



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2024 – 08:27 PM EST

PDB ID : 5S5Z  
Title : Tubulin-Z2856434944-complex  
Authors : Muehlethaler, T.; Gioia, D.; Protá, A.E.; Sharpe, M.E.; Cavalli, A.; Steinmetz, M.O.  
Deposited on : 2020-11-08  
Resolution : 2.55 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

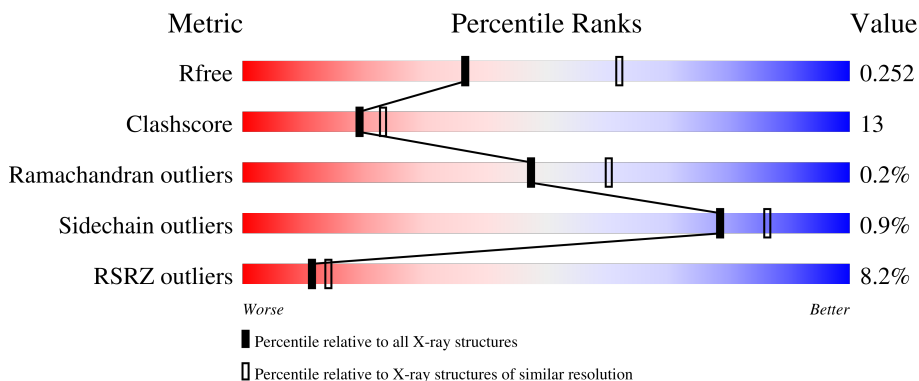
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.55 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	1284 (2.56-2.52)
Clashscore	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)

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	 6% 70% 27% •
1	C	451	 2% 76% 22% •
2	B	445	 3% 63% 31% 5%
2	D	445	 10% 68% 27% 5%
3	E	143	 8% 69% 16% • 14%

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Mol	Chain	Length	Quality of chain
4	F	384	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
9	MES	B	504	-	-	-	X

## 2 Entry composition i

There are 12 unique types of molecules in this entry. The entry contains 17859 atoms, of which 48 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	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
			Total	C	N	O	S			
2	B	423	Total	C	N	O	S	2	1	0
			3349	2103	575	644	27			
2	D	422	Total	C	N	O	S	6	0	0
			3314	2083	563	641	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	348	Total	C	N	O	S	0	0	0
			2848	1826	487	521	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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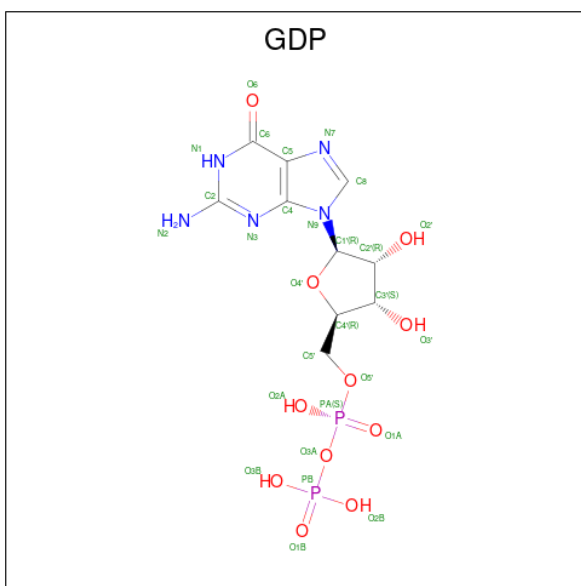
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	F	1	Total	Mg	0	0
			1	1		

- 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<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>11</sub>P<sub>2</sub>).



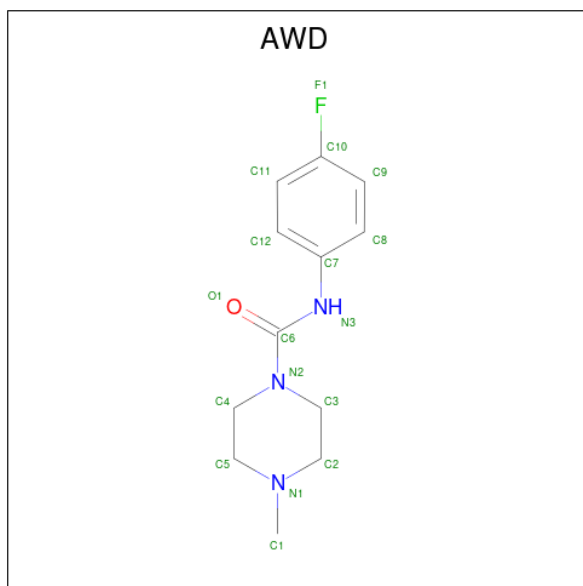
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	B	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
8	D	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

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



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-fluorophenyl)-4-methyl-piperazine-1-carboxamide (three-letter code: AWD) (formula: C<sub>12</sub>H<sub>16</sub>FN<sub>3</sub>O) (labeled as "Ligand of Interest" by depositor).



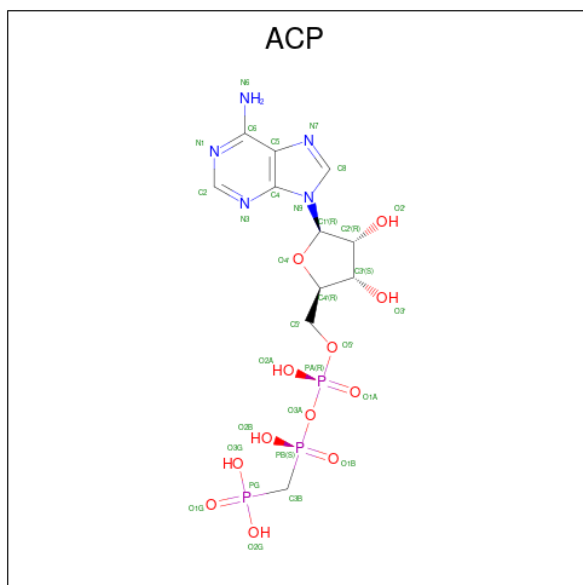
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	F	H	N			O
10	B	1	33	12	1	16	3	1	0	0
10	B	1	33	12	1	16	3	1	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	F	H	N			O
10	B	1	33	12	1	16	3	1	0	0

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



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

- Molecule 12 is water.

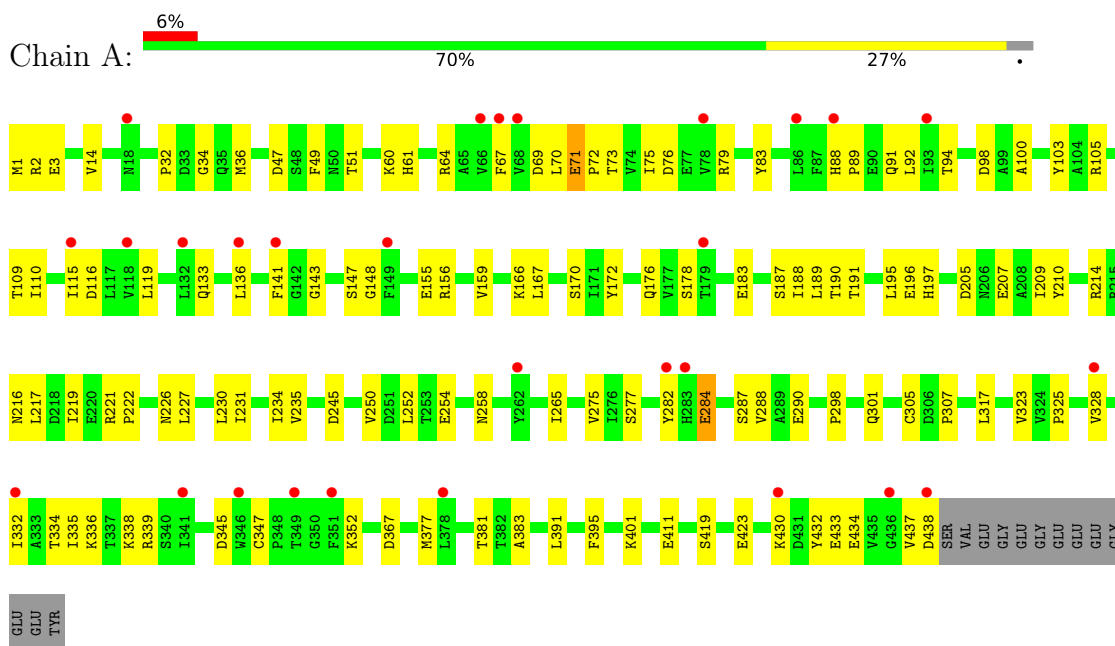
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	23	Total	O	0	0
			23	23		
12	B	43	Total	O	0	0
			43	43		
12	C	114	Total	O	0	0
			114	114		
12	D	10	Total	O	0	0
			10	10		
12	E	4	Total	O	0	0
			4	4		
12	F	2	Total	O	0	0
			2	2		



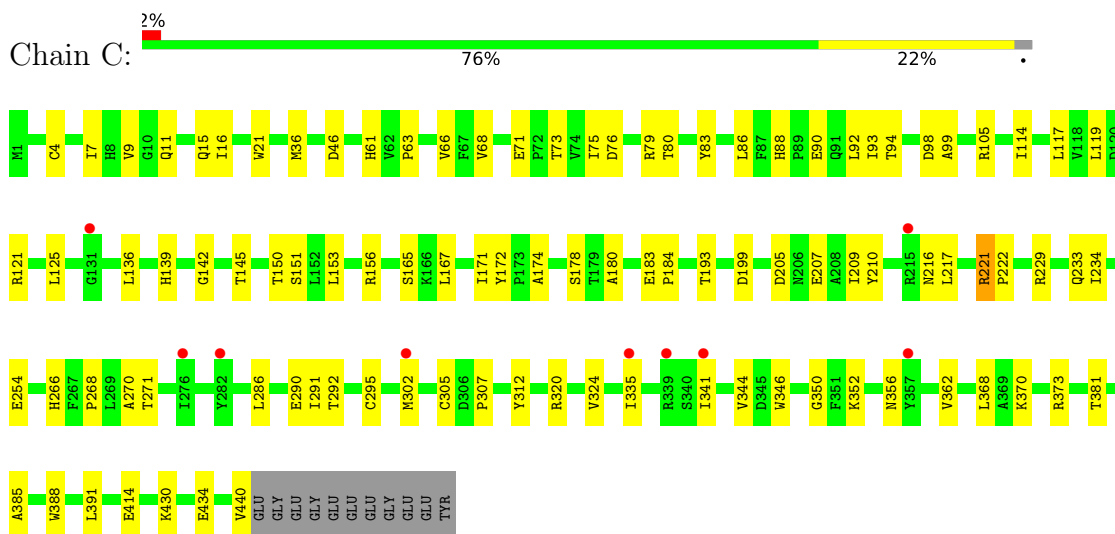
### 3 Residue-property plots i

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.

