



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2024 – 09:36 PM EST

PDB ID : 5S5F  
Title : Tubulin-Z87615031-complex  
Authors : Muehlethaler, T.; Gioia, D.; Prota, A.E.; Sharpe, M.E.; Cavalli, A.; Steinmetz, M.O.  
Deposited on : 2020-11-08  
Resolution : 2.24 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
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) : 2.36

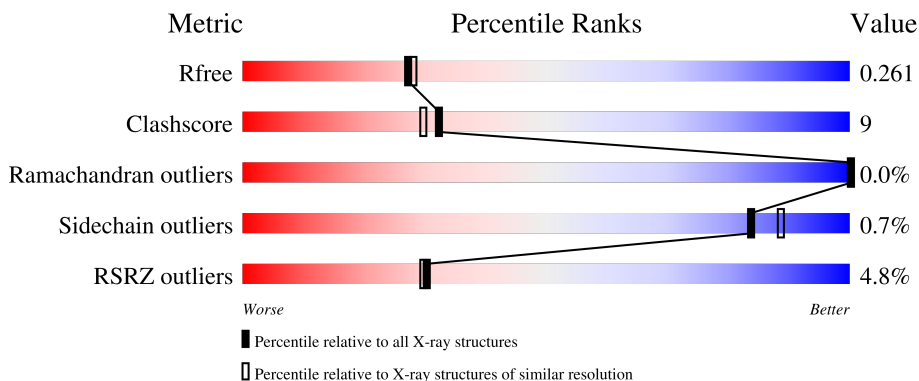
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.24 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.



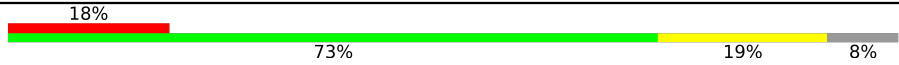
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	2391 (2.26-2.22)
Clashscore	141614	2539 (2.26-2.22)
Ramachandran outliers	138981	2489 (2.26-2.22)
Sidechain outliers	138945	2490 (2.26-2.22)
RSRZ outliers	127900	2353 (2.26-2.22)

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 style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 78%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 18%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: grey; margin-right: 5px;"></div> </div> <p style="margin-left: 20px;">2%      78%      18%      ..</p>
1	C	451	<div style="display: flex; align-items: center;"> <div style="width: 78%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 20%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: grey; margin-right: 5px;"></div> </div> <p style="margin-left: 20px;">78%      20%      .</p>
2	B	445	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 72%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 22%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: grey; margin-right: 5px;"></div> </div> <p style="margin-left: 20px;">2%      72%      22%      5%</p>
2	D	445	<div style="display: flex; align-items: center;"> <div style="width: 3%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 78%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 18%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey; margin-right: 5px;"></div> </div> <p style="margin-left: 20px;">3%      78%      18%      .</p>
3	E	143	<div style="display: flex; align-items: center;"> <div style="width: 5%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 70%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 16%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 9%; height: 10px; background-color: grey; margin-right: 5px;"></div> </div> <p style="margin-left: 20px;">5%      70%      16%      14%</p>

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Mol	Chain	Length	Quality of chain
4	F	384	 <p>A horizontal bar chart showing the quality of chain. The bar is divided into four segments: 18% red, 73% green, 19% yellow, and 8% grey. The percentages are labeled above each segment.</p>

## 2 Entry composition i

There are 12 unique types of molecules in this entry. The entry contains 18097 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
			Total	C	N	O	S			
1	A	437	Total	C	N	O	S	0	0	0
			3416	2163	581	650	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
			Total	C	N	O	S			
2	B	421	Total	C	N	O	S	1	1	0
			3326	2091	569	639	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
			Total	C	N	O	S			
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

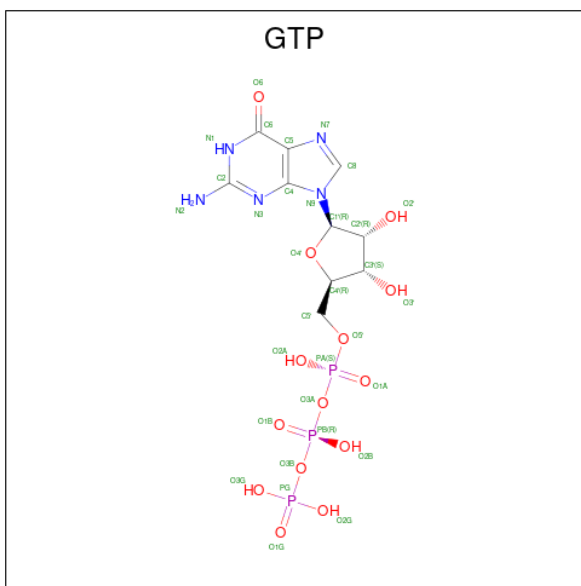
- Molecule 4 is a protein called Tubulin-Tyrosine Ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
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
			Total	C	N	O	P		
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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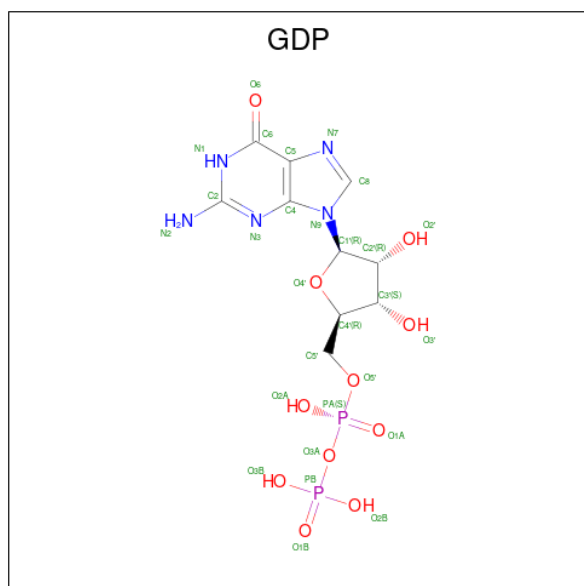
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	F	1	Total	Mg	0	0
			1	1		

- 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	1	Total	Ca	0	0
			1	1		
7	C	1	Total	Ca	0	0
			1	1		

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



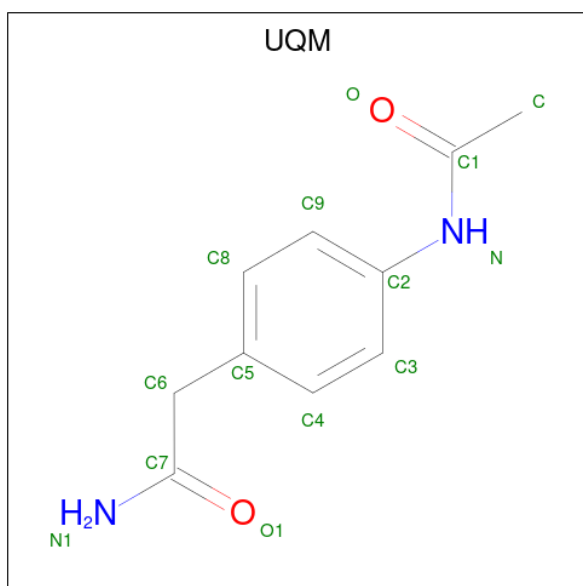
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
8	B	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
8	D	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

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



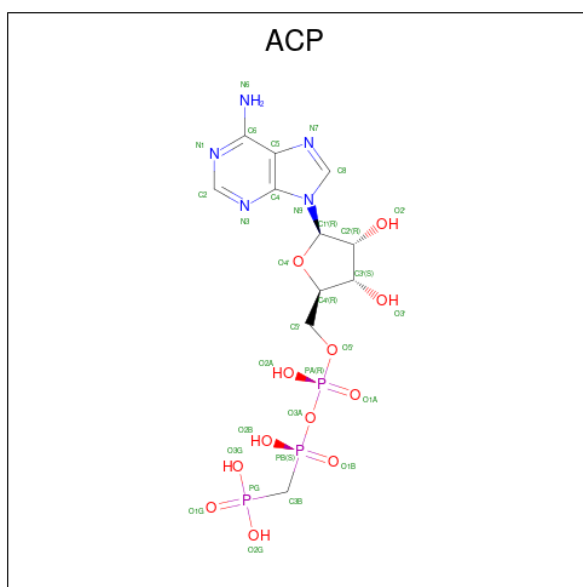
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
9	B	1	12	6	1	4	1	0	0

- Molecule 10 is N-[4-(2-amino-2-oxoethyl)phenyl]acetamide (three-letter code: UQM) (formula:  $C_{10}H_{12}N_2O_2$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	N	O		
10	C	1	26	10	12	2	2	0	0

- Molecule 11 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (three-letter code: ACP) (formula:  $C_{11}H_{18}N_5O_{12}P_3$ ).



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

- Molecule 12 is water.

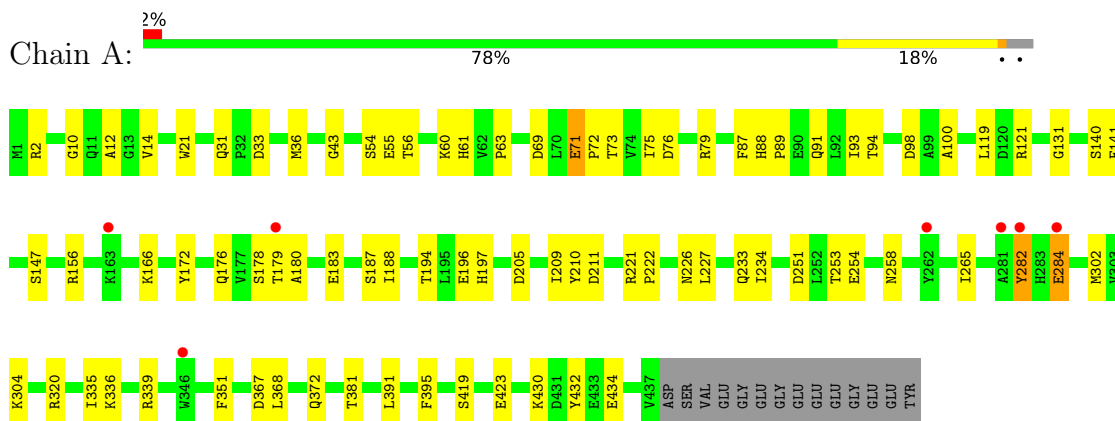
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	81	Total	O	0	0
			81	81		
12	B	105	Total	O	0	0
			105	105		
12	C	212	Total	O	0	0
			212	212		
12	D	45	Total	O	0	0
			45	45		
12	E	16	Total	O	0	0
			16	16		
12	F	16	Total	O	0	0
			16	16		



