



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 21, 2021 – 12:06 PM EDT

PDB ID : 5S5A  
Title : Tubulin-Z1449748885-complex  
Authors : Muehlethaler, T.; Gioia, D.; Protá, A.E.; Sharpe, M.E.; Cavalli, A.; Steinmetz, M.O.  
Deposited on : 2020-11-08  
Resolution : 2.35 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.20  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.20

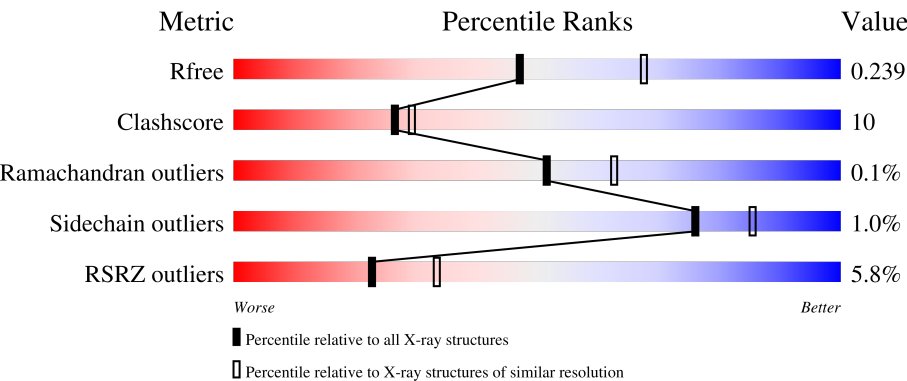
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.35 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.




Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R <sub>free</sub>	130704	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

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

Mol	Chain	Length	Quality of chain
1	A	451	<div><div>3%</div><div><div></div><div></div><div></div><div></div></div><div>73%24%..</div></div>
1	C	451	<div><div>3%</div><div><div></div><div></div><div></div><div></div></div><div>77%20%.</div></div>
2	B	445	<div><div>4%</div><div><div></div><div></div><div></div><div></div></div><div>76%21%.</div></div>
2	D	445	<div><div>5%</div><div><div></div><div></div><div></div><div></div></div><div>73%24%..</div></div>
3	E	143	<div><div>9%</div><div><div></div><div></div><div></div><div></div></div><div>69%17%14%</div></div>

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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

There are 12 unique types of molecules in this entry. The entry contains 18104 atoms, of which 52 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Tubulin alpha-1B chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	438	Total	C	N	O	S	0	0	0
			3424	2167	582	653	22			
1	C	440	Total	C	N	O	S	0	1	0
			3443	2178	585	657	23			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	428	Total	C	N	O	S	1	1	0
			3376	2119	580	650	27			
2	D	431	Total	C	N	O	S	5	0	0
			3368	2113	575	653	27			

- Molecule 3 is a protein called Stathmin-4.

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	352	Total	C	N	O	S	0	0	0
			2877	1843	495	525	14			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	379	HIS	-	expression tag	UNP E1BQ43
F	380	HIS	-	expression tag	UNP E1BQ43
F	381	HIS	-	expression tag	UNP E1BQ43
F	382	HIS	-	expression tag	UNP E1BQ43
F	383	HIS	-	expression tag	UNP E1BQ43
F	384	HIS	-	expression tag	UNP E1BQ43

- Molecule 5 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula:  $C_{10}H_{16}N_5O_{14}P_3$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
5	C	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

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

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

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	F	1	Total	Mg	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>).



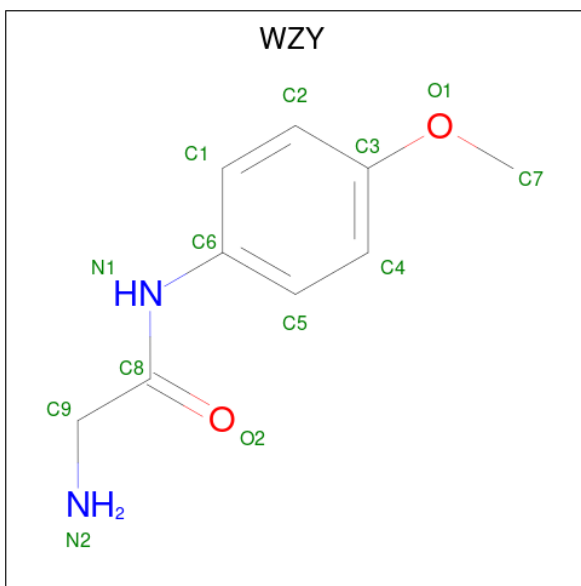
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	B	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
8	D	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- 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
9	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 10 is N-(4-methoxyphenyl)glycinamide (three-letter code: WZY) (formula:  $C_9H_{12}N_2O_2$ ) (labeled as "Ligand of Interest" by depositor).



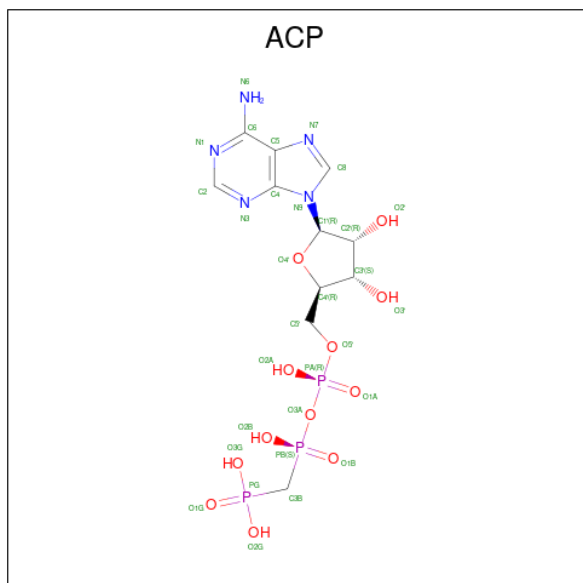
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	B	1	Total	C	H	N	O	0	0
			26	9	13	2	2		
10	C	1	Total	C	H	N	O	0	0
			26	9	13	2	2		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	D	1	Total	C	H	N	O	0	0
			26	9	13	2	2		
10	E	1	Total	C	H	N	O	0	0
			26	9	13	2	2		

- 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.

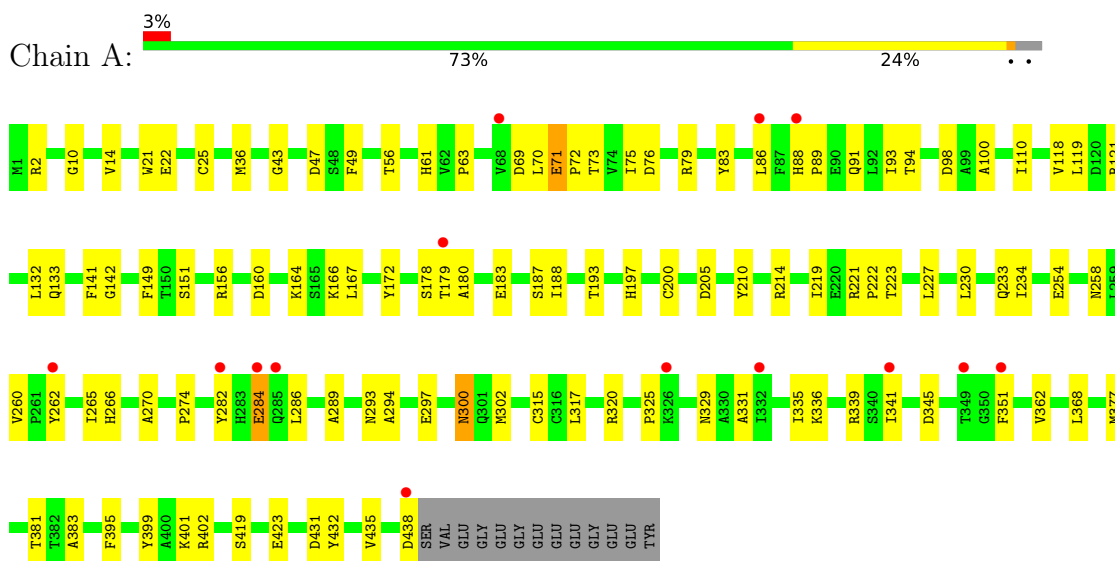
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	58	Total	O	0	0
			58	58		
12	B	62	Total	O	0	0
			62	62		
12	C	160	Total	O	0	0
			160	160		
12	D	30	Total	O	0	0
			30	30		
12	E	11	Total	O	0	0
			11	11		
12	F	5	Total	O	0	0
			5	5		



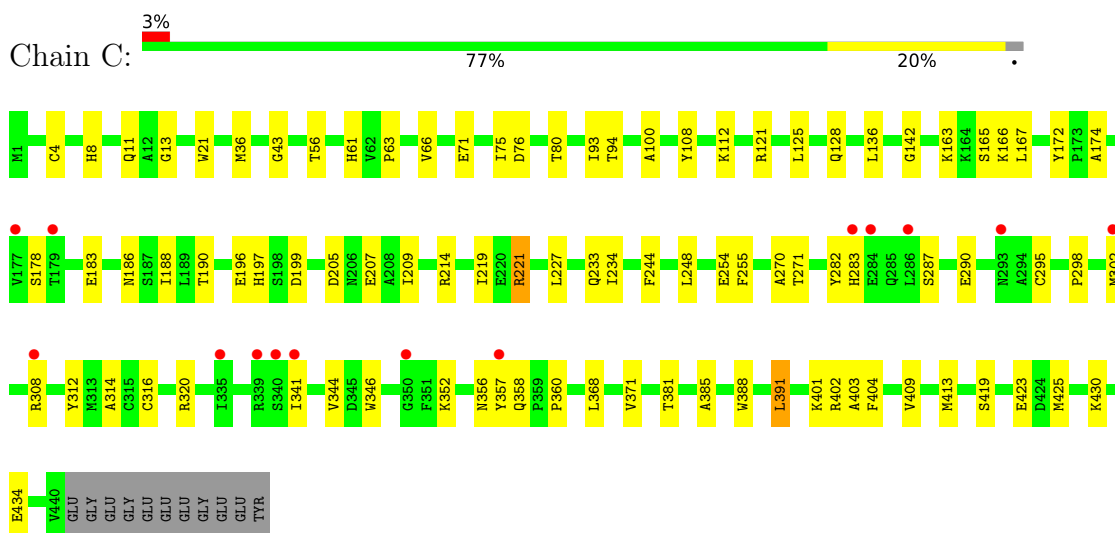
### 3 Residue-property plots [i](#)

