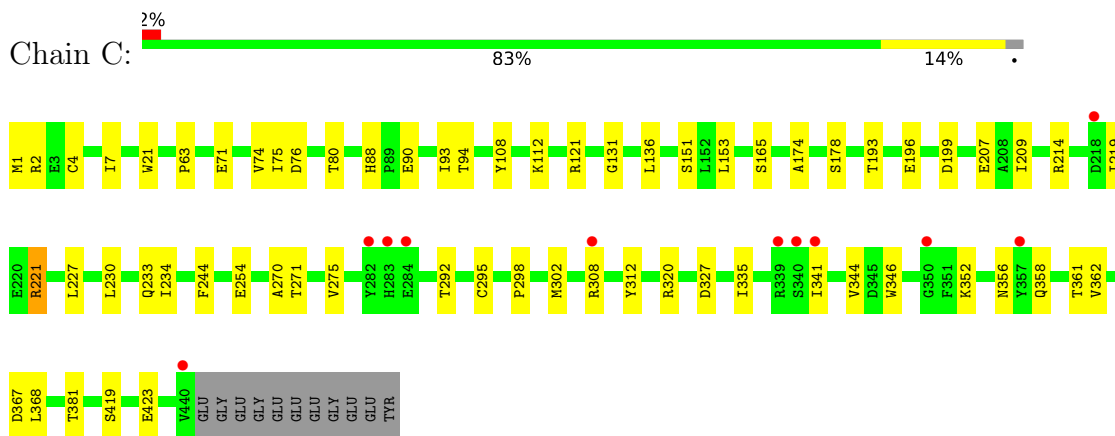
### 3 Residue-property plots

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

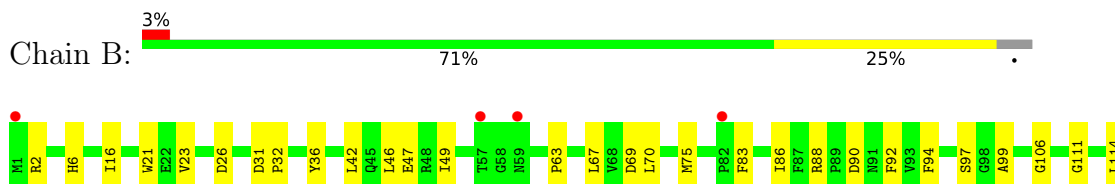
#### • Molecule 1: Tubulin alpha-1B chain

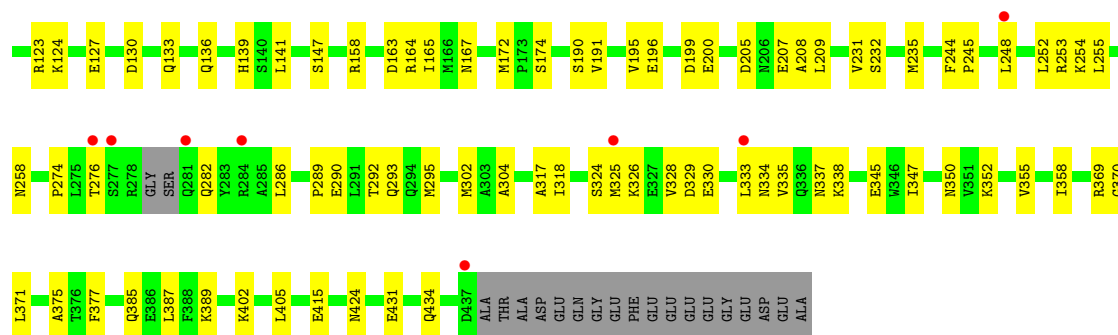


#### • Molecule 1: Tubulin alpha-1B chain

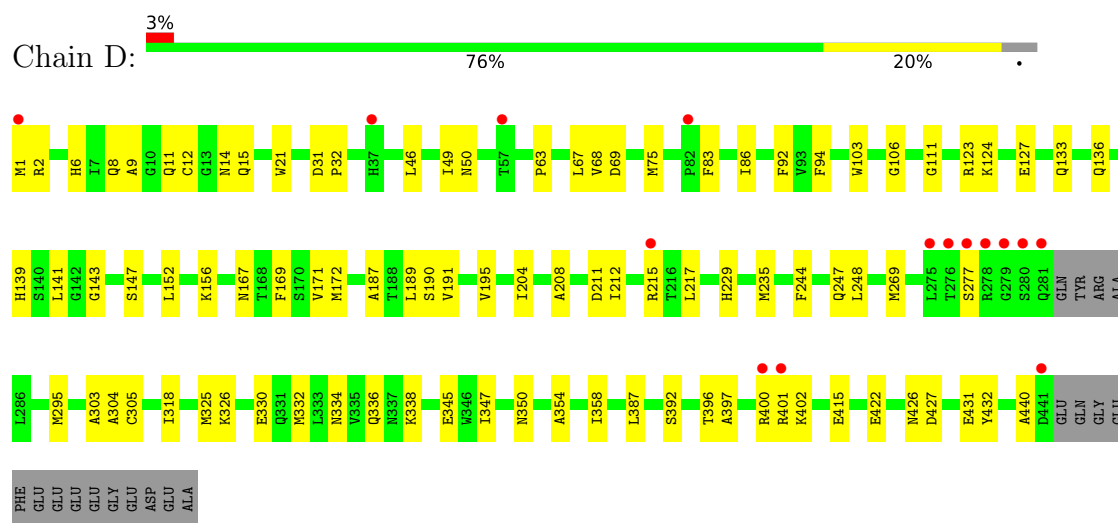


#### • Molecule 2: Tubulin beta-2B chain

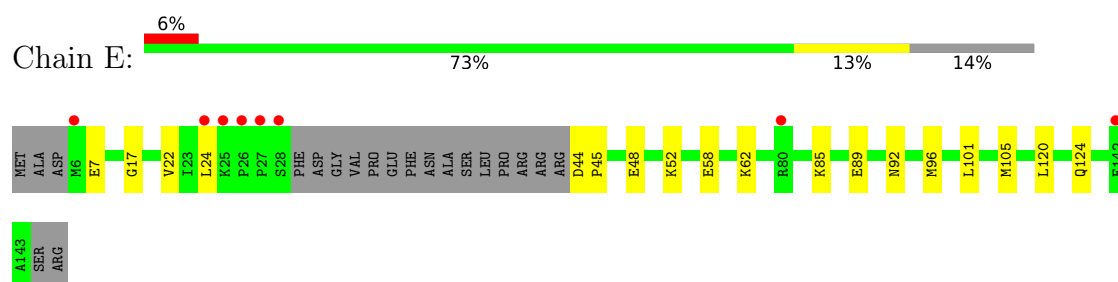




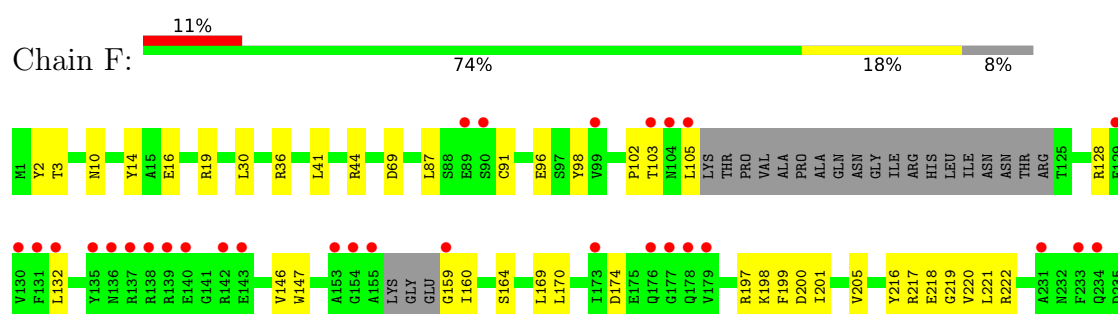
• Molecule 2: Tubulin beta-2B chain

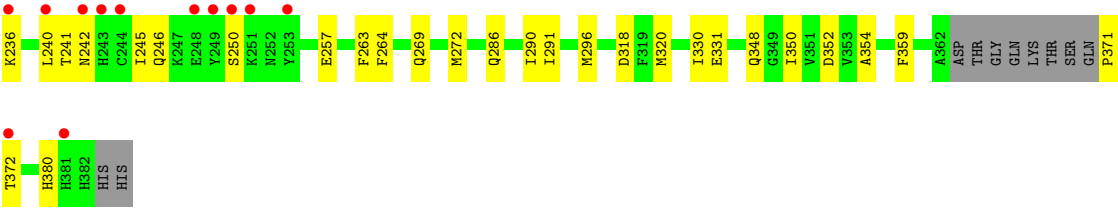


• Molecule 3: Stathmin-4



• 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, $\alpha$ , $\beta$ , $\gamma$	105.19Å 158.92Å 179.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	62.70 – 2.25 118.94 – 2.25	Depositor EDS
% Data completeness (in resolution range)	99.4 (62.70-2.25) 99.4 (118.94-2.25)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.99 (at 2.25Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, $R_{free}$	0.205 , 0.234 0.205 , 0.235	Depositor DCC
$R_{free}$ test set	7020 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	50.8	Xtriage
Anisotropy	0.198	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 40.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	18083	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.43% 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: X1J, CA, GTP, MG, MES, GDP, ACP

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	0.25	0/3502	0.42	0/4754
1	C	0.26	0/3521	0.43	0/4780
2	B	0.25	0/3433	0.41	0/4647
2	D	0.25	0/3421	0.41	0/4633
3	E	0.24	0/1022	0.35	0/1356
4	F	0.24	0/2944	0.40	0/3978
All	All	0.25	0/17843	0.41	0/24148

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	3424	0	3334	68	0
1	C	3443	0	3352	44	0
2	B	3359	0	3235	79	0
2	D	3348	0	3224	59	0
3	E	1014	0	1029	12	0
4	F	2877	0	2839	48	0
5	A	32	0	12	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	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
6	F	1	0	0	0	0
7	A	2	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
8	D	28	0	12	2	0
9	B	12	0	12	3	0
10	C	13	12	0	0	0
11	F	31	0	14	5	0
12	A	69	0	0	4	0
12	B	89	0	0	3	0
12	C	199	0	0	4	0
12	D	35	0	0	1	0
12	E	12	0	0	1	0
12	F	17	0	0	0	0
All	All	18071	12	17087	301	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 9.