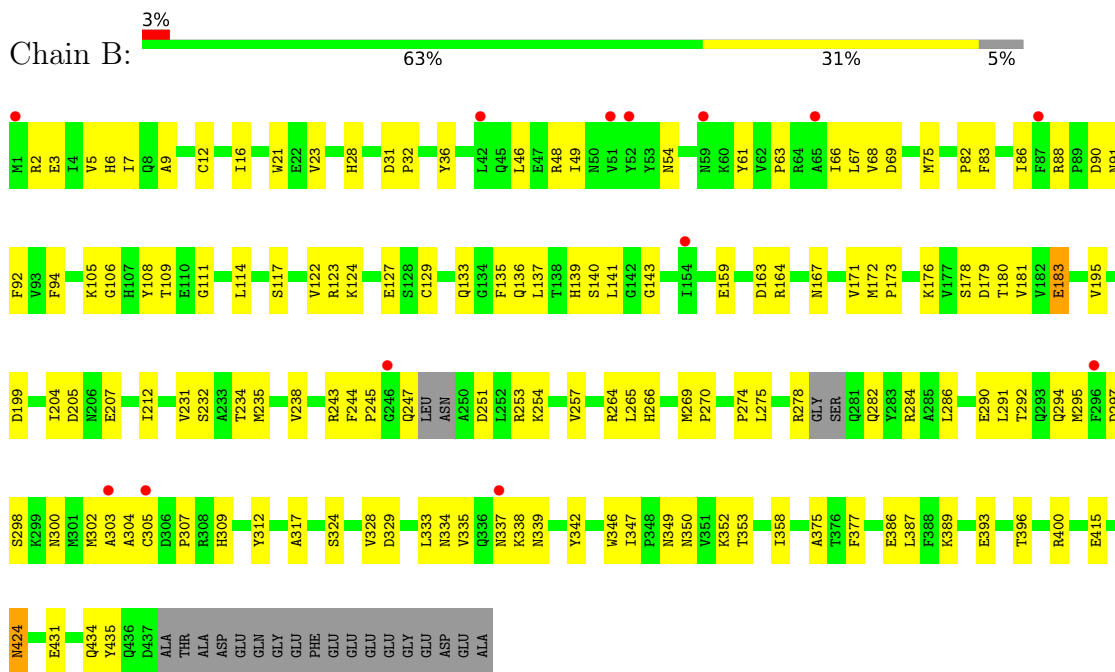
- Molecule 1: Tubulin alpha-1B chain



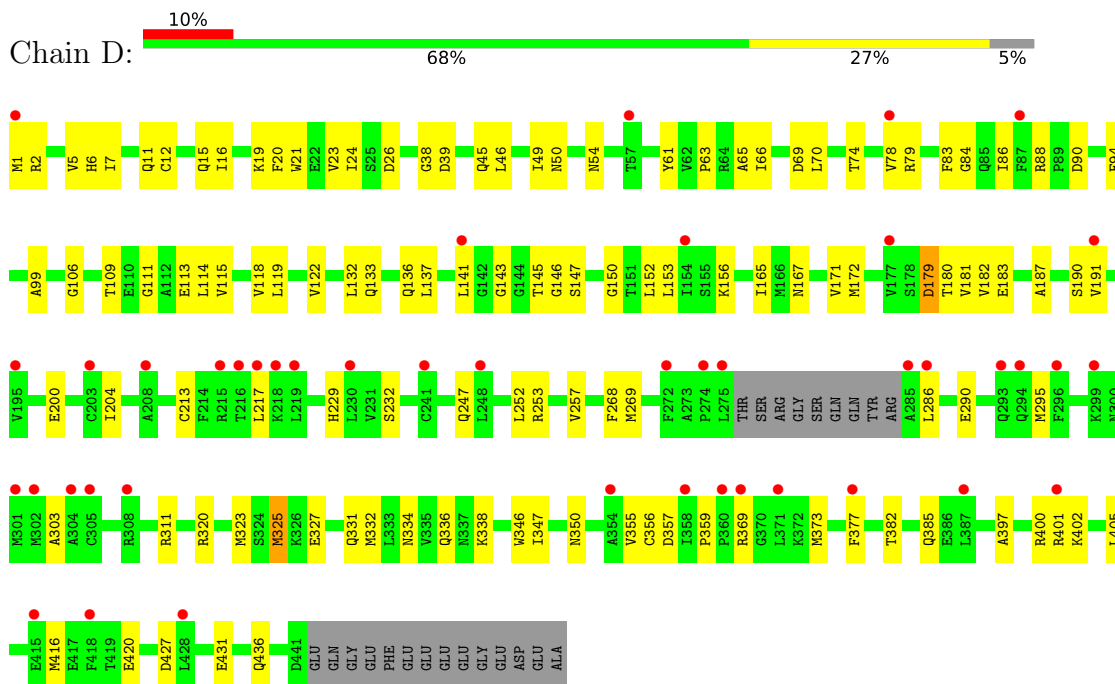
- Molecule 1: Tubulin alpha-1B chain



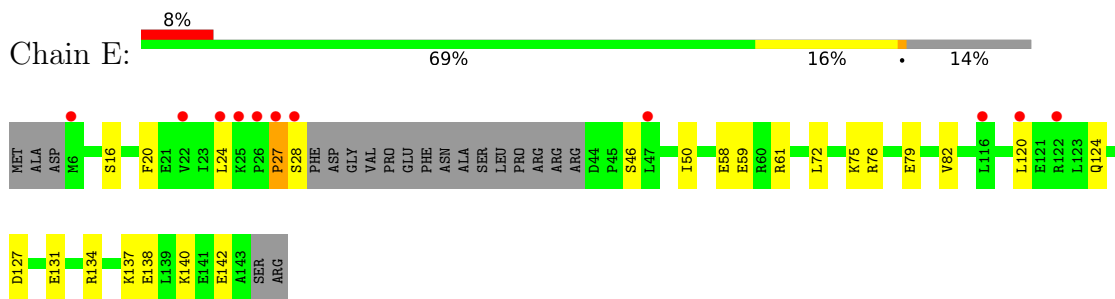
- Molecule 2: Tubulin beta-2B chain



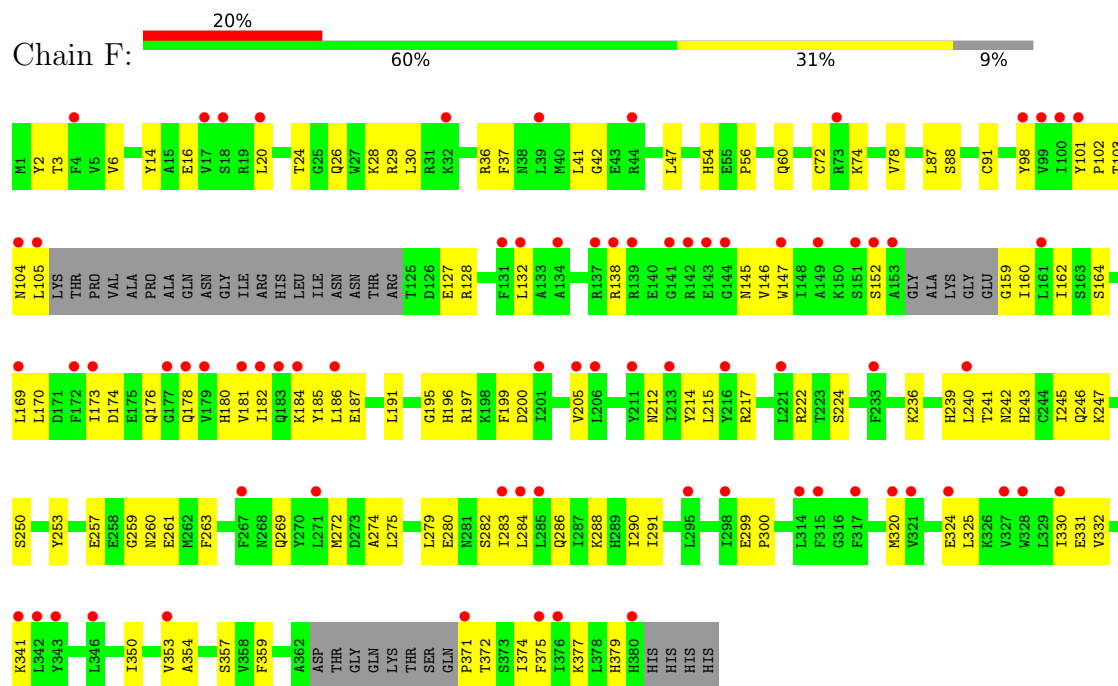
• Molecule 2: Tubulin beta-2B chain



• 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, $\alpha$ , $\beta$ , $\gamma$	105.18Å 158.03Å 182.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	91.08 – 2.55 91.08 – 2.55	Depositor EDS
% Data completeness (in resolution range)	99.5 (91.08-2.55) 99.5 (91.08-2.55)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.16 (at 2.55Å)	Xtrriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, $R_{free}$	0.209 , 0.253 0.210 , 0.252	Depositor DCC
$R_{free}$ test set	4911 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	68.9	Xtrriage
Anisotropy	0.173	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 49.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	17859	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	86.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.06% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, GDP, MES, GTP, AWD, ACP, 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	0.26	0/3502	0.42	0/4754
1	C	0.26	0/3521	0.43	0/4780
2	B	0.26	0/3422	0.42	0/4630
2	D	0.25	0/3387	0.41	0/4588
3	E	0.25	0/1022	0.35	0/1356
4	F	0.25	0/2913	0.41	0/3936
All	All	0.26	0/17767	0.41	0/24044

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	3424	0	3335	90	0
1	C	3443	0	3352	73	0
2	B	3349	0	3230	108	0
2	D	3314	0	3194	85	0
3	E	1014	0	1029	18	0
4	F	2848	0	2817	90	0
5	A	32	0	12	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	32	0	12	1	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	4	0
8	D	28	0	12	4	0
9	B	12	0	12	3	0
10	B	51	48	0	5	0
11	F	31	0	14	3	0
12	A	23	0	0	0	0
12	B	43	0	0	2	0
12	C	114	0	0	3	0
12	D	10	0	0	0	0
12	E	4	0	0	0	0
12	F	2	0	0	0	0
All	All	17811	48	17031	447	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 13.