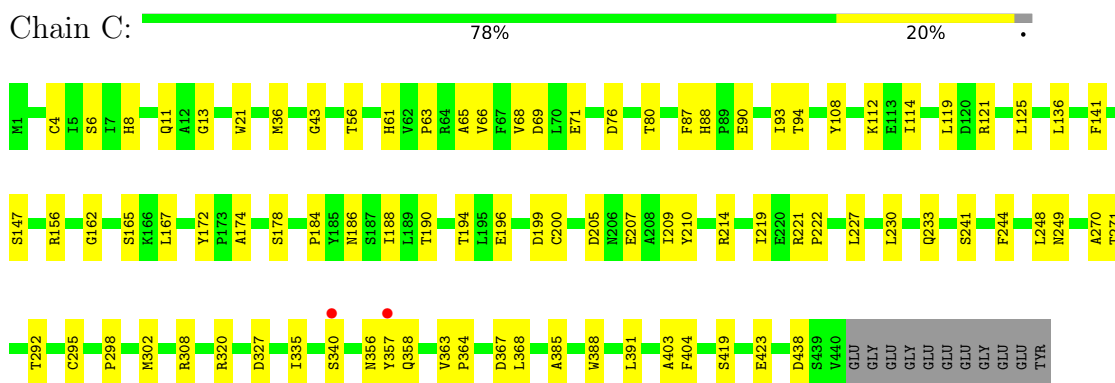
### 3 Residue-property plots [i](#)

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

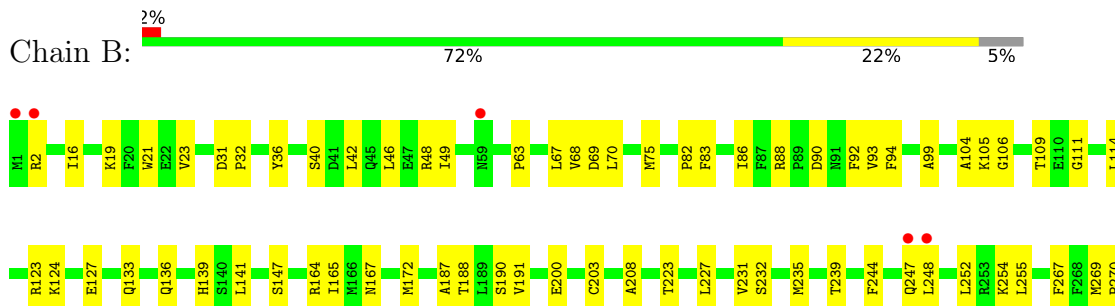
- Molecule 1: Tubulin alpha-1B chain

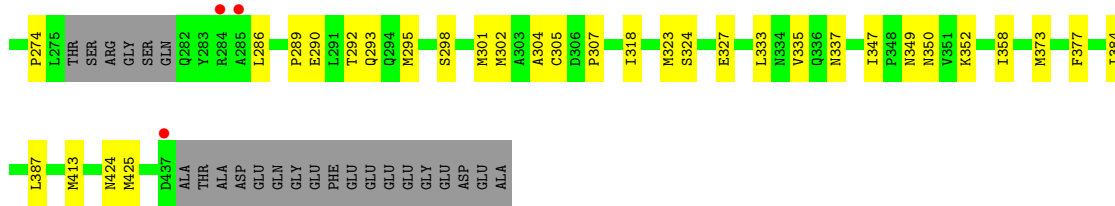


- Molecule 1: Tubulin alpha-1B chain

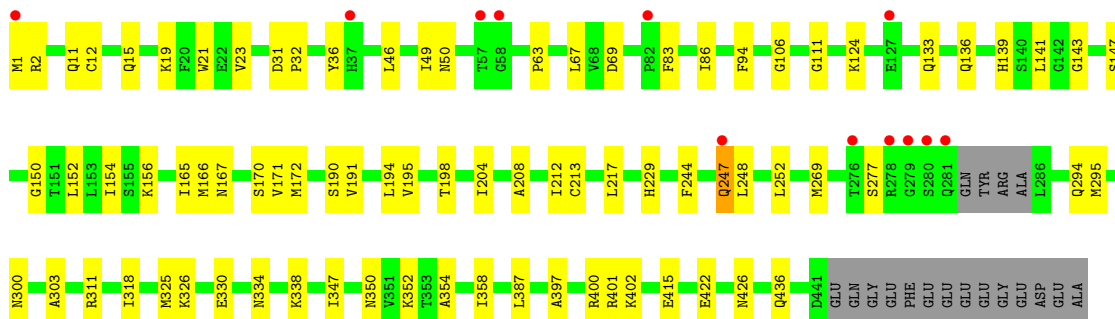
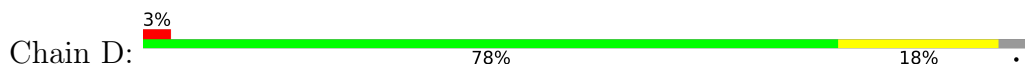


- Molecule 2: Tubulin beta-2B chain





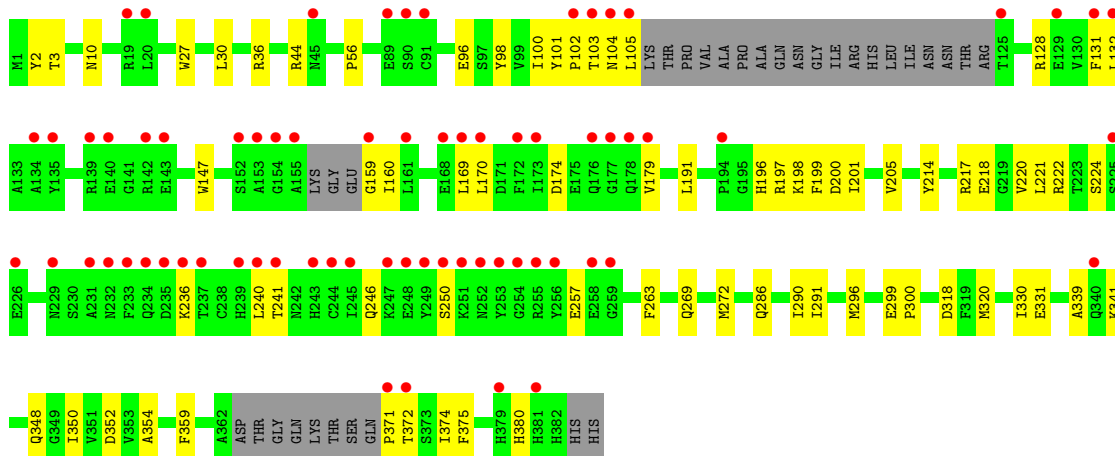
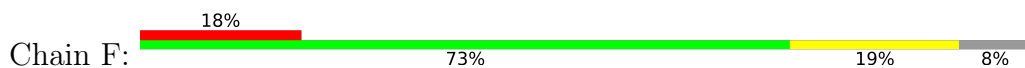
• Molecule 2: Tubulin beta-2B chain



• 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, $\alpha$ , $\beta$ , $\gamma$	104.83Å 158.37Å 179.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	72.43 – 2.24 72.43 – 2.24	Depositor EDS
% Data completeness (in resolution range)	97.1 (72.43-2.24) 97.1 (72.43-2.24)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	11.25 (at 2.25Å)	Xtrriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, $R_{free}$	0.236 , 0.262 0.235 , 0.261	Depositor DCC
$R_{free}$ test set	1952 reflections (1.40%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	24.3	Xtrriage
Anisotropy	0.215	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 36.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	18097	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	50.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.29% 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: MES, ACP, GTP, MG, GDP, UQM, CA

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	0/3494	0.42	0/4743
1	C	0.26	0/3521	0.43	0/4780
2	B	0.25	0/3400	0.42	0/4603
2	D	0.25	0/3421	0.42	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	0/17802	0.41	0/24093