All (301) 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:C:221:ARG:HG3	2:D:325:MET:HG2	1.38	1.01
2:B:16:ILE:HD13	2:B:231:VAL:HG11	1.56	0.88
2:D:217:LEU:HA	2:D:277:SER:HB3	1.56	0.87
1:C:209:ILE:HD11	1:C:302:MET:CE	2.10	0.82
4:F:10:ASN:HB2	4:F:44:ARG:HH22	1.45	0.81
4:F:102:PRO:HG2	4:F:105:LEU:HD13	1.64	0.80
4:F:241:THR:OG1	11:F:401:ACP:O3'	2.01	0.78
4:F:331:GLU:OE2	11:F:401:ACP:O3G	2.02	0.78
2:D:334:ASN:HD21	2:D:338:LYS:HE3	1.48	0.78
4:F:318:ASP:OD2	11:F:401:ACP:O2G	2.02	0.77
1:A:335:ILE:HG23	1:A:339:ARG:HG3	1.65	0.76
1:A:250:VAL:HG12	1:A:254:GLU:OE1	1.86	0.75
1:C:209:ILE:HD11	1:C:302:MET:HE3	1.67	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:GLU:OE2	1:A:73:THR:OG1	2.06	0.72
2:D:136:GLN:HA	2:D:167:ASN:O	1.88	0.72
4:F:236:LYS:HB3	4:F:240:LEU:HD13	1.73	0.69
2:B:83:PHE:O	2:B:86:ILE:HG22	1.93	0.69
1:C:76:ASP:O	1:C:80:THR:HG22	1.93	0.69
1:A:293:ASN:OD1	1:A:339:ARG:NH2	2.24	0.68
2:D:21:TRP:CZ3	2:D:63:PRO:HB3	2.30	0.67
1:C:4[A]:CYS:SG	1:C:136:LEU:HG	2.35	0.66
2:B:136:GLN:HA	2:B:167:ASN:O	1.96	0.65
3:E:44:ASP:OD2	12:E:201:HOH:O	2.14	0.65
1:A:179:THR:HA	2:B:352:LYS:HD2	1.78	0.65
4:F:371:PRO:HA	4:F:372:THR:O	1.97	0.65
2:B:88:ARG:NH1	2:B:90:ASP:HB2	2.12	0.65
2:B:147:SER:HG	2:B:190:SER:HG	1.45	0.65
2:B:67:LEU:HD22	2:B:92:PHE:CE2	2.32	0.64
2:D:269:MET:HG3	2:D:303:ALA:HB3	1.79	0.64
3:E:48:GLU:HG2	3:E:52:LYS:HE3	1.78	0.64
1:C:234:ILE:HD13	1:C:302:MET:HE1	1.78	0.64
4:F:128:ARG:NH2	4:F:174:ASP:OD1	2.32	0.63
1:C:234:ILE:HD13	1:C:302:MET:CE	2.29	0.63
1:C:270:ALA:O	1:C:302:MET:HG2	1.98	0.63
1:A:179:THR:HG21	2:B:248:LEU:CB	2.28	0.63
4:F:320:MET:HG3	4:F:330:ILE:HD11	1.81	0.63
2:D:171:VAL:HA	2:D:204:ILE:O	1.99	0.62
2:D:1:MET:HG3	2:D:50:ASN:HB2	1.80	0.62
2:D:106:GLY:O	2:D:111:GLY:HA3	2.00	0.62
2:B:209:LEU:HD23	2:B:302:MET:HG2	1.82	0.61
2:D:83:PHE:O	2:D:86:ILE:HG22	2.00	0.61
2:D:334:ASN:ND2	2:D:338:LYS:HE3	2.14	0.61
2:B:2:ARG:HB2	2:B:133:GLN:CG	2.30	0.61
2:B:164:ARG:HD2	12:B:665:HOH:O	1.99	0.61
1:C:209:ILE:HG22	1:C:227:LEU:HD22	1.82	0.60
4:F:147:TRP:HB2	4:F:169:LEU:HD11	1.83	0.60
4:F:371:PRO:HA	4:F:372:THR:HB	1.83	0.60
2:D:347:ILE:HG22	2:D:350:ASN:HB3	1.84	0.60
2:D:427:ASP:O	2:D:431:GLU:HG3	2.02	0.59
2:B:253[A]:ARG:NH1	9:B:504:MES:O2S	2.35	0.59
1:A:71:GLU:HG2	1:A:72:PRO:HD2	1.84	0.59
4:F:197:ARG:NH1	4:F:257:GLU:OE2	2.23	0.59
1:A:75:ILE:HD12	1:A:94:THR:HG22	1.83	0.58
1:C:367:ASP:OD1	12:C:601:HOH:O	2.17	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:88:ARG:HH11	2:B:90:ASP:HB2	1.68	0.58
1:A:300:ASN:HB3	12:A:601:HOH:O	2.04	0.58
2:B:69:ASP:O	2:B:94:PHE:HA	2.04	0.58
4:F:132:LEU:HD21	4:F:170:LEU:HD11	1.86	0.58
2:D:69:ASP:O	2:D:94:PHE:HA	2.04	0.57
4:F:371:PRO:CA	4:F:372:THR:HB	2.34	0.57
2:B:337:ASN:OD1	4:F:36:ARG:HD3	2.04	0.57
1:C:209:ILE:HD11	1:C:302:MET:HE1	1.82	0.57
1:C:320:ARG:HA	1:C:356:ASN:O	2.03	0.57
1:C:292:THR:HG22	1:C:335:ILE:HD12	1.85	0.57
1:A:36:MET:HB3	1:A:61:HIS:CE1	2.39	0.57
4:F:159:GLY:C	4:F:160:ILE:HD12	2.25	0.57
2:D:152:LEU:O	2:D:156:LYS:HG2	2.03	0.57
1:C:93:ILE:HD11	1:C:121:ARG:HG3	1.87	0.56
1:A:21:TRP:CZ3	1:A:63:PRO:HB3	2.41	0.56
1:C:298:PRO:HG2	1:C:308:ARG:NH2	2.20	0.56
1:A:100:ALA:HA	2:B:254:LYS:HG3	1.88	0.56
2:D:21:TRP:CE3	2:D:63:PRO:HB3	2.40	0.56
1:A:88:HIS:HB2	1:A:89:PRO:HD2	1.88	0.56
4:F:246:GLN:O	4:F:250:SER:HB3	2.05	0.56
2:B:172:MET:HG3	2:B:387:LEU:HD11	1.88	0.55
1:C:214:ARG:HG2	1:C:219:ILE:O	2.06	0.55
4:F:3:THR:HB	4:F:30:LEU:HD11	1.88	0.55
1:C:254:GLU:HG2	1:C:352:LYS:HE2	1.88	0.55
1:A:210:TYR:CE1	1:A:222:PRO:HD2	2.42	0.55
2:B:274:PRO:HB3	2:B:286:LEU:CD2	2.37	0.55
1:C:233:GLN:HG3	1:C:368:LEU:CD1	2.36	0.55
2:B:209:LEU:CD2	2:B:302:MET:HG2	2.36	0.55
2:B:274:PRO:HB3	2:B:286:LEU:HD22	1.89	0.55
3:E:85:LYS:O	3:E:89:GLU:HG3	2.06	0.55
1:C:327:ASP:OD2	12:C:602:HOH:O	2.18	0.55
4:F:371:PRO:HA	4:F:372:THR:C	2.27	0.55
1:A:187:SER:HB3	1:A:391:LEU:HD21	1.89	0.54
1:A:294:ALA:O	1:A:300:ASN:ND2	2.40	0.54
1:A:336:LYS:HG3	3:E:24:LEU:HD13	1.90	0.54
2:D:172:MET:HG3	2:D:387:LEU:HD11	1.88	0.54
2:B:124:LYS:HD3	2:B:124:LYS:C	2.27	0.54
2:D:187:ALA:O	2:D:191:VAL:HG23	2.08	0.54
1:A:69:ASP:O	1:A:94:THR:HA	2.06	0.54
1:C:419:SER:O	1:C:423:GLU:HG3	2.07	0.54
4:F:14:TYR:HB3	4:F:41:LEU:HD13	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:87:LEU:O	4:F:91:CYS:HB2	2.07	0.54
1:A:214:ARG:HG2	1:A:219:ILE:O	2.08	0.54
1:A:227:LEU:O	1:A:231:ILE:HG13	2.08	0.54
1:A:381:THR:HG22	1:A:383:ALA:H	1.73	0.54
3:E:92:ASN:O	3:E:96:MET:HG2	2.08	0.54
4:F:296:MET:SD	4:F:380:HIS:HB2	2.48	0.53
2:B:123:ARG:O	2:B:127:GLU:HG3	2.09	0.53