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

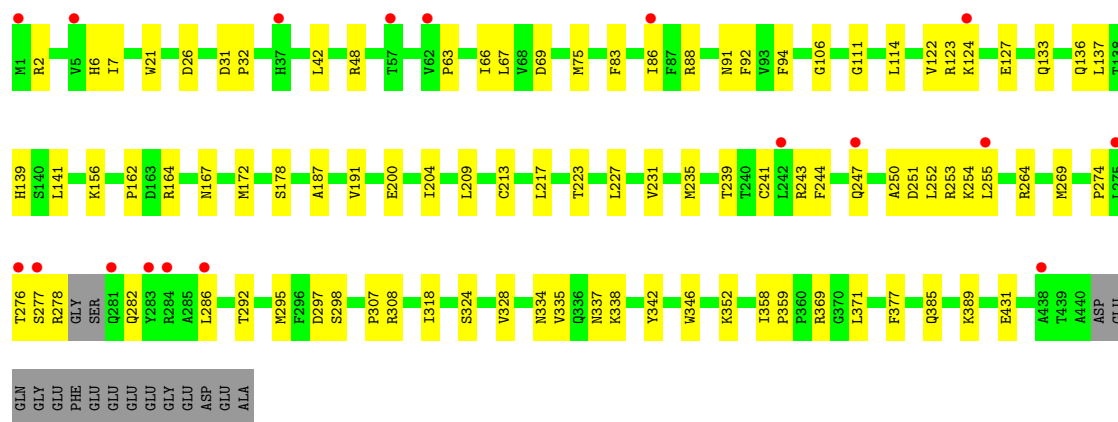


- Molecule 1: Tubulin alpha-1B chain

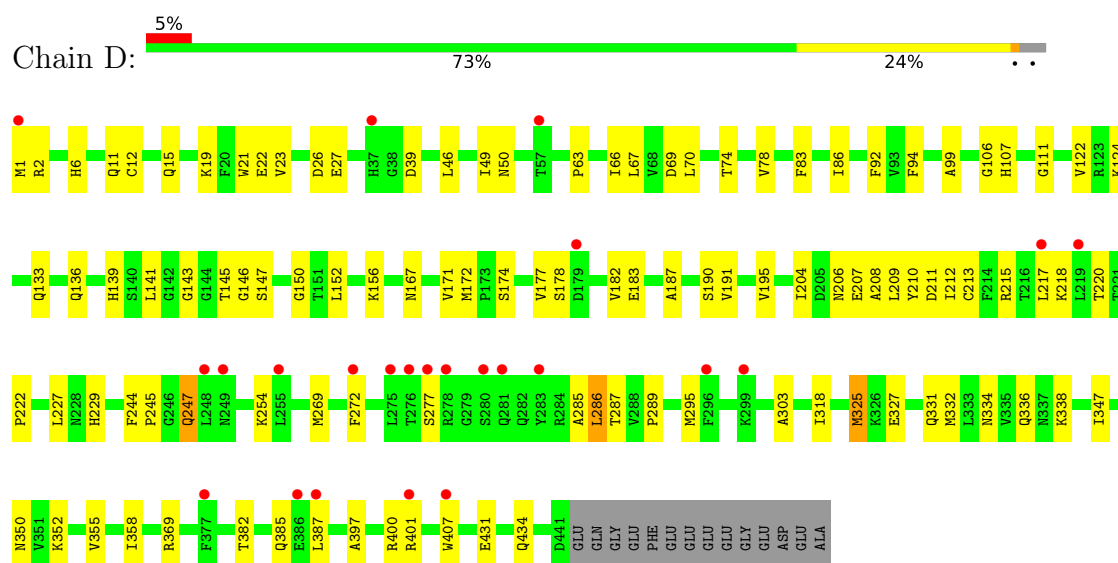


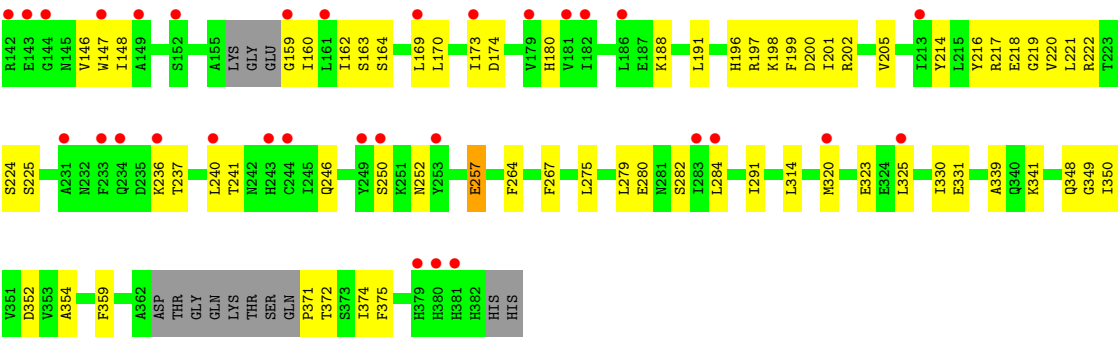
- Molecule 2: Tubulin beta-2B chain





• Molecule 2: Tubulin beta-2B chain





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	104.59Å 158.16Å 179.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	63.08 – 2.35 118.67 – 2.35	Depositor EDS
% Data completeness (in resolution range)	99.8 (63.08-2.35) 99.8 (118.67-2.35)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.26 (at 2.34Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, $R_{free}$	0.205 , 0.237 0.206 , 0.239	Depositor DCC
$R_{free}$ test set	6345 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	60.2	Xtriage
Anisotropy	0.256	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 50.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	18104	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.56% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GDP, MES, ACP, GTP, WZY, MG, 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	0/3502	0.42	0/4754
1	C	0.26	0/3521	0.43	0/4780
2	B	0.25	0/3450	0.42	0/4671
2	D	0.25	0/3442	0.41	0/4664
3	E	0.25	0/1022	0.35	0/1356
4	F	0.24	0/2944	0.40	0/3978
All	All	0.25	0/17881	0.41	0/24203

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3424	0	3334	81	0
1	C	3443	0	3352	68	0
2	B	3376	0	3252	70	0
2	D	3368	0	3236	80	0
3	E	1014	0	1029	16	0
4	F	2877	0	2839	60	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	3	0
9	B	12	0	12	3	0
10	B	13	13	0	1	0
10	C	13	13	0	0	0
10	D	13	13	0	0	0
10	E	13	13	0	0	0
11	F	31	0	14	2	0
12	A	58	0	0	3	0
12	B	62	0	0	3	0
12	C	160	0	0	4	0
12	D	30	0	0	4	0
12	E	11	0	0	2	0
12	F	5	0	0	0	0
All	All	18052	52	17116	358	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 10.