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

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	3416	0	3330	60	0
1	C	3443	0	3352	58	0
2	B	3326	0	3202	70	0
2	D	3348	0	3224	56	0
3	E	1014	0	1029	15	0
4	F	2877	0	2839	56	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	1	0
10	C	14	12	0	2	0
11	F	31	0	14	5	0
12	A	81	0	0	2	0
12	B	105	0	0	3	0
12	C	212	0	0	4	0
12	D	45	0	0	1	0
12	E	16	0	0	2	0
12	F	16	0	0	0	0
All	All	18085	12	17050	306	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 (306) 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)
4:F:102:PRO:HG2	4:F:105:LEU:HD13	1.50	0.91
1:C:221:ARG:HG3	2:D:325:MET:HG2	1.51	0.91
1:C:327:ASP:OD2	12:C:601:HOH:O	1.94	0.85
1:C:209:ILE:HD11	1:C:302:MET:HE3	1.60	0.84
2:D:217:LEU:HA	2:D:277:SER:HB3	1.57	0.84
2:D:334:ASN:HD21	2:D:338:LYS:HE3	1.46	0.80
2:D:2:ARG:NH1	12:D:601:HOH:O	2.13	0.80
4:F:241:THR:OG1	11:F:401:ACP:O3'	2.00	0.79
1:A:335:ILE:HG23	1:A:339:ARG:HG3	1.66	0.77
2:D:397:ALA:O	2:D:401:ARG:NH1	2.20	0.75
4:F:10:ASN:HB2	4:F:44:ARG:HH22	1.53	0.74
1:C:367:ASP:OD1	12:C:602:HOH:O	2.07	0.73
2:B:83:PHE:O	2:B:86:ILE:HG22	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:76:ASP:O	1:C:80:THR:HG22	1.90	0.71
4:F:236:LYS:HB3	4:F:240:LEU:HD13	1.73	0.71
1:A:71:GLU:OE2	1:A:73:THR:OG1	2.07	0.70
4:F:331:GLU:OE2	11:F:401:ACP:O3G	2.08	0.70
2:D:1:MET:HG3	2:D:50:ASN:HB2	1.73	0.70
2:D:136:GLN:HA	2:D:167:ASN:O	1.90	0.69
2:B:274:PRO:HB3	2:B:286:LEU:HD22	1.76	0.68
1:A:179:THR:HA	2:B:352:LYS:HD2	1.77	0.67
4:F:102:PRO:HG2	4:F:105:LEU:CD1	2.24	0.67
1:A:209:ILE:HG22	1:A:227:LEU:HD22	1.77	0.66
3:E:44:ASP:OD2	12:E:201:HOH:O	2.11	0.66
4:F:147:TRP:HB2	4:F:169:LEU:HD11	1.78	0.66
1:C:438:ASP:OD1	12:C:603:HOH:O	2.14	0.66
2:B:136:GLN:HA	2:B:167:ASN:O	1.95	0.66
1:C:270:ALA:O	1:C:302:MET:HG2	1.96	0.65
4:F:371:PRO:HA	4:F:372:THR:O	1.97	0.65
2:D:397:ALA:HA	2:D:400:ARG:NH1	2.11	0.65
2:B:69:ASP:O	2:B:94:PHE:HA	1.98	0.64
2:D:334:ASN:ND2	2:D:338:LYS:HE3	2.12	0.64
2:B:88:ARG:HH11	2:B:90:ASP:HB2	1.63	0.64
2:B:147:SER:HG	2:B:190:SER:HG	1.45	0.63
1:C:298:PRO:HG2	1:C:308:ARG:NH2	2.13	0.63
2:D:172:MET:HG3	2:D:387:LEU:HD11	1.81	0.63
1:A:75:ILE:HD12	1:A:94:THR:HG22	1.82	0.62
2:B:147:SER:OG	2:B:190:SER:OG	2.18	0.62
1:A:336:LYS:HG3	3:E:24:LEU:HD13	1.81	0.61
1:C:93:ILE:HD11	1:C:121:ARG:HG3	1.81	0.61
4:F:132:LEU:HD21	4:F:170:LEU:HD11	1.82	0.61
1:A:254:GLU:HG2	1:A:258:ASN:ND2	2.16	0.61
2:B:88:ARG:NH1	2:B:90:ASP:HB2	2.16	0.60
2:D:347:ILE:HG22	2:D:350:ASN:HB3	1.83	0.60
1:C:209:ILE:HD11	1:C:302:MET:CE	2.29	0.60
1:A:100:ALA:HA	2:B:254:LYS:HG3	1.84	0.59
1:A:179:THR:HG21	2:B:248:LEU:CB	2.32	0.59
1:A:88:HIS:HB2	1:A:89:PRO:HD2	1.85	0.59
2:D:21:TRP:CZ3	2:D:63:PRO:HB3	2.37	0.59
1:C:162:GLY:HA2	3:E:94:ILE:HD11	1.84	0.59
1:C:4[A]:CYS:SG	1:C:136:LEU:HG	2.42	0.59
4:F:371:PRO:CA	4:F:372:THR:HB	2.33	0.59
2:B:2:ARG:HB2	2:B:133:GLN:CG	2.32	0.59
4:F:197:ARG:NH1	4:F:257:GLU:OE2	2.26	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:269:GLN:HA	4:F:272:MET:HE2	1.84	0.59
2:B:274:PRO:HB3	2:B:286:LEU:CD2	2.33	0.58
2:D:152:LEU:O	2:D:156:LYS:HG2	2.02	0.58
3:E:85:LYS:NZ	12:E:202:HOH:O	2.35	0.58
1:C:320:ARG:HA	1:C:356:ASN:O	2.04	0.58
2:D:83:PHE:O	2:D:86:ILE:HG22	2.04	0.58
2:B:295:MET:CG	2:B:377:PHE:HB2	2.34	0.57
2:B:21:TRP:CZ3	2:B:63:PRO:HB3	2.39	0.57
2:B:67:LEU:HD22	2:B:92:PHE:CE2	2.40	0.57
2:D:171:VAL:HA	2:D:204:ILE:O	2.05	0.57
2:B:23:VAL:HG21	2:B:232:SER:HB3	1.87	0.56
4:F:246:GLN:O	4:F:250:SER:HB3	2.06	0.56
4:F:371:PRO:HA	4:F:372:THR:C	2.23	0.56
4:F:159:GLY:C	4:F:160:ILE:HD12	2.26	0.56
2:B:244:PHE:CE1	2:B:358:ILE:HD12	2.42	0.55
2:B:36:TYR:CD1	2:B:46:LEU:HD21	2.41	0.55
1:A:21:TRP:CZ3	1:A:63:PRO:HB3	2.42	0.55
1:C:271:THR:HG21	1:C:295:CYS:O	2.06	0.55
2:B:2:ARG:HB2	2:B:133:GLN:HG3	1.88	0.55
4:F:350:ILE:O	4:F:354:ALA:HB3	2.07	0.55
2:B:106:GLY:O	2:B:111:GLY:HA3	2.07	0.55
3:E:85:LYS:O	3:E:89:GLU:HG3	2.06	0.55
1:A:187:SER:HB3	1:A:391:LEU:HD21	1.87	0.55
1:A:69:ASP:O	1:A:94:THR:HA	2.06	0.54
2:B:42:LEU:H	2:B:42:LEU:HD12	1.71	0.54
2:B:424:ASN:HB3	12:B:629:HOH:O	2.08	0.54
1:A:36:MET:HB3	1:A:61:HIS:CE1	2.42	0.54
2:B:208:ALA:HB2	2:B:304:ALA:HB2	1.89	0.54
4:F:318:ASP:OD2	11:F:401:ACP:O2G	2.26	0.54
2:D:69:ASP:O	2:D:94:PHE:HA	2.08	0.53
2:B:16:ILE:HD13	2:B:231:VAL:HG11	1.89	0.53
4:F:371:PRO:HA	4:F:372:THR:HB	1.89	0.53
2:B:46:LEU:HA	2:B:49:ILE:HB	1.91	0.53
2:B:141:LEU:HD12	2:B:172:MET:SD	2.49	0.53
2:D:269:MET:HG3	2:D:303:ALA:HB3	1.91	0.53
1:A:335:ILE:HG23	1:A:339:ARG:CG	2.38	0.53
2:D:21:TRP:CE3	2:D:63:PRO:HB3	2.43	0.53
2:B:165:ILE:HG21	2:B:252:LEU:HB3	1.91	0.53
4:F:147:TRP:HB2	4:F:169:LEU:CD1	2.38	0.52
1:A:178:SER:OG	1:A:183:GLU:OE1	2.19	0.52
2:D:19:LYS:O	2:D:23:VAL:HG23	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:348:GLN:NE2	4:F:352:ASP:OD1	2.41	0.52
2:B:124:LYS:HD3	2:B:124:LYS:C	2.30	0.52
2:B:298:SER:HA	2:B:301:MET:HG3	1.91	0.52
2:D:1:MET:HG3	2:D:50:ASN:CB	2.39	0.52
1:A:187:SER:CB	1:A:391:LEU:HD21	2.41	0.51
2:B:75:MET:HE3	2:B:92:PHE:CD2	2.45	0.51
2:B:200:GLU:OE2	2:B:255:LEU:HG	2.11	0.51
2:B:289:PRO:O	2:B:293:GLN:HG3	2.10	0.51
4:F:128:ARG:NH2	4:F:174:ASP:OD1	2.44	0.51
2:B:172:MET:HG3	2:B:387:LEU:HD11	1.93	0.51
2:D:11:GLN:O	2:D:15:GLN:HG2	2.11	0.51
2:B:123:ARG:O	2:B:127:GLU:HG3	2.11	0.51
4:F:320:MET:HG3	4:F:330:ILE:HD11	1.93	0.51
1:C:66:VAL:HG23	1:C:125:LEU:CD1	2.42	0.50
1:A:166:LYS:HE2	1:A:197:HIS:O	2.11	0.50
2:B:75:MET:HE3	2:B:92:PHE:HD2	1.77	0.50
2:D:147:SER:HB2	2:D:190:SER:OG	2.11	0.50
2:D:106:GLY:O	2:D:111:GLY:HA3	2.12	0.50
2:D:165:ILE:HG21	2:D:252:LEU:HB3	1.93	0.50
1:C:249:ASN:OD1	1:C:356:ASN:ND2	2.39	0.50
2:B:247:GLN:N	2:B:247:GLN:OE1	2.45	0.50
1:C:419:SER:O	1:C:423:GLU:HG3	2.11	0.50
2:D:402:LYS:HE2	2:D:415:GLU:OE1	2.11	0.50
2:B:223:THR:O	2:B:227:LEU:HD13	2.12	0.50
2:B:295:MET:HG2	2:B:377:PHE:HB2	1.94	0.50
4:F:296:MET:SD	4:F:380:HIS:HB2	2.51	0.50
4:F:200:ASP:OD1	4:F:222:ARG:HB2	2.12	0.50
2:D:191:VAL:O	2:D:195:VAL:HG23	2.12	0.49
4:F:269:GLN:HA	4:F:272:MET:CE	2.43	0.49
3:E:72:LEU:O	3:E:76:ARG:HG2	2.12	0.49
1:A:98:ASP:HB2	5:A:501:GTP:O2G	2.13	0.49
4:F:197:ARG:HB2	4:F:224:SER:O	2.12	0.49
1:C:174:ALA:O	1:C:178:SER:HB3	2.13	0.49
1:A:226:ASN:ND2	1:A:367:ASP:OD2	2.45	0.49
2:B:349:ASN:O	2:B:352:LYS:HE2	2.13	0.49
1:C:172:TYR:HB3	1:C:205:ASP:HA	1.95	0.49
4:F:198:LYS:HG2	4:F:199:PHE:H	1.78	0.49
2:B:82:PRO:O	12:B:601:HOH:O	2.20	0.48
1:A:2:ARG:HB3	1:A:131:GLY:O	2.13	0.48
1:A:31:GLN:HB2	1:A:33:ASP:OD1	2.13	0.48
1:C:233:GLN:HG3	1:C:368:LEU:CD1	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:ILE:HD11	1:A:121:ARG:HG3	1.96	0.48
2:D:36:TYR:CD1	2:D:46:LEU:HD21	2.49	0.48
4:F:3:THR:HB	4:F:30:LEU:HD11	1.95	0.48
2:D:31:ASP:HB2	2:D:32:PRO:CD	2.43	0.48
4:F:220:VAL:HG11	4:F:339:ALA:HB2	1.95	0.48
2:B:164:ARG:HD2	12:B:649:HOH:O	2.14	0.48
2:B:286:LEU:HD12	2:B:290:GLU:OE1	2.14	0.48
2:D:124:LYS:C	2:D:124:LYS:HD3	2.34	0.48
9:B:504:MES:H51	9:B:504:MES:H81	1.54	0.47
3:E:120:LEU:O	3:E:124:GLN:HG3	2.15	0.47
1:C:21:TRP:CZ3	1:C:63:PRO:HB3	2.48	0.47
1:A:188:ILE:HD12	1:A:395:PHE:HB2	1.96	0.47
2:D:2:ARG:HB3	2:D:133:GLN:CG	2.45	0.47
4:F:10:ASN:CB	4:F:44:ARG:HH22	2.23	0.47
2:D:12:CYS:HB2	8:D:501:GDP:C8	2.49	0.47