All (447) 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	1.02
1:C:254:GLU:HG2	1:C:352:LYS:HE2	1.48	0.96
2:D:295:MET:HE2	2:D:377:PHE:HB2	1.48	0.95
1:A:335:ILE:HG23	1:A:339:ARG:HG3	1.49	0.94
1:A:2:ARG:HB2	1:A:133:GLN:HE21	1.33	0.91
4:F:236:LYS:HB3	4:F:240:LEU:HD13	1.54	0.87
4:F:132:LEU:HD21	4:F:170:LEU:HD11	1.57	0.86
1:C:11:GLN:HE22	2:D:247:GLN:HE22	1.23	0.84
1:A:71:GLU:OE2	1:A:73:THR:OG1	1.97	0.82
4:F:128:ARG:NH2	4:F:174:ASP:OD1	2.13	0.82
2:D:179:ASP:OD1	2:D:179:ASP:N	2.15	0.79
1:C:209:ILE:HD11	1:C:302:MET:HE3	1.63	0.79
2:D:397:ALA:O	2:D:401:ARG:NH1	2.15	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:331:GLU:OE2	11:F:401:ACP:O3G	2.02	0.77
2:D:136:GLN:HA	2:D:167:ASN:O	1.84	0.77
1:C:76:ASP:O	1:C:80:THR:HG22	1.85	0.75
2:B:173:PRO:HB2	2:B:183:GLU:HG2	1.68	0.74
4:F:146:VAL:HG22	4:F:164:SER:HB3	1.69	0.73
2:B:274:PRO:HB3	2:B:286:LEU:HD22	1.69	0.72
2:D:69:ASP:O	2:D:94:PHE:HA	1.89	0.72
4:F:102:PRO:HG2	4:F:105:LEU:HD13	1.72	0.71
2:B:75:MET:HE3	2:B:92:PHE:HD2	1.54	0.71
1:C:254:GLU:HG2	1:C:352:LYS:CE	2.20	0.71
2:D:311:ARG:NH1	2:D:436:GLN:O	2.22	0.71
4:F:214:TYR:HB3	4:F:375:PHE:HB3	1.71	0.71
2:D:152:LEU:O	2:D:156:LYS:HG2	1.90	0.70
4:F:241:THR:HG1	11:F:401:ACP:HO3'	1.27	0.70
4:F:102:PRO:HG2	4:F:105:LEU:CD1	2.22	0.69
4:F:147:TRP:HB2	4:F:169:LEU:HD11	1.75	0.69
2:B:176:LYS:HE2	2:B:207:GLU:OE2	1.92	0.69
1:A:433:GLU:HG3	1:A:437:VAL:HG21	1.74	0.68
2:B:173:PRO:CB	2:B:183:GLU:HG2	2.23	0.68
2:D:145:THR:N	8:D:501:GDP:O2B	2.26	0.68
4:F:14:TYR:HB3	4:F:41:LEU:HD13	1.76	0.68
2:B:23:VAL:HG21	2:B:232:SER:HB3	1.73	0.68
1:C:270:ALA:O	1:C:302:MET:HG2	1.93	0.68
2:D:213:CYS:HA	2:D:217:LEU:HB2	1.74	0.68
1:A:209:ILE:HG23	1:A:230:LEU:HD23	1.74	0.67
1:C:136:LEU:HD23	1:C:167:LEU:HB2	1.77	0.67
1:A:71:GLU:HG2	1:A:72:PRO:HD2	1.77	0.67
2:D:347:ILE:HG22	2:D:350:ASN:HB3	1.76	0.67
1:C:165:SER:HA	1:C:199:ASP:OD2	1.96	0.66
1:C:362:VAL:HG22	1:C:370:LYS:HD3	1.77	0.66
2:B:337:ASN:OD1	4:F:36:ARG:HD3	1.95	0.66
2:D:83:PHE:O	2:D:86:ILE:HG22	1.96	0.66
2:D:332:MET:O	2:D:336:GLN:HG3	1.94	0.66
4:F:246:GLN:O	4:F:250:SER:HB3	1.95	0.66
2:B:164:ARG:O	9:B:504:MES:H31	1.96	0.66
1:A:119:LEU:HD11	1:A:156:ARG:HB3	1.78	0.65
2:B:136:GLN:HA	2:B:167:ASN:O	1.95	0.65
1:A:381:THR:HG22	1:A:383:ALA:H	1.61	0.65
2:B:251:ASP:HB3	2:B:254:LYS:HB2	1.79	0.65
1:C:180:ALA:O	1:C:183:GLU:HG3	1.97	0.65
1:C:11:GLN:HE22	2:D:247:GLN:NE2	1.94	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:234:ILE:HG12	1:C:302:MET:HE2	1.80	0.64
2:D:171:VAL:HA	2:D:204:ILE:O	1.97	0.64
1:C:430:LYS:HE2	1:C:434:GLU:OE2	1.98	0.64
1:A:1:MET:HG2	1:A:51:THR:HG22	1.81	0.63
1:A:250:VAL:HG12	1:A:254:GLU:OE1	1.98	0.63
1:A:334:THR:O	1:A:338:LYS:HG3	1.99	0.63
2:B:69:ASP:O	2:B:94:PHE:HA	1.98	0.63
4:F:162:ILE:HD11	4:F:240:LEU:HD11	1.80	0.63
1:C:21:TRP:CZ3	1:C:63:PRO:HB3	2.34	0.62
1:C:117:LEU:HD11	1:C:121:ARG:NH2	2.14	0.62
2:B:295:MET:HG2	2:B:377:PHE:HB2	1.81	0.62
2:D:88:ARG:NH1	2:D:90:ASP:HB2	2.14	0.62
1:A:3:GLU:HG2	1:A:64:ARG:NH1	2.15	0.62
1:A:105:ARG:NH1	1:A:411:GLU:OE2	2.32	0.62
2:B:2:ARG:HB2	2:B:133:GLN:CG	2.29	0.62
4:F:243:HIS:HE2	4:F:253:TYR:HH	1.48	0.62
2:B:286:LEU:HD23	2:B:291:LEU:HD23	1.82	0.62
4:F:102:PRO:HB2	4:F:104:ASN:OD1	2.00	0.62
2:B:247:GLN:N	2:B:247:GLN:OE1	2.33	0.61
3:E:120:LEU:O	3:E:124:GLN:HG3	2.00	0.61
4:F:200:ASP:OD1	4:F:222:ARG:HB2	2.00	0.61
1:C:229:ARG:HG3	12:C:653:HOH:O	2.00	0.61
2:B:123:ARG:O	2:B:127:GLU:HG3	2.01	0.61
2:D:5:VAL:HG23	2:D:132:LEU:HD11	1.81	0.61
4:F:197:ARG:NH1	4:F:257:GLU:OE2	2.19	0.61
2:B:324:SER:O	2:B:328:VAL:HG23	2.01	0.60
2:B:292:THR:HG22	2:B:335:VAL:HG21	1.83	0.60
4:F:2:TYR:CE1	4:F:359:PHE:HB3	2.36	0.60
2:B:88:ARG:HD3	2:B:91:ASN:OD1	2.02	0.60
1:A:430:LYS:O	1:A:434:GLU:HG3	2.02	0.60
1:A:14:VAL:HG13	1:A:67:PHE:HD2	1.66	0.59
4:F:128:ARG:O	4:F:132:LEU:HG	2.02	0.59
2:B:141:LEU:HD12	2:B:172:MET:SD	2.42	0.59
2:D:106:GLY:O	2:D:111:GLY:HA3	2.02	0.59
2:D:147:SER:HB2	2:D:190:SER:OG	2.01	0.59
4:F:371:PRO:HA	4:F:372:THR:C	2.21	0.59
1:A:245:ASP:HB3	3:E:16:SER:OG	2.02	0.59
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.20	0.59
2:D:1:MET:HE2	2:D:50:ASN:HB2	1.84	0.59
1:A:34:GLY:HA3	1:A:60:LYS:HG3	1.85	0.59
4:F:280:GLU:OE1	4:F:284:LEU:HD23	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:191:LEU:HD12	4:F:196:HIS:CE1	2.38	0.58
1:A:88:HIS:HB2	1:A:89:PRO:HD2	1.85	0.58
2:B:159:GLU:HB2	3:E:72:LEU:HD13	1.85	0.58
2:D:12:CYS:HB2	8:D:501:GDP:C8	2.38	0.58
2:B:83:PHE:O	2:B:86:ILE:HG22	2.04	0.58
2:D:70:LEU:HD12	2:D:99:ALA:HB2	1.86	0.58
4:F:371:PRO:HA	4:F:372:THR:HB	1.84	0.58
1:A:69:ASP:O	1:A:94:THR:HA	2.02	0.58
1:C:16:ILE:CD1	1:C:171:ILE:HD11	2.34	0.58
2:D:180:THR:O	2:D:183:GLU:HG3	2.04	0.57
2:D:323:MET:HE1	2:D:373:MET:HB3	1.85	0.57
3:E:138:GLU:O	3:E:142:GLU:HG3	2.05	0.57
1:A:14:VAL:HG13	1:A:67:PHE:CD2	2.39	0.57
4:F:205:VAL:CG2	4:F:291:ILE:HD13	2.35	0.57
1:C:142:GLY:HA3	1:C:183:GLU:OE1	2.04	0.56
2:D:286:LEU:HD12	2:D:290:GLU:OE1	2.05	0.56
2:D:416:MET:O	2:D:420:GLU:HG3	2.06	0.56
1:A:36:MET:HB3	1:A:61:HIS:CE1	2.40	0.56
1:A:178:SER:OG	1:A:183:GLU:OE1	2.17	0.56
2:D:143:GLY:HA3	8:D:501:GDP:O3A	2.05	0.56
4:F:197:ARG:HB2	4:F:224:SER:O	2.06	0.56
2:B:295:MET:CG	2:B:377:PHE:HB2	2.35	0.56
1:C:66:VAL:HG23	1:C:125:LEU:CD1	2.35	0.56
2:D:7:ILE:O	2:D:137:LEU:HD12	2.05	0.56
1:A:155:GLU:O	1:A:159:VAL:HG23	2.06	0.55
2:B:2:ARG:HB2	2:B:133:GLN:HG3	1.88	0.55
1:A:88:HIS:NE2	1:A:91:GLN:HG3	2.21	0.55
1:A:100:ALA:HA	2:B:254:LYS:HG3	1.88	0.55
2:D:1:MET:CE	2:D:50:ASN:HB2	2.36	0.55
2:B:295:MET:SD	2:B:375:ALA:HB1	2.47	0.55
4:F:6:VAL:HB	4:F:29:ARG:NH2	2.22	0.55
1:A:70:LEU:HD13	1:A:110:ILE:HG21	1.89	0.55
1:C:7:ILE:HG21	1:C:153:LEU:HD21	1.89	0.54
2:B:264:ARG:HD3	2:B:431:GLU:OE1	2.07	0.54
1:C:172:TYR:CE2	1:C:391:LEU:HD22	2.43	0.54
4:F:222:ARG:O	4:F:241:THR:HB	2.07	0.54
4:F:3:THR:HA	4:F:28:LYS:O	2.07	0.54
1:A:79:ARG:HG2	1:A:92:LEU:HD12	1.89	0.54
2:B:36:TYR:CD1	2:B:46:LEU:HD21	2.42	0.53
1:A:335:ILE:CG2	1:A:339:ARG:HG3	2.31	0.53
2:B:179:ASP:HA	10:B:505:AWD:C8	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:205:ASP:OD2	2:B:304:ALA:HB3	2.08	0.53
2:D:334:ASN:HD21	2:D:338:LYS:HE3	1.74	0.53
2:D:269:MET:HG3	2:D:303:ALA:HB3	1.91	0.53
4:F:259:GLY:O	4:F:261:GLU:HG3	2.09	0.53
1:C:139:HIS:CD2	1:C:150:THR:HG21	2.44	0.53
1:A:1:MET:HG2	1:A:51:THR:CG2	2.39	0.53
2:B:286:LEU:HD23	2:B:291:LEU:CD2	2.38	0.53
2:B:172:MET:HG3	2:B:387:LEU:HD11	1.90	0.53
2:B:312:TYR:CE1	2:B:377:PHE:HZ	2.27	0.53
2:D:26:ASP:OD2	2:D:369:ARG:HD2	2.09	0.53
1:A:210:TYR:CE1	1:A:222:PRO:HD2	2.44	0.52
2:D:20:PHE:CZ	2:D:24:ILE:HD13	2.44	0.52
2:D:187:ALA:O	2:D:191:VAL:HG23	2.09	0.52
2:D:334:ASN:ND2	2:D:338:LYS:HE3	2.24	0.52
2:B:180:THR:HB	2:B:183:GLU:OE1	2.09	0.52
1:C:71:GLU:HG2	1:C:98:ASP:HB3	1.92	0.52
2:B:28:HIS:HB3	2:B:49:ILE:HD13	1.91	0.52
2:B:212:ILE:HG23	2:B:275:LEU:HD13	1.90	0.52
2:B:274:PRO:HB3	2:B:286:LEU:CD2	2.36	0.52
4:F:205:VAL:HG21	4:F:291:ILE:HD13	1.90	0.52
2:B:21:TRP:CZ3	2:B:63:PRO:HB3	2.44	0.52
1:C:385:ALA:HA	1:C:388:TRP:CD1	2.45	0.52
2:D:382:THR:O	2:D:385:GLN:HG2	2.10	0.52
1:C:151:SER:HB2	1:C:193:THR:CG2	2.39	0.52
4:F:286:GLN:O	4:F:290:ILE:HG13	2.10	0.52
2:B:349:ASN:O	2:B:352:LYS:HE2	2.09	0.52
1:C:312:TYR:CE1	1:C:341:ILE:HG23	2.45	0.52
4:F:242:ASN:HD22	4:F:245:ILE:HD12	1.75	0.52
1:A:325:PRO:HB3	3:E:20:PHE:CE1	2.45	0.51
2:B:12:CYS:HB2	8:B:501:GDP:C8	2.46	0.51
2:B:275:LEU:HD11	2:B:300:ASN:HA	1.92	0.51
2:B:124:LYS:HD3	2:B:124:LYS:C	2.31	0.51
2:D:115:VAL:HG23	2:D:153:LEU:HD23	1.91	0.51
2:B:46:LEU:O	2:B:49:ILE:HG22	2.11	0.51
1:A:71:GLU:HG2	1:A:72:PRO:CD	2.40	0.51
2:B:171:VAL:HA	2:B:204:ILE:O	2.11	0.51
1:C:4[A]:CYS:SG	1:C:136:LEU:HG	2.50	0.51
2:D:327:GLU:O	2:D:331:GLN:HG2	2.11	0.51
2:B:3:GLU:OE1	2:B:129:CYS:HB3	2.11	0.51
2:D:200:GLU:HB2	2:D:268:PHE:CE2	2.45	0.51
1:A:76:ASP:OD1	1:A:79:ARG:NH1	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:93:ILE:HG22	1:C:114:ILE:HD11	1.93	0.51
4:F:147:TRP:HB2	4:F:169:LEU:CD1	2.41	0.51
2:D:1:MET:HG3	2:D:50:ASN:OD1	2.11	0.50
2:D:402:LYS:HB3	2:D:405:LEU:HD12	1.93	0.50
4:F:16:GLU:O	4:F:20:LEU:HG	2.10	0.50
1:A:265:ILE:HG23	1:A:432:TYR:CE1	2.47	0.50
1:A:191:THR:O	1:A:195:LEU:HB2	2.11	0.50
2:B:48:ARG:HB2	2:B:243:ARG:O	2.10	0.50
2:B:199:ASP:O	2:B:266:HIS:HB2	2.11	0.50
1:A:2:ARG:HB2	1:A:133:GLN:NE2	2.14	0.50
1:C:414:GLU:HB3	12:C:674:HOH:O	2.10	0.50
2:B:183:GLU:OE2	8:B:501:GDP:O3'	2.22	0.50
1:A:143:GLY:HA3	5:A:501:GTP:O3A	2.11	0.50
1:A:103:TYR:CD1	1:A:189:LEU:HD13	2.46	0.50
1:C:79:ARG:HG2	1:C:92:LEU:HD12	1.94	0.50
2:B:88:ARG:NH1	2:B:90:ASP:HB2	2.27	0.50
4:F:371:PRO:HA	4:F:372:THR:O	2.12	0.50
4:F:241:THR:OG1	11:F:401:ACP:O3'	2.03	0.50
1:A:411:GLU:O	3:E:61:ARG:HD3	2.12	0.49
1:C:178:SER:HB2	1:C:183:GLU:OE2	2.11	0.49
2:B:396:THR:HG23	12:B:629:HOH:O	2.12	0.49
4:F:74:LYS:HB3	4:F:181:VAL:HG21	1.94	0.49
4:F:162:ILE:HD11	4:F:240:LEU:CD1	2.42	0.49
4:F:74:LYS:O	4:F:78:VAL:HG23	2.12	0.49
4:F:282:SER:HB2	4:F:325:LEU:HD13	1.93	0.49
2:D:74:THR:O	2:D:78:VAL:HG23	2.12	0.49
1:C:136:LEU:CD2	1:C:167:LEU:HB2	2.43	0.49
2:D:21:TRP:CZ3	2:D:63:PRO:HB3	2.47	0.49
2:D:79:ARG:O	2:D:84:GLY:HA3	2.13	0.49
2:D:325:MET:CE	2:D:355:VAL:HG21	2.42	0.49
2:B:282:GLN:N	2:B:282:GLN:OE1	2.41	0.49
4:F:279:LEU:HD12	4:F:283:ILE:HB	1.93	0.49
2:B:269:MET:HG2	2:B:303:ALA:CB	2.43	0.49
2:D:2:ARG:HB3	2:D:133:GLN:CG	2.41	0.49
2:D:180:THR:HB	2:D:183:GLU:HG3	1.94	0.49
4:F:103:THR:HG23	4:F:128:ARG:NH2	2.27	0.49
2:B:334:ASN:HD21	2:B:338:LYS:HD2	1.77	0.49
2:D:397:ALA:HA	2:D:400:ARG:NH1	2.27	0.49
4:F:98:TYR:HA	4:F:127:GLU:OE1	2.13	0.49
4:F:24:THR:O	4:F:26:GLN:HG3	2.13	0.49
4:F:246:GLN:HB3	4:F:260:ASN:ND2	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:371:PRO:CA	4:F:372:THR:HB	2.43	0.48
1:A:167:LEU:HD13	1:A:252:LEU:HD22	1.95	0.48
1:A:345:ASP:HB3	3:E:28:SER:HB2	1.94	0.48
2:B:253[B]:ARG:O	2:B:257:VAL:HG23	2.13	0.48
1:C:83:TYR:HD2	1:C:86:LEU:HD22	1.78	0.48