All (358) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:381:THR:HG22	1:A:383:ALA:H	1.20	1.07
1:C:221:ARG:HG3	2:D:325:MET:HG2	1.37	1.06
4:F:102:PRO:HG2	4:F:105:LEU:HD13	1.47	0.93
1:C:209:ILE:HD11	1:C:302:MET:CE	2.04	0.88
4:F:236:LYS:HB3	4:F:240:LEU:HD13	1.58	0.84
1:C:209:ILE:HG22	1:C:227:LEU:HD22	1.61	0.83
1:A:297:GLU:HB2	1:A:300:ASN:HD21	1.43	0.82
1:A:71:GLU:OE2	1:A:73:THR:OG1	1.97	0.82
2:B:167:ASN:OD1	2:B:200:GLU:HB2	1.79	0.82
1:A:335:ILE:HG23	1:A:339:ARG:HG3	1.61	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:217:LEU:HA	2:D:277:SER:HB3	1.63	0.80
4:F:241:THR:OG1	11:F:401:ACP:O3'	1.98	0.80
1:A:294:ALA:O	1:A:300:ASN:ND2	2.18	0.76
1:A:300:ASN:OD1	12:A:601:HOH:O	2.02	0.76
2:D:334:ASN:HD21	2:D:338:LYS:HE3	1.51	0.76
4:F:10:ASN:HB2	4:F:44:ARG:HH22	1.51	0.76
1:C:76:ASP:O	1:C:80:THR:HG22	1.87	0.74
1:C:270:ALA:O	1:C:302:MET:HG2	1.89	0.73
1:C:209:ILE:HD11	1:C:302:MET:HE3	1.69	0.73
2:D:177:VAL:HG21	2:D:206:ASN:HB3	1.71	0.72
2:D:347:ILE:HG22	2:D:350:ASN:HB3	1.71	0.72
2:D:136:GLN:HA	2:D:167:ASN:O	1.89	0.71
4:F:197:ARG:NH1	4:F:257:GLU:OE2	2.24	0.71
1:C:209:ILE:HD11	1:C:302:MET:HE1	1.71	0.70
2:D:83:PHE:O	2:D:86:ILE:HG22	1.93	0.69
1:A:71:GLU:HG2	1:A:72:PRO:HD2	1.75	0.69
1:C:312:TYR:CD1	1:C:341:ILE:HG23	2.27	0.69
2:D:431:GLU:OE1	12:D:601:HOH:O	2.10	0.68
1:C:234:ILE:HD13	1:C:302:MET:SD	2.33	0.68
4:F:102:PRO:HG2	4:F:105:LEU:CD1	2.23	0.68
2:B:83:PHE:O	2:B:86:ILE:HG22	1.94	0.68
4:F:331:GLU:OE2	11:F:401:ACP:O3G	2.12	0.68
1:A:179:THR:HA	2:B:352:LYS:HD2	1.75	0.67
1:A:75:ILE:HD12	1:A:94:THR:HG22	1.77	0.66
1:A:88:HIS:CD2	1:A:91:GLN:HG3	2.31	0.66
2:D:11:GLN:O	2:D:15:GLN:HG2	1.96	0.66
4:F:371:PRO:HA	4:F:372:THR:HB	1.77	0.66
4:F:348:GLN:NE2	4:F:352:ASP:OD1	2.28	0.66
2:D:434:GLN:OE1	12:D:602:HOH:O	2.14	0.65
2:B:2:ARG:HB2	2:B:133:GLN:CG	2.27	0.65
2:B:69:ASP:O	2:B:94:PHE:HA	1.98	0.64
2:B:67:LEU:HD22	2:B:92:PHE:CE2	2.33	0.64
2:B:337:ASN:OD1	4:F:36:ARG:HD3	1.97	0.64
1:C:282:TYR:O	1:C:283:HIS:HB2	1.98	0.64
2:B:2:ARG:HB2	2:B:133:GLN:HG3	1.81	0.63
1:A:351:PHE:HE1	3:E:24:LEU:HD11	1.64	0.63
1:C:234:ILE:HD13	1:C:302:MET:CE	2.28	0.63
1:C:4[A]:CYS:SG	1:C:136:LEU:HG	2.39	0.63
2:B:274:PRO:HB3	2:B:286:LEU:HD22	1.81	0.62
4:F:371:PRO:HA	4:F:372:THR:O	1.99	0.62
2:B:204:ILE:HD13	2:B:231:VAL:HG13	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:254:GLU:HG2	1:C:352:LYS:HE2	1.80	0.62
2:D:397:ALA:HA	2:D:400:ARG:NH1	2.14	0.61
4:F:188:LYS:HD3	4:F:323:GLU:OE2	2.00	0.61
1:A:180:ALA:HB3	1:A:183:GLU:HG3	1.80	0.61
1:C:270:ALA:HB3	1:C:302:MET:HG3	1.82	0.61
2:D:215:ARG:O	2:D:218:LYS:HE3	2.00	0.61
1:C:320:ARG:HA	1:C:356:ASN:O	2.01	0.60
1:A:2:ARG:HB2	1:A:133:GLN:HE21	1.66	0.60
1:C:221:ARG:CG	2:D:325:MET:HG2	2.24	0.60
2:D:325:MET:CE	2:D:355:VAL:HG21	2.32	0.60
2:D:285:ALA:O	2:D:286:LEU:HB2	2.02	0.59
4:F:246:GLN:O	4:F:250:SER:HB3	2.01	0.59
2:B:253[A]:ARG:NH1	9:B:504:MES:O2S	2.35	0.59
2:D:21:TRP:CZ3	2:D:63:PRO:HB3	2.37	0.59
2:D:147:SER:HB2	2:D:190:SER:OG	2.02	0.59
4:F:280:GLU:OE1	4:F:284:LEU:HD23	2.02	0.59
1:A:166:LYS:HE2	1:A:197:HIS:O	2.03	0.58
1:C:172:TYR:HB3	1:C:205:ASP:HA	1.85	0.58
2:D:70:LEU:HD12	2:D:99:ALA:HB2	1.85	0.58
1:A:36:MET:HB3	1:A:61:HIS:CE1	2.39	0.58
2:D:334:ASN:ND2	2:D:338:LYS:HE3	2.18	0.58
1:A:71:GLU:HG2	1:A:72:PRO:CD	2.33	0.58
2:B:324:SER:O	2:B:328:VAL:HG23	2.04	0.58
2:D:325:MET:HE1	2:D:355:VAL:HG21	1.86	0.57
4:F:371:PRO:CA	4:F:372:THR:HB	2.33	0.57
2:B:136:GLN:HA	2:B:167:ASN:O	2.03	0.57
1:C:298:PRO:HG2	1:C:308:ARG:NH2	2.20	0.57
4:F:314:LEU:HD22	4:F:350:ILE:HD11	1.87	0.57
1:A:335:ILE:CG2	1:A:339:ARG:HG3	2.32	0.57
1:C:93:ILE:HD11	1:C:121:ARG:HG3	1.86	0.57
2:D:69:ASP:O	2:D:94:PHE:HA	2.04	0.57
2:B:264:ARG:NE	2:B:431:GLU:OE2	2.36	0.56
1:A:233:GLN:HG3	1:A:368:LEU:HD12	1.85	0.56
1:A:431:ASP:O	1:A:435:VAL:HG23	2.05	0.56
1:C:165:SER:HA	1:C:199:ASP:OD2	2.05	0.56
2:D:2:ARG:HB3	2:D:133:GLN:CG	2.35	0.56
1:A:69:ASP:O	1:A:94:THR:HA	2.05	0.56
2:B:292:THR:HG22	2:B:335:VAL:HG21	1.88	0.56
1:A:43:GLY:HA2	1:A:56:THR:O	2.06	0.56
4:F:128:ARG:NH2	4:F:174:ASP:OD1	2.39	0.56
2:B:31:ASP:HB2	2:B:32:PRO:CD	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:205:VAL:HG21	4:F:291:ILE:HD13	1.89	0.55
1:A:223:THR:HB	2:B:247:GLN:HE22	1.72	0.55
1:C:214:ARG:HG2	1:C:219:ILE:O	2.07	0.55
2:D:152:LEU:O	2:D:156:LYS:HG2	2.07	0.55
2:B:278:ARG:HG2	2:B:282:GLN:NE2	2.21	0.55
4:F:220:VAL:HG11	4:F:339:ALA:HB2	1.89	0.55
2:D:12:CYS:HB2	8:D:501:GDP:C8	2.41	0.55
4:F:200:ASP:OD1	4:F:222:ARG:HB2	2.06	0.55
1:C:8:HIS:HB3	1:C:13:GLY:O	2.07	0.55
1:A:88:HIS:HB2	1:A:89:PRO:HD2	1.89	0.55
4:F:371:PRO:HA	4:F:372:THR:C	2.27	0.55
2:B:231:VAL:O	2:B:235:MET:HG3	2.08	0.54
4:F:236:LYS:HB3	4:F:240:LEU:CD1	2.32	0.54
1:C:75:ILE:HD12	1:C:94:THR:HG22	1.87	0.54
2:B:164:ARG:O	9:B:504:MES:H31	2.07	0.54
1:A:172:TYR:HB3	1:A:205:ASP:HA	1.88	0.54
1:C:172:TYR:CE2	1:C:391:LEU:HD22	2.43	0.54
1:C:271:THR:HG21	1:C:295:CYS:O	2.07	0.54
1:A:93:ILE:HD11	1:A:121:ARG:HG3	1.89	0.54
2:D:213:CYS:O	2:D:217:LEU:HB2	2.08	0.54
2:D:287:THR:HB	2:D:289:PRO:HD2	1.88	0.54
2:D:397:ALA:O	2:D:401:ARG:NH1	2.41	0.54
1:A:188:ILE:HD12	1:A:395:PHE:CD2	2.43	0.54
1:C:21:TRP:CZ3	1:C:63:PRO:HB3	2.43	0.54
2:D:2:ARG:HB3	2:D:133:GLN:HG2	1.89	0.54
4:F:216:TYR:CE2	4:F:218:GLU:HB2	2.43	0.53
4:F:214:TYR:HB3	4:F:375:PHE:HB3	1.90	0.53
1:C:11:GLN:HE22	2:D:247:GLN:NE2	2.06	0.53
2:B:308:ARG:HA	2:B:342:TYR:CE1	2.44	0.53
1:A:71:GLU:HG3	2:B:2:ARG:NH2	2.24	0.53
2:B:141:LEU:HD12	2:B:172:MET:SD	2.49	0.53
1:A:233:GLN:HG3	1:A:368:LEU:CD1	2.37	0.53
2:D:22:GLU:HG2	2:D:83:PHE:CD1	2.44	0.53
4:F:159:GLY:C	4:F:160:ILE:HD12	2.30	0.53
4:F:350:ILE:O	4:F:354:ALA:HB3	2.09	0.53
1:A:100:ALA:HA	2:B:254:LYS:HG3	1.91	0.52
1:C:360:PRO:HG2	1:C:371:VAL:HG23	1.90	0.52
4:F:14:TYR:HB3	4:F:41:LEU:HD13	1.89	0.52
4:F:100:ILE:HD12	4:F:128:ARG:HA	1.90	0.52
4:F:217:ARG:NH2	4:F:374:ILE:HA	2.24	0.52
2:D:106:GLY:O	2:D:111:GLY:HA3	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:146:GLY:O	2:D:150:GLY:HA3	2.10	0.52
2:B:295:MET:CG	2:B:377:PHE:HB2	2.39	0.52
1:A:21:TRP:CZ3	1:A:63:PRO:HB3	2.44	0.52
3:E:12:ASN:HB3	12:E:307:HOH:O	2.09	0.52
3:E:128:LYS:O	3:E:128:LYS:HD3	2.09	0.52
1:A:419:SER:O	1:A:423:GLU:HG3	2.10	0.52
2:D:46:LEU:HA	2:D:49:ILE:HB	1.92	0.52
2:D:187:ALA:O	2:D:191:VAL:HG23	2.10	0.52
3:E:45:PRO:HA	3:E:49:GLU:OE1	2.10	0.52
1:C:186:ASN:O	1:C:190:THR:HG22	2.10	0.51
2:D:69:ASP:HA	2:D:145:THR:HG21	1.91	0.51
1:A:98:ASP:HB2	5:A:501:GTP:O2G	2.10	0.51
2:D:332:MET:O	2:D:336:GLN:HG3	2.10	0.51
2:B:75:MET:HE3	2:B:92:PHE:HD2	1.73	0.51
1:C:174:ALA:HB1	1:C:207:GLU:HB2	1.92	0.51
2:D:19:LYS:O	2:D:23:VAL:HG23	2.10	0.51
2:D:204:ILE:HG22	2:D:209:LEU:HD11	1.93	0.51
2:D:211:ASP:O	2:D:215:ARG:HB2	2.10	0.51
3:E:85:LYS:NZ	12:E:304:HOH:O	2.43	0.51
2:D:269:MET:HG3	2:D:303:ALA:HB3	1.92	0.50
2:D:327:GLU:O	2:D:331:GLN:HG2	2.10	0.50
2:D:178:SER:HB3	2:D:183:GLU:OE2	2.11	0.50
2:B:385:GLN:OE1	2:B:389:LYS:HE3	2.11	0.50
1:C:166:LYS:HE2	1:C:197:HIS:O	2.12	0.50
1:C:174:ALA:CB	1:C:207:GLU:HB2	2.41	0.50
1:C:234:ILE:HD13	1:C:302:MET:HE1	1.92	0.50
4:F:146:VAL:HG22	4:F:164:SER:HB3	1.94	0.50
4:F:341:LYS:HG2	4:F:341:LYS:O	2.12	0.50
4:F:197:ARG:HB2	4:F:224:SER:O	2.12	0.50
1:A:76:ASP:OD1	1:A:79:ARG:NH1	2.44	0.49
1:A:151:SER:HB2	1:A:193:THR:OG1	2.11	0.49
2:D:26:ASP:OD2	2:D:369:ARG:HD2	2.11	0.49
1:A:88:HIS:NE2	1:A:91:GLN:HG3	2.27	0.49
2:B:123:ARG:O	2:B:127:GLU:HG3	2.13	0.49
2:B:213:CYS:HA	2:B:217:LEU:HD12	1.94	0.49
2:B:241:CYS:HB3	2:B:250:ALA:HB2	1.93	0.49
2:B:42:LEU:H	2:B:42:LEU:HD12	1.78	0.49
2:D:213:CYS:HA	2:D:217:LEU:HD12	1.94	0.49
1:A:320:ARG:HG3	12:A:646:HOH:O	2.11	0.49
2:B:178:SER:N	10:B:505:WZY:O2	2.27	0.49
1:C:234:ILE:CD1	1:C:302:MET:HE1	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:385:ALA:HA	1:C:388:TRP:CD1	2.48	0.49
2:D:1:MET:HG3	2:D:50:ASN:HB2	1.94	0.49
1:A:289:ALA:HA	1:A:331:ALA:HB1	1.95	0.49
4:F:198:LYS:HG2	4:F:199:PHE:H	1.76	0.49
1:A:142:GLY:HA3	1:A:183:GLU:OE2	2.13	0.49
1:C:233:GLN:HG3	1:C:368:LEU:CD1	2.42	0.49
1:C:36:MET:HB3	1:C:61:HIS:CE1	2.48	0.49
2:D:191:VAL:O	2:D:195:VAL:HG23	2.13	0.49
1:C:244:PHE:CD1	1:C:358:GLN:HG2	2.48	0.49
1:A:119:LEU:HD12	1:A:156:ARG:NH2	2.27	0.48
2:B:164:ARG:HD2	12:B:655:HOH:O	2.14	0.48
4:F:205:VAL:CG2	4:F:291:ILE:HD13	2.43	0.48
1:A:254:GLU:HG2	1:A:258:ASN:ND2	2.29	0.48
2:D:318:ILE:N	2:D:318:ILE:HD12	2.28	0.48
1:A:214:ARG:HG2	1:A:219:ILE:O	2.13	0.48
2:B:106:GLY:O	2:B:111:GLY:HA3	2.13	0.48
1:C:66:VAL:HG23	1:C:125:LEU:CD1	2.44	0.48
1:A:345:ASP:HB3	3:E:28:SER:HB2	1.94	0.48
1:C:221:ARG:HG3	2:D:325:MET:CG	2.26	0.48
1:C:136:LEU:HD23	1:C:167:LEU:HB2	1.96	0.48
4:F:162:ILE:HD11	4:F:240:LEU:HD11	1.95	0.48
2:D:67:LEU:N	2:D:67:LEU:HD12	2.28	0.47
2:D:208:ALA:O	2:D:212:ILE:HG13	2.13	0.47
1:A:317:LEU:HD23	1:A:377:MET:HG3	1.96	0.47
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.32	0.47
1:C:287:SER:OG	1:C:290:GLU:HG3	2.14	0.47
2:D:124:LYS:C	2:D:124:LYS:HD3	2.34	0.47
12:B:629:HOH:O	1:C:163:LYS:HD2	2.14	0.47
1:C:108:TYR:O	1:C:112:LYS:HG2	2.14	0.47
1:C:196:GLU:HG2	12:C:663:HOH:O	2.15	0.47
2:D:382:THR:O	2:D:385:GLN:HG2	2.14	0.47
2:B:297:ASP:OD1	2:B:298:SER:N	2.47	0.47
2:D:107:HIS:O	2:D:152:LEU:HD22	2.14	0.47
4:F:163:SER:HB3	4:F:169:LEU:HD21	1.96	0.47
1:C:430:LYS:HE2	1:C:434:GLU:OE2	2.15	0.47
1:A:336:LYS:HD2	1:A:341:ILE:HD12	1.96	0.47
4:F:147:TRP:HB2	4:F:169:LEU:HD11	1.97	0.47
1:A:71:GLU:HG2	1:A:72:PRO:N	2.29	0.47
1:A:293:ASN:OD1	1:A:339:ARG:NH2	2.47	0.47
1:A:325:PRO:HB3	3:E:20:PHE:CE1	2.50	0.47
2:B:318:ILE:N	2:B:318:ILE:HD12	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:72:LEU:O	3:E:76:ARG:HG2	2.14	0.47
4:F:147:TRP:HB2	4:F:169:LEU:CD1	2.45	0.47
1:A:118:VAL:HG21	1:A:149:PHE:CZ	2.50	0.47
2:D:141:LEU:HA	2:D:147:SER:HB3	1.97	0.47
4:F:191:LEU:HD13	4:F:196:HIS:CD2	2.50	0.47
1:C:270:ALA:HB3	1:C:302:MET:CG	2.45	0.46
2:D:145:THR:HB	8:D:501:GDP:O2B	2.15	0.46
1:C:401:LYS:NZ	12:C:608:HOH:O	2.47	0.46
2:D:143:GLY:HA3	8:D:501:GDP:O3A	2.16	0.46
1:A:381:THR:HG22	1:A:383:ALA:N	2.05	0.46
2:B:295:MET:HG3	2:B:377:PHE:HB2	1.98	0.46
1:C:419:SER:O	1:C:423:GLU:HG3	2.14	0.46
4:F:216:TYR:CZ	4:F:218:GLU:HB2	2.50	0.46
1:A:274:PRO:HB3	1:A:286:LEU:HD12	1.98	0.46
1:A:315:CYS:HG	1:A:351:PHE:HD2	1.62	0.46
1:C:142:GLY:HA3	1:C:183:GLU:OE1	2.16	0.46
2:B:114:LEU:O	2:B:114:LEU:HG	2.15	0.46
2:B:204:ILE:CG2	2:B:209:LEU:HD11	2.45	0.46
2:D:171:VAL:HA	2:D:204:ILE:O	2.16	0.46
4:F:101:TYR:N	4:F:126:ASP:OD1	2.31	0.46
2:B:26:ASP:OD1	2:B:369:ARG:NH2	2.49	0.46
1:C:178:SER:OG	2:D:352:LYS:NZ	2.49	0.46
1:C:205:ASP:HB3	1:C:302:MET:O	2.15	0.46
1:A:289:ALA:HA	1:A:331:ALA:CB	2.46	0.46
1:C:188:ILE:HG13	1:C:425:MET:HG3	1.97	0.46
2:D:6:HIS:CD2	2:D:21:TRP:HE1	2.34	0.46
1:A:297:GLU:HB2	1:A:300:ASN:ND2	2.22	0.45
1:A:141:PHE:HB3	1:A:187:SER:OG	2.16	0.45
1:A:438:ASP:OD1	1:A:438:ASP:N	2.49	0.45
1:A:10:GLY:O	1:A:14:VAL:HG23	2.15	0.45
2:D:141:LEU:HD12	2:D:172:MET:SD	2.56	0.45
4:F:100:ILE:CD1	4:F:128:ARG:HA	2.45	0.45
2:B:334:ASN:ND2	2:B:338:LYS:HD2	2.32	0.45
2:D:74:THR:O	2:D:78:VAL:HG23	2.17	0.45
2:D:244:PHE:CE1	2:D:358:ILE:HD12	2.52	0.45
4:F:2:TYR:O	4:F:27:TRP:HA	2.16	0.45
1:A:362:VAL:HG22	12:A:602:HOH:O	2.16	0.45
1:C:344:VAL:HG21	1:C:346:TRP:CE2	2.52	0.45
1:C:43:GLY:HA2	1:C:56:THR:O	2.17	0.45
1:C:401:LYS:O	1:C:402:ARG:HB2	2.17	0.45
3:E:101:LEU:O	3:E:105:MET:HG2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:31:ASP:HB2	2:B:32:PRO:HD2	1.98	0.45
4:F:202:ARG:HB3	4:F:220:VAL:CG2	2.47	0.45
2:B:67:LEU:N	2:B:67:LEU:HD12	2.32	0.44
3:E:92:ASN:O	3:E:96:MET:HG2	2.16	0.44
4:F:173:ILE:HD13	4:F:180:HIS:HB2	1.97	0.44
1:A:132:LEU:O	1:A:164:LYS:NZ	2.51	0.44
1:C:100:ALA:HA	2:D:254:LYS:HG3	1.98	0.44
2:D:347:ILE:CG2	2:D:350:ASN:HB3	2.45	0.44
1:A:335:ILE:HG23	1:A:339:ARG:CG	2.40	0.44
2:B:276:THR:HG22	2:B:277:SER:O	2.18	0.44
2:B:334:ASN:HD21	2:B:338:LYS:HD2	1.83	0.44
1:C:255:PHE:CD1	1:C:316:CYS:HB3	2.53	0.44
1:A:22:GLU:HG3	1:A:83:TYR:HE1	1.82	0.43
2:D:210:TYR:CE2	2:D:222:PRO:HG2	2.53	0.43
1:A:234:ILE:HD12	1:A:234:ILE:N	2.33	0.43
4:F:267:PHE:CE2	4:F:279:LEU:HD13	2.53	0.43
1:A:118:VAL:HG21	1:A:149:PHE:HZ	1.83	0.43
1:A:21:TRP:CE3	1:A:63:PRO:HB3	2.53	0.43
1:A:25:CYS:SG	1:A:86:LEU:HD11	2.59	0.43
2:D:66:ILE:HD12	2:D:122:VAL:HG22	2.01	0.43
2:D:220:THR:O	2:D:222:PRO:HD3	2.18	0.43
4:F:282:SER:HB2	4:F:325:LEU:HD13	2.00	0.43
1:A:119:LEU:HD13	1:A:160:ASP:OD2	2.19	0.43
2:B:88:ARG:NH2	2:B:124:LYS:HE3	2.33	0.43
2:D:295:MET:HE2	2:D:295:MET:HB2	1.73	0.43
4:F:148:ILE:HD11	4:F:160:ILE:HG21	2.00	0.43
2:D:325:MET:HE1	2:D:355:VAL:CG2	2.49	0.43
2:B:42:LEU:HD12	2:B:42:LEU:N	2.34	0.43
4:F:201:ILE:HG12	4:F:221:LEU:HG	2.00	0.43
1:A:70:LEU:HD13	1:A:110:ILE:HG21	2.00	0.43
2:B:124:LYS:HD3	2:B:124:LYS:C	2.39	0.43
2:B:278:ARG:HG2	2:B:282:GLN:HE22	1.83	0.43
2:D:1:MET:HB3	2:D:1:MET:HE3	1.89	0.43
2:B:359:PRO:HB2	2:B:371:LEU:O	2.18	0.42
1:C:75:ILE:HB	1:C:94:THR:CG2	2.48	0.42
1:A:284:GLU:CD	1:A:284:GLU:H	2.21	0.42
1:C:174:ALA:HB2	1:C:207:GLU:N	2.35	0.42
2:D:177:VAL:HG11	2:D:206:ASN:ND2	2.34	0.42
2:B:223:THR:O	2:B:227:LEU:HD13	2.20	0.42
2:B:244:PHE:CD1	2:B:358:ILE:HD12	2.54	0.42
2:D:182:VAL:HG11	2:D:407:TRP:CE3	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:213:CYS:HA	2:D:217:LEU:HB2	2.02	0.42
1:A:210:TYR:CE1	1:A:222:PRO:HD2	2.55	0.42
2:B:7:ILE:O	2:B:137:LEU:HA	2.20	0.42
1:A:260:VAL:HG11	1:A:266:HIS:HB3	2.02	0.42
2:D:19:LYS:HE3	12:D:620:HOH:O	2.19	0.42
1:A:47:ASP:HB2	1:A:49:PHE:CE2	2.55	0.42
1:A:329:ASN:HB3	3:E:6:MET:CE	2.49	0.42
2:B:66:ILE:HD12	2:B:122:VAL:HG22	2.02	0.42
2:B:156:LYS:HE3	12:B:641:HOH:O	2.19	0.42
2:B:200:GLU:OE2	2:B:255:LEU:HG	2.20	0.42
4:F:240:LEU:HD12	4:F:240:LEU:N	2.35	0.42
1:A:399:TYR:O	1:A:402:ARG:NH1	2.51	0.42
2:D:387:LEU:HD23	2:D:387:LEU:C	2.40	0.42
2:B:251:ASP:HB3	2:B:254:LYS:HB2	2.01	0.41
2:D:67:LEU:HD22	2:D:92:PHE:CE2	2.55	0.41
2:D:174:SER:OG	2:D:207:GLU:OE1	2.35	0.41
3:E:7:GLU:O	3:E:22:VAL:HA	2.20	0.41
3:E:123:LEU:O	3:E:126:LYS:HB2	2.21	0.41
1:A:223:THR:HB	2:B:247:GLN:NE2	2.34	0.41
3:E:44:ASP:HB3	3:E:45:PRO:HD2	2.03	0.41
4:F:2:TYR:CE1	4:F:359:PHE:HB3	2.55	0.41
4:F:237:THR:O	4:F:246:GLN:NE2	2.46	0.41
1:A:401:LYS:HG3	2:B:346:TRP:CE3	2.55	0.41
2:B:75:MET:HE3	2:B:92:PHE:CD2	2.53	0.41
2:B:123:ARG:HB2	2:B:123:ARG:CZ	2.51	0.41
1:C:409:VAL:HA	1:C:413:MET:O	2.21	0.41
1:A:167:LEU:HG	1:A:200:CYS:HB3	2.03	0.41
1:A:265:ILE:HG23	1:A:432:TYR:CE1	2.54	0.41
4:F:236:LYS:O	4:F:240:LEU:HD13	2.21	0.41
4:F:349:GLY:HA3	4:F:374:ILE:HD11	2.01	0.41
2:B:187:ALA:O	2:B:191:VAL:HG23	2.21	0.41
1:C:128:GLN:NE2	12:C:615:HOH:O	2.54	0.41
2:B:162:PRO:O	9:B:504:MES:H72	2.21	0.41
1:C:66:VAL:HG23	1:C:125:LEU:HD11	2.03	0.41
1:A:22:GLU:HG3	1:A:83:TYR:CE1	2.56	0.41
1:A:75:ILE:HD12	1:A:94:THR:CG2	2.49	0.41
2:B:133:GLN:OE1	2:B:252:LEU:HG	2.21	0.41
1:C:75:ILE:HB	1:C:94:THR:HG21	2.03	0.41
4:F:163:SER:HB3	4:F:169:LEU:CD2	2.50	0.41
4:F:320:MET:HG3	4:F:330:ILE:HD11	2.03	0.41
1:A:230:LEU:O	1:A:234:ILE:HD13	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:60:ARG:O	3:E:64:GLN:HG3	2.20	0.41
4:F:219:GLY:HA3	4:F:264:PHE:CZ	2.56	0.41
2:B:88:ARG:HD3	2:B:91:ASN:OD1	2.21	0.40
1:C:391:LEU:HD12	1:C:391:LEU:HA	1.90	0.40
2:B:269:MET:HE1	2:B:307:PRO:HG3	2.03	0.40
1:C:248:LEU:HD12	1:C:357:TYR:OH	2.21	0.40
2:B:63:PRO:HD2	2:B:86:ILE:O	2.21	0.40
1:C:403:ALA:O	1:C:404:PHE:HB2	2.21	0.40
2:D:213:CYS:SG	2:D:227:LEU:HD23	2.61	0.40
4:F:132:LEU:HD21	4:F:170:LEU:HD11	2.02	0.40
4:F:225:SER:O	4:F:252:ASN:HB2	2.21	0.40
1:A:223:THR:O	1:A:227:LEU:HG	2.22	0.40
2:B:88:ARG:CZ	2:B:124:LYS:HE3	2.52	0.40
2:B:239:THR:O	2:B:243:ARG:HG3	2.22	0.40
2:D:23:VAL:O	2:D:27:GLU:HG3	2.21	0.40
2:D:272:PHE:HE2	12:D:624:HOH:O	2.03	0.40
1:A:270:ALA:HB3	1:A:302:MET:CG	2.52	0.40
1:C:314:ALA:HB2	12:C:632:HOH:O	2.22	0.40
3:E:75:LYS:NZ	3:E:79:GLU:OE2	2.40	0.40
4:F:275:LEU:N	4:F:275:LEU:HD22	2.37	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%)	426 (98%)	10 (2%)	0	100	100
1	C	439/451 (97%)	429 (98%)	10 (2%)	0	100	100
2	B	425/445 (96%)	410 (96%)	15 (4%)	0	100	100
2	D	429/445 (96%)	413 (96%)	14 (3%)	2 (0%)	29	32