4:F:2:TYR:CE1	4:F:359:PHE:HB3	2.43	0.53
4:F:147:TRP:HB2	4:F:169:LEU:CD1	2.38	0.53
4:F:216:TYR:CE2	4:F:218:GLU:HB2	2.43	0.53
2:D:11:GLN:O	2:D:15:GLN:HG2	2.09	0.53
1:C:271:THR:HG21	1:C:295:CYS:O	2.07	0.53
2:D:397:ALA:O	2:D:401:ARG:NH1	2.41	0.53
2:B:415:GLU:HG3	12:B:648:HOH:O	2.09	0.53
1:C:196:GLU:HG2	12:C:669:HOH:O	2.09	0.53
1:A:98:ASP:HB2	5:A:501:GTP:O2G	2.09	0.52
1:A:96:LYS:NZ	2:B:130:ASP:OD1	2.39	0.52
1:A:187:SER:CB	1:A:391:LEU:HD21	2.38	0.52
1:C:244:PHE:CD1	1:C:358:GLN:HG2	2.44	0.52
2:D:392:SER:O	2:D:396:THR:HG22	2.10	0.52
3:E:101:LEU:O	3:E:105:MET:HG2	2.09	0.52
2:B:36:TYR:CD1	2:B:46:LEU:HD21	2.45	0.52
2:B:345:GLU:OE1	2:B:345:GLU:N	2.36	0.52
2:D:143:GLY:HA3	8:D:501:GDP:O3A	2.10	0.52
3:E:48:GLU:CG	3:E:52:LYS:HE3	2.40	0.52
2:B:46:LEU:HA	2:B:49:ILE:HB	1.92	0.51
2:D:9:ALA:HA	2:D:68:VAL:O	2.10	0.51
2:D:12:CYS:HB2	8:D:501:GDP:C8	2.46	0.51
2:B:244:PHE:CE1	2:B:358:ILE:HD12	2.46	0.51
1:A:172:TYR:HB3	1:A:205:ASP:HA	1.92	0.51
2:D:1:MET:HG3	2:D:50:ASN:CB	2.41	0.51
2:D:6:HIS:CD2	2:D:21:TRP:HE1	2.29	0.51
1:C:292:THR:HG22	1:C:335:ILE:CD1	2.41	0.51
2:D:397:ALA:HA	2:D:400:ARG:NH1	2.25	0.51
2:D:318:ILE:N	2:D:318:ILE:HD12	2.26	0.50
1:A:166:LYS:HE2	1:A:197:HIS:O	2.11	0.50
2:B:295:MET:CG	2:B:377:PHE:HB2	2.41	0.50
2:B:31:ASP:HB2	2:B:32:PRO:CD	2.42	0.50
1:A:188:ILE:HD12	1:A:395:PHE:HB2	1.92	0.50
2:B:370:GLY:O	2:B:371:LEU:HD23	2.11	0.50
2:B:47:GLU:HG2	2:B:245:PRO:HG3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:419:SER:O	1:A:423:GLU:HG3	2.12	0.49
2:B:318:ILE:N	2:B:318:ILE:HD12	2.27	0.49
4:F:16:GLU:OE2	4:F:19:ARG:NH2	2.41	0.49
1:A:22:GLU:HG3	1:A:83:TYR:CE1	2.47	0.49
1:A:76:ASP:OD1	1:A:79:ARG:NH1	2.45	0.49
4:F:201:ILE:HG12	4:F:221:LEU:HG	1.93	0.49
4:F:10:ASN:CB	4:F:44:ARG:HH22	2.22	0.49
2:B:141:LEU:HD12	2:B:172:MET:SD	2.53	0.49
2:D:248:LEU:HD23	2:D:354:ALA:HB2	1.92	0.49
2:B:347:ILE:HG22	2:B:350:ASN:HB3	1.94	0.49
1:A:271:THR:HG21	1:A:295:CYS:HA	1.95	0.49
1:C:174:ALA:CB	1:C:207:GLU:HB2	2.43	0.49
1:A:71:GLU:HG2	1:A:72:PRO:CD	2.42	0.49
4:F:320:MET:CG	4:F:330:ILE:HD11	2.42	0.49
4:F:348:GLN:NE2	4:F:352:ASP:OD1	2.45	0.49
2:B:106:GLY:O	2:B:111:GLY:HA3	2.12	0.48
2:B:286:LEU:HD12	2:B:290:GLU:OE1	2.13	0.48
1:A:217:LEU:HD21	1:A:368:LEU:HD23	1.96	0.48
1:C:21:TRP:CZ3	1:C:63:PRO:HB3	2.48	0.48
4:F:220:VAL:HG12	4:F:263:PHE:CE1	2.48	0.48
4:F:286:GLN:O	4:F:290:ILE:HG13	2.14	0.48
2:B:199:ASP:OD1	9:B:504:MES:H62	2.13	0.48
2:D:402:LYS:HE2	2:D:415:GLU:OE1	2.12	0.48
4:F:200:ASP:OD1	4:F:222:ARG:HB2	2.12	0.48
1:A:274:PRO:HB3	1:A:286:LEU:HD12	1.95	0.48
4:F:350:ILE:O	4:F:354:ALA:HB3	2.13	0.48
1:A:196:GLU:OE1	1:A:196:GLU:HA	2.13	0.48
2:B:431:GLU:O	2:B:434:GLN:HG2	2.13	0.48
2:B:292:THR:HG22	2:B:335:VAL:HG21	1.96	0.47
2:B:165:ILE:HG21	2:B:252:LEU:HB3	1.97	0.47
2:D:432:TYR:OH	12:D:601:HOH:O	2.20	0.47
3:E:120:LEU:O	3:E:124:GLN:HG3	2.14	0.47
1:A:70:LEU:HD13	1:A:110:ILE:HG21	1.96	0.47
2:D:147:SER:HB2	2:D:190:SER:OG	2.14	0.47
1:A:284:GLU:CD	1:A:284:GLU:H	2.17	0.47
1:A:289:ALA:HA	1:A:331:ALA:CB	2.44	0.47
2:B:114:LEU:O	2:B:114:LEU:HG	2.15	0.47
2:B:163:ASP:O	2:B:253[A]:ARG:NH2	2.46	0.47
1:C:75:ILE:HD12	1:C:94:THR:HG22	1.96	0.47
2:D:1:MET:CE	2:D:50:ASN:HB2	2.43	0.47
4:F:205:VAL:HG21	4:F:291:ILE:HD13	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:21:TRP:CZ3	2:B:63:PRO:HB3	2.50	0.47
2:D:67:LEU:N	2:D:67:LEU:HD12	2.30	0.47
2:B:67:LEU:N	2:B:67:LEU:HD12	2.30	0.47
2:B:295:MET:HG2	2:B:377:PHE:HB2	1.97	0.46
3:E:44:ASP:HB3	3:E:45:PRO:HD2	1.97	0.46
2:B:70:LEU:HD12	2:B:99:ALA:HB2	1.97	0.46
2:B:97:SER:HA	1:C:2:ARG:NH1	2.30	0.46
2:B:326:LYS:O	2:B:330:GLU:HG3	2.16	0.46
2:B:385:GLN:OE1	2:B:389:LYS:HE3	2.15	0.46
1:C:1:MET:O	1:C:2:ARG:HB2	2.15	0.46
2:D:303:ALA:O	2:D:305:CYS:N	2.43	0.46
1:C:165:SER:HA	1:C:199:ASP:OD2	2.15	0.46
2:D:326:LYS:O	2:D:330:GLU:HG3	2.15	0.46
4:F:269:GLN:HA	4:F:272:MET:HE2	1.98	0.46
11:F:401:ACP:O3G	11:F:401:ACP:O1B	2.33	0.46
4:F:242:ASN:HD22	4:F:245:ILE:HD12	1.80	0.46
2:D:141:LEU:HA	2:D:147:SER:HB3	1.97	0.46
2:D:332:MET:O	2:D:336:GLN:HG3	2.16	0.46
4:F:146:VAL:HG22	4:F:164:SER:HB3	1.98	0.46
2:D:124:LYS:C	2:D:124:LYS:HD3	2.36	0.46
2:B:42:LEU:H	2:B:42:LEU:HD12	1.81	0.46
1:C:230:LEU:O	1:C:234:ILE:HD12	2.16	0.45
1:A:180:ALA:HA	2:B:258:ASN:OD1	2.16	0.45
4:F:96:GLU:OE2	4:F:98:TYR:OH	2.27	0.45
2:B:424:ASN:HB3	12:B:629:HOH:O	2.16	0.45
1:A:48:SER:O	1:A:51:THR:HG23	2.16	0.45
2:B:334:ASN:HD21	2:B:338:LYS:HD2	1.82	0.45
1:A:88:HIS:CD2	1:A:91:GLN:HG3	2.52	0.45
1:A:265:ILE:HG23	1:A:432:TYR:CE1	2.52	0.45
1:A:271:THR:HG23	1:A:300:ASN:HD22	1.82	0.45