2:D:19:LYS:O	2:D:23:VAL:HG23	2.12	0.48
1:A:3:GLU:HG2	1:A:64:ARG:CZ	2.43	0.48
4:F:159:GLY:C	4:F:160:ILE:HD12	2.33	0.48
2:B:46:LEU:HA	2:B:49:ILE:HB	1.95	0.48
2:B:309:HIS:ND1	2:B:386:GLU:OE2	2.34	0.48
2:B:317:ALA:HB3	2:B:353:THR:HG23	1.94	0.48
2:D:12:CYS:O	2:D:16:ILE:HG12	2.14	0.48
2:B:9:ALA:HA	2:B:68:VAL:O	2.12	0.48
2:B:212:ILE:CG2	2:B:275:LEU:HD13	2.44	0.48
2:B:297:ASP:OD1	2:B:298:SER:N	2.46	0.48
2:B:305:CYS:O	2:B:307:PRO:HD3	2.12	0.48
1:C:21:TRP:CE3	1:C:63:PRO:HB3	2.48	0.48
1:C:66:VAL:HG23	1:C:125:LEU:HD11	1.95	0.48
2:B:294:GLN:O	2:B:300:ASN:HB2	2.14	0.48
2:D:70:LEU:HG	2:D:145:THR:HG23	1.96	0.48
1:A:75:ILE:HB	1:A:94:THR:CG2	2.44	0.48
1:C:320:ARG:HA	1:C:356:ASN:O	2.13	0.48
2:D:118:VAL:O	2:D:122:VAL:HG23	2.14	0.48
4:F:215:LEU:HD22	4:F:288:LYS:HG2	1.96	0.48
1:A:70:LEU:HD13	1:A:110:ILE:CG2	2.43	0.48
1:A:187:SER:HB3	1:A:391:LEU:HD21	1.96	0.48
1:A:217:LEU:HA	1:A:277:SER:HB2	1.96	0.48
1:A:347:CYS:C	3:E:27:PRO:HB3	2.35	0.48
1:C:291:ILE:HD13	1:C:373:ARG:HG3	1.95	0.47
1:A:254:GLU:HG2	1:A:258:ASN:ND2	2.29	0.47
2:B:31:ASP:HB2	2:B:32:PRO:CD	2.44	0.47
2:B:389:LYS:O	2:B:393:GLU:HG3	2.13	0.47
1:A:88:HIS:CD2	1:A:91:GLN:HG3	2.49	0.47
1:A:401:LYS:HG3	2:B:346:TRP:CE3	2.49	0.47
2:B:5:VAL:HB	2:B:135:PHE:HD2	1.78	0.47
2:B:347:ILE:HG22	2:B:350:ASN:HB3	1.95	0.47
1:A:32:PRO:HA	1:A:83:TYR:CD2	2.49	0.47
1:A:317:LEU:HD23	1:A:377:MET:HG3	1.97	0.47
1:A:328:VAL:O	1:A:332:ILE:HG13	2.15	0.47
2:B:178:SER:HB3	10:B:507:AWD:C1	2.45	0.47
1:C:292:THR:HG22	1:C:335:ILE:CD1	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:209:ILE:HG22	1:A:227:LEU:HD22	1.96	0.47
4:F:320:MET:CG	4:F:330:ILE:HD11	2.45	0.47
1:A:136:LEU:HD21	1:A:252:LEU:HD21	1.97	0.47
2:B:31:ASP:HB2	2:B:32:PRO:HD2	1.97	0.47
2:D:54:ASN:O	2:D:61:TYR:HA	2.15	0.47
1:A:172:TYR:CZ	1:A:391:LEU:HD13	2.50	0.46
2:D:427:ASP:O	2:D:431:GLU:HG3	2.15	0.46
4:F:299:GLU:HB3	4:F:300:PRO:HD3	1.96	0.46
1:A:47:ASP:HB2	1:A:49:PHE:CE2	2.50	0.46
2:B:75:MET:HE3	2:B:92:PHE:CD2	2.43	0.46
1:C:90:GLU:HB3	1:C:121:ARG:HD2	1.98	0.46
2:B:204:ILE:HD13	2:B:231:VAL:HG13	1.97	0.46
2:B:234:THR:O	2:B:238:VAL:HG13	2.16	0.46
1:C:71:GLU:OE1	1:C:73:THR:OG1	2.21	0.46
4:F:169:LEU:O	4:F:173:ILE:HG13	2.16	0.46
2:B:163:ASP:O	2:B:253[B]:ARG:NH1	2.48	0.46
1:A:265:ILE:HG23	1:A:432:TYR:CZ	2.51	0.46
4:F:101:TYR:HD2	4:F:105:LEU:CD2	2.29	0.46
2:B:143:GLY:HA3	8:B:501:GDP:O3A	2.16	0.46
4:F:173:ILE:HD11	4:F:182:ILE:HD11	1.98	0.46
1:A:234:ILE:HD12	1:A:234:ILE:N	2.31	0.45
2:B:253[A]:ARG:O	2:B:257:VAL:HG23	2.15	0.45
2:D:180:THR:HB	2:D:183:GLU:CG	2.46	0.45
4:F:274:ALA:HB3	4:F:275:LEU:HD22	1.99	0.45
10:B:505:AWD:O1	1:C:350:GLY:HA3	2.15	0.45
1:C:216:ASN:O	1:C:217:LEU:HD23	2.15	0.45
1:C:440:VAL:HG12	1:C:440:VAL:O	2.15	0.45
2:D:295:MET:CE	2:D:377:PHE:HB2	2.33	0.45
4:F:263:PHE:CE1	4:F:341:LYS:HE2	2.51	0.45
2:B:179:ASP:HA	10:B:505:AWD:C7	2.46	0.45
2:B:195:VAL:HG11	2:B:424:ASN:HD21	1.81	0.45
1:A:207:GLU:OE2	4:F:54:HIS:ND1	2.49	0.45
4:F:372:THR:O	4:F:372:THR:HG22	2.15	0.45
1:A:98:ASP:HB2	5:A:501:GTP:O2G	2.16	0.45
1:A:188:ILE:HD12	1:A:395:PHE:HB2	1.97	0.45
1:A:231:ILE:O	1:A:235:VAL:HG23	2.17	0.45
4:F:42:GLY:HA3	4:F:47:LEU:CD1	2.45	0.45
4:F:138:ARG:HD2	4:F:145:ASN:OD1	2.16	0.45
2:B:106:GLY:O	2:B:111:GLY:HA3	2.17	0.45
2:B:270:PRO:HG2	2:B:302:MET:HB2	1.99	0.45
1:C:119:LEU:HD11	1:C:156:ARG:HB3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:185:TYR:OH	4:F:239:HIS:HB3	2.16	0.45
4:F:371:PRO:HA	4:F:372:THR:CB	2.45	0.45
4:F:341:LYS:HG2	4:F:341:LYS:O	2.17	0.45
2:B:108:TYR:CG	3:E:82:VAL:HG11	2.52	0.45
2:B:329:ASP:O	2:B:333:LEU:HG	2.17	0.45
2:D:46:LEU:HA	2:D:49:ILE:HB	1.98	0.45
1:A:141:PHE:CE1	1:A:170:SER:HB3	2.52	0.45
2:B:334:ASN:ND2	2:B:338:LYS:HD2	2.31	0.45
1:C:174:ALA:HB1	1:C:207:GLU:HB2	1.98	0.45
1:C:271:THR:HG21	1:C:295:CYS:O	2.17	0.45
1:A:226:ASN:ND2	1:A:367:ASP:OD2	2.47	0.44
1:A:305:CYS:O	1:A:307:PRO:HD3	2.16	0.44
1:C:234:ILE:HD12	1:C:234:ILE:H	1.83	0.44
3:E:72:LEU:O	3:E:76:ARG:HG2	2.17	0.44
2:B:183:GLU:OE2	8:B:501:GDP:C3'	2.65	0.44
2:D:347:ILE:CG2	2:D:350:ASN:HB3	2.45	0.44
4:F:242:ASN:HD22	4:F:245:ILE:CD1	2.30	0.44
2:B:16:ILE:HD13	2:B:231:VAL:HG11	2.00	0.44
2:B:244:PHE:HB3	2:B:245:PRO:HD2	1.99	0.44
1:C:172:TYR:HB3	1:C:205:ASP:HA	2.00	0.44
1:C:344:VAL:HG21	1:C:346:TRP:CE2	2.53	0.44
2:D:146:GLY:O	2:D:150:GLY:HA3	2.18	0.44
2:D:357:ASP:O	2:D:359:PRO:HD3	2.18	0.44
4:F:199:PHE:HA	4:F:241:THR:HG21	2.00	0.44
2:B:5:VAL:HB	2:B:135:PHE:CD2	2.52	0.44
2:B:431:GLU:O	2:B:434:GLN:HG2	2.18	0.44
2:D:21:TRP:CE3	2:D:63:PRO:HB3	2.52	0.44
4:F:72:CYS:HA	4:F:332:VAL:O	2.17	0.44
4:F:324:GLU:OE1	4:F:324:GLU:HA	2.18	0.44
2:B:181:VAL:HG12	10:B:505:AWD:F1	2.08	0.44
1:A:214:ARG:HG2	1:A:219:ILE:O	2.18	0.44
1:A:49:PHE:HE1	1:A:61:HIS:HD2	1.65	0.44
1:A:103:TYR:CE2	1:A:148:GLY:HA2	2.53	0.44
2:D:109:THR:O	2:D:113:GLU:HG2	2.18	0.44
4:F:87:LEU:O	4:F:88:SER:OG	2.24	0.44
2:B:7:ILE:O	2:B:137:LEU:HA	2.18	0.43
2:B:66:ILE:HD12	2:B:122:VAL:HG22	2.00	0.43
4:F:176:GLN:HB3	4:F:178:GLN:NE2	2.33	0.43
2:B:415:GLU:HG3	12:B:619:HOH:O	2.17	0.43
4:F:214:TYR:HB3	4:F:375:PHE:CB	2.45	0.43
4:F:377:LYS:HD3	4:F:379:HIS:CE1	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:339:ASN:HB3	2:B:342:TYR:HD2	1.82	0.43
2:D:5:VAL:HG23	2:D:132:LEU:CD1	2.48	0.43
1:C:233:GLN:HG3	1:C:368:LEU:HD12	2.00	0.43
1:C:335:ILE:HG22	1:C:341:ILE:HD11	2.01	0.43
2:D:11:GLN:O	2:D:15:GLN:HG2	2.18	0.43
2:D:23:VAL:HG21	2:D:232:SER:HB2	1.99	0.43
2:D:253:ARG:O	2:D:257:VAL:HG23	2.18	0.43
1:A:75:ILE:HB	1:A:94:THR:HG21	2.00	0.43
1:A:176:GLN:HG3	4:F:56:PRO:HB3	2.01	0.43
3:E:58:GLU:HA	3:E:61:ARG:NH2	2.33	0.43
2:B:2:ARG:HD2	2:B:48:ARG:HH12	1.83	0.43
1:C:9:VAL:HG12	1:C:145:THR:HG22	2.01	0.43
1:C:210:TYR:CZ	1:C:222:PRO:HD2	2.54	0.43
4:F:217:ARG:NH2	4:F:374:ILE:HA	2.33	0.43
1:A:287:SER:OG	1:A:290:GLU:HG3	2.18	0.43
2:D:38:GLY:HA3	2:D:45:GLN:OE1	2.18	0.43
4:F:3:THR:HB	4:F:30:LEU:HD11	2.01	0.43
1:A:258:ASN:OD1	1:A:352:LYS:HE2	2.19	0.43
2:B:163:ASP:O	2:B:253[A]:ARG:NH2	2.42	0.43
2:D:320:ARG:HA	2:D:356:CYS:O	2.19	0.43
1:C:75:ILE:HD12	1:C:94:THR:HG22	2.00	0.42
1:C:99:ALA:O	1:C:105:ARG:HD3	2.18	0.42
1:A:336:LYS:HG3	3:E:24:LEU:CD1	2.49	0.42
1:C:15:GLN:NE2	5:C:501:GTP:O6	2.48	0.42
3:E:127:ASP:O	3:E:131:GLU:HG2	2.20	0.42
4:F:2:TYR:CZ	4:F:359:PHE:HB3	2.54	0.42
1:A:166:LYS:HE2	1:A:197:HIS:O	2.19	0.42
1:A:196:GLU:OE1	1:A:196:GLU:HA	2.18	0.42
2:B:253[A]:ARG:NH1	9:B:504:MES:O2S	2.51	0.42
9:B:504:MES:H81	9:B:504:MES:H51	1.80	0.42
1:C:151:SER:HB2	1:C:193:THR:HG21	2.02	0.42
3:E:75:LYS:O	3:E:79:GLU:HG3	2.19	0.42
4:F:195:GLY:HA3	4:F:197:ARG:HD3	2.02	0.42
1:A:172:TYR:HB3	1:A:205:ASP:HA	2.02	0.42
4:F:184:LYS:NZ	4:F:187:GLU:HG3	2.33	0.42
4:F:263:PHE:CZ	4:F:341:LYS:HE2	2.54	0.42
1:C:391:LEU:HD12	1:C:391:LEU:HA	1.89	0.42
4:F:102:PRO:HG2	4:F:105:LEU:HD11	1.99	0.42
1:C:266:HIS:O	1:C:268:PRO:HD3	2.19	0.42
2:D:7:ILE:O	2:D:137:LEU:HA	2.20	0.42
2:B:244:PHE:CE1	2:B:358:ILE:HD12	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:284:ARG:NH2	2:B:290:GLU:OE2	2.53	0.42
1:C:234:ILE:HG12	1:C:302:MET:CE	2.48	0.42
2:D:6:HIS:CD2	2:D:21:TRP:HE1	2.37	0.42
1:C:174:ALA:CB	1:C:207:GLU:HB2	2.50	0.42
2:D:66:ILE:CD1	2:D:122:VAL:HG22	2.50	0.42
1:A:336:LYS:HG3	3:E:24:LEU:HD13	2.00	0.42
1:A:437:VAL:HG12	1:A:438:ASP:N	2.35	0.42
1:C:36:MET:HB3	1:C:61:HIS:CE1	2.54	0.42
2:D:1:MET:HG3	2:D:50:ASN:CG	2.39	0.42
1:A:419:SER:O	1:A:423:GLU:HG3	2.20	0.42
2:B:114:LEU:O	2:B:114:LEU:HG	2.20	0.42
2:D:21:TRP:CZ2	2:D:65:ALA:HB2	2.55	0.42
2:D:181:VAL:HG13	2:D:182:VAL:HG13	2.02	0.42
1:C:209:ILE:HD11	1:C:302:MET:CE	2.43	0.41
3:E:137:LYS:O	3:E:140:LYS:HG2	2.20	0.41
4:F:350:ILE:O	4:F:354:ALA:HB3	2.19	0.41
2:B:265:LEU:HD11	2:B:435:TYR:CD2	2.54	0.41
1:C:305:CYS:O	1:C:307:PRO:HD3	2.21	0.41
2:D:20:PHE:O	2:D:24:ILE:HG12	2.21	0.41
1:A:209:ILE:HG22	1:A:227:LEU:CD2	2.50	0.41
1:A:284:GLU:CD	1:A:284:GLU:H	2.23	0.41
1:C:183:GLU:N	1:C:184:PRO:CD	2.84	0.41
1:A:176:GLN:CG	4:F:56:PRO:HB3	2.51	0.41
1:A:216:ASN:HD22	1:A:275:VAL:HB	1.85	0.41
2:D:114:LEU:O	2:D:114:LEU:HG	2.20	0.41
1:C:88:HIS:HE1	1:C:90:GLU:HG3	1.85	0.41
1:C:234:ILE:CG1	1:C:302:MET:HE2	2.48	0.41
2:B:231:VAL:O	2:B:235:MET:HG3	2.20	0.41
2:B:396:THR:O	2:B:400:ARG:HG2	2.21	0.41
2:D:325:MET:HE2	2:D:355:VAL:HG21	2.03	0.41
1:A:115:ILE:HG23	1:A:116:ASP:N	2.36	0.41
1:A:147:SER:HB2	1:A:190:THR:HB	2.02	0.41
1:A:433:GLU:HG3	1:A:437:VAL:CG2	2.49	0.41
3:E:46:SER:O	3:E:50:ILE:HG13	2.20	0.41
4:F:160:ILE:HD12	4:F:160:ILE:N	2.36	0.41
4:F:178:GLN:NE2	4:F:180:HIS:HE1	2.18	0.41
2:B:105:LYS:HA	2:B:109:THR:OG1	2.20	0.41
1:C:46:ASP:N	1:C:46:ASP:OD1	2.54	0.41
1:C:286:LEU:HA	1:C:290:GLU:OE1	2.21	0.41
4:F:247:LYS:HG3	4:F:253:TYR:CE2	2.55	0.41
4:F:269:GLN:HA	4:F:272:MET:HE2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:320:MET:HG3	4:F:330:ILE:HD11	2.02	0.41
4:F:353:VAL:O	4:F:357:SER:OG	2.26	0.41
1:A:288:VAL:HG22	1:A:323:VAL:HG22	2.02	0.41
2:B:67:LEU:HD22	2:B:92:PHE:CE2	2.56	0.41
2:D:115:VAL:O	2:D:119:LEU:HG	2.21	0.41
3:E:131:GLU:CD	3:E:134:ARG:HH21	2.24	0.41
4:F:212:ASN:HB2	4:F:214:TYR:CE2	2.55	0.41
1:A:298:PRO:HA	1:A:301:GLN:CD	2.41	0.40
2:B:334:ASN:OD1	2:B:338:LYS:HD3	2.21	0.40
1:C:66:VAL:HG12	1:C:68:VAL:CG2	2.50	0.40
4:F:74:LYS:HG2	4:F:152:SER:OG	2.21	0.40
2:B:12:CYS:SG	2:B:140:SER:HB3	2.61	0.40
1:C:174:ALA:HB2	1:C:207:GLU:N	2.36	0.40
2:D:1:MET:HE2	2:D:1:MET:HB3	1.89	0.40
2:D:165:ILE:HG21	2:D:252:LEU:HB3	2.03	0.40
2:B:54:ASN:O	2:B:61:TYR:HA	2.21	0.40
2:D:320:ARG:O	2:D:373:MET:HA	2.22	0.40
2:D:346:TRP:CE3	2:D:347:ILE:HG13	2.56	0.40
1:C:324:VAL:HG22	12:C:626:HOH:O	2.22	0.40
2:D:141:LEU:HD12	2:D:172:MET:SD	2.62	0.40
4:F:37:PHE:O	4:F:60:GLN:HG2	2.21	0.40
1:A:34:GLY:O	1:A:61:HIS:N	2.48	0.40
2:B:434:GLN:HG3	2:B:435:TYR:N	2.37	0.40
2:D:183:GLU:OE1	8:D:501:GDP:O3'	2.35	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%)	420 (96%)	15 (3%)	1 (0%)	47 60