2:D:46:LEU:HA	2:D:49:ILE:HB	1.97	0.47
2:D:318:ILE:N	2:D:318:ILE:HD12	2.30	0.47
4:F:198:LYS:HZ1	11:F:401:ACP:C2	2.28	0.47
1:A:172:TYR:HB3	1:A:205:ASP:HA	1.97	0.47
2:B:270:PRO:HG2	2:B:302:MET:HB2	1.96	0.47
1:A:71:GLU:HG2	1:A:72:PRO:N	2.29	0.47
1:A:211:ASP:OD2	1:A:304:LYS:NZ	2.34	0.47
1:A:265:ILE:HG23	1:A:432:TYR:CE1	2.50	0.47
1:A:55:GLU:HA	1:A:60:LYS:O	2.15	0.47
2:B:31:ASP:HB2	2:B:32:PRO:CD	2.45	0.46
2:D:294:GLN:HG2	2:D:300:ASN:ND2	2.29	0.46
1:A:284:GLU:CD	1:A:284:GLU:H	2.17	0.46
1:A:43:GLY:HA2	1:A:56:THR:O	2.16	0.46
1:A:419:SER:O	1:A:423:GLU:HG3	2.16	0.46
2:D:208:ALA:O	2:D:212:ILE:HG13	2.15	0.46
1:A:12:ALA:CB	1:A:140:SER:HB3	2.46	0.46
1:A:75:ILE:HB	1:A:94:THR:HG21	1.97	0.46
1:A:351:PHE:HE1	3:E:24:LEU:HD11	1.81	0.46
1:C:214:ARG:HG2	1:C:219:ILE:O	2.16	0.46
1:C:244:PHE:CD1	1:C:358:GLN:HG2	2.51	0.46
2:D:2:ARG:HB3	2:D:133:GLN:HG2	1.98	0.45
1:C:209:ILE:HG22	1:C:227:LEU:HD22	1.98	0.45
1:A:75:ILE:HB	1:A:94:THR:CG2	2.47	0.45
2:B:40:SER:OG	2:B:42:LEU:HD13	2.16	0.45
2:B:19:LYS:HB3	2:B:232:SER:OG	2.17	0.45
1:C:241:SER:HA	1:C:249:ASN:OD1	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:341:LYS:HG2	4:F:341:LYS:O	2.16	0.45
1:A:194:THR:O	1:A:194:THR:HG22	2.16	0.45
3:E:60:ARG:O	3:E:64:GLN:HG3	2.16	0.45
3:E:101:LEU:O	3:E:105:MET:HG2	2.16	0.45
2:D:31:ASP:HB2	2:D:32:PRO:HD2	1.99	0.45
1:C:363:VAL:HG13	1:C:364:PRO:HD2	1.98	0.45
2:D:248:LEU:HD23	2:D:354:ALA:HB2	1.98	0.45
2:B:187:ALA:O	2:B:191:VAL:HG23	2.17	0.45
1:C:174:ALA:CB	1:C:207:GLU:HB2	2.47	0.45
3:E:92:ASN:O	3:E:96:MET:HG2	2.17	0.45
1:A:10:GLY:O	1:A:14:VAL:HG23	2.17	0.45
2:B:67:LEU:N	2:B:67:LEU:HD12	2.32	0.45
2:D:387:LEU:HD23	2:D:387:LEU:C	2.37	0.45
4:F:191:LEU:HD12	4:F:196:HIS:CE1	2.52	0.45
1:C:165:SER:HA	1:C:199:ASP:OD2	2.16	0.44
4:F:201:ILE:HG12	4:F:221:LEU:HG	1.99	0.44
4:F:217:ARG:HG3	4:F:218:GLU:HG2	1.99	0.44
1:A:251:ASP:OD1	1:A:253:THR:HB	2.17	0.44
2:B:337:ASN:OD1	4:F:36:ARG:HD3	2.18	0.44
2:B:70:LEU:HD12	2:B:99:ALA:HB2	2.00	0.44
2:B:235:MET:O	2:B:239:THR:HG23	2.16	0.44
1:A:233:GLN:HG3	1:A:368:LEU:CD1	2.47	0.44
2:B:203:CYS:SG	2:B:267:PHE:HB3	2.57	0.44
1:C:196:GLU:HG2	12:C:640:HOH:O	2.17	0.44
1:C:248:LEU:HD12	1:C:357:TYR:OH	2.18	0.44
2:D:248:LEU:HD11	2:D:352:LYS:HB3	1.99	0.44
1:A:71:GLU:HG2	1:A:72:PRO:HD2	1.99	0.44
4:F:205:VAL:HG21	4:F:291:ILE:HD13	2.00	0.44
1:A:119:LEU:HD11	1:A:156:ARG:HB3	1.99	0.44
1:C:8:HIS:HB3	1:C:13:GLY:O	2.18	0.44
2:D:141:LEU:HD21	2:D:170:SER:HB3	1.99	0.44
3:E:45:PRO:HA	3:E:49:GLU:OE1	2.18	0.44
1:A:54:SER:O	1:A:61:HIS:HA	2.17	0.44
1:C:11:GLN:HE22	2:D:247:GLN:CD	2.21	0.44
2:D:213:CYS:HA	2:D:217:LEU:HB2	1.99	0.44
2:B:21:TRP:CE3	2:B:63:PRO:HB3	2.53	0.43
4:F:100:ILE:CD1	4:F:128:ARG:HA	2.48	0.43
4:F:131:PHE:CD2	4:F:132:LEU:HD23	2.53	0.43
2:B:68:VAL:HA	2:B:93:VAL:O	2.18	0.43
2:B:269:MET:HG2	2:B:384:ILE:HD13	1.99	0.43
1:C:43:GLY:HA2	1:C:56:THR:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:67:LEU:N	2:D:67:LEU:HD12	2.32	0.43
2:D:311:ARG:NH1	2:D:436:GLN:O	2.51	0.43
4:F:96:GLU:OE2	4:F:98:TYR:OH	2.32	0.43
2:B:333:LEU:O	2:B:337:ASN:ND2	2.50	0.43
2:D:295:MET:HB2	2:D:295:MET:HE3	1.69	0.43
4:F:286:GLN:O	4:F:290:ILE:HG13	2.18	0.43
1:A:320:ARG:HG3	12:A:668:HOH:O	2.18	0.43
1:A:430:LYS:HE2	1:A:434:GLU:OE2	2.19	0.43
2:B:347:ILE:HG22	2:B:350:ASN:HB3	1.99	0.43
1:C:210:TYR:CZ	1:C:222:PRO:HD2	2.54	0.43
2:D:154:ILE:HG23	2:D:166:MET:HG2	2.01	0.43
4:F:2:TYR:CE1	4:F:359:PHE:HB3	2.54	0.43
4:F:371:PRO:N	4:F:372:THR:HB	2.33	0.43
1:A:21:TRP:CE3	1:A:63:PRO:HB3	2.54	0.43
1:A:196:GLU:OE1	1:A:196:GLU:HA	2.17	0.43
2:B:292:THR:HG22	2:B:335:VAL:HG21	2.01	0.43
1:C:108:TYR:O	1:C:112:LYS:HG2	2.19	0.43
4:F:299:GLU:HB3	4:F:300:PRO:HD3	1.99	0.43
4:F:320:MET:CG	4:F:330:ILE:HD11	2.49	0.43
2:B:42:LEU:HD12	2:B:42:LEU:N	2.33	0.43
2:B:305:CYS:O	2:B:307:PRO:HD3	2.19	0.43
1:C:93:ILE:HG22	1:C:114:ILE:HD11	2.01	0.43
2:D:2:ARG:HB2	2:D:133:GLN:HE21	1.83	0.43
3:E:75:LYS:NZ	3:E:79:GLU:OE2	2.38	0.43
1:A:12:ALA:HB3	1:A:140:SER:HB3	2.01	0.42
1:C:209:ILE:HG23	1:C:230:LEU:HD23	2.00	0.42
3:E:11:LEU:HD11	3:E:18:GLN:OE1	2.19	0.42
4:F:103:THR:HG23	4:F:128:ARG:NH2	2.33	0.42
2:D:143:GLY:HA3	8:D:501:GDP:O3A	2.20	0.42
2:B:318:ILE:N	2:B:318:ILE:HD12	2.34	0.42
1:A:372:GLN:OE1	1:A:372:GLN:HA	2.19	0.42
2:B:188:THR:HG23	2:B:425:MET:HE2	2.01	0.42
1:A:176:GLN:HG3	4:F:56:PRO:HB3	2.01	0.42
1:C:66:VAL:HG23	1:C:125:LEU:HD12	2.01	0.42
2:D:194:LEU:HD22	2:D:198:THR:HG21	2.01	0.42
2:D:422:GLU:HG2	2:D:426:ASN:ND2	2.35	0.42
1:A:320:ARG:HD2	12:A:660:HOH:O	2.20	0.42
2:B:105:LYS:HA	2:B:109:THR:OG1	2.19	0.42
1:C:119:LEU:HD11	1:C:156:ARG:HB3	2.01	0.42
1:C:194:THR:O	1:C:194:THR:HG22	2.20	0.42
4:F:102:PRO:HB2	4:F:104:ASN:OD1	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:209:ILE:HD11	1:A:302:MET:SD	2.60	0.42
4:F:2:TYR:HB2	4:F:27:TRP:CD2	2.55	0.42
1:C:11:GLN:HE22	2:D:247:GLN:NE2	2.18	0.41
1:C:385:ALA:HA	1:C:388:TRP:CD1	2.54	0.41
4:F:199:PHE:HA	4:F:241:THR:HG21	2.02	0.41
1:A:71:GLU:HG2	1:A:72:PRO:CD	2.50	0.41
4:F:320:MET:HE3	4:F:320:MET:HB3	1.96	0.41
1:A:76:ASP:OD1	1:A:79:ARG:NH1	2.53	0.41
1:A:234:ILE:HD12	1:A:234:ILE:N	2.35	0.41
1:C:186:ASN:O	1:C:190:THR:HG22	2.21	0.41
1:C:391:LEU:HD12	1:C:391:LEU:HA	1.94	0.41
2:B:235:MET:HE2	2:B:235:MET:HB3	1.90	0.41
1:C:69:ASP:O	1:C:94:THR:HA	2.20	0.41
1:C:88:HIS:HE1	1:C:90:GLU:HG3	1.86	0.41
1:C:292:THR:HG22	1:C:335:ILE:CD1	2.50	0.41
4:F:217:ARG:NH2	4:F:374:ILE:HA	2.36	0.41
1:A:75:ILE:HD12	1:A:94:THR:CG2	2.49	0.41
1:A:141:PHE:O	1:A:147:SER:HB3	2.20	0.41
1:C:93:ILE:CD1	1:C:121:ARG:HG3	2.48	0.41
4:F:220:VAL:HG12	4:F:263:PHE:CE1	2.56	0.41
2:B:324:SER:HB3	2:B:327:GLU:HB3	2.03	0.41
2:D:150:GLY:O	2:D:154:ILE:HG13	2.20	0.41
2:D:244:PHE:CE1	2:D:358:ILE:HD12	2.56	0.41
1:A:210:TYR:CE1	1:A:222:PRO:HD2	2.56	0.41
2:B:104:ALA:HB2	2:B:413:MET:SD	2.60	0.41
1:C:36:MET:HB3	1:C:61:HIS:CE1	2.55	0.41
1:C:66:VAL:HG12	1:C:68:VAL:HG23	2.03	0.41
1:A:180:ALA:HB3	1:A:183:GLU:HG3	2.02	0.41
4:F:101:TYR:CD2	4:F:179:VAL:HG22	2.56	0.41
4:F:371:PRO:HA	4:F:372:THR:CB	2.50	0.41
1:C:6:SER:O	1:C:65:ALA:HA	2.20	0.40
1:C:165:SER:HB3	10:C:504:UQM:C7	2.51	0.40
3:E:7:GLU:O	3:E:22:VAL:HA	2.20	0.40
1:A:88:HIS:CD2	1:A:91:GLN:HG3	2.56	0.40
2:D:141:LEU:HD12	2:D:172:MET:SD	2.61	0.40
1:C:167:LEU:HG	1:C:200:CYS:HB3	2.02	0.40
1:C:403:ALA:O	1:C:404:PHE:HB2	2.22	0.40
11:F:401:ACP:O3G	11:F:401:ACP:O1B	2.40	0.40
2:B:31:ASP:HB2	2:B:32:PRO:HD2	2.02	0.40
2:B:323:MET:HB3	2:B:373:MET:CE	2.52	0.40
1:C:63:PRO:HG2	1:C:87:PHE:CE1	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:165:SER:HB3	10:C:504:UQM:N1	2.37	0.40
2:D:326:LYS:O	2:D:330:GLU:HG3	2.22	0.40
2:B:114:LEU:HG	2:B:114:LEU:O	2.21	0.40
1:C:141:PHE:O	1:C:147:SER:HB3	2.21	0.40
1:C:184:PRO:O	1:C:188:ILE:HD13	2.21	0.40
4:F:214:TYR:HB3	4:F:375:PHE:HB3	2.02	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	435/451 (96%)	426 (98%)	8 (2%)	1 (0%)	47	53
1	C	439/451 (97%)	427 (97%)	12 (3%)	0	100	100
2	B	418/445 (94%)	409 (98%)	9 (2%)	0	100	100
2	D	423/445 (95%)	414 (98%)	9 (2%)	0	100	100
3	E	119/143 (83%)	118 (99%)	1 (1%)	0	100	100
4	F	344/384 (90%)	332 (96%)	12 (4%)	0	100	100
All	All	2178/2319 (94%)	2126 (98%)	51 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	282	TYR