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	E	119/143 (83%)	119 (100%)	0	0	100	100
4	F	344/384 (90%)	327 (95%)	17 (5%)	0	100	100
All	All	2192/2319 (94%)	2124 (97%)	66 (3%)	2 (0%)	51	63

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	286	LEU
2	D	245	PRO

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	369/379 (97%)	362 (98%)	7 (2%)	57	68
1	C	372/379 (98%)	368 (99%)	4 (1%)	73	84
2	B	369/383 (96%)	367 (100%)	2 (0%)	88	94
2	D	368/383 (96%)	363 (99%)	5 (1%)	67	78
3	E	110/127 (87%)	110 (100%)	0	100	100
4	F	315/342 (92%)	314 (100%)	1 (0%)	92	96
All	All	1903/1993 (96%)	1884 (99%)	19 (1%)	76	85

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	GLU
1	A	178	SER
1	A	221	ARG
1	A	262	TYR
1	A	282	TYR
1	A	284	GLU
1	A	300	ASN
2	B	48	ARG

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Mol	Chain	Res	Type
2	B	139	HIS
1	C	71	GLU
1	C	221	ARG
1	C	381	THR
1	C	391	LEU
2	D	39	ASP
2	D	139	HIS
2	D	229	HIS
2	D	247	GLN
2	D	325	MET
4	F	257	GLU

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	300	ASN
2	B	15	GLN
2	B	247	GLN
2	B	282	GLN
2	B	294	GLN
1	C	11	GLN
2	D	294	GLN
2	D	300	ASN
4	F	180	HIS
4	F	229	ASN
4	F	269	GLN
4	F	333	ASN
4	F	348	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry

Of 19 ligands modelled in this entry, 9 are monoatomic - leaving 10 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	1.18	2 (8%)	31,47,47	1.93	7 (22%)
10	WZY	B	505	-	12,13,13	0.14	0	14,16,16	0.32	0
10	WZY	E	201	-	12,13,13	0.15	0	14,16,16	0.59	0
9	MES	B	504	-	12,12,12	2.27	1 (8%)	14,16,16	2.11	7 (50%)
10	WZY	C	504	-	12,13,13	0.13	0	14,16,16	0.42	0
8	GDP	B	501	6	24,30,30	1.14	2 (8%)	31,47,47	1.90	7 (22%)
5	GTP	C	501	6	26,34,34	0.98	1 (3%)	33,54,54	1.67	6 (18%)
5	GTP	A	501	6	26,34,34	0.99	1 (3%)	33,54,54	1.75	7 (21%)
11	ACP	F	401	6	27,33,33	1.42	5 (18%)	32,52,52	1.50	4 (12%)
10	WZY	D	503	-	12,13,13	0.14	0	14,16,16	0.44	0

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	-	6/12/32/32	0/3/3/3
10	WZY	B	505	-	-	4/8/8/8	0/1/1/1
10	WZY	E	201	-	-	0/8/8/8	0/1/1/1
9	MES	B	504	-	-	4/6/14/14	0/1/1/1
10	WZY	C	504	-	-	0/8/8/8	0/1/1/1
8	GDP	B	501	6	-	3/12/32/32	0/3/3/3
5	GTP	C	501	6	-	7/18/38/38	0/3/3/3
5	GTP	A	501	6	-	6/18/38/38	0/3/3/3
11	ACP	F	401	6	-	11/15/38/38	0/3/3/3
10	WZY	D	503	-	-	2/8/8/8	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	504	MES	C8-S	-7.55	1.66	1.77
8	D	501	GDP	C6-C5	4.13	1.48	1.41
8	B	501	GDP	C6-C5	4.01	1.48	1.41
5	A	501	GTP	C6-N1	3.19	1.38	1.33
5	C	501	GTP	C6-N1	3.11	1.38	1.33
11	F	401	ACP	PG-O2G	3.01	1.61	1.54
11	F	401	ACP	PB-O3A	3.01	1.61	1.58
11	F	401	ACP	PG-O3G	2.95	1.61	1.54
11	F	401	ACP	C5-C4	2.49	1.47	1.40
8	D	501	GDP	C5-C4	2.41	1.47	1.40
11	F	401	ACP	PB-O2B	2.28	1.61	1.56
8	B	501	GDP	C5-C4	2.27	1.46	1.40