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	439/451 (97%)	427 (97%)	12 (3%)	0	100	100
2	B	418/445 (94%)	404 (97%)	13 (3%)	1 (0%)	47	60
2	D	418/445 (94%)	401 (96%)	17 (4%)	0	100	100
3	E	119/143 (83%)	118 (99%)	0	1 (1%)	19	27
4	F	340/384 (88%)	324 (95%)	15 (4%)	1 (0%)	41	51
All	All	2170/2319 (94%)	2094 (96%)	72 (3%)	4 (0%)	47	60

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	109	THR
4	F	186	LEU
3	E	27	PRO
2	B	82	PRO

### 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%)	365 (99%)	4 (1%)	73	83
1	C	372/379 (98%)	370 (100%)	2 (0%)	88	93
2	B	368/383 (96%)	363 (99%)	5 (1%)	67	79
2	D	364/383 (95%)	360 (99%)	4 (1%)	73	83
3	E	110/127 (87%)	109 (99%)	1 (1%)	78	86
4	F	313/342 (92%)	312 (100%)	1 (0%)	92	96
All	All	1896/1993 (95%)	1879 (99%)	17 (1%)	78	86

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	GLU
1	A	221	ARG

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Mol	Chain	Res	Type
1	A	282	TYR
1	A	284	GLU
2	B	117	SER
2	B	139	HIS
2	B	183	GLU
2	B	278	ARG
2	B	424	ASN
1	C	221	ARG
1	C	381	THR
2	D	39	ASP
2	D	179	ASP
2	D	229	HIS
2	D	325	MET
3	E	59	GLU
4	F	91	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	HIS
1	A	329	ASN
2	B	294	GLN
2	B	300	ASN
2	B	424	ASN
1	C	256	GLN
2	D	247	GLN
3	E	115	HIS
4	F	180	HIS
4	F	229	ASN
4	F	242	ASN
4	F	333	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 9 are monoatomic - leaving 9 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	GTP	C	501	6	26,34,34	1.13	2 (7%)	32,54,54	1.45	5 (15%)
5	GTP	A	501	6	26,34,34	1.13	2 (7%)	32,54,54	1.37	5 (15%)
10	AWD	B	506	-	18,18,18	0.20	0	24,24,24	0.47	0
11	ACP	F	401	6	27,33,33	1.42	5 (18%)	32,52,52	1.48	4 (12%)
10	AWD	B	507	-	18,18,18	0.18	0	24,24,24	0.35	0
9	MES	B	504	-	12,12,12	2.28	1 (8%)	14,16,16	2.04	7 (50%)
8	GDP	B	501	6	24,30,30	0.94	1 (4%)	30,47,47	1.10	3 (10%)
10	AWD	B	505	-	18,18,18	0.19	0	24,24,24	0.34	0
8	GDP	D	501	6	24,30,30	0.94	1 (4%)	30,47,47	1.24	4 (13%)

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
5	GTP	C	501	6	-	4/18/38/38	0/3/3/3
5	GTP	A	501	6	-	6/18/38/38	0/3/3/3
10	AWD	B	506	-	-	1/8/18/18	0/2/2/2
11	ACP	F	401	6	-	9/15/38/38	0/3/3/3
10	AWD	B	507	-	-	4/8/18/18	0/2/2/2
9	MES	B	504	-	-	4/6/14/14	0/1/1/1
8	GDP	B	501	6	-	3/12/32/32	0/3/3/3
10	AWD	B	505	-	-	1/8/18/18	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	GDP	D	501	6	-	2/12/32/32	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	-7.60	1.66	1.77
5	C	501	GTP	C5-C6	-3.98	1.39	1.47
5	A	501	GTP	C5-C6	-3.91	1.39	1.47
11	F	401	ACP	PG-O2G	3.02	1.61	1.54
11	F	401	ACP	PG-O3G	3.01	1.61	1.54
11	F	401	ACP	PB-O3A	3.00	1.61	1.58
11	F	401	ACP	C5-C4	2.50	1.47	1.40
8	D	501	GDP	C6-N1	-2.41	1.34	1.37
8	B	501	GDP	C6-N1	-2.37	1.34	1.37
11	F	401	ACP	PB-O2B	2.28	1.61	1.56
5	A	501	GTP	C2-N3	2.14	1.38	1.33
5	C	501	GTP	C2-N3	2.09	1.38	1.33

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	504	MES	C5-N4-C3	3.83	117.45	108.83
11	F	401	ACP	PB-O3A-PA	-3.77	120.59	132.56
11	F	401	ACP	C3'-C2'-C1'	3.74	106.61	100.98
9	B	504	MES	C6-C5-N4	-3.40	104.94	110.10
5	C	501	GTP	PA-O3A-PB	-3.16	121.98	132.83
5	A	501	GTP	C8-N7-C5	3.16	109.01	102.99
11	F	401	ACP	N3-C2-N1	-3.15	123.75	128.68
5	A	501	GTP	C5-C6-N1	3.15	119.52	113.95
5	C	501	GTP	C5-C6-N1	3.13	119.47	113.95
5	C	501	GTP	C8-N7-C5	3.06	108.81	102.99
5	C	501	GTP	PB-O3B-PG	-3.02	122.47	132.83
8	D	501	GDP	PA-O3A-PB	-2.98	122.60	132.83
8	D	501	GDP	C3'-C2'-C1'	2.79	105.18	100.98
5	C	501	GTP	C2-N1-C6	-2.75	120.04	125.10
5	A	501	GTP	C2-N1-C6	-2.74	120.04	125.10
5	A	501	GTP	PA-O3A-PB	-2.72	123.51	132.83
8	B	501	GDP	C8-N7-C5	2.53	107.81	102.99
11	F	401	ACP	C4-C5-N7	-2.50	106.79	109.40
9	B	504	MES	O1S-S-C8	2.47	109.89	106.92
8	D	501	GDP	C8-N7-C5	2.36	107.49	102.99
9	B	504	MES	C7-N4-C5	2.33	117.18	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	501	GDP	C5-C6-N1	2.31	118.02	113.95
8	D	501	GDP	C5-C6-N1	2.27	117.96	113.95
8	B	501	GDP	PA-O3A-PB	-2.24	125.13	132.83
9	B	504	MES	O3S-S-C8	2.15	109.25	105.77
9	B	504	MES	C7-N4-C3	2.13	116.69	111.23
9	B	504	MES	O2S-S-C8	2.06	109.40	106.92
5	A	501	GTP	O6-C6-C5	-2.02	120.42	124.37

There are no chirality outliers.

All (34) 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-O3A
8	D	501	GDP	C5'-O5'-PA-O2A
9	B	504	MES	C8-C7-N4-C5
10	B	507	AWD	N3-C6-N2-C4
10	B	507	AWD	N3-C6-N2-C3
10	B	507	AWD	O1-C6-N2-C4
10	B	507	AWD	O1-C6-N2-C3
11	F	401	ACP	PB-C3B-PG-O1G
11	F	401	ACP	PB-C3B-PG-O2G
11	F	401	ACP	PB-C3B-PG-O3G
11	F	401	ACP	PG-C3B-PB-O1B
11	F	401	ACP	PG-C3B-PB-O3A
11	F	401	ACP	C5'-O5'-PA-O1A
11	F	401	ACP	C5'-O5'-PA-O2A
5	C	501	GTP	PB-O3B-PG-O2G
10	B	506	AWD	N2-C6-N3-C7
9	B	504	MES	C7-C8-S-O1S
9	B	504	MES	C7-C8-S-O2S
9	B	504	MES	C7-C8-S-O3S
5	A	501	GTP	PB-O3B-PG-O1G
5	A	501	GTP	PB-O3B-PG-O2G
5	A	501	GTP	PB-O3B-PG-O3G
11	F	401	ACP	PB-O3A-PA-O2A
5	A	501	GTP	C5'-O5'-PA-O3A

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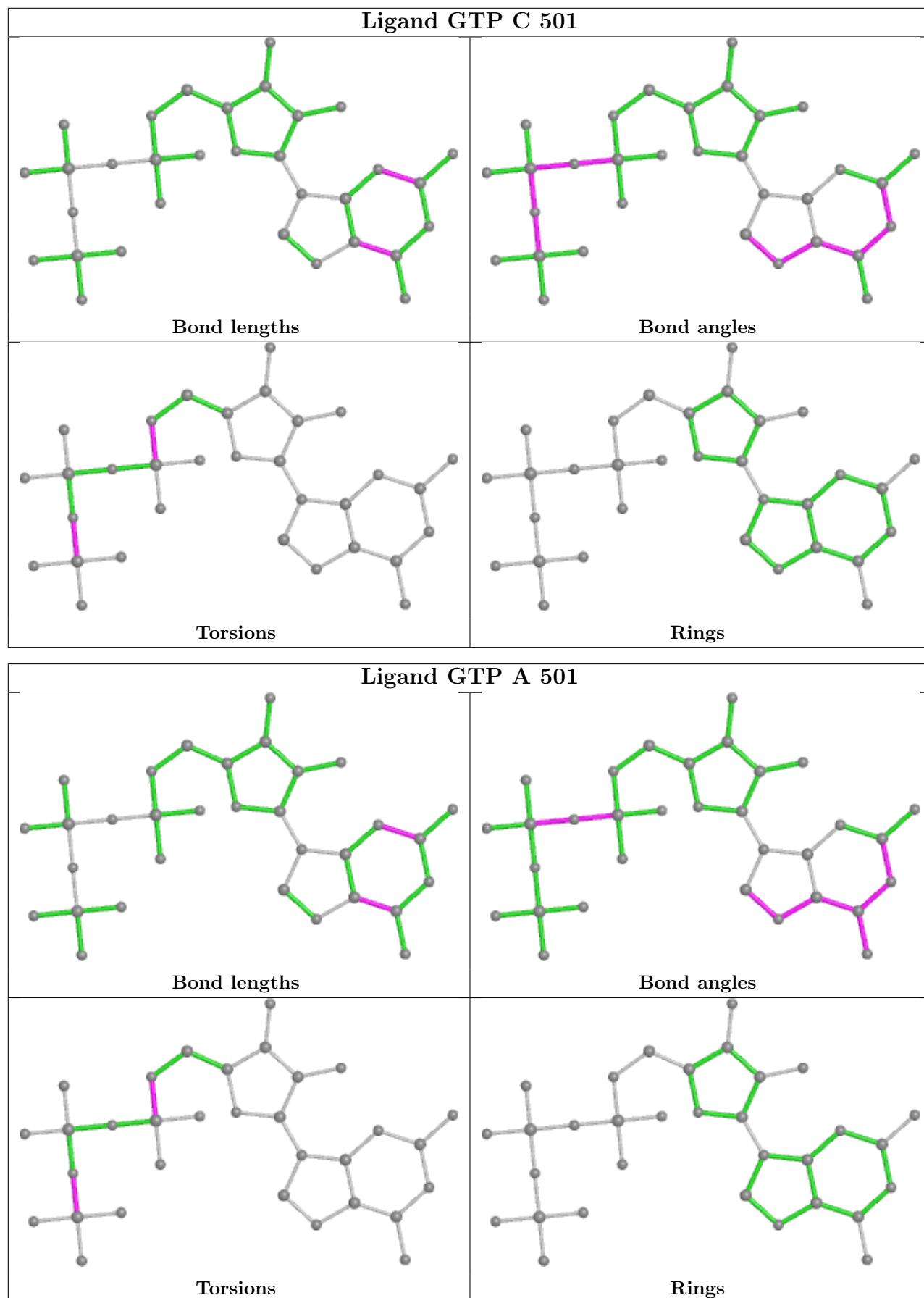
Mol	Chain	Res	Type	Atoms
5	C	501	GTP	C5'-O5'-PA-O3A
8	B	501	GDP	C5'-O5'-PA-O3A
11	F	401	ACP	C5'-O5'-PA-O3A
10	B	505	AWD	O1-C6-N2-C4

There are no ring outliers.