### 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	368/379 (97%)	362 (98%)	6 (2%)	62	70
1	C	372/379 (98%)	370 (100%)	2 (0%)	88	92
2	B	364/383 (95%)	362 (100%)	2 (0%)	88	92
2	D	368/383 (96%)	365 (99%)	3 (1%)	81	87
3	E	110/127 (87%)	110 (100%)	0	100	100
4	F	315/342 (92%)	315 (100%)	0	100	100
All	All	1897/1993 (95%)	1884 (99%)	13 (1%)	84	88

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

Mol	Chain	Res	Type
1	A	71	GLU
1	A	87	PHE
1	A	221	ARG
1	A	282	TYR
1	A	284	GLU
1	A	381	THR
2	B	48	ARG
2	B	139	HIS
1	C	71	GLU
1	C	340	SER
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 (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	88	HIS
1	A	301	GLN
2	B	15	GLN
2	B	282	GLN
2	B	294	GLN
1	C	11	GLN
2	D	294	GLN
2	D	300	ASN

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Mol	Chain	Res	Type
4	F	196	HIS
4	F	229	ASN
4	F	269	GLN
4	F	333	ASN
4	F	380	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

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
8	GDP	D	501	6	24,30,30	0.94	1 (4%)	30,47,47	1.12	3 (10%)
10	UQM	C	504	-	14,14,14	1.22	1 (7%)	18,18,18	0.68	0
9	MES	B	504	-	12,12,12	2.26	1 (8%)	14,16,16	2.01	6 (42%)
5	GTP	A	501	6	26,34,34	1.16	2 (7%)	32,54,54	1.42	6 (18%)
8	GDP	B	501	6	24,30,30	0.93	1 (4%)	30,47,47	1.14	4 (13%)
11	ACP	F	401	6	27,33,33	1.42	5 (18%)	32,52,52	1.47	4 (12%)
5	GTP	C	501	6	26,34,34	1.09	2 (7%)	32,54,54	1.33	5 (15%)

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

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

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	504	MES	C8-S	-7.53	1.66	1.77
5	A	501	GTP	C5-C6	-4.14	1.39	1.47
5	C	501	GTP	C5-C6	-3.76	1.39	1.47
10	C	504	UQM	C1-N	3.48	1.42	1.36
11	F	401	ACP	PB-O3A	3.04	1.61	1.58
11	F	401	ACP	PG-O3G	2.97	1.61	1.54
11	F	401	ACP	PG-O2G	2.95	1.61	1.54
11	F	401	ACP	C5-C4	2.57	1.47	1.40
11	F	401	ACP	PB-O2B	2.28	1.61	1.56
8	D	501	GDP	C6-N1	-2.19	1.34	1.37
8	B	501	GDP	C6-N1	-2.18	1.34	1.37
5	C	501	GTP	C2-N3	2.14	1.38	1.33
5	A	501	GTP	C2-N3	2.05	1.38	1.33

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	F	401	ACP	PB-O3A-PA	-3.84	120.37	132.56
9	B	504	MES	C5-N4-C3	3.71	117.18	108.83
11	F	401	ACP	C3'-C2'-C1'	3.43	106.14	100.98
9	B	504	MES	C6-C5-N4	-3.30	105.09	110.10
5	A	501	GTP	C5-C6-N1	3.25	119.69	113.95
11	F	401	ACP	N3-C2-N1	-3.19	123.69	128.68
5	C	501	GTP	C8-N7-C5	3.17	109.03	102.99
5	C	501	GTP	C5-C6-N1	2.97	119.20	113.95
5	A	501	GTP	C8-N7-C5	2.96	108.63	102.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	501	GTP	C2-N1-C6	-2.81	119.93	125.10
8	B	501	GDP	PA-O3A-PB	-2.78	123.29	132.83
5	A	501	GTP	PA-O3A-PB	-2.72	123.51	132.83
5	C	501	GTP	C2-N1-C6	-2.71	120.11	125.10
8	D	501	GDP	PA-O3A-PB	-2.67	123.66	132.83
11	F	401	ACP	C4-C5-N7	-2.63	106.66	109.40
5	C	501	GTP	PA-O3A-PB	-2.62	123.83	132.83
9	B	504	MES	O2S-S-C8	2.47	109.89	106.92
5	A	501	GTP	O6-C6-C5	-2.44	119.61	124.37
8	B	501	GDP	C5-C6-N1	2.43	118.24	113.95
5	C	501	GTP	PB-O3B-PG	-2.40	124.60	132.83
8	D	501	GDP	C8-N7-C5	2.33	107.43	102.99
8	D	501	GDP	C5-C6-N1	2.33	118.07	113.95
8	B	501	GDP	C8-N7-C5	2.31	107.40	102.99
5	A	501	GTP	PB-O3B-PG	-2.26	125.06	132.83
9	B	504	MES	C7-N4-C5	2.21	116.88	111.23
9	B	504	MES	O1S-S-C8	2.17	109.52	106.92
9	B	504	MES	O3S-S-C8	2.15	109.25	105.77
8	B	501	GDP	O6-C6-C5	-2.04	120.39	124.37

There are no chirality outliers.

All (39) 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	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
9	B	504	MES	C7-C8-S-O3S
11	F	401	ACP	PB-C3B-PG-O1G
11	F	401	ACP	PB-C3B-PG-O2G
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	C5'-O5'-PA-O1A
11	F	401	ACP	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
11	F	401	ACP	C3'-C4'-C5'-O5'
5	C	501	GTP	PB-O3B-PG-O1G
11	F	401	ACP	C5'-O5'-PA-O3A
11	F	401	ACP	C5'-O5'-PA-O2A
9	B	504	MES	C7-C8-S-O1S
11	F	401	ACP	PB-C3B-PG-O3G
5	C	501	GTP	PB-O3A-PA-O2A
5	A	501	GTP	PB-O3B-PG-O1G
5	A	501	GTP	PB-O3B-PG-O2G
5	A	501	GTP	PB-O3B-PG-O3G
5	C	501	GTP	PB-O3B-PG-O2G
5	C	501	GTP	PB-O3B-PG-O3G
11	F	401	ACP	PB-O3A-PA-O2A
5	A	501	GTP	C5'-O5'-PA-O3A
5	C	501	GTP	C5'-O5'-PA-O3A
8	B	501	GDP	C5'-O5'-PA-O3A
8	D	501	GDP	C5'-O5'-PA-O3A
5	A	501	GTP	C4'-C5'-O5'-PA
5	A	501	GTP	PB-O3A-PA-O2A
5	C	501	GTP	PB-O3A-PA-O1A
8	B	501	GDP	PB-O3A-PA-O2A