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	501	GTP	N3-C2-N1	-5.39	120.03	127.22
5	C	501	GTP	N3-C2-N1	-5.03	120.52	127.22
8	D	501	GDP	C2-N3-C4	5.00	121.07	115.36
8	B	501	GDP	C2-N3-C4	4.86	120.91	115.36
9	B	504	MES	C5-N4-C3	4.23	118.36	108.83
5	A	501	GTP	C2-N3-C4	4.13	120.07	115.36
8	B	501	GDP	C6-C5-C4	-4.12	116.86	120.80
8	B	501	GDP	C6-N1-C2	4.07	122.39	115.93
8	D	501	GDP	C6-N1-C2	4.05	122.36	115.93
11	F	401	ACP	PA-O3A-PB	-4.00	119.89	132.56
8	D	501	GDP	C5-C6-N1	-3.98	117.99	123.43
8	D	501	GDP	C6-C5-C4	-3.85	117.12	120.80
8	B	501	GDP	C5-C6-N1	-3.84	118.17	123.43
5	C	501	GTP	C2-N3-C4	3.81	119.71	115.36
11	F	401	ACP	C3'-C2'-C1'	3.62	106.43	100.98
8	B	501	GDP	N3-C2-N1	-3.51	122.55	127.22
9	B	504	MES	C6-C5-N4	-3.47	104.83	110.10
8	D	501	GDP	N3-C2-N1	-3.37	122.72	127.22
11	F	401	ACP	N3-C2-N1	-3.23	123.63	128.68
5	C	501	GTP	C5-C6-N1	-3.18	119.08	123.43
5	A	501	GTP	C5-C6-N1	-3.00	119.33	123.43
8	D	501	GDP	PA-O3A-PB	-2.94	122.75	132.83
5	A	501	GTP	PA-O3A-PB	-2.87	122.98	132.83
5	C	501	GTP	PB-O3B-PG	-2.82	123.14	132.83
5	C	501	GTP	PA-O3A-PB	-2.80	123.22	132.83
8	D	501	GDP	C4-C5-N7	-2.78	106.50	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	501	GTP	PB-O3B-PG	-2.72	123.48	132.83
5	A	501	GTP	C6-N1-C2	2.69	120.20	115.93
8	B	501	GDP	C4-C5-N7	-2.68	106.61	109.40
8	B	501	GDP	PA-O3A-PB	-2.66	123.71	132.83
5	C	501	GTP	C6-N1-C2	2.57	120.01	115.93
11	F	401	ACP	C4-C5-N7	-2.56	106.73	109.40
9	B	504	MES	C7-N4-C5	2.31	117.14	111.23
9	B	504	MES	O1S-S-C8	2.28	109.67	106.92
9	B	504	MES	O3S-S-C8	2.26	109.42	105.77
5	A	501	GTP	N2-C2-N1	2.25	120.76	117.25
9	B	504	MES	C2-C3-N4	-2.22	106.74	110.10
9	B	504	MES	C7-N4-C3	2.17	116.79	111.23

There are no chirality outliers.

All (43) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	501	GTP	PB-O3B-PG-O2G
5	A	501	GTP	C5'-O5'-PA-O1A
5	A	501	GTP	C5'-O5'-PA-O2A
5	C	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O2A
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-O1S
10	B	505	WZY	N1-C8-C9-N2
10	B	505	WZY	O2-C8-C9-N2
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	C5'-O5'-PA-O2A
9	B	504	MES	C7-C8-S-O3S
10	D	503	WZY	O2-C8-C9-N2
10	D	503	WZY	N1-C8-C9-N2
5	C	501	GTP	PB-O3B-PG-O1G
8	D	501	GDP	PA-O3A-PB-O1B
11	F	401	ACP	C5'-O5'-PA-O3A
9	B	504	MES	C7-C8-S-O2S

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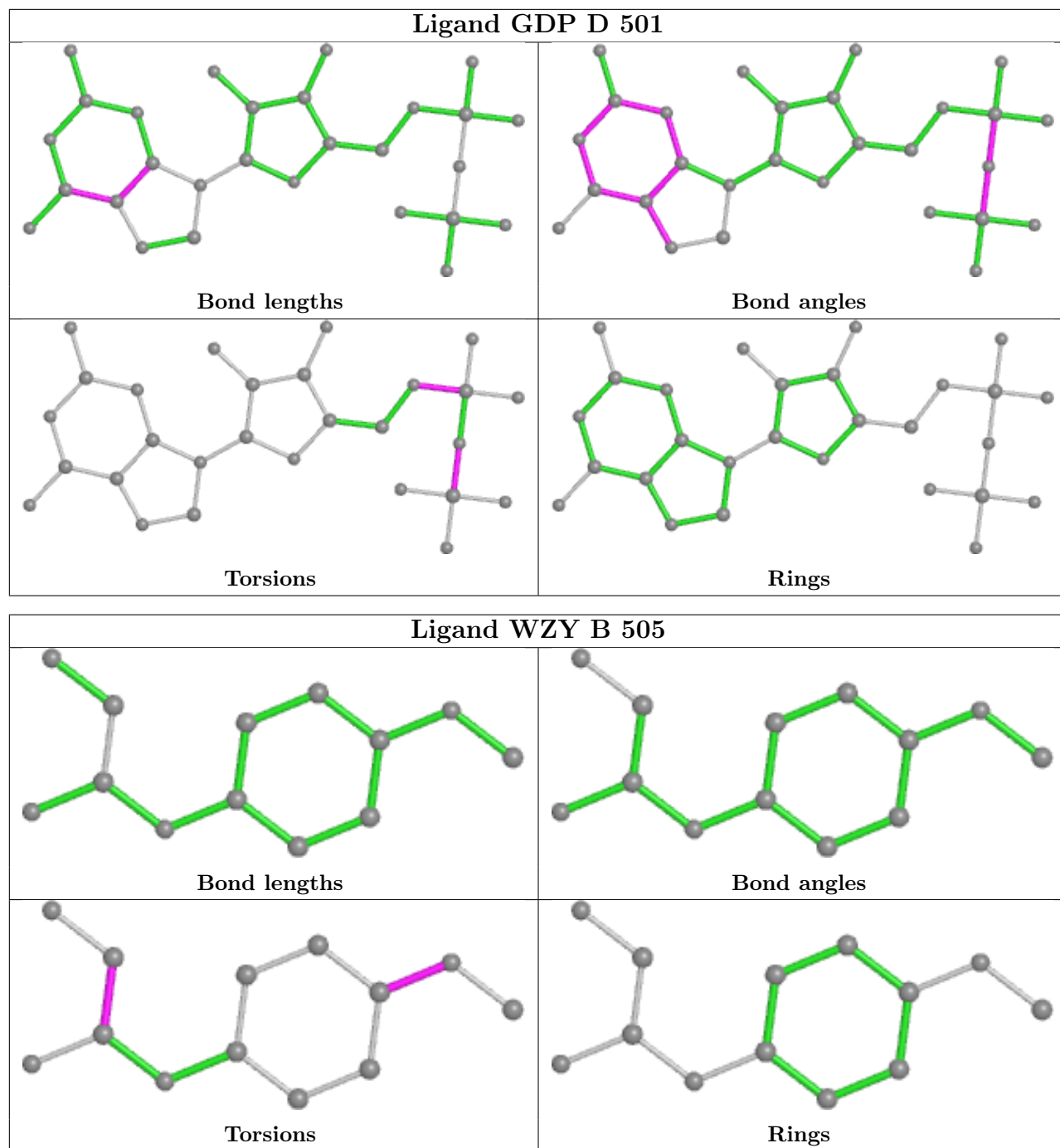
Mol	Chain	Res	Type	Atoms
11	F	401	ACP	PB-C3B-PG-O2G
11	F	401	ACP	PB-C3B-PG-O3G
5	A	501	GTP	C4'-C5'-O5'-PA
10	B	505	WZY	C4-C3-O1-C7
10	B	505	WZY	C2-C3-O1-C7
11	F	401	ACP	C3'-C4'-C5'-O5'
11	F	401	ACP	PB-C3B-PG-O1G
5	C	501	GTP	PB-O3B-PG-O2G
5	C	501	GTP	PB-O3B-PG-O3G
8	D	501	GDP	PA-O3A-PB-O2B
8	D	501	GDP	PA-O3A-PB-O3B
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	PB-O3A-PA-O2A
5	C	501	GTP	PB-O3A-PA-O2A

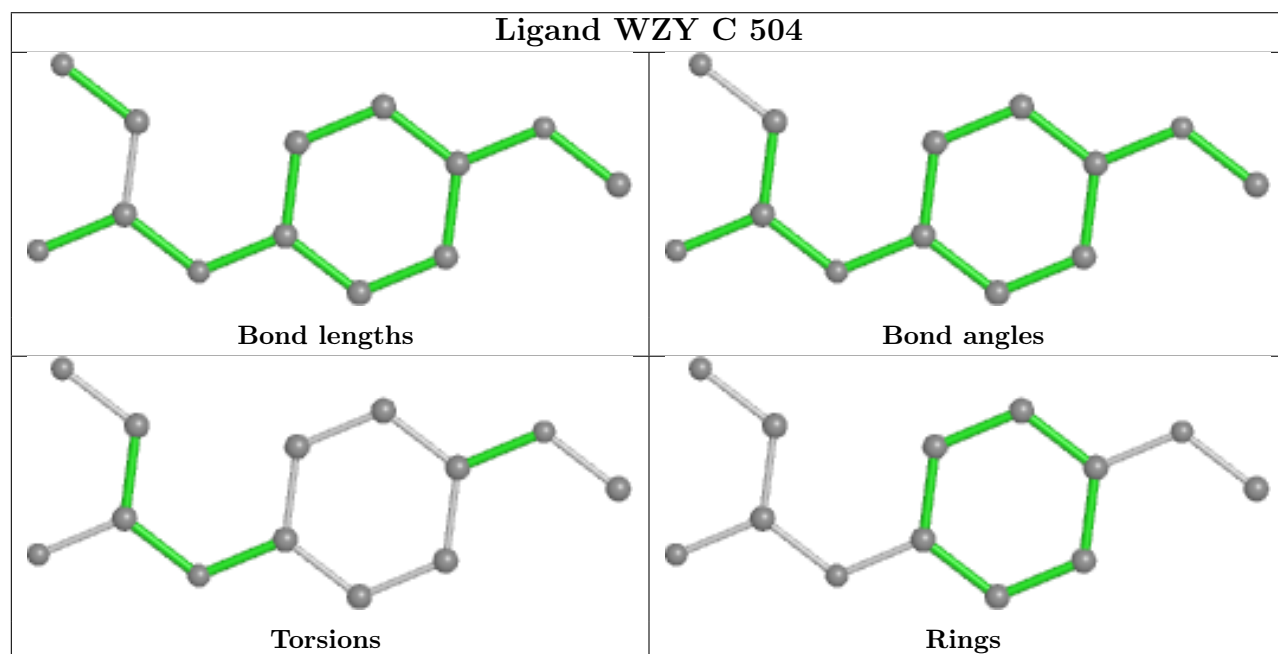
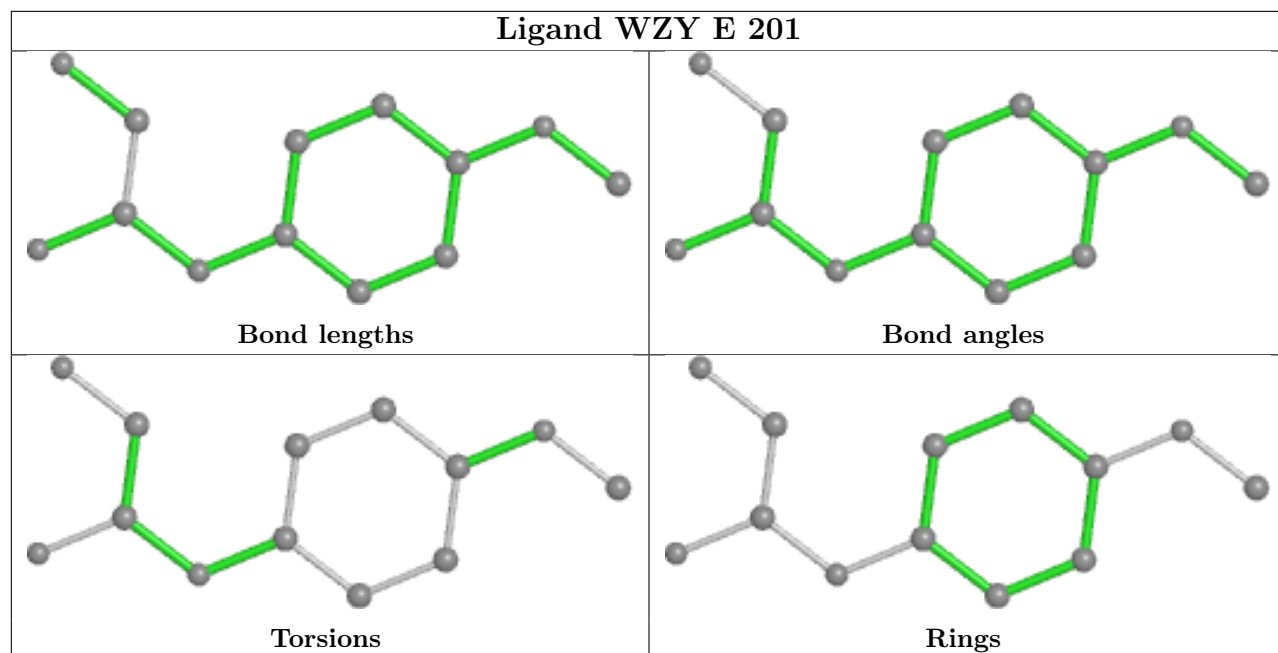
There are no ring outliers.