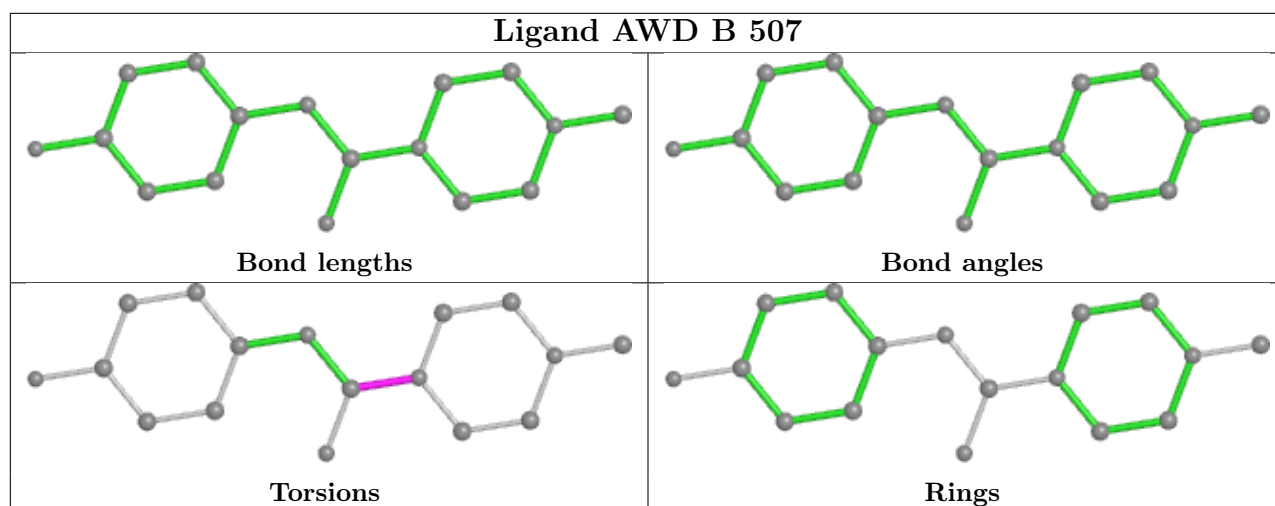
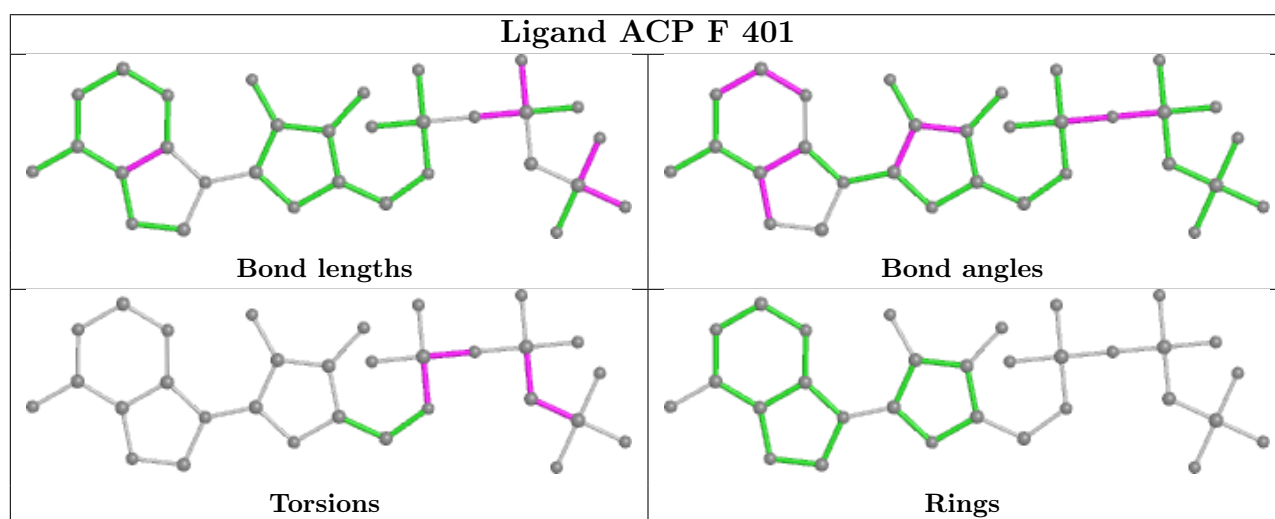
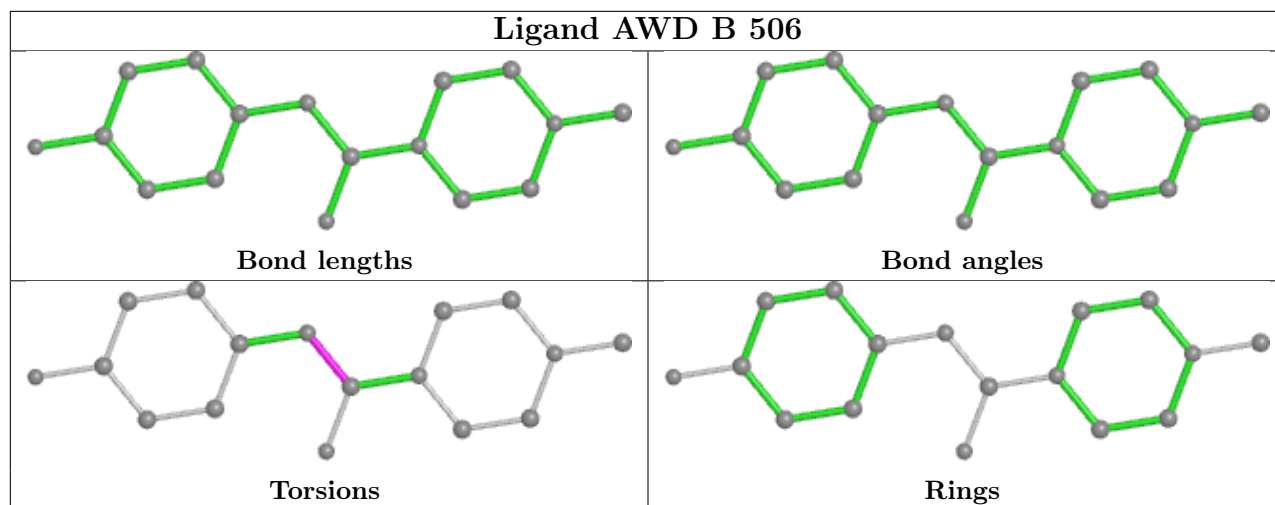
8 monomers are involved in 22 short contacts:

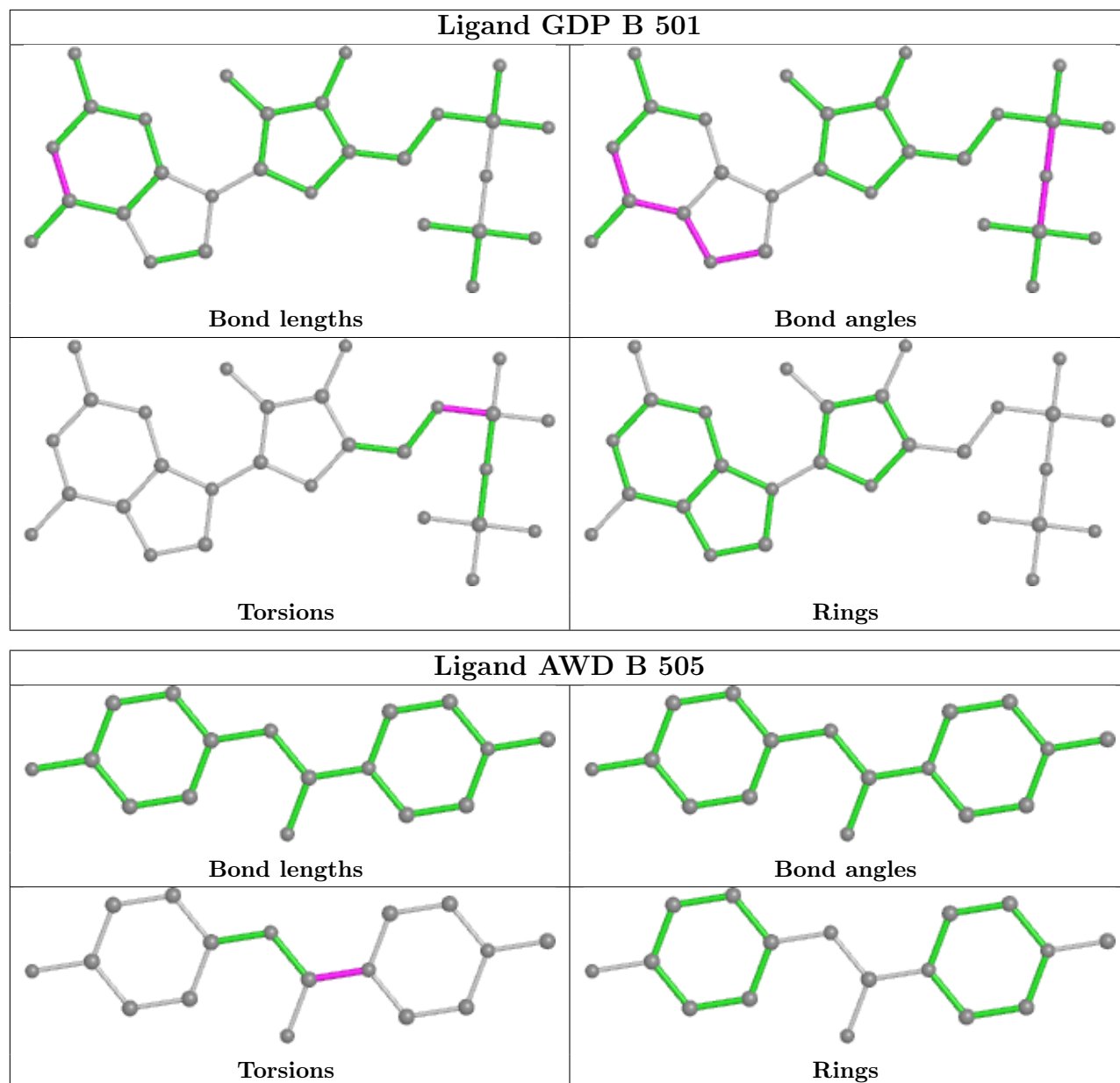
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	501	GTP	1	0
5	A	501	GTP	2	0
11	F	401	ACP	3	0
10	B	507	AWD	1	0
9	B	504	MES	3	0
8	B	501	GDP	4	0
10	B	505	AWD	4	0
8	D	501	GDP	4	0