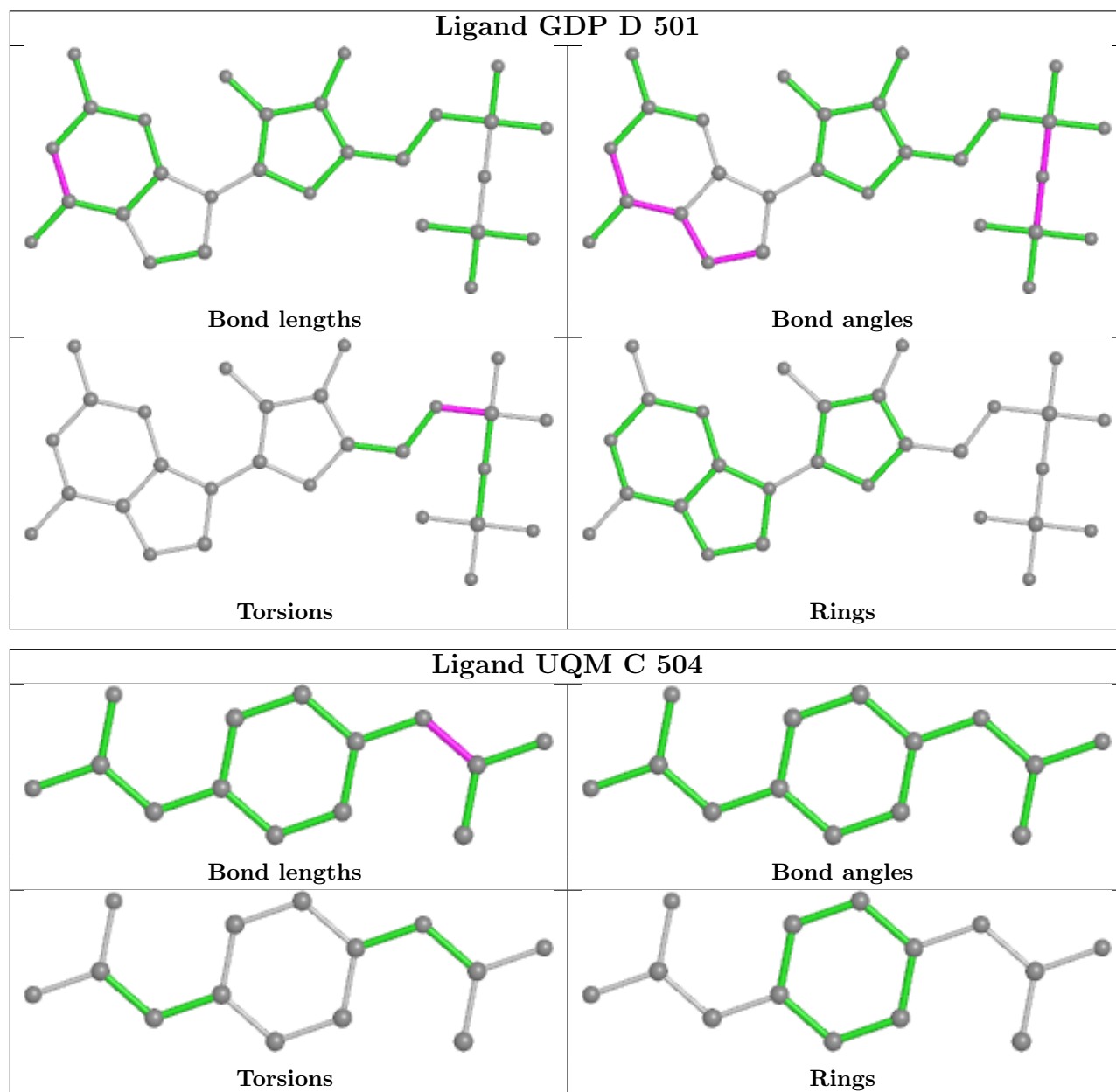
There are no ring outliers.

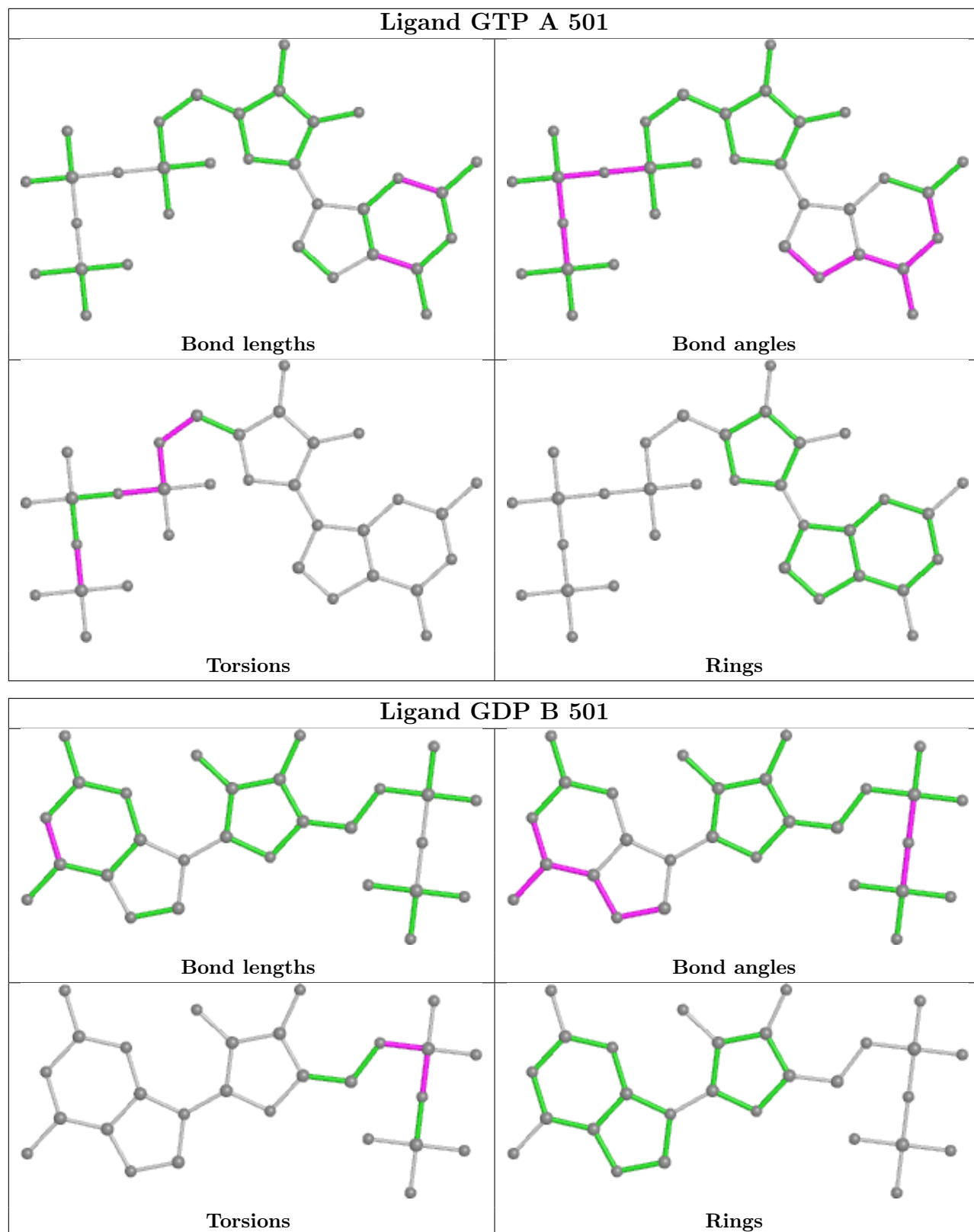
5 monomers are involved in 11 short contacts:

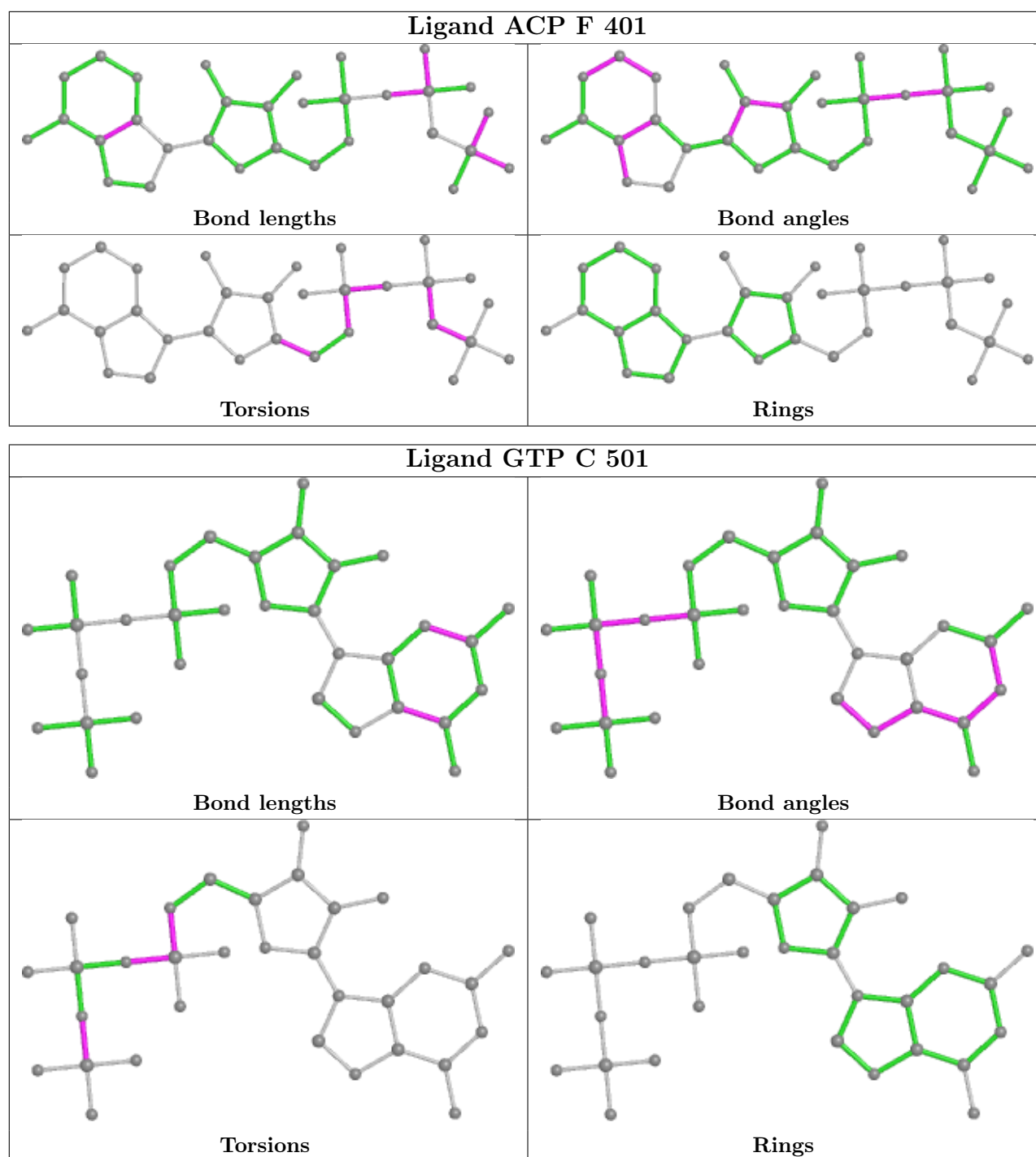
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	D	501	GDP	2	0
10	C	504	UQM	2	0
9	B	504	MES	1	0
5	A	501	GTP	1	0
11	F	401	ACP	5	0

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.