2:B:231:VAL:O	2:B:235:MET:HG3	2.17	0.45
2:B:402:LYS:HB3	2:B:405:LEU:HD12	1.98	0.45
2:D:244:PHE:CE1	2:D:358:ILE:HD12	2.52	0.45
1:A:66:VAL:HG23	1:A:125:LEU:HD12	1.98	0.44
2:D:103:TRP:CE3	2:D:189:LEU:HD13	2.52	0.44
2:D:123:ARG:O	2:D:127:GLU:HG3	2.16	0.44
1:A:74:VAL:HB	12:A:604:HOH:O	2.17	0.44
4:F:103:THR:HG23	4:F:128:ARG:NH2	2.32	0.44
4:F:198:LYS:HG2	4:F:199:PHE:H	1.83	0.44
2:B:205:ASP:OD1	2:B:207:GLU:N	2.47	0.44
2:D:345:GLU:HG3	2:D:440:ALA:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:286:LEU:HD12	2:B:286:LEU:HA	1.89	0.44
2:B:174:SER:OG	2:B:207:GLU:HB2	2.17	0.44
2:B:324:SER:O	2:B:328:VAL:HG23	2.17	0.44
2:D:208:ALA:O	2:D:212:ILE:HG13	2.17	0.44
1:A:141:PHE:HB3	1:A:187:SER:OG	2.18	0.44
1:C:108:TYR:O	1:C:112:LYS:HG2	2.18	0.44
2:D:211:ASP:O	2:D:215:ARG:HB2	2.18	0.44
1:A:31:GLN:HB2	1:A:33:ASP:OD1	2.18	0.43
2:B:23:VAL:HG21	2:B:232:SER:HB3	2.00	0.43
2:B:276:THR:HG21	2:B:282:GLN:HA	2.00	0.43
2:B:289:PRO:O	2:B:293:GLN:HG3	2.18	0.43
1:A:22:GLU:HG3	1:A:83:TYR:HE1	1.81	0.43
2:B:208:ALA:HB2	2:B:304:ALA:HB2	2.00	0.43
2:D:191:VAL:O	2:D:195:VAL:HG23	2.18	0.43
3:E:58:GLU:HG2	3:E:62:LYS:HE3	2.01	0.43
4:F:219:GLY:HA3	4:F:264:PHE:CZ	2.53	0.43
1:A:21:TRP:CE3	1:A:63:PRO:HB3	2.54	0.43
2:B:329:ASP:O	2:B:333:LEU:HG	2.18	0.43
1:C:151:SER:HB2	1:C:193:THR:CG2	2.49	0.43
1:C:174:ALA:O	1:C:178:SER:HB3	2.19	0.43
2:B:164:ARG:O	9:B:504:MES:H31	2.18	0.43
2:B:191:VAL:O	2:B:195:VAL:HG23	2.18	0.43
1:C:7:ILE:HG21	1:C:153:LEU:HD21	2.01	0.43
2:D:2:ARG:HB3	2:D:133:GLN:CG	2.49	0.43
2:D:295:MET:HB2	2:D:295:MET:HE3	1.82	0.43
1:C:1:MET:HE3	1:C:131:GLY:HA3	2.00	0.43
1:C:312:TYR:CD1	1:C:341:ILE:HG23	2.53	0.43
1:C:74:VAL:HB	12:C:657:HOH:O	2.17	0.42
1:C:275:VAL:HG13	1:C:368:LEU:HD21	2.01	0.42
2:D:8:GLN:NE2	2:D:14:ASN:HA	2.34	0.42
4:F:217:ARG:HG3	4:F:218:GLU:HG2	2.00	0.42
2:B:325:MET:HE2	2:B:355:VAL:HG21	2.02	0.42
1:A:75:ILE:HB	1:A:94:THR:HG21	2.02	0.42
2:B:158:ARG:NH1	2:B:196:GLU:O	2.53	0.42
1:C:88:HIS:HE1	1:C:90:GLU:HG3	1.83	0.42
2:D:345:GLU:H	2:D:345:GLU:HG2	1.69	0.42
1:A:141:PHE:CE1	1:A:170:SER:HB3	2.54	0.42
2:B:200:GLU:OE2	2:B:255:LEU:HG	2.19	0.42
1:C:174:ALA:HB1	1:C:207:GLU:HB2	2.01	0.42
2:D:46:LEU:HA	2:D:49:ILE:HB	2.02	0.42
2:B:75:MET:HE3	2:B:92:PHE:HD2	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:387:LEU:C	2:B:387:LEU:HD23	2.40	0.42
2:D:75:MET:HE3	2:D:92:PHE:CD2	2.54	0.42
4:F:371:PRO:HA	4:F:372:THR:CB	2.45	0.42
2:D:31:ASP:HB2	2:D:32:PRO:HD2	2.01	0.42
4:F:242:ASN:OD1	11:F:401:ACP:H5'1	2.19	0.42
1:A:289:ALA:HA	1:A:331:ALA:HB1	2.01	0.42
2:D:1:MET:HE2	2:D:50:ASN:HB2	2.01	0.42
4:F:69:ASP:OD1	4:F:69:ASP:N	2.53	0.41
1:A:180:ALA:HB3	1:A:183:GLU:HG3	2.03	0.41
1:A:233:GLN:HG3	1:A:368:LEU:HD12	2.01	0.41
1:A:233:GLN:HG3	1:A:368:LEU:CD1	2.50	0.41
2:B:75:MET:HE3	2:B:92:PHE:CD2	2.55	0.41
1:A:75:ILE:HB	1:A:94:THR:CG2	2.50	0.41
2:D:387:LEU:HD23	2:D:387:LEU:C	2.40	0.41
1:A:188:ILE:HD11	1:A:392:ASP:HA	2.02	0.41
1:A:320:ARG:HD2	12:A:645:HOH:O	2.20	0.41
1:A:10:GLY:O	1:A:14:VAL:HG23	2.20	0.41
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.39	0.41
1:C:312:TYR:CE1	1:C:341:ILE:HG23	2.55	0.41
4:F:160:ILE:HD12	4:F:160:ILE:N	2.35	0.41
4:F:269:GLN:HA	4:F:272:MET:CE	2.51	0.41
1:A:2:ARG:HB3	1:A:131:GLY:O	2.21	0.41
1:A:193:THR:HG23	12:A:640:HOH:O	2.20	0.41
1:A:271:THR:CG2	1:A:295:CYS:HA	2.51	0.41
1:A:409:VAL:HA	1:A:413:MET:O	2.21	0.41
2:B:26:ASP:OD1	2:B:369:ARG:NH2	2.54	0.41
2:B:31:ASP:HB2	2:B:32:PRO:HD2	2.02	0.41
1:A:71:GLU:HG2	1:A:72:PRO:N	2.36	0.41
1:A:357:TYR:CE2	3:E:17:GLY:HA2	2.56	0.41
2:B:317:ALA:C	2:B:318:ILE:HD12	2.42	0.41
2:D:31:ASP:HB2	2:D:32:PRO:CD	2.51	0.40
1:A:134:GLY:HA3	1:A:165:SER:O	2.20	0.40
1:A:234:ILE:HD12	1:A:234:ILE:N	2.36	0.40
2:B:21:TRP:CE3	2:B:63:PRO:HB3	2.57	0.40
1:C:344:VAL:HG21	1:C:346:TRP:CE2	2.56	0.40
2:D:169:PHE:CE2	2:D:235:MET:HG2	2.56	0.40
1:A:141:PHE:O	1:A:147:SER:HB3	2.22	0.40
2:D:141:LEU:HD12	2:D:172:MET:SD	2.61	0.40
2:B:295:MET:SD	2:B:375:ALA:HB1	2.62	0.40
1:C:361:THR:HG22	1:C:362:VAL:N	2.37	0.40
2:D:422:GLU:HG2	2:D:426:ASN:ND2	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:7:GLU:O	3:E:22:VAL:HA	2.21	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	436/451 (97%)	428 (98%)	8 (2%)	0	100	100
1	C	439/451 (97%)	430 (98%)	9 (2%)	0	100	100
2	B	422/445 (95%)	415 (98%)	7 (2%)	0	100	100
2	D	423/445 (95%)	415 (98%)	7 (2%)	1 (0%)	47	55
3	E	119/143 (83%)	119 (100%)	0	0	100	100
4	F	344/384 (90%)	331 (96%)	13 (4%)	0	100	100
All	All	2183/2319 (94%)	2138 (98%)	44 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	304	ALA