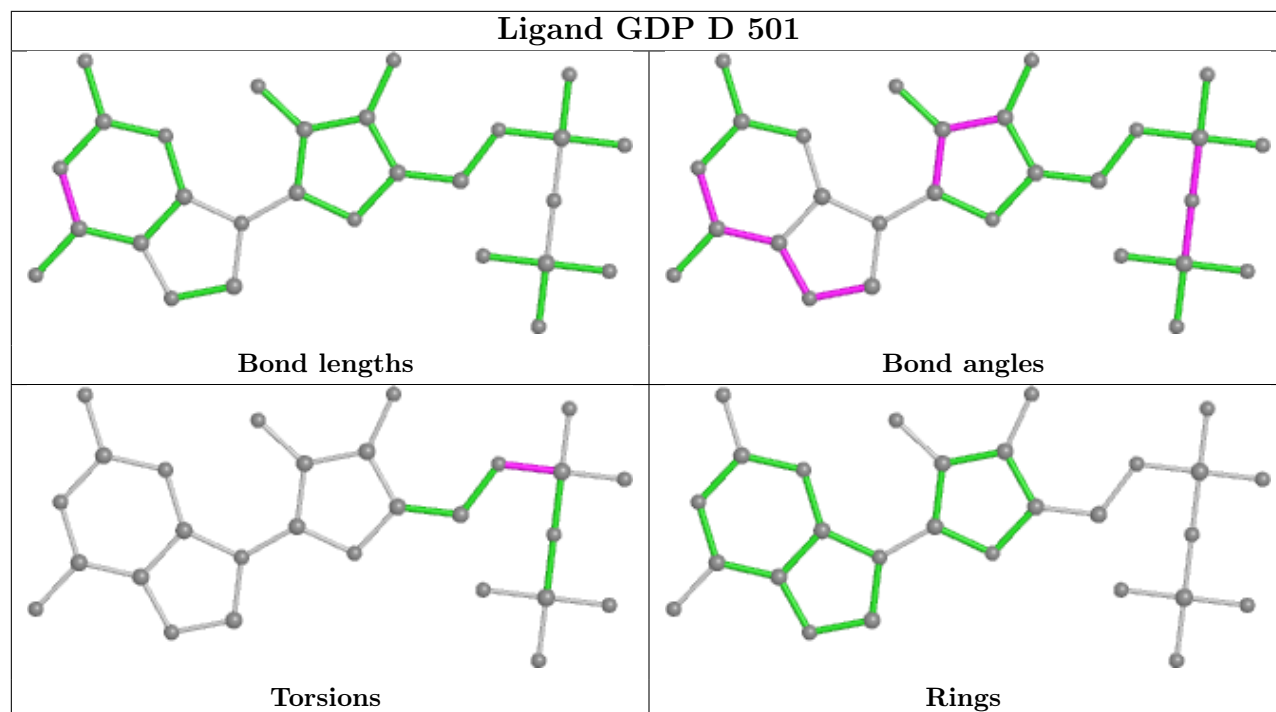
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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	438/451 (97%)	0.44	28 (6%) 19 22	57, 79, 117, 190	0
1	C	440/451 (97%)	0.44	9 (2%) 65 72	47, 62, 85, 131	0
2	B	423/445 (95%)	0.55	13 (3%) 49 56	51, 73, 122, 174	2 (0%)
2	D	422/445 (94%)	0.60	44 (10%) 6 8	63, 90, 127, 152	5 (1%)
3	E	123/143 (86%)	0.59	11 (8%) 9 11	62, 92, 136, 166	0
4	F	348/384 (90%)	1.14	75 (21%) 0 0	72, 105, 167, 186	0
All	All	2194/2319 (94%)	0.61	180 (8%) 11 14	47, 82, 137, 190	7 (0%)

All (180) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	143	GLU	9.3
4	F	169	LEU	7.1
2	D	275	LEU	6.4
2	D	285	ALA	6.3
2	D	272	PHE	6.1
2	B	303	ALA	5.8
4	F	240	LEU	5.6
4	F	152	SER	5.5
4	F	142	ARG	5.4
4	F	179	VAL	5.1
4	F	173	ILE	5.1
2	D	387	LEU	5.1
4	F	315	PHE	4.9
4	F	181	VAL	4.9
2	D	218	LYS	4.8
4	F	131	PHE	4.7
4	F	314	LEU	4.7
4	F	186	LEU	4.7
4	F	283	ILE	4.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	179	THR	4.4
4	F	177	GLY	4.4
4	F	346	LEU	4.3
3	E	6	MET	4.2
1	A	78	VAL	4.2
4	F	147	TRP	4.2
4	F	182	ILE	4.2
1	A	282	TYR	4.2
2	D	216	THR	4.0
3	E	22	VAL	3.9
1	A	351	PHE	3.8
2	D	418	PHE	3.8
3	E	27	PRO	3.8
1	A	86	LEU	3.8
4	F	99	VAL	3.7
4	F	317	PHE	3.6
4	F	132	LEU	3.6
1	A	346	TRP	3.6
2	D	293	GLN	3.6
4	F	144	GLY	3.6
4	F	149	ALA	3.6
1	A	93	ILE	3.5
4	F	101	TYR	3.5
4	F	376	ILE	3.5
4	F	295	LEU	3.4
4	F	267	PHE	3.4
4	F	98	TYR	3.4
4	F	285	LEU	3.4
2	D	401	ARG	3.4
3	E	116	LEU	3.4
2	D	215	ARG	3.4
4	F	39	LEU	3.3
4	F	137	ARG	3.3
4	F	172	PHE	3.3
2	D	286	LEU	3.3
2	D	371	LEU	3.2
2	D	195	VAL	3.2
4	F	161	LEU	3.2
3	E	24	LEU	3.2
4	F	327	VAL	3.2
4	F	206	LEU	3.2
4	F	371	PRO	3.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
4	F	17	VAL	3.1
2	D	294	GLN	3.1
4	F	284	LEU	3.1
2	D	299	LYS	3.1
4	F	138	ARG	3.1
4	F	380	HIS	3.0
2	D	296	PHE	3.0
4	F	330	ILE	3.0
2	D	177	VAL	3.0
4	F	320	MET	3.0
3	E	25	LYS	3.0
1	C	357	TYR	3.0
1	A	430	LYS	3.0
3	E	26	PRO	3.0
4	F	134	ALA	3.0
2	D	274	PRO	2.9
4	F	178	GLN	2.9
2	B	65	ALA	2.9
3	E	120	LEU	2.9
2	B	1	MET	2.8
2	D	191	VAL	2.8
1	A	68	VAL	2.7
2	B	246	GLY	2.7
2	B	154	ILE	2.7
4	F	4	PHE	2.7
4	F	213	ILE	2.7
4	F	343	TYR	2.7
3	E	28	SER	2.7
2	B	59	ASN	2.7
1	A	118	VAL	2.6
1	A	67	PHE	2.6
2	D	208	ALA	2.6
2	D	219	LEU	2.6
4	F	44	ARG	2.6
1	A	341	ILE	2.6
2	D	308	ARG	2.6
4	F	141	GLY	2.6
2	D	304	ALA	2.5
4	F	105	LEU	2.5
4	F	205	VAL	2.5
4	F	233	PHE	2.5
1	A	88	HIS	2.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
4	F	298	ILE	2.5
4	F	153	ALA	2.5
1	C	131	GLY	2.5
1	A	438	ASP	2.5
4	F	100	ILE	2.5
1	A	283	HIS	2.4
4	F	73	ARG	2.4
4	F	342	LEU	2.4
1	A	436	GLY	2.4
2	D	369	ARG	2.4
2	D	203	CYS	2.4
2	B	52	TYR	2.4
4	F	32	LYS	2.4
1	C	302	MET	2.4
1	C	339	ARG	2.4
4	F	183	GLN	2.4
2	D	305	CYS	2.4
4	F	221	LEU	2.4
2	D	248	LEU	2.4
1	A	149	PHE	2.3
1	A	115	ILE	2.3
1	C	335	ILE	2.3
4	F	151	SER	2.3
4	F	211	TYR	2.3
2	D	78	VAL	2.3
2	D	1	MET	2.3
1	A	332	ILE	2.3
2	B	305	CYS	2.3
4	F	139	ARG	2.3
2	D	87	PHE	2.3
4	F	184	LYS	2.3
4	F	321	VAL	2.2
4	F	375	PHE	2.2
1	A	378	LEU	2.2
2	D	428	LEU	2.2
3	E	122	ARG	2.2
4	F	341	LYS	2.2
4	F	216	TYR	2.2
1	A	66	VAL	2.2
2	D	141	LEU	2.2
2	D	301	MET	2.2
2	D	217	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	136	LEU	2.2
2	B	337	ASN	2.2
4	F	271	LEU	2.2
1	A	262	TYR	2.2
1	C	215	ARG	2.2
1	C	276	ILE	2.2
2	D	377	PHE	2.2
2	D	241	CYS	2.2
3	E	47	LEU	2.2
4	F	328	TRP	2.2
2	B	296	PHE	2.2
2	D	230	LEU	2.2
1	C	282	TYR	2.1
1	A	141	PHE	2.1
4	F	20	LEU	2.1
4	F	353	VAL	2.1
1	C	341	ILE	2.1
4	F	201	ILE	2.1
2	B	42	LEU	2.1
2	B	87	PHE	2.1
2	D	302	MET	2.1
1	A	328	VAL	2.1
2	D	57	THR	2.1
4	F	324	GLU	2.1
2	D	358	ILE	2.1
4	F	104	ASN	2.1
1	A	349	THR	2.1
2	B	51	VAL	2.0
1	A	132	LEU	2.0
2	D	354	ALA	2.0
2	D	415	GLU	2.0
4	F	18	SER	2.0
2	D	360	PRO	2.0
1	A	18	ASN	2.0
2	D	154	ILE	2.0

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

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



### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 6.4 Ligands [i](#)

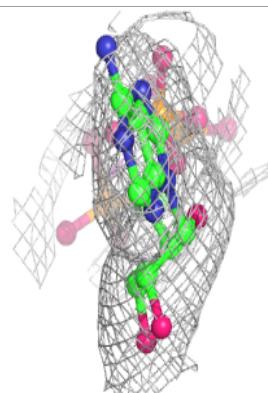
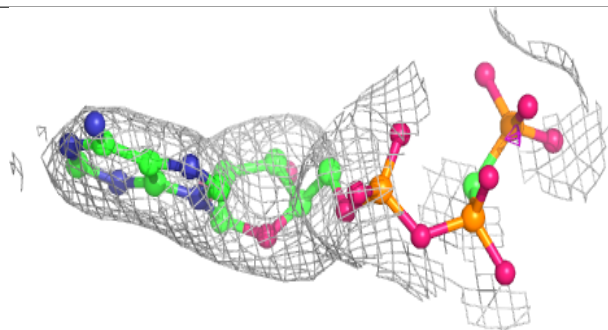
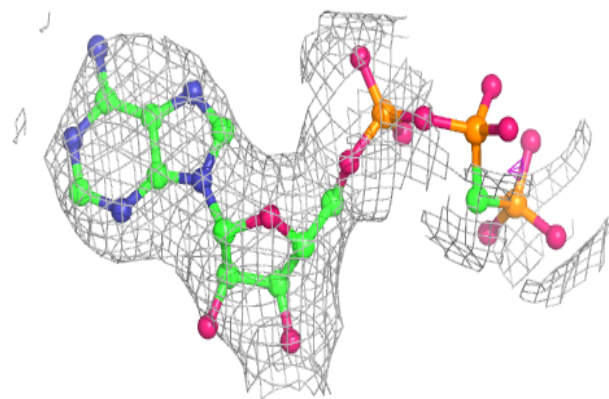
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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	0.32	0.52	183,189,199,200	0
7	CA	A	504	1/1	0.80	0.15	110,110,110,110	0
7	CA	A	503	1/1	0.80	0.14	134,134,134,134	0
6	MG	B	502	1/1	0.82	0.18	89,89,89,89	0
11	ACP	F	401	31/31	0.85	0.16	117,128,134,136	0
7	CA	B	503	1/1	0.86	0.28	114,114,114,114	0
6	MG	D	502	1/1	0.87	0.22	92,92,92,92	0
10	AWD	B	506	17/17	0.89	0.18	59,73,86,86	0
10	AWD	B	507	17/17	0.91	0.26	54,64,71,77	33
6	MG	F	402	1/1	0.92	0.06	120,120,120,120	0
8	GDP	D	501	28/28	0.95	0.17	81,88,101,103	0
10	AWD	B	505	17/17	0.96	0.15	54,67,78,82	33
7	CA	C	503	1/1	0.96	0.16	80,80,80,80	0
5	GTP	A	501	32/32	0.97	0.15	57,63,68,70	0
6	MG	A	502	1/1	0.98	0.11	62,62,62,62	0
5	GTP	C	501	32/32	0.98	0.19	45,54,59,60	0
8	GDP	B	501	28/28	0.98	0.21	48,58,62,64	0
6	MG	C	502	1/1	0.99	0.14	55,55,55,55	0

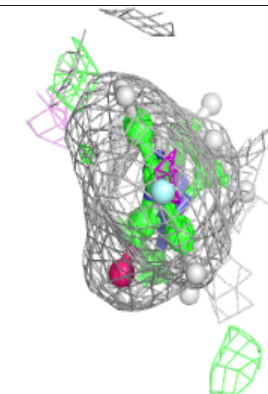
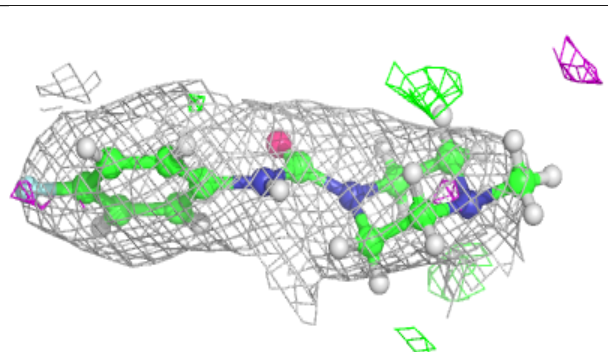
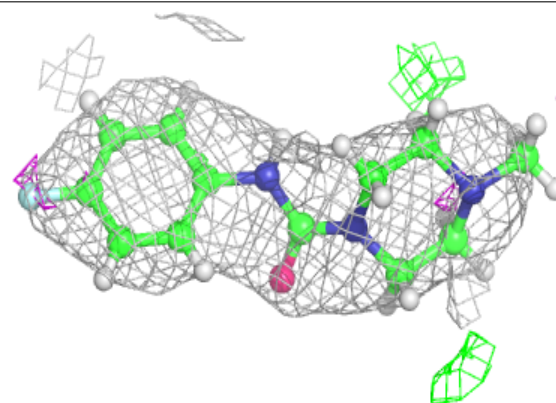
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