## 5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	437/451 (96%)	-0.10	7 (1%) 72 73	26, 45, 83, 135	0
1	C	440/451 (97%)	-0.18	2 (0%) 91 91	20, 33, 54, 96	0
2	B	421/445 (94%)	0.05	8 (1%) 66 68	19, 42, 78, 119	2 (0%)
2	D	427/445 (95%)	-0.07	12 (2%) 53 53	25, 47, 76, 115	4 (0%)
3	E	123/143 (86%)	0.29	7 (5%) 23 23	31, 51, 96, 136	0
4	F	352/384 (91%)	0.84	69 (19%) 1 1	38, 67, 129, 160	0
All	All	2200/2319 (94%)	0.09	105 (4%) 30 30	19, 45, 95, 160	6 (0%)

All (105) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	249	TYR	8.4
4	F	251	LYS	7.0
4	F	105	LEU	6.2
4	F	231	ALA	6.2
4	F	90	SER	6.0
3	E	26	PRO	5.9
4	F	253	TYR	5.9
4	F	372	THR	5.7
4	F	103	THR	5.7
4	F	173	ILE	5.6
2	B	1	MET	5.4
3	E	27	PRO	5.1
4	F	234	GLN	5.1
4	F	240	LEU	5.1
4	F	252	ASN	5.0
4	F	104	ASN	5.0
2	B	284	ARG	4.9
1	A	179	THR	4.9
4	F	155	ALA	4.8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
4	F	250	SER	4.8
2	D	57	THR	4.7
4	F	243	HIS	4.6
4	F	248	GLU	4.5
4	F	371	PRO	4.5
1	A	282	TYR	4.5
4	F	232	ASN	4.4
4	F	233	PHE	4.3
4	F	244	CYS	4.2
2	B	59	ASN	4.2
1	A	262	TYR	4.2
4	F	89	GLU	4.2
2	D	278	ARG	4.1
4	F	259	GLY	4.1
4	F	177	GLY	4.0
3	E	142	GLU	3.8
1	A	281	ALA	3.8
4	F	179	VAL	3.7
4	F	247	LYS	3.7
4	F	245	ILE	3.7
2	D	281	GLN	3.7
4	F	154	GLY	3.6
1	A	284	GLU	3.5
4	F	236	LYS	3.5
4	F	153	ALA	3.4
1	A	346	TRP	3.4
4	F	176	GLN	3.4
4	F	256	TYR	3.4
4	F	125	THR	3.4
4	F	254	GLY	3.3
2	D	279	GLY	3.2
4	F	258	GLU	3.1
3	E	28	SER	3.1
4	F	168	GLU	3.1
4	F	255	ARG	3.1
2	D	276	THR	3.0
3	E	6	MET	3.0
4	F	142	ARG	3.0
4	F	169	LEU	3.0
4	F	102	PRO	2.9
2	D	127	GLU	2.8
2	D	280	SER	2.8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
4	F	135	TYR	2.8
4	F	225	SER	2.8
4	F	178	GLN	2.7
4	F	140	GLU	2.7
4	F	172	PHE	2.7
2	B	437	ASP	2.7
2	D	1	MET	2.6
1	A	163	LYS	2.6
4	F	45	ASN	2.6
4	F	131	PHE	2.6
2	B	248	LEU	2.5
4	F	381	HIS	2.5
4	F	235	ASP	2.5
1	C	340	SER	2.4
4	F	19	ARG	2.4
4	F	143	GLU	2.4
2	D	37	HIS	2.3
4	F	226	GLU	2.3
4	F	340	GLN	2.3
2	B	285	ALA	2.3
4	F	134	ALA	2.3
4	F	229	ASN	2.3
4	F	194	PRO	2.3
4	F	241	THR	2.2
2	D	82	PRO	2.2
3	E	139	LEU	2.2
4	F	239	HIS	2.2
3	E	48	GLU	2.2
2	B	247	GLN	2.2
4	F	379	HIS	2.2
4	F	20	LEU	2.2
4	F	161	LEU	2.2
2	D	58	GLY	2.2
2	D	247	GLN	2.1
1	C	357	TYR	2.1
4	F	129	GLU	2.1
4	F	132	LEU	2.1
4	F	152	SER	2.1
2	B	2	ARG	2.1
4	F	170	LEU	2.0
4	F	159	GLY	2.0
4	F	237	THR	2.0

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Mol	Chain	Res	Type	RSRZ
4	F	91	CYS	2.0
4	F	139	ARG	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](#)

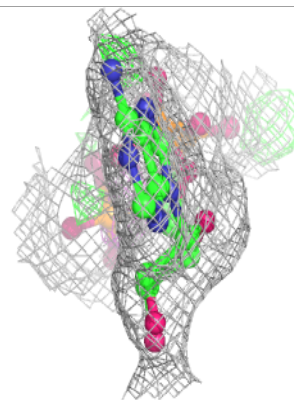
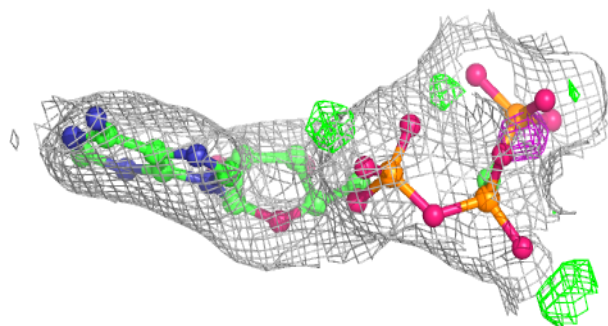
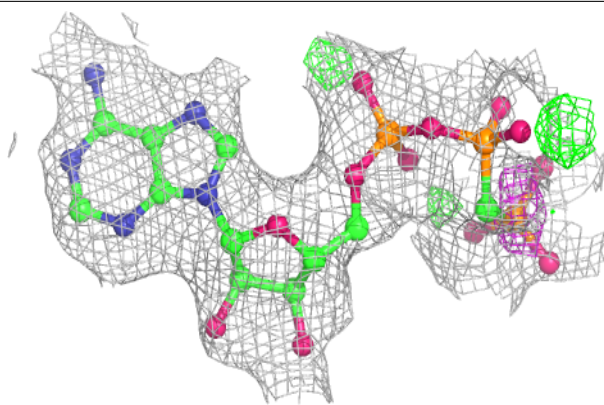
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<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
9	MES	B	504	12/12	0.74	0.20	83,85,94,100	0
11	ACP	F	401	31/31	0.82	0.14	67,75,88,94	0
10	UQM	C	504	14/14	0.88	0.18	24,34,46,54	26
7	CA	B	503	1/1	0.91	0.13	78,78,78,78	0
7	CA	A	504	1/1	0.91	0.14	77,77,77,77	0
6	MG	D	502	1/1	0.92	0.06	47,47,47,47	0
7	CA	A	503	1/1	0.93	0.07	77,77,77,77	0
6	MG	F	402	1/1	0.94	0.08	70,70,70,70	0
8	GDP	D	501	28/28	0.95	0.12	40,44,54,55	0
6	MG	A	502	1/1	0.97	0.09	28,28,28,28	0
5	GTP	A	501	32/32	0.98	0.13	26,30,34,36	0
6	MG	B	502	1/1	0.98	0.16	19,19,19,19	0
6	MG	C	502	1/1	0.98	0.11	23,23,23,23	0
5	GTP	C	501	32/32	0.98	0.14	21,24,27,28	0
7	CA	C	503	1/1	0.99	0.05	48,48,48,48	0
8	GDP	B	501	28/28	0.99	0.12	21,27,30,31	0

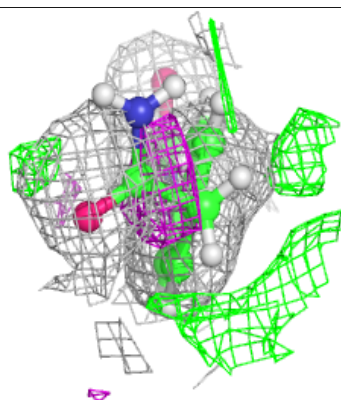
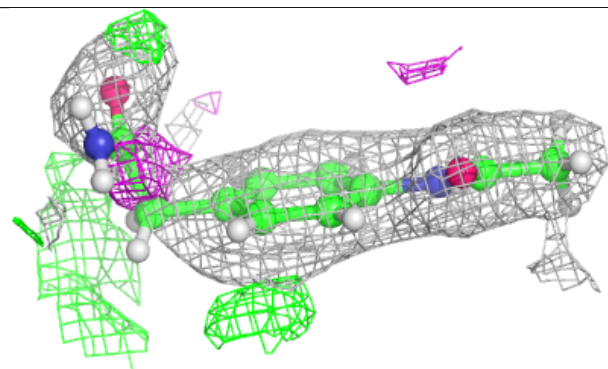
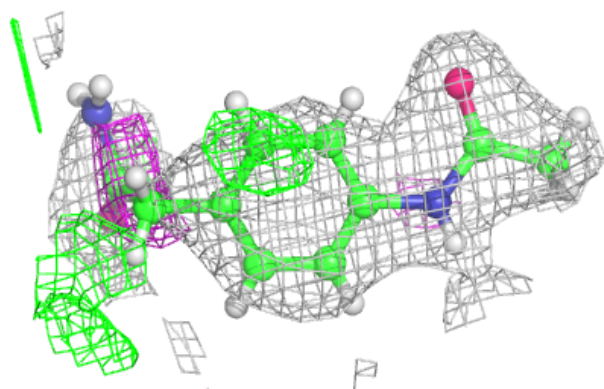
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