### 5.3.2 Protein sidechains [i](#)

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	369/379 (97%)	363 (98%)	6 (2%)	62	73
1	C	372/379 (98%)	369 (99%)	3 (1%)	81	88
2	B	368/383 (96%)	367 (100%)	1 (0%)	92	95
2	D	368/383 (96%)	365 (99%)	3 (1%)	81	88
3	E	110/127 (87%)	110 (100%)	0	100	100
4	F	315/342 (92%)	315 (100%)	0	100	100
All	All	1902/1993 (95%)	1889 (99%)	13 (1%)	84	90

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	GLU
1	A	219	ILE
1	A	221	ARG
1	A	282	TYR
1	A	284	GLU
1	A	300	ASN
2	B	139	HIS
1	C	71	GLU
1	C	221	ARG
1	C	381	THR
2	D	139	HIS
2	D	229	HIS
2	D	247	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	88	HIS
1	A	300	ASN
1	A	301	GLN
2	B	15	GLN
2	B	294	GLN
1	C	11	GLN
1	C	133	GLN
1	C	300	ASN
2	D	294	GLN
2	D	300	ASN
2	D	334	ASN
4	F	229	ASN

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Mol	Chain	Res	Type
4	F	333	ASN
4	F	380	HIS

### 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 16 ligands modelled in this entry, 9 are monoatomic - leaving 7 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
10	X1J	C	504	-	14,14,14	0.27	0	17,20,20	0.80	1 (5%)
8	GDP	D	501	6	24,30,30	1.18	2 (8%)	31,47,47	1.91	7 (22%)
5	GTP	A	501	6	26,34,34	0.97	1 (3%)	33,54,54	1.72	7 (21%)
9	MES	B	504	-	12,12,12	2.23	1 (8%)	14,16,16	2.00	6 (42%)
5	GTP	C	501	6	26,34,34	0.97	1 (3%)	33,54,54	1.68	6 (18%)
8	GDP	B	501	6	24,30,30	1.14	2 (8%)	31,47,47	1.87	7 (22%)
11	ACP	F	401	6	27,33,33	1.42	5 (18%)	32,52,52	1.44	4 (12%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the



Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.  
'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	X1J	C	504	-	-	0/4/12/12	0/2/2/2
8	GDP	D	501	6	-	4/12/32/32	0/3/3/3
5	GTP	A	501	6	-	8/18/38/38	0/3/3/3
9	MES	B	504	-	-	4/6/14/14	0/1/1/1
5	GTP	C	501	6	-	7/18/38/38	0/3/3/3
8	GDP	B	501	6	-	3/12/32/32	0/3/3/3
11	ACP	F	401	6	-	9/15/38/38	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	504	MES	C8-S	-7.47	1.66	1.77
8	D	501	GDP	C6-C5	4.08	1.48	1.41
8	B	501	GDP	C6-C5	3.91	1.48	1.41
5	C	501	GTP	C6-N1	3.17	1.38	1.33
5	A	501	GTP	C6-N1	3.04	1.38	1.33
11	F	401	ACP	PG-O3G	2.99	1.61	1.54
11	F	401	ACP	PB-O3A	2.99	1.61	1.58
11	F	401	ACP	PG-O2G	2.98	1.61	1.54
11	F	401	ACP	C5-C4	2.52	1.47	1.40
8	D	501	GDP	C5-C4	2.44	1.47	1.40
8	B	501	GDP	C5-C4	2.28	1.47	1.40
11	F	401	ACP	PB-O2B	2.24	1.61	1.56

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	501	GTP	N3-C2-N1	-5.32	120.13	127.22
5	C	501	GTP	N3-C2-N1	-5.28	120.18	127.22
8	B	501	GDP	C2-N3-C4	4.85	120.89	115.36
8	D	501	GDP	C2-N3-C4	4.83	120.88	115.36
8	B	501	GDP	C6-C5-C4	-4.21	116.78	120.80
5	A	501	GTP	C2-N3-C4	4.18	120.13	115.36
8	D	501	GDP	C6-N1-C2	4.14	122.50	115.93
8	D	501	GDP	C6-C5-C4	-4.09	116.89	120.80
5	C	501	GTP	C2-N3-C4	4.09	120.03	115.36
8	B	501	GDP	C6-N1-C2	4.03	122.33	115.93
8	D	501	GDP	C5-C6-N1	-3.96	118.01	123.43
11	F	401	ACP	PA-O3A-PB	-3.90	120.18	132.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	501	GDP	C5-C6-N1	-3.75	118.30	123.43
9	B	504	MES	C5-N4-C3	3.72	117.21	108.83
8	B	501	GDP	N3-C2-N1	-3.53	122.51	127.22
8	D	501	GDP	N3-C2-N1	-3.45	122.62	127.22
11	F	401	ACP	C3'-C2'-C1'	3.42	106.13	100.98
9	B	504	MES	C6-C5-N4	-3.21	105.24	110.10
11	F	401	ACP	N3-C2-N1	-3.14	123.78	128.68
5	C	501	GTP	C5-C6-N1	-3.05	119.26	123.43
5	A	501	GTP	C5-C6-N1	-2.91	119.45	123.43
5	A	501	GTP	PA-O3A-PB	-2.91	122.85	132.83
5	A	501	GTP	PB-O3B-PG	-2.80	123.22	132.83
8	D	501	GDP	PA-O3A-PB	-2.71	123.53	132.83
8	D	501	GDP	C4-C5-N7	-2.70	106.58	109.40
5	C	501	GTP	PB-O3B-PG	-2.68	123.63	132.83
5	C	501	GTP	PA-O3A-PB	-2.61	123.86	132.83
5	A	501	GTP	C6-N1-C2	2.59	120.05	115.93
5	C	501	GTP	C6-N1-C2	2.59	120.04	115.93
9	B	504	MES	O1S-S-C8	2.58	110.02	106.92
11	F	401	ACP	C4-C5-N7	-2.56	106.73	109.40
8	B	501	GDP	PA-O3A-PB	-2.52	124.19	132.83
8	B	501	GDP	C4-C5-N7	-2.44	106.86	109.40
9	B	504	MES	C7-N4-C5	2.32	117.17	111.23
9	B	504	MES	O2S-S-C8	2.22	109.59	106.92
9	B	504	MES	O3S-S-C8	2.19	109.32	105.77
10	C	504	X1J	C3-C4-C5	-2.13	119.09	121.18
5	A	501	GTP	N2-C2-N1	2.02	120.39	117.25

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
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
8	B	501	GDP	C5'-O5'-PA-O1A
8	B	501	GDP	C5'-O5'-PA-O2A
8	D	501	GDP	PA-O3A-PB-O3B
8	D	501	GDP	C5'-O5'-PA-O1A
8	D	501	GDP	C5'-O5'-PA-O2A
9	B	504	MES	C8-C7-N4-C5
9	B	504	MES	C7-C8-S-O2S

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Mol	Chain	Res	Type	Atoms
9	B	504	MES	C7-C8-S-O3S
11	F	401	ACP	PB-C3B-PG-O1G
11	F	401	ACP	PG-C3B-PB-O1B
11	F	401	ACP	PG-C3B-PB-O2B
11	F	401	ACP	PG-C3B-PB-O3A
11	F	401	ACP	O4'-C4'-C5'-O5'
11	F	401	ACP	C3'-C4'-C5'-O5'
5	A	501	GTP	PB-O3B-PG-O1G
5	C	501	GTP	PB-O3B-PG-O3G
8	D	501	GDP	C5'-O5'-PA-O3A
9	B	504	MES	C7-C8-S-O1S
11	F	401	ACP	PB-C3B-PG-O2G
11	F	401	ACP	PB-C3B-PG-O3G
5	A	501	GTP	C4'-C5'-O5'-PA
5	C	501	GTP	PB-O3A-PA-O2A
11	F	401	ACP	PB-O3A-PA-O2A
5	C	501	GTP	C4'-C5'-O5'-PA
5	A	501	GTP	PB-O3B-PG-O2G
5	A	501	GTP	PB-O3B-PG-O3G
5	A	501	GTP	C5'-O5'-PA-O3A
5	C	501	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

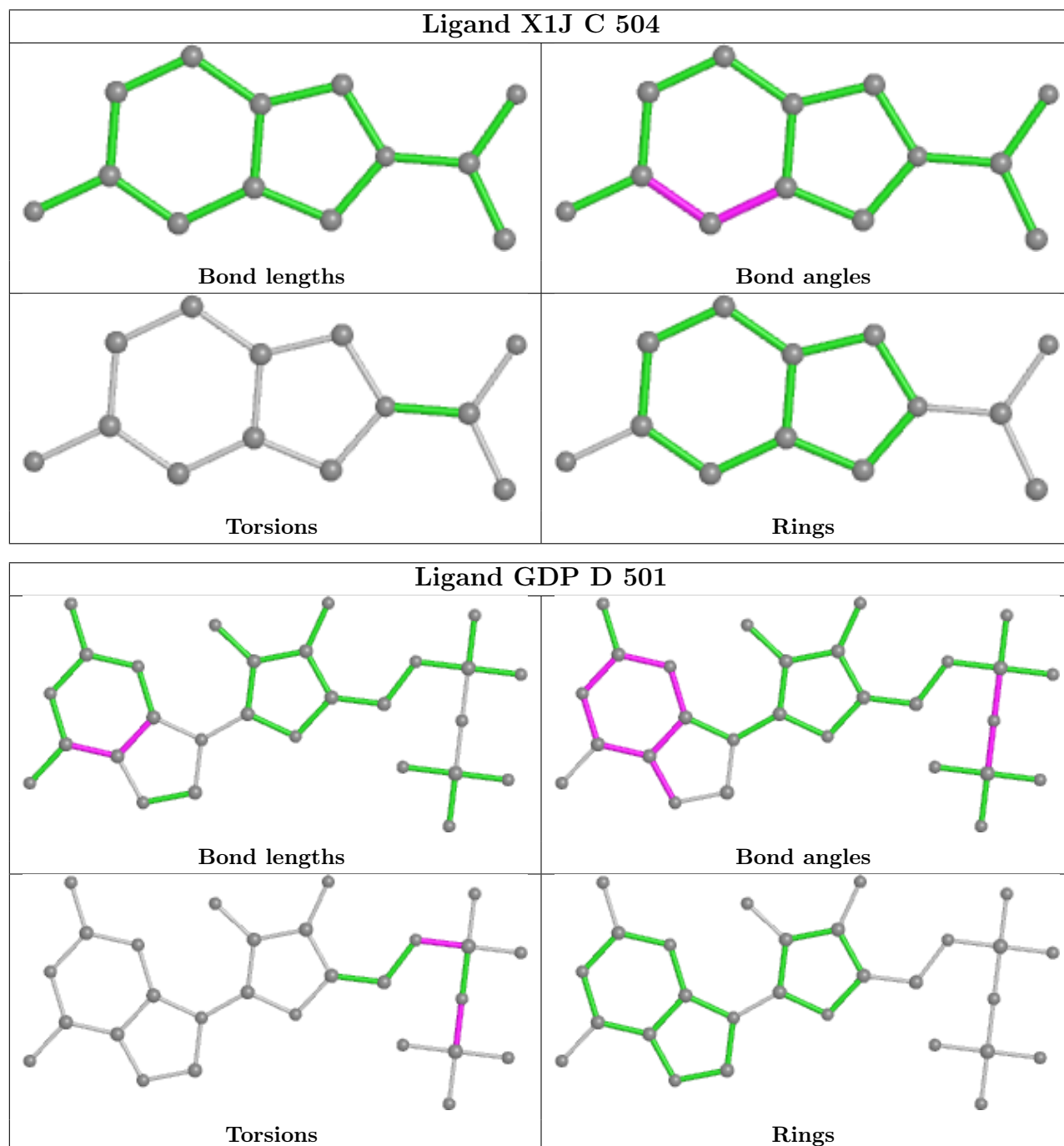
There are no ring outliers.