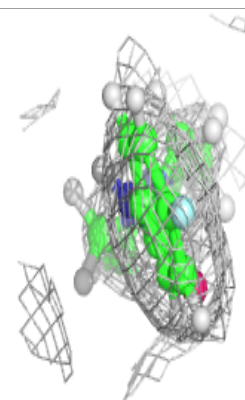
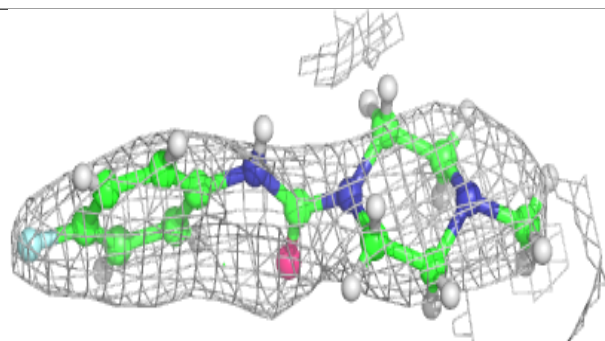
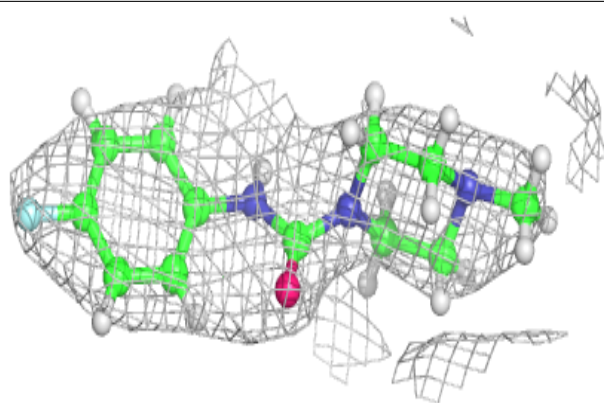
**Electron density around AWD B 506:**

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

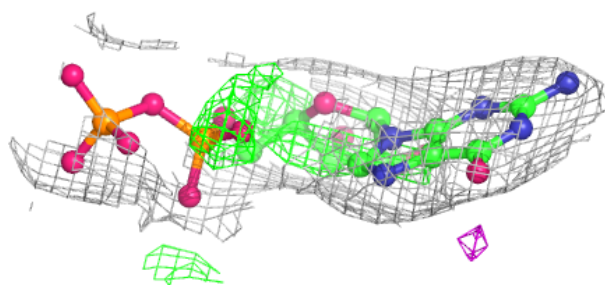
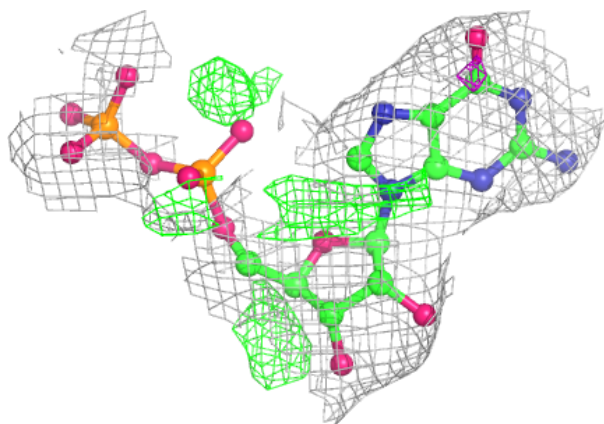


**Electron density around AWD B 507:**

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

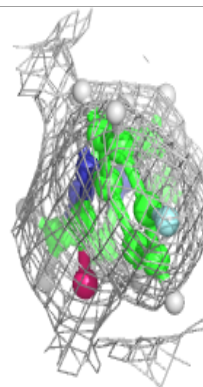
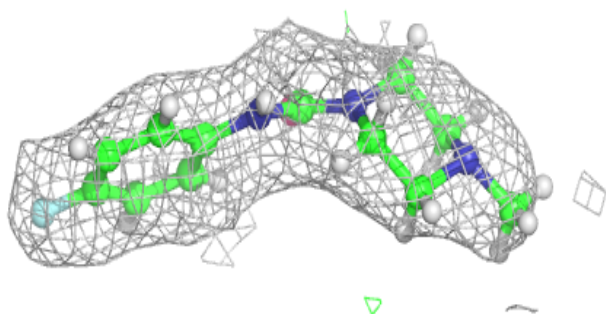
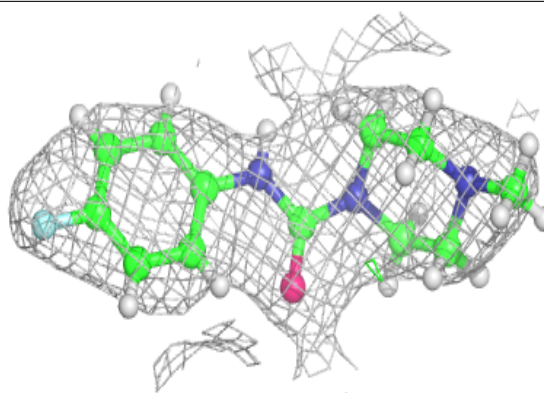
**Electron density around GDP D 501:**

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

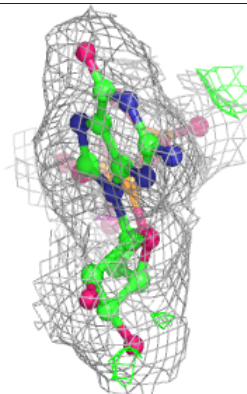
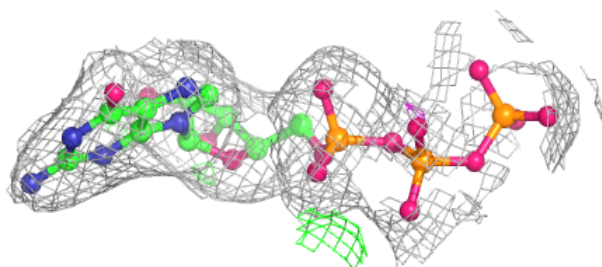
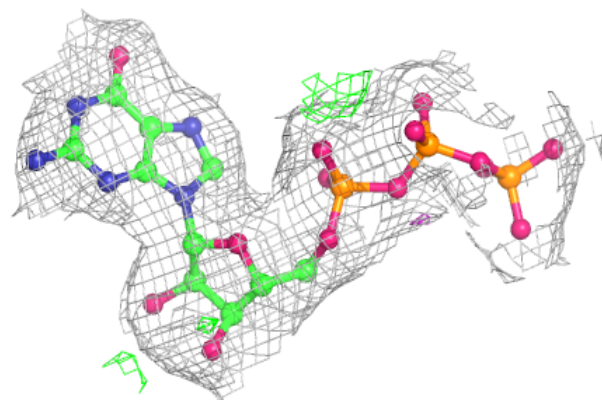


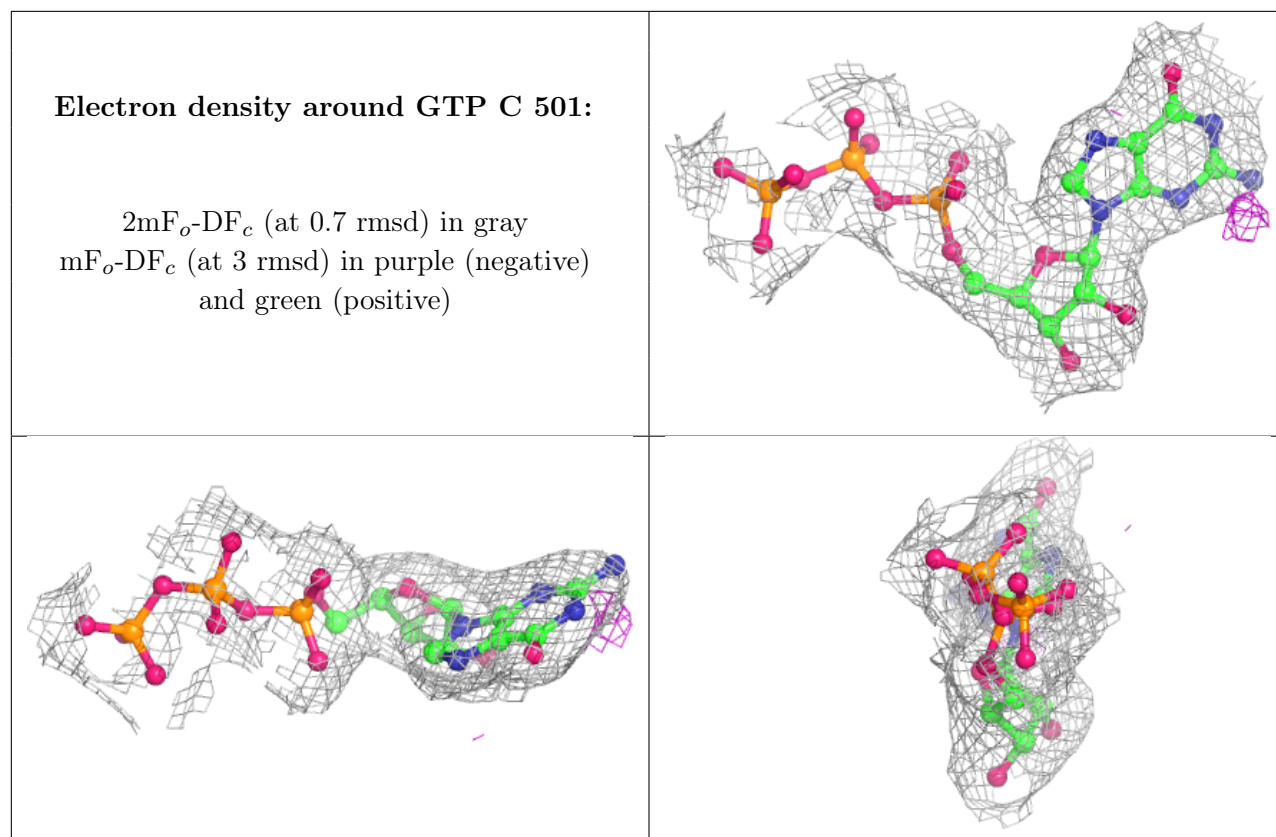
**Electron density around AWD B 505:**

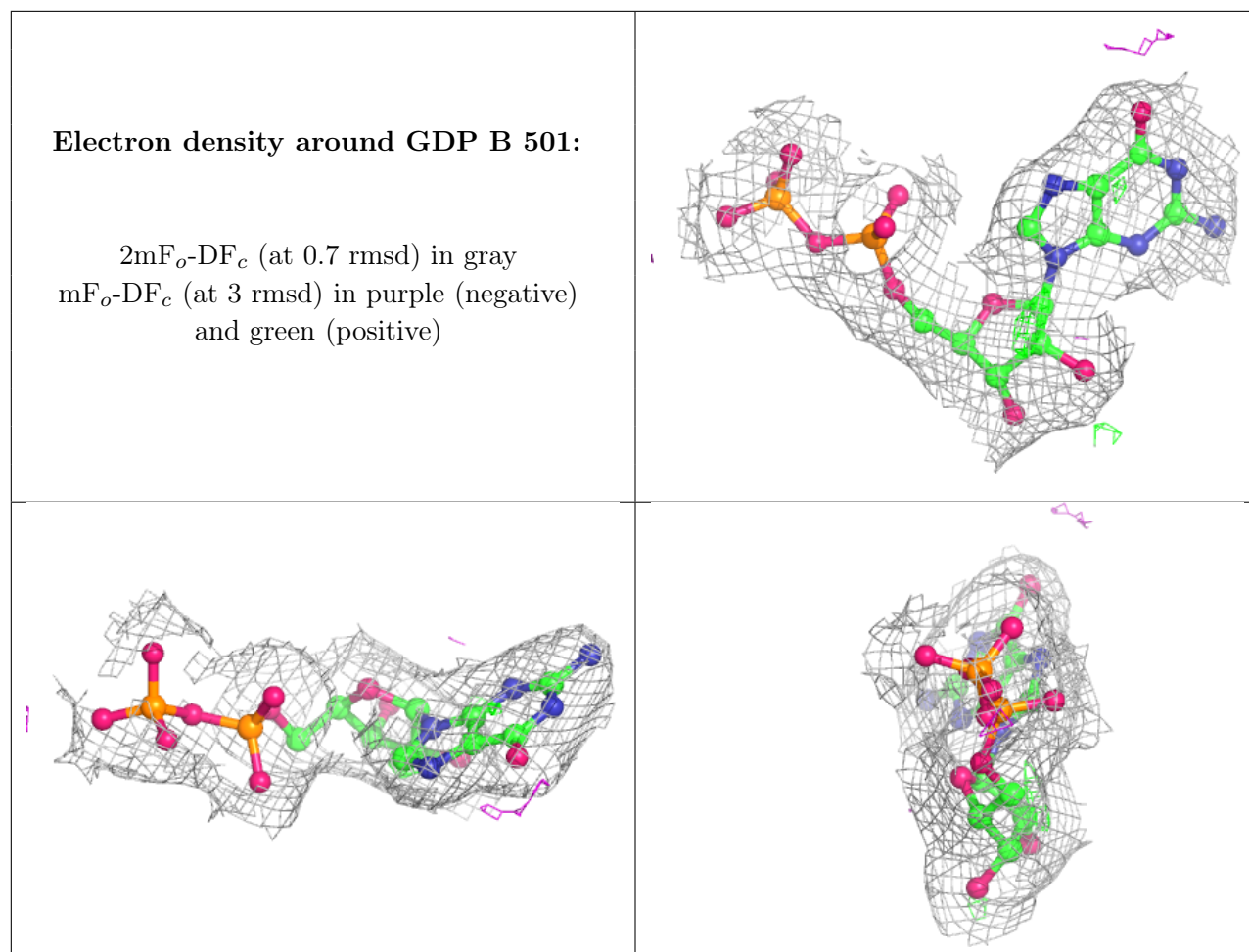
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around 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.