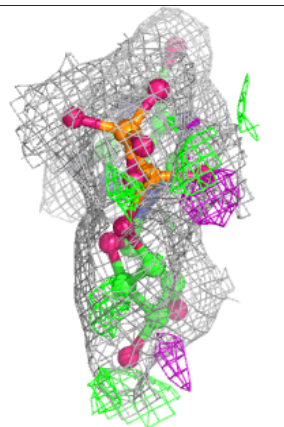
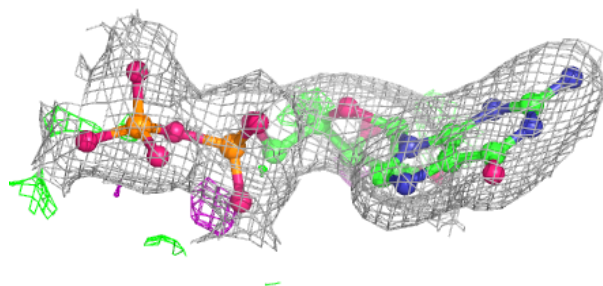
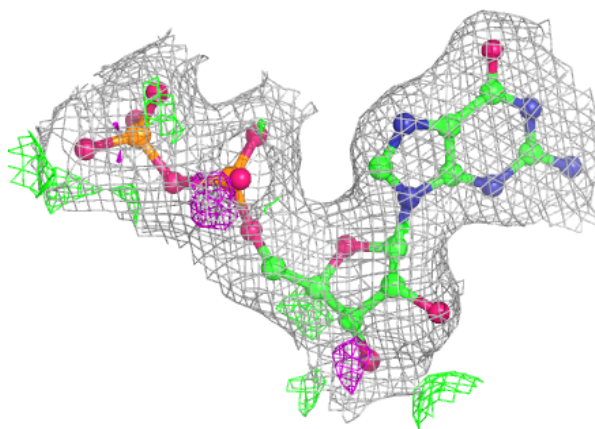
**Electron density around UQM C 504:**

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

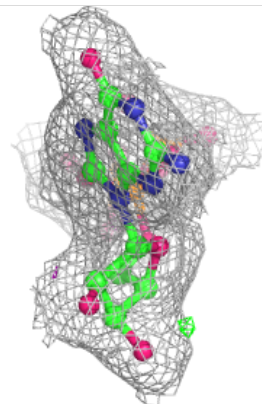
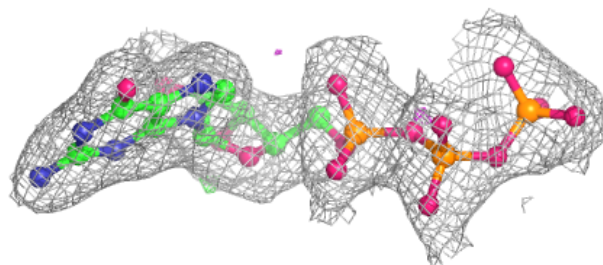
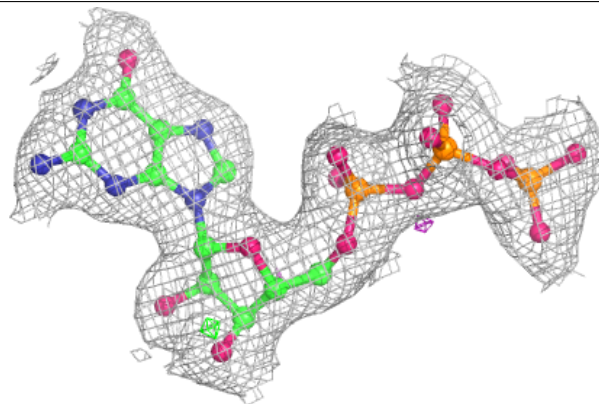


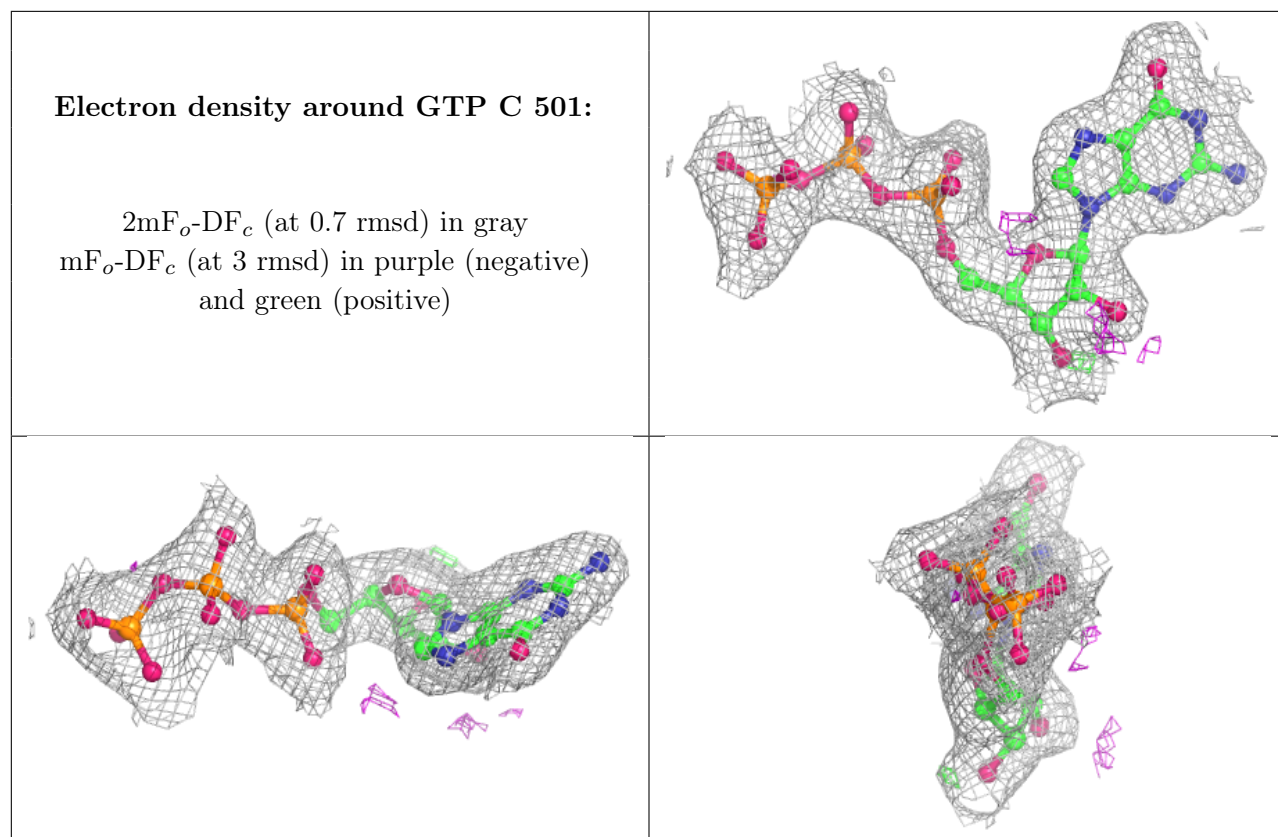
**Electron density around GDP D 501:**

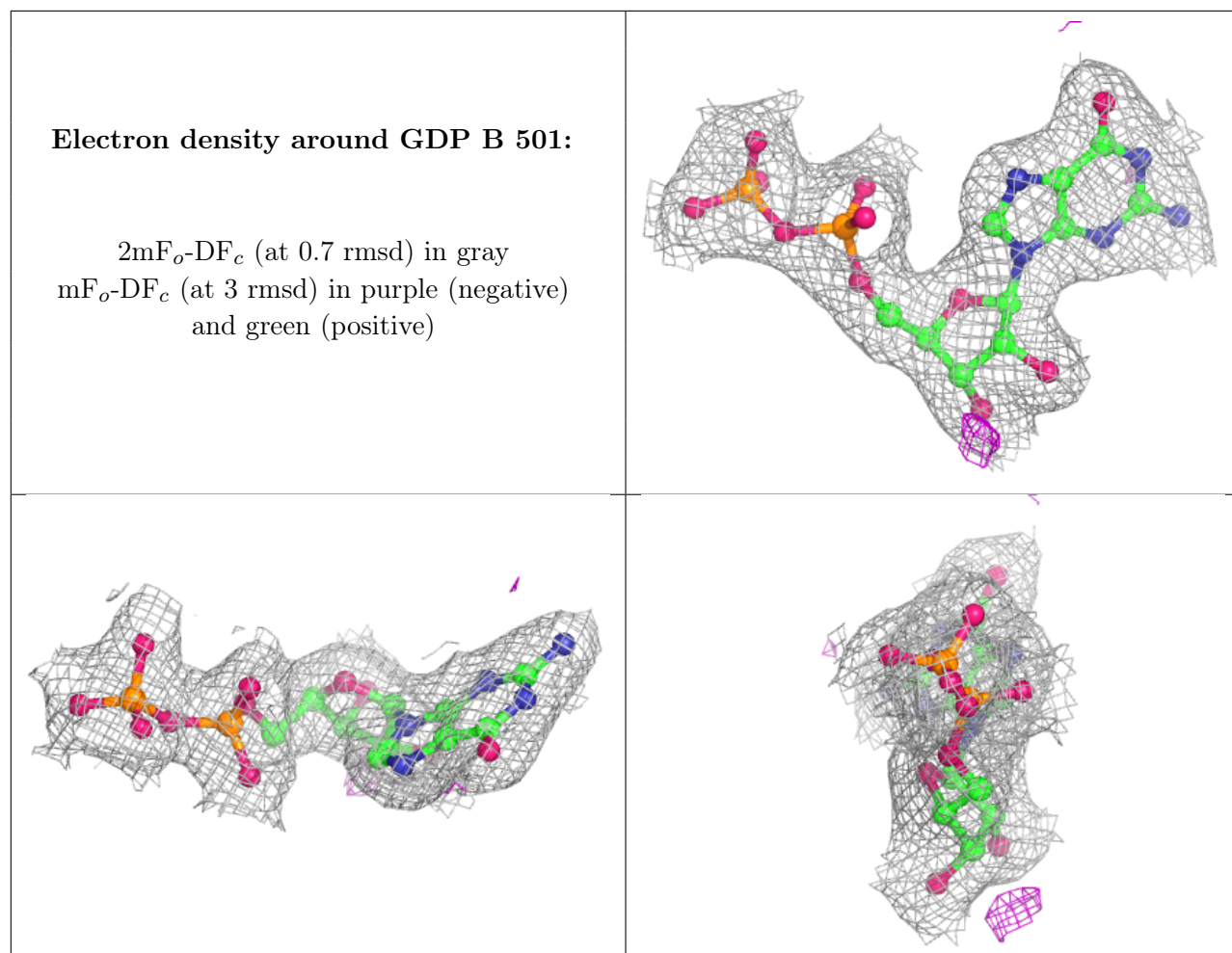
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**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)







## 6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.