4 monomers are involved in 11 short contacts:

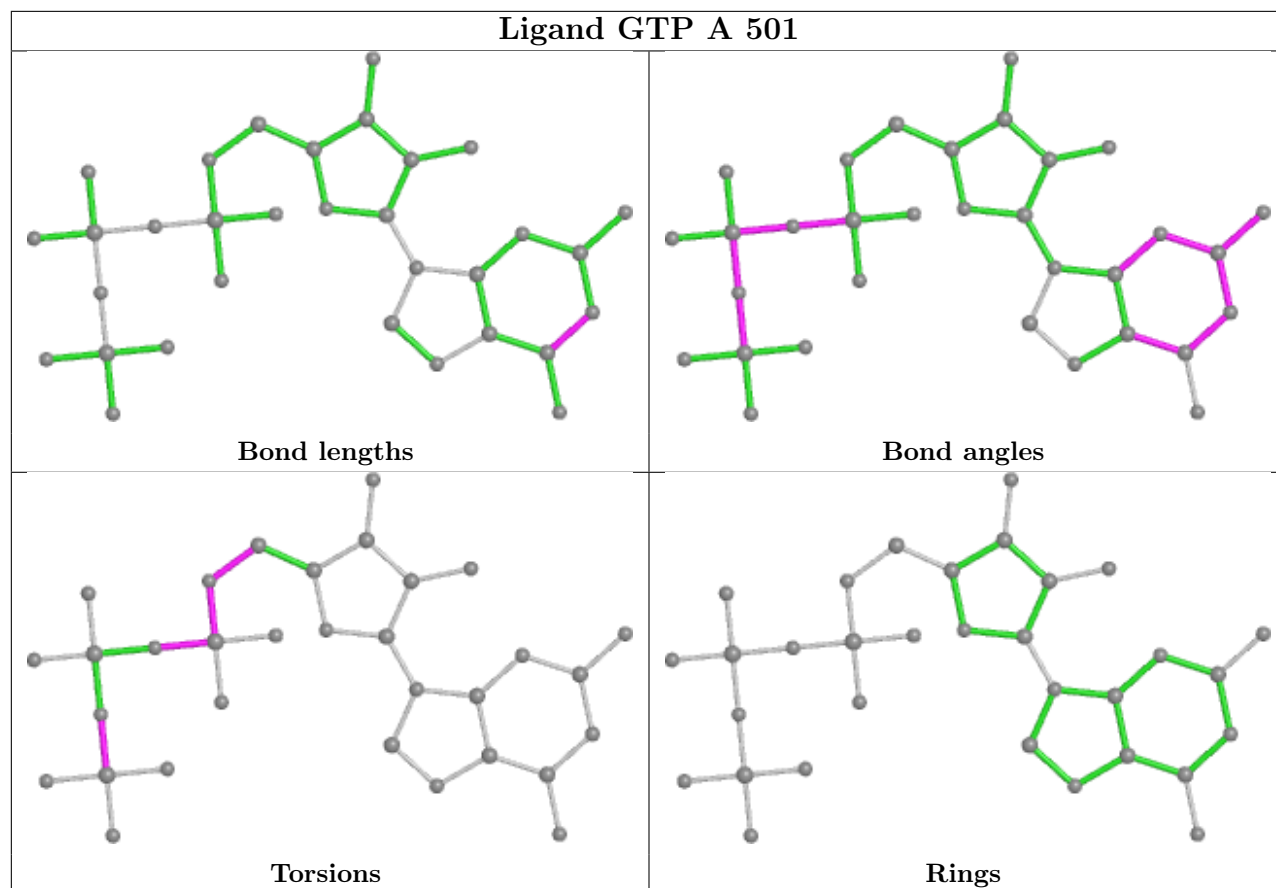
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	D	501	GDP	2	0
5	A	501	GTP	1	0
9	B	504	MES	3	0
11	F	401	ACP	5	0

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

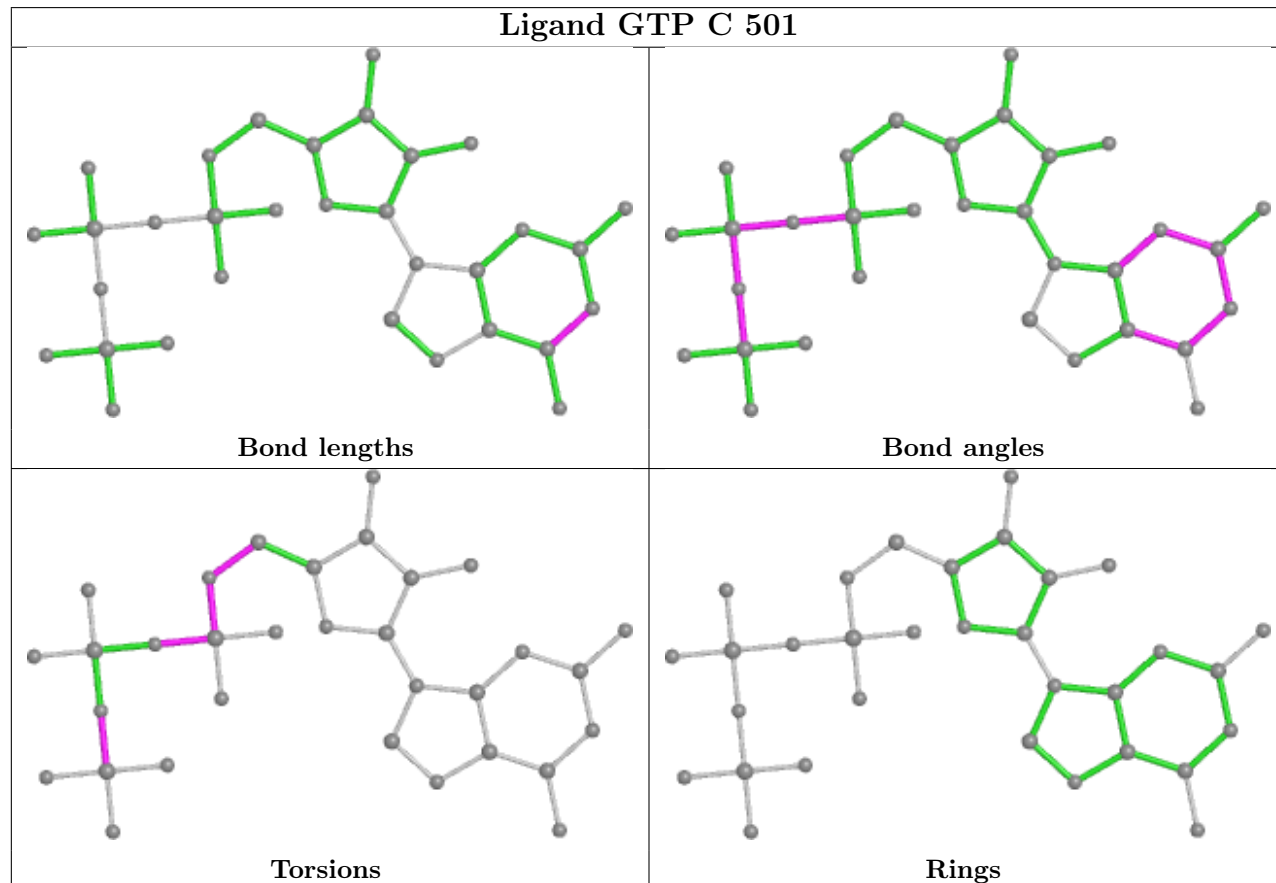
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