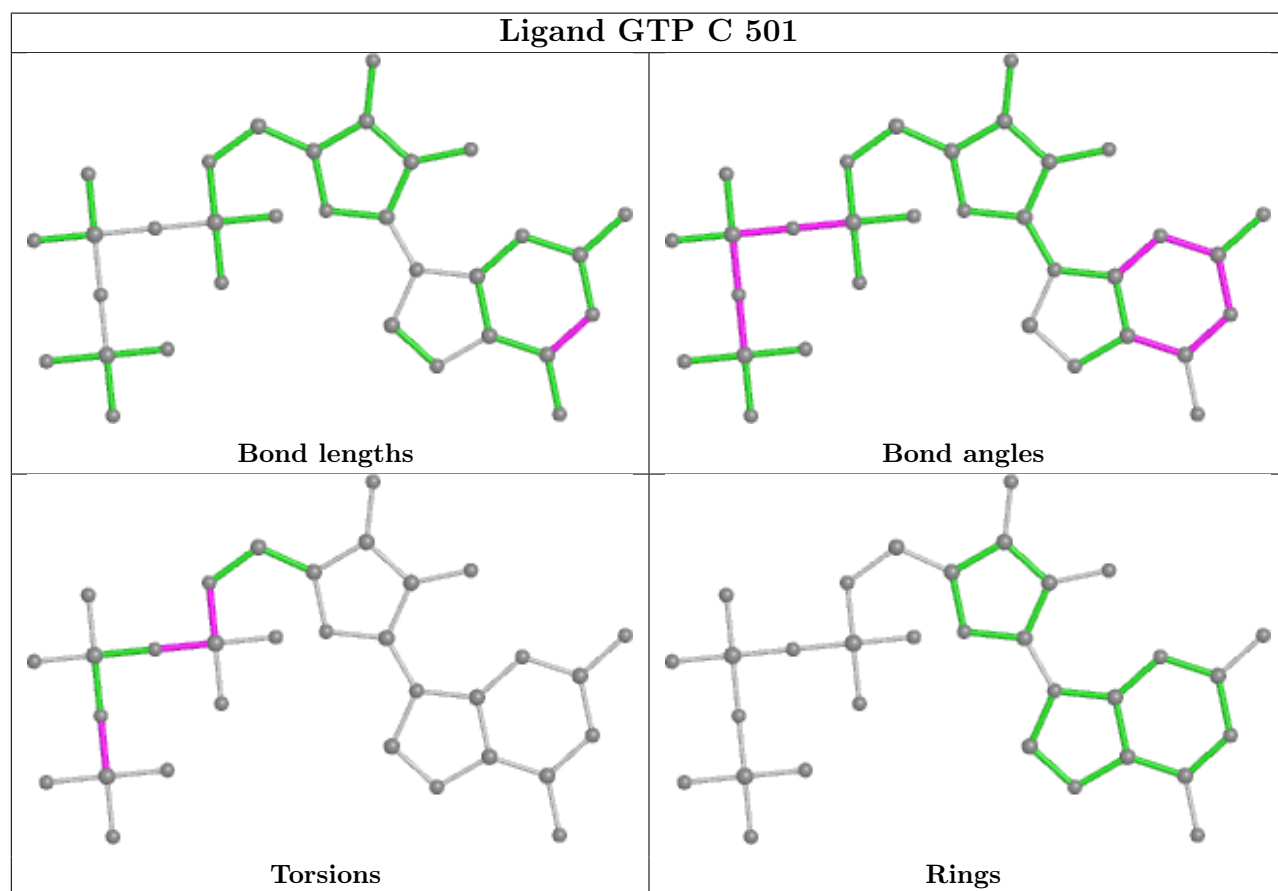
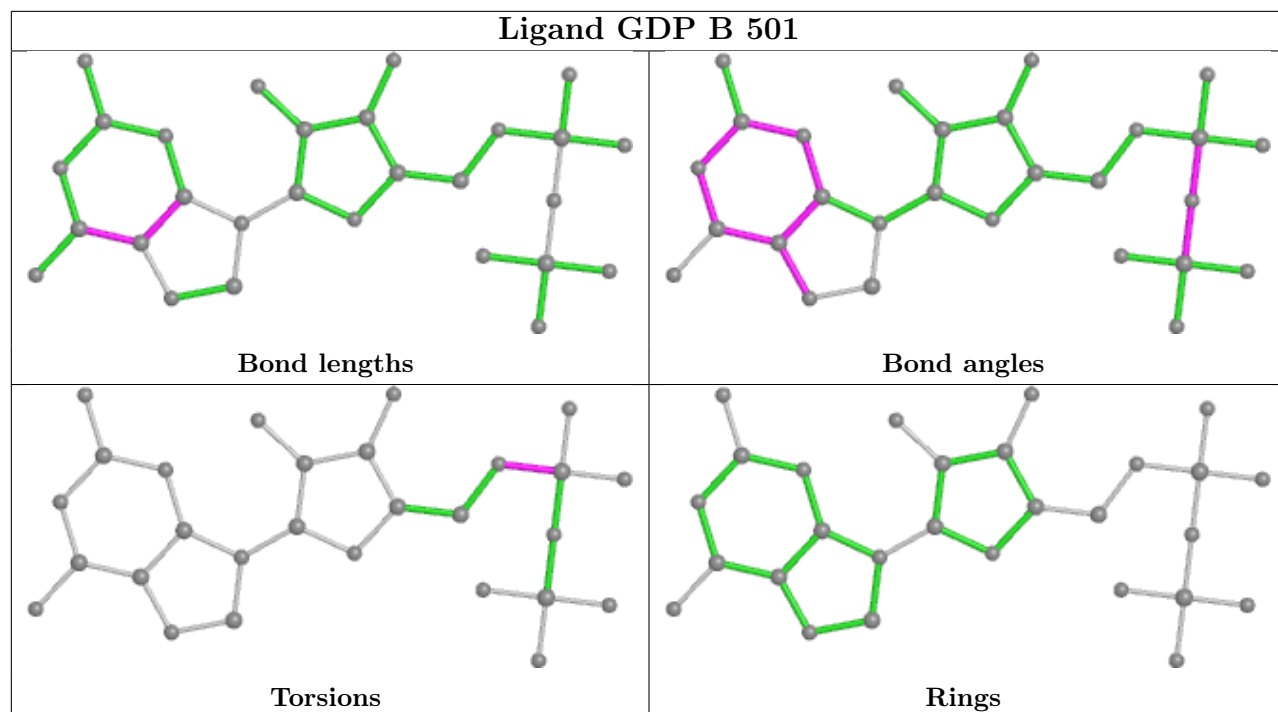
5 monomers are involved in 10 short contacts:

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

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

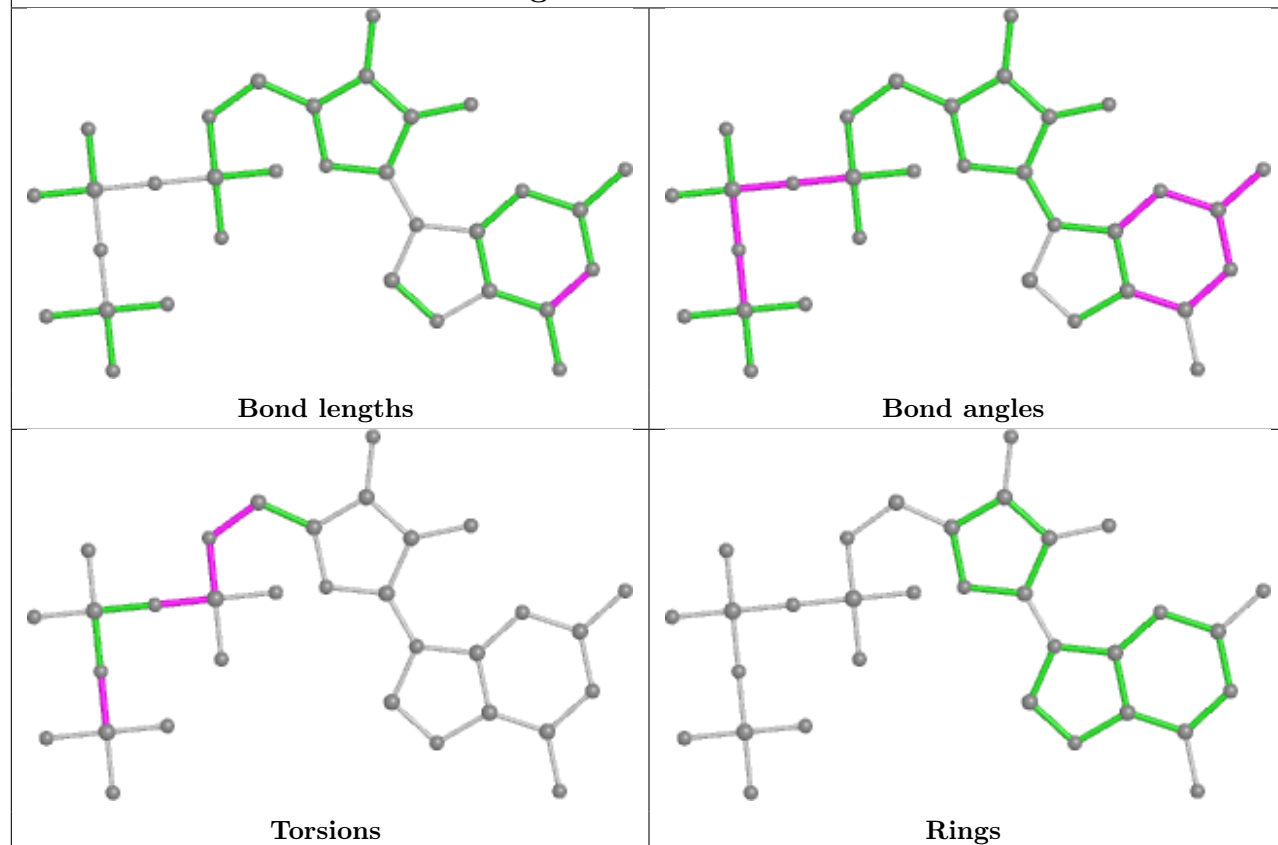




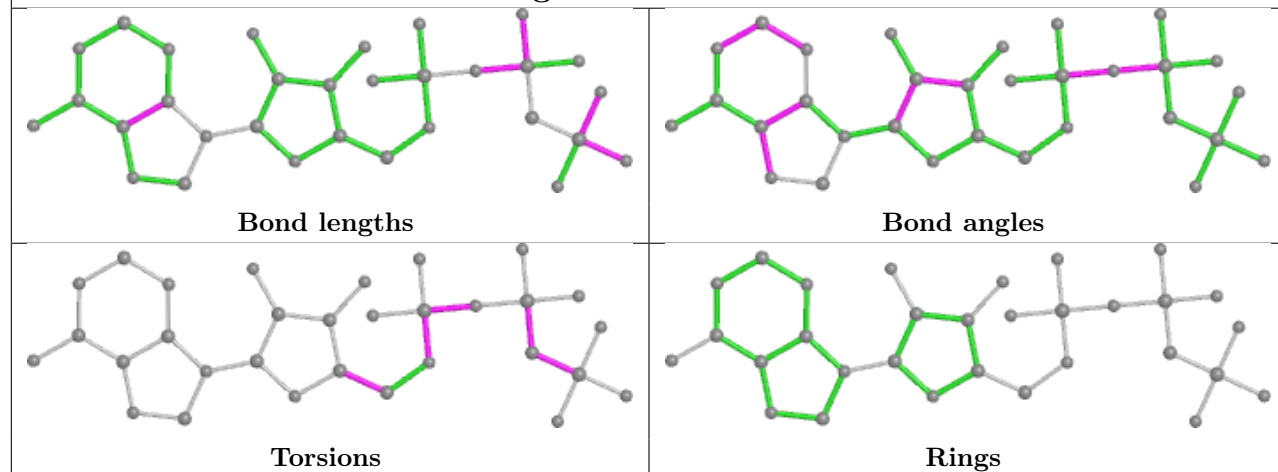


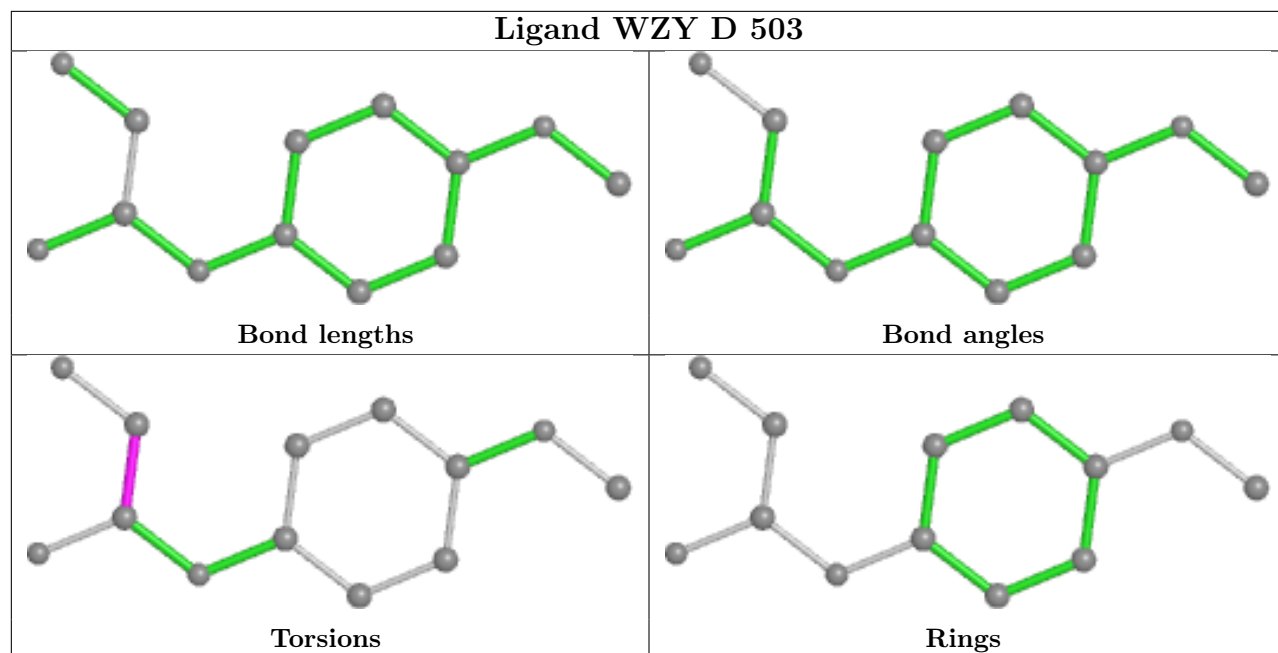


## Ligand GTP A 501



## Ligand ACP F 401





## 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%)	0.39	14 (3%)	47	59	51, 69, 109, 184	0
1	C	440/451 (97%)	0.38	14 (3%)	47	59	45, 58, 83, 131	0
2	B	428/445 (96%)	0.53	18 (4%)	36	48	48, 67, 116, 164	1 (0%)
2	D	431/445 (96%)	0.47	24 (5%)	24	35	55, 78, 114, 192	4 (0%)
3	E	123/143 (86%)	0.80	13 (10%)	6	9	57, 79, 129, 163	0
4	F	352/384 (91%)	0.74	46 (13%)	3	5	67, 103, 169, 206	0
All	All	2212/2319 (95%)	0.51	129 (5%)	23	33	45, 73, 135, 206	5 (0%)

All (129) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	E	24	LEU	7.3
2	B	281	GLN	6.9
4	F	240	LEU	6.6
2	D	278	ARG	5.6
1	A	179	THR	5.4
2	B	284	ARG	5.3
3	E	27	PRO	5.0
4	F	105	LEU	4.9
3	E	25	LYS	4.8
4	F	143	GLU	4.6
1	C	357	TYR	4.6
4	F	381	HIS	4.5
2	D	248	LEU	4.4
4	F	169	LEU	4.4
3	E	6	MET	4.3
2	B	1	MET	4.2
1	A	282	TYR	4.2
2	B	277	SER	4.1
2	D	1	MET	4.1

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Mol	Chain	Res	Type	RSRZ
4	F	131	PHE	4.1
2	D	276	THR	4.0
4	F	152	SER	3.9
4	F	182	ILE	3.8
4	F	173	ILE	3.8
2	B	57	THR	3.8
1	A	351	PHE	3.7
1	C	286	LEU	3.7
3	E	142	GLU	3.6
4	F	249	TYR	3.6
4	F	234	GLN	3.6
3	E	26	PRO	3.6
4	F	100	ILE	3.5
1	A	326	LYS	3.5
2	B	276	THR	3.5
4	F	236	LYS	3.5
1	A	88	HIS	3.4
4	F	99	VAL	3.3
2	D	272	PHE	3.3
4	F	142	ARG	3.3
2	B	283	TYR	3.3
2	D	179	ASP	3.3
1	A	262	TYR	3.3
3	E	22	VAL	3.2
4	F	179	VAL	3.2
4	F	233	PHE	3.2
1	C	341	ILE	3.1
4	F	379	HIS	3.1
4	F	380	HIS	3.1
4	F	161	LEU	3.0
4	F	138	ARG	3.0
4	F	144	GLY	3.0
1	A	349	THR	3.0
2	D	387	LEU	3.0
3	E	123	LEU	3.0
4	F	231	ALA	2.9
2	D	401	ARG	2.9
2	D	283	TYR	2.9
1	A	341	ILE	2.9
2	D	386	GLU	2.9
4	F	149	ALA	2.9
1	C	308	ARG	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	302	MET	2.8
2	D	407	TRP	2.8
4	F	325	LEU	2.8
1	C	335	ILE	2.7
2	D	299	LYS	2.7
4	F	213	ILE	2.7
1	C	284	GLU	2.6
2	D	377	PHE	2.6
1	C	339	ARG	2.6
2	D	280	SER	2.6
4	F	90	SER	2.5
1	A	285	GLN	2.5
2	D	249	ASN	2.5
3	E	139	LEU	2.5
2	D	57	THR	2.4
4	F	31	ARG	2.4
4	F	250	SER	2.4
2	B	275	LEU	2.4
4	F	253	TYR	2.4
4	F	284	LEU	2.4
4	F	135	TYR	2.4
2	D	217	LEU	2.4
3	E	128	LYS	2.4
2	D	277	SER	2.4
1	C	350	GLY	2.4
1	A	68	VAL	2.4
2	D	296	PHE	2.4
2	D	255	LEU	2.3
2	D	275	LEU	2.3
4	F	186	LEU	2.3
2	D	37	HIS	2.3
4	F	132	LEU	2.3
4	F	244	CYS	2.3
1	C	179	THR	2.3
4	F	89	GLU	2.2
2	B	247	GLN	2.2
2	B	242	LEU	2.2
4	F	101	TYR	2.2
1	A	284	GLU	2.2
4	F	127	GLU	2.2
2	B	62	VAL	2.2
3	E	116	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	438	ASP	2.2
4	F	140	GLU	2.2
1	C	283	HIS	2.2
1	A	86	LEU	2.2
4	F	243	HIS	2.2
4	F	137	ARG	2.2
1	A	332	ILE	2.2
1	C	293	ASN	2.1
2	B	286	LEU	2.1
4	F	147	TRP	2.1
2	B	438	ALA	2.1
2	D	281	GLN	2.1
3	E	120	LEU	2.1
4	F	320	MET	2.1
4	F	181	VAL	2.1
2	D	219	LEU	2.1
2	B	124	LYS	2.1
4	F	283	ILE	2.0
3	E	130	ALA	2.0
1	C	340	SER	2.0
1	C	177	VAL	2.0
2	B	5	VAL	2.0
2	B	37	HIS	2.0
2	B	86	ILE	2.0
2	B	255	LEU	2.0
4	F	159	GLY	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](#)

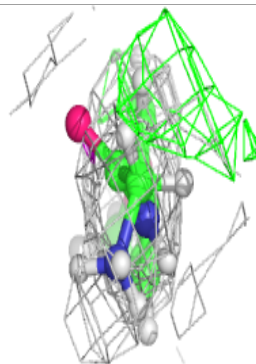
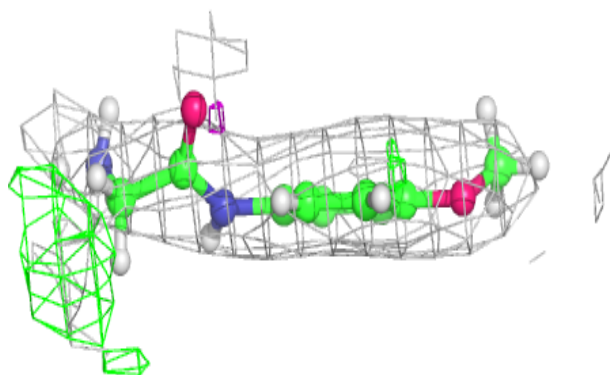
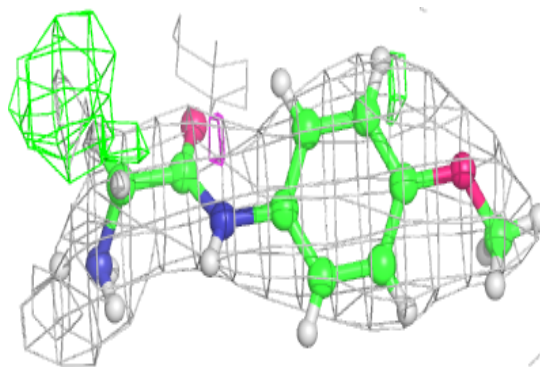
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
9	MES	B	504	12/12	0.61	0.44	65,84,94,102	0
10	WZY	B	505	13/13	0.79	0.23	61,73,90,92	26
10	WZY	C	504	13/13	0.84	0.22	71,79,93,95	26
10	WZY	E	201	13/13	0.84	0.28	67,73,88,88	26
11	ACP	F	401	31/31	0.84	0.13	98,109,119,124	0
10	WZY	D	503	13/13	0.91	0.18	59,71,82,83	26
6	MG	B	502	1/1	0.93	0.15	45,45,45,45	0
7	CA	B	503	1/1	0.93	0.10	96,96,96,96	0
6	MG	F	402	1/1	0.95	0.06	99,99,99,99	0
7	CA	A	504	1/1	0.95	0.05	96,96,96,96	0
6	MG	D	502	1/1	0.95	0.16	79,79,79,79	0
8	GDP	D	501	28/28	0.96	0.17	67,72,81,85	0
7	CA	C	503	1/1	0.97	0.13	70,70,70,70	0
7	CA	A	503	1/1	0.97	0.13	94,94,94,94	0
5	GTP	C	501	32/32	0.98	0.17	42,50,55,60	0
6	MG	A	502	1/1	0.98	0.20	53,53,53,53	0
8	GDP	B	501	28/28	0.98	0.16	43,52,55,60	0
5	GTP	A	501	32/32	0.98	0.15	46,54,60,62	0
6	MG	C	502	1/1	0.98	0.15	47,47,47,47	0

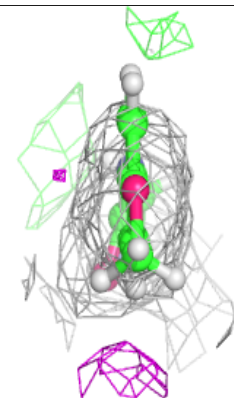
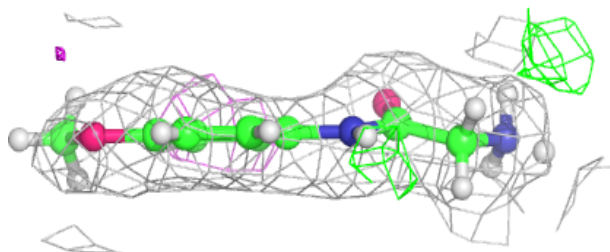
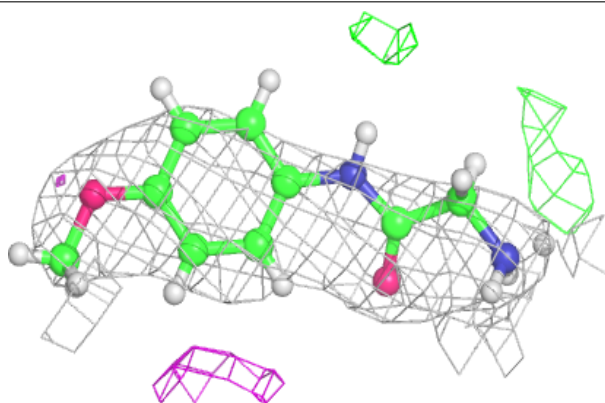
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around WZY 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 WZY C 504:**

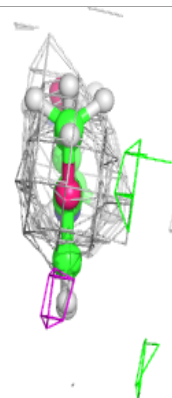
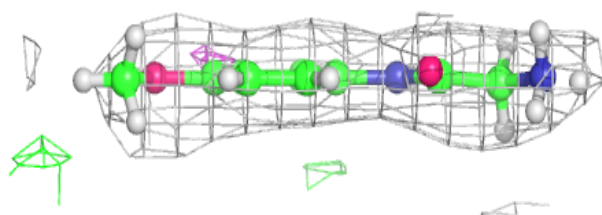
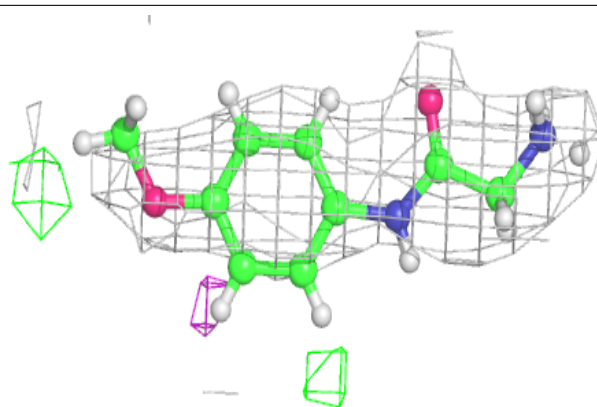
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