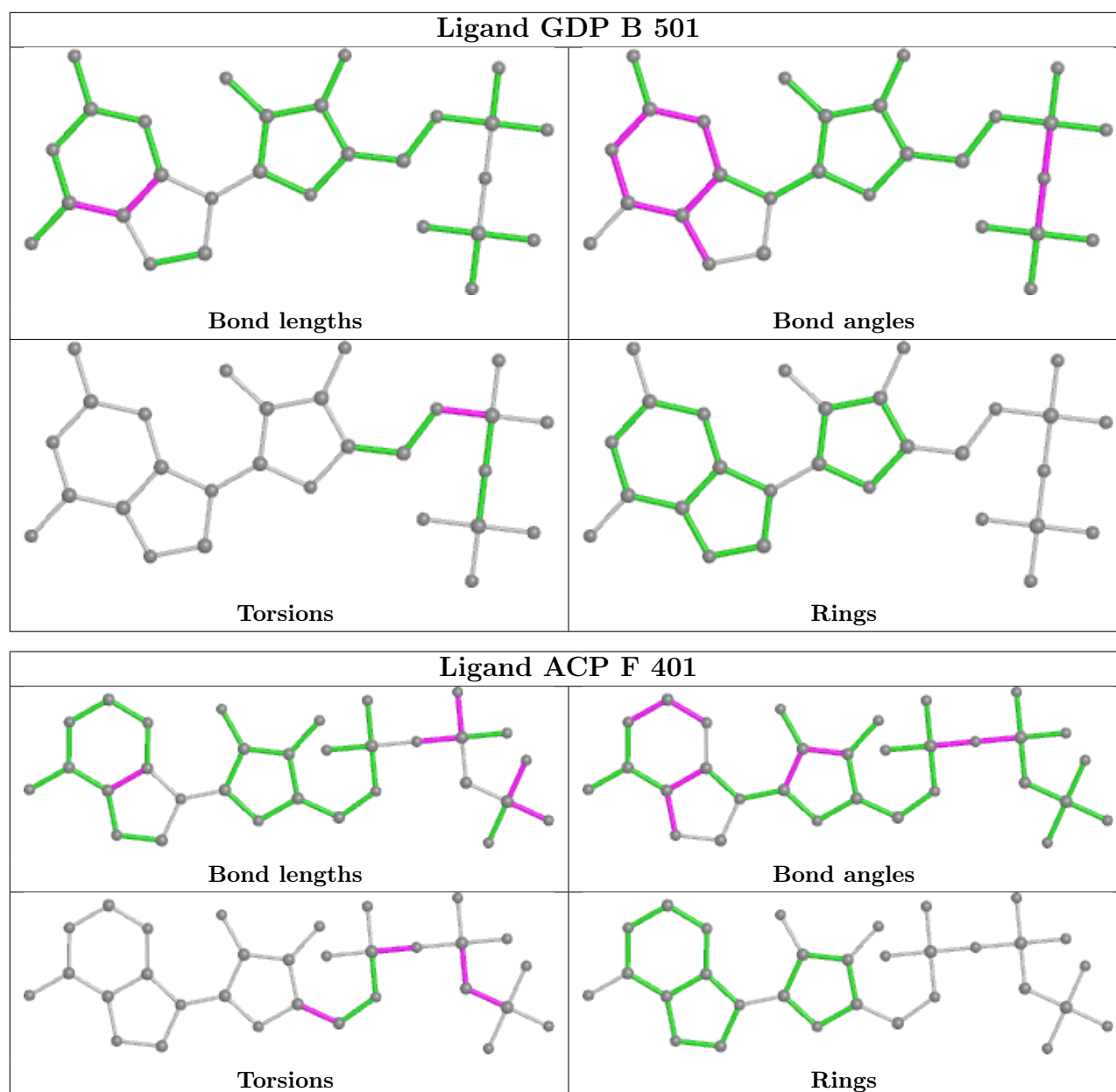


## Ligand GTP A 501



## Ligand GTP C 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	438/451 (97%)	0.22	10 (2%) 60 63	39, 57, 91, 156	0
1	C	440/451 (97%)	0.21	11 (2%) 57 60	34, 46, 68, 106	0
2	B	425/445 (95%)	0.33	12 (2%) 53 55	36, 58, 101, 143	2 (0%)
2	D	427/445 (95%)	0.21	15 (3%) 44 46	40, 62, 94, 138	4 (0%)
3	E	123/143 (86%)	0.60	8 (6%) 18 20	48, 66, 110, 138	0
4	F	352/384 (91%)	0.57	42 (11%) 4 3	49, 81, 146, 181	0
All	All	2205/2319 (95%)	0.31	98 (4%) 34 37	34, 59, 114, 181	6 (0%)

All (98) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	179	THR	8.2
3	E	26	PRO	7.8
2	D	281	GLN	6.9
4	F	173	ILE	6.7
3	E	27	PRO	6.3
4	F	143	GLU	5.5
2	B	281	GLN	5.4
4	F	105	LEU	5.4
2	D	280	SER	5.3
4	F	177	GLY	5.2
1	A	282	TYR	5.0
2	D	278	ARG	5.0
4	F	240	LEU	4.9
2	B	1	MET	4.8
4	F	90	SER	4.6
4	F	244	CYS	4.6
2	D	276	THR	4.6
4	F	176	GLN	4.5
3	E	28	SER	4.5

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Mol	Chain	Res	Type	RSRZ
4	F	249	TYR	4.4
4	F	103	THR	4.3
2	B	276	THR	4.3
1	A	438	ASP	4.1
4	F	89	GLU	4.0
2	D	82	PRO	4.0
4	F	243	HIS	3.9
4	F	137	ARG	3.7
1	A	262	TYR	3.6
4	F	251	LYS	3.5
1	A	281	ALA	3.5
3	E	25	LYS	3.5
2	D	215	ARG	3.5
4	F	153	ALA	3.5
1	A	340	SER	3.5
2	D	57	THR	3.4
2	D	277	SER	3.4
4	F	154	GLY	3.4
3	E	6	MET	3.3
4	F	253	TYR	3.3
4	F	142	ARG	3.2
4	F	155	ALA	3.1
4	F	381	HIS	3.1
2	B	57	THR	3.1
4	F	135	TYR	3.0
4	F	129	GLU	3.0
1	A	285	GLN	3.0
3	E	142	GLU	2.9
2	B	437	ASP	2.9
4	F	248	GLU	2.9
4	F	136	ASN	2.9
4	F	131	PHE	2.9
1	C	308	ARG	2.9
1	C	282	TYR	2.8
2	B	59	ASN	2.8
1	C	284	GLU	2.7
4	F	104	ASN	2.7
2	B	248	LEU	2.6
4	F	138	ARG	2.6
2	B	82	PRO	2.6
4	F	159	GLY	2.6
1	A	346	TRP	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	341	ILE	2.6
1	C	218	ASP	2.6
2	B	284	ARG	2.6
1	C	340	SER	2.5
3	E	24	LEU	2.5
4	F	140	GLU	2.5
1	A	345	ASP	2.5
4	F	130	VAL	2.5
4	F	132	LEU	2.5
2	D	37	HIS	2.5
2	D	400	ARG	2.4
1	A	88	HIS	2.4
4	F	372	THR	2.4
2	D	279	GLY	2.4
4	F	236	LYS	2.4
4	F	178	GLN	2.4
4	F	250	SER	2.4
2	D	441	ASP	2.3
4	F	99	VAL	2.3
1	C	283	HIS	2.3
1	C	339	ARG	2.3
4	F	242	ASN	2.3
1	C	350	GLY	2.3
4	F	179	VAL	2.3
2	B	325	MET	2.2
2	D	401	ARG	2.2
2	B	333	LEU	2.2
3	E	80	ARG	2.2
1	C	357	TYR	2.2
2	D	1	MET	2.2
1	C	440	VAL	2.1
4	F	233	PHE	2.1
2	B	277	SER	2.1
2	D	275	LEU	2.1
4	F	139	ARG	2.1
4	F	234	GLN	2.0
4	F	231	ALA	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 ⓘ

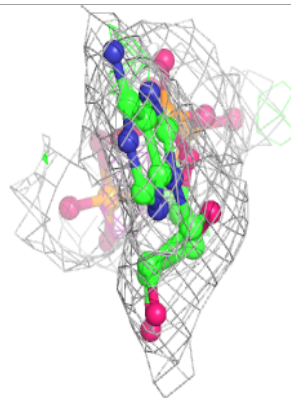
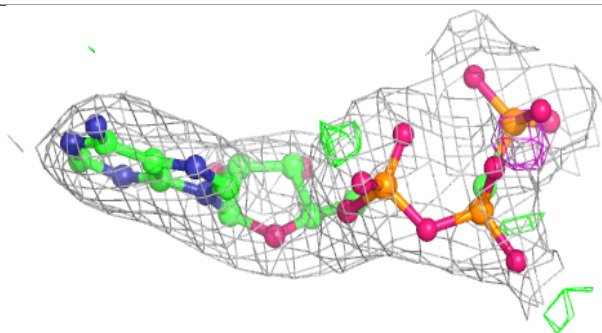
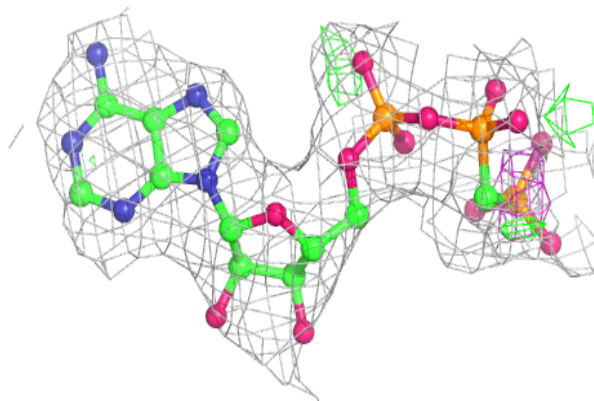
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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	CA	B	503	1/1	0.76	0.10	93,93,93,93	0
11	ACP	F	401	31/31	0.82	0.15	78,90,100,106	0
9	MES	B	504	12/12	0.86	0.20	86,92,102,109	0
7	CA	A	504	1/1	0.87	0.07	87,87,87,87	0
10	X1J	C	504	13/13	0.89	0.19	59,71,88,88	0
6	MG	D	502	1/1	0.89	0.13	55,55,55,55	0
7	CA	A	503	1/1	0.90	0.07	78,78,78,78	0
6	MG	F	402	1/1	0.93	0.10	79,79,79,79	0
8	GDP	D	501	28/28	0.95	0.14	53,59,66,67	0
6	MG	C	502	1/1	0.96	0.11	38,38,38,38	0
5	GTP	A	501	32/32	0.96	0.15	38,45,49,51	0
6	MG	A	502	1/1	0.97	0.10	40,40,40,40	0
6	MG	B	502	1/1	0.98	0.17	34,34,34,34	0
7	CA	C	503	1/1	0.98	0.09	52,52,52,52	0
5	GTP	C	501	32/32	0.98	0.16	34,37,40,41	0
8	GDP	B	501	28/28	0.99	0.15	36,42,47,51	0

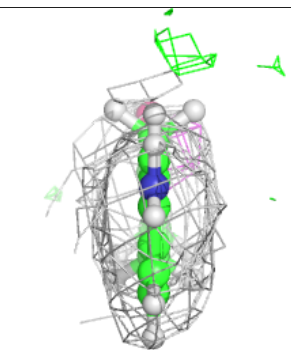
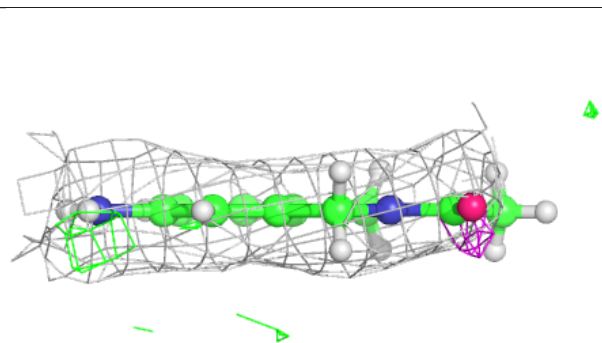
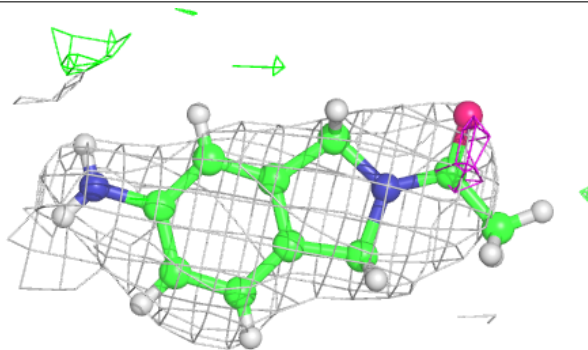
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

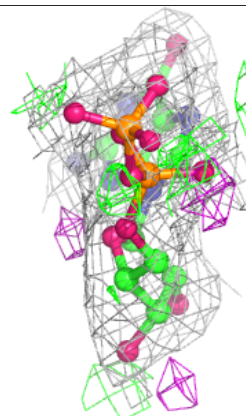
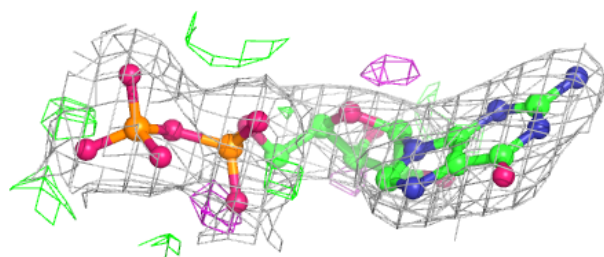
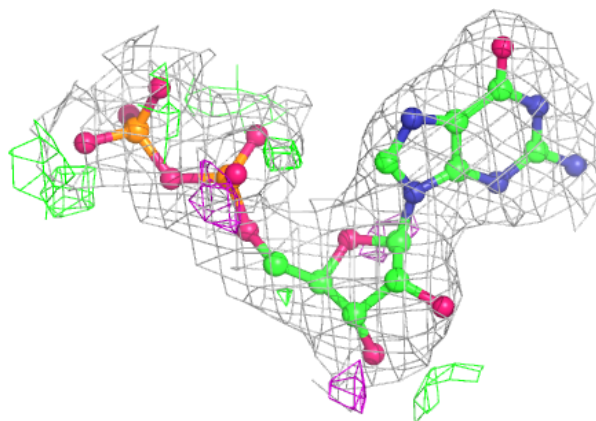
**Electron density around X1J C 504:**

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

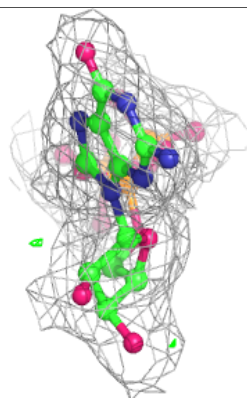
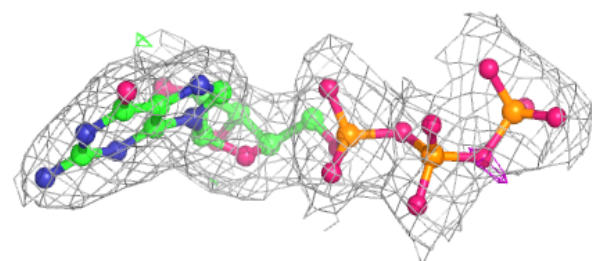
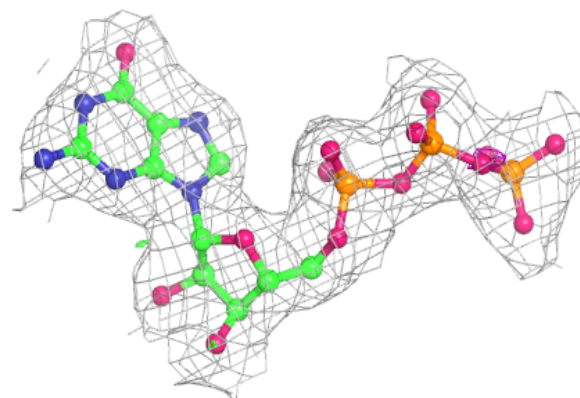


**Electron density around GDP D 501:**

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

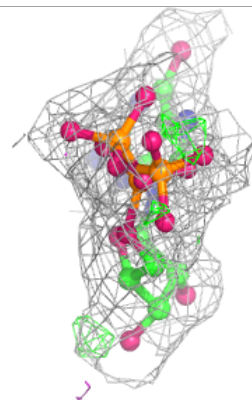
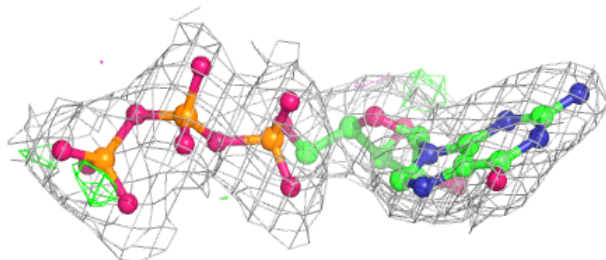
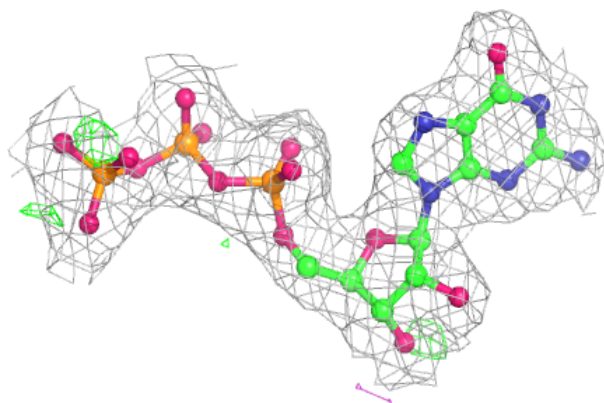
**Electron density around GTP A 501:**

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



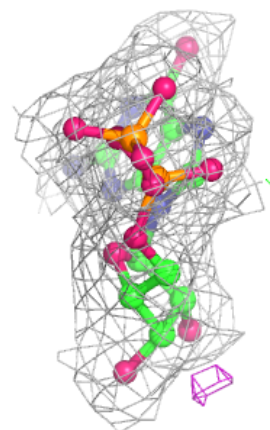
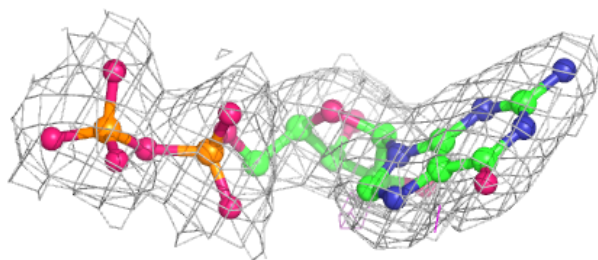
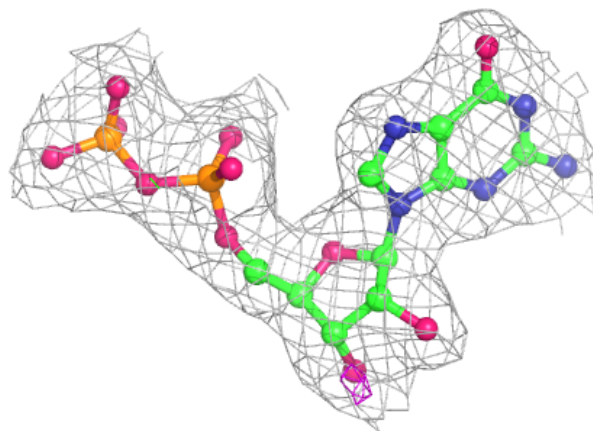
**Electron density around GTP C 501:**

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



**Electron density around 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.