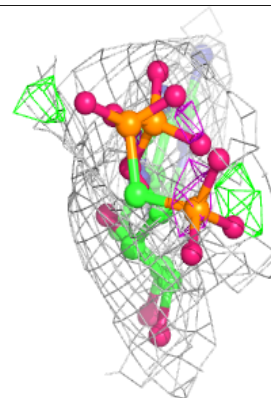
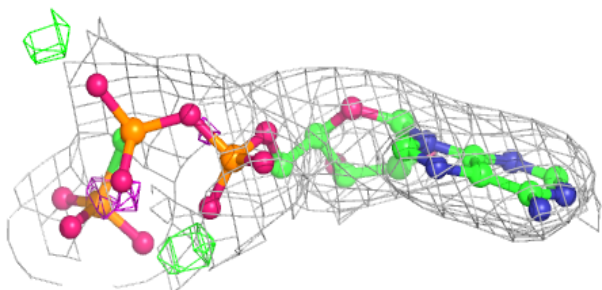
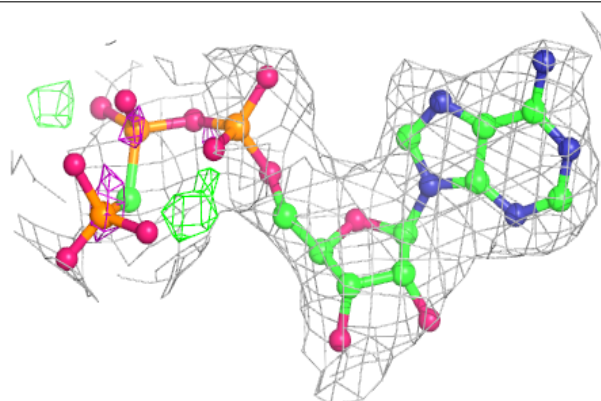


**Electron density around WZY E 201:**

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

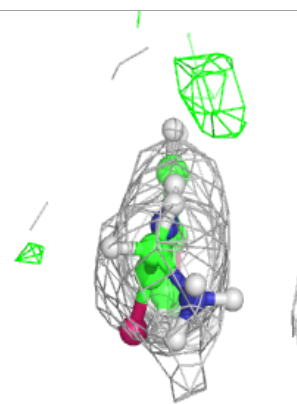
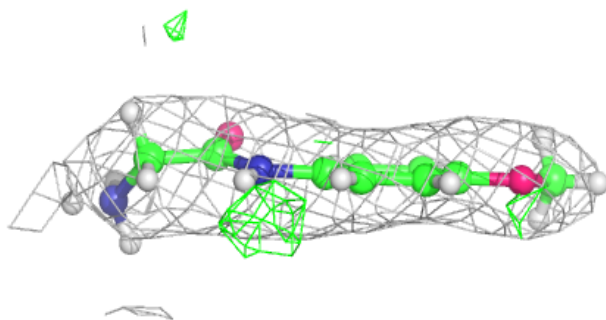
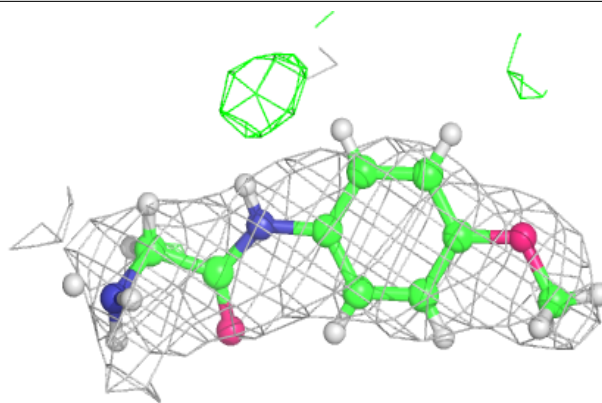
**Electron density around ACP F 401:**

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



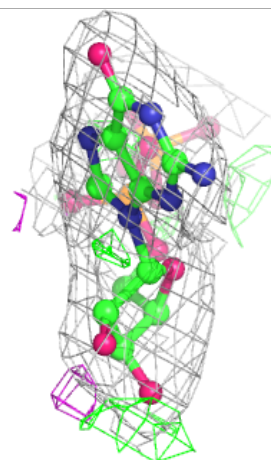
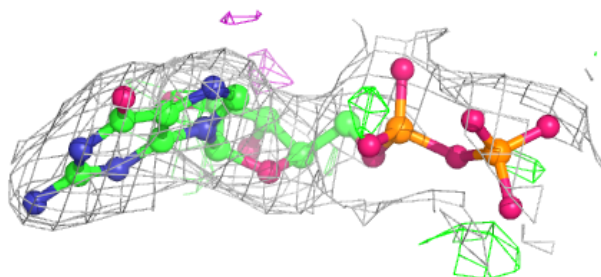
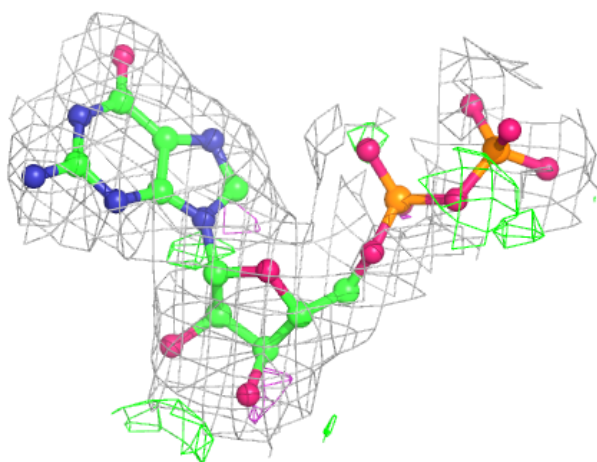
**Electron density around WZY D 503:**

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



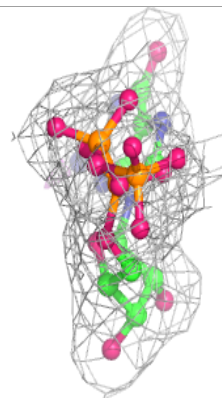
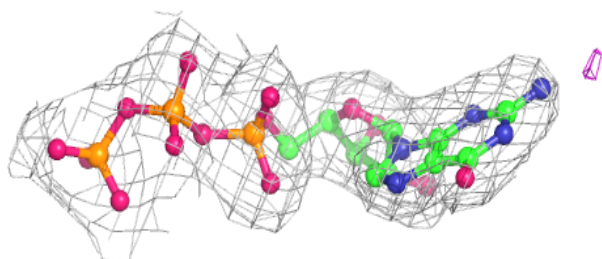
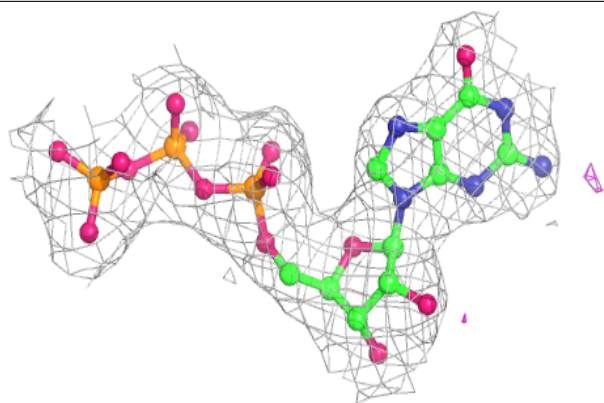
**Electron density around GDP D 501:**

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

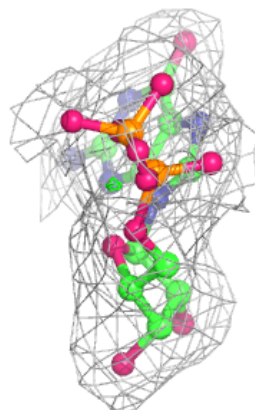
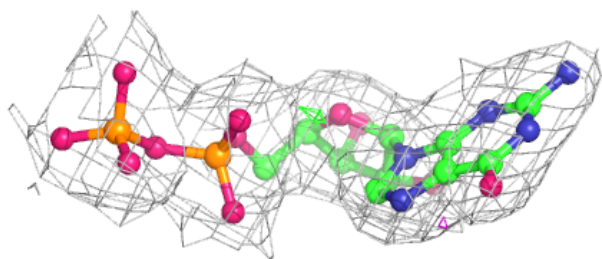
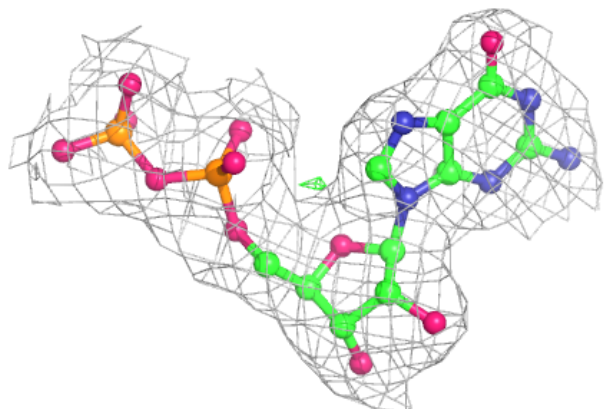


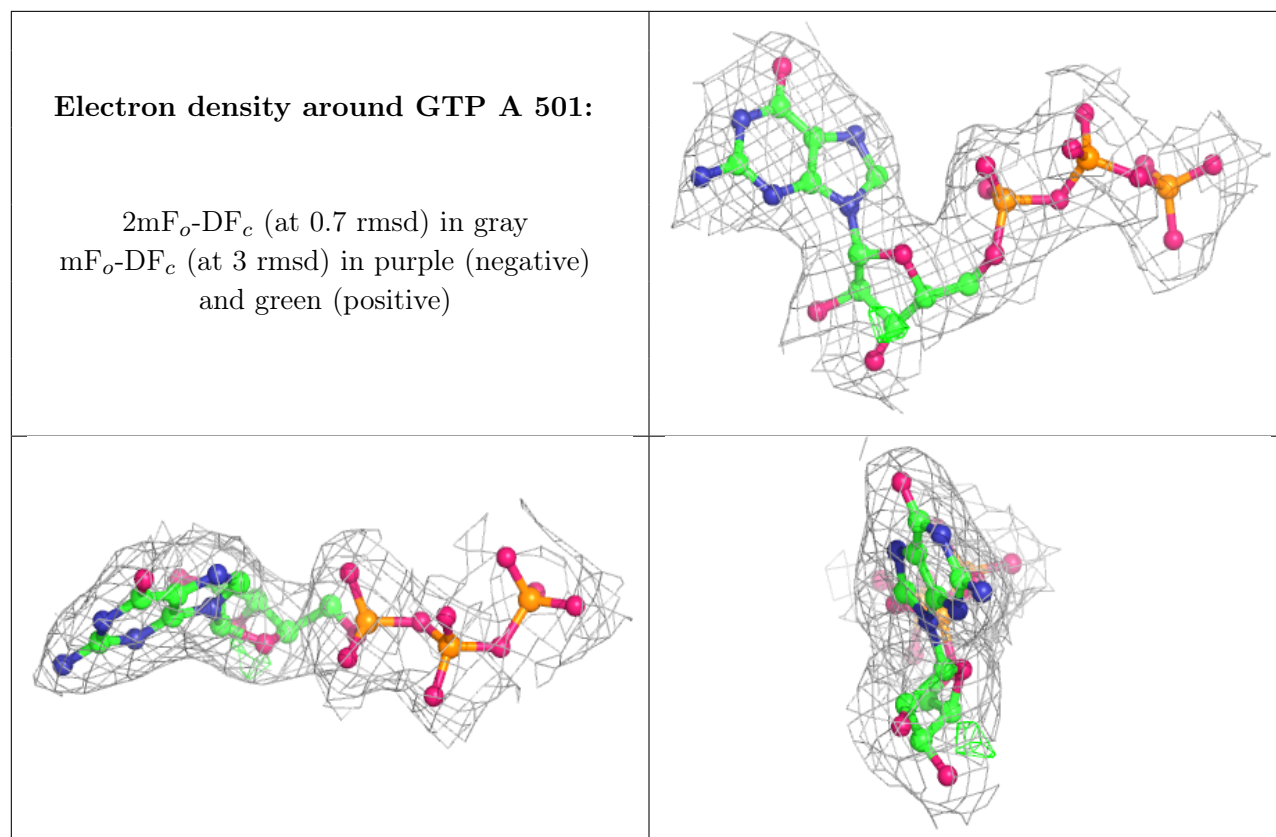
**Electron density around GTP C 501:**

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

**Electron density around GDP B 501:**

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





## 6.5 Other polymers [i](#)

There are no such residues in this entry.