



# Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 06:01 pm BST

PDB ID : 6HX8  
Title : Tubulin-STX3451 complex  
Authors : Dohle, W.; Protá, A.E.; Menchon, G.; Hamel, E.; Steinmetz, M.O.; Potter, B.V.L.  
Deposited on : 2018-10-16  
Resolution : 2.40 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 : 2.11  
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) : 2.11

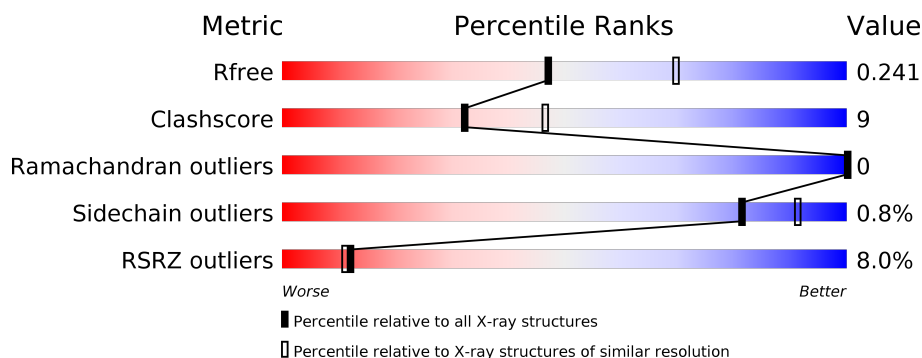
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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 on 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>79%</div> <div>18%</div> <div>•</div> </div>
1	C	451	<div> <div>0%</div> <div>86%</div> <div>11%</div> <div>•</div> </div>
2	B	445	<div> <div>2%</div> <div>78%</div> <div>16%</div> <div>5%</div> </div>
2	D	445	<div> <div>7%</div> <div>71%</div> <div>22%</div> <div>• 6%</div> </div>
3	E	143	<div> <div>9%</div> <div>69%</div> <div>17%</div> <div>14%</div> </div>
4	F	384	<div> <div>27%</div> <div>57%</div> <div>26%</div> <div>18%</div> </div>

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	GXN	D	503	-	-	-	X

## 2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 17785 atoms, of which 46 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	437	Total	C	N	O	S	0	5	0
			3445	2181	585	654	25			
1	C	440	Total	C	N	O	S	0	8	0
			3476	2199	587	665	25			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	422	Total	C	N	O	S	0	6	0
			3372	2119	579	647	27			
2	D	420	Total	C	N	O	S	0	1	0
			3303	2078	560	638	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	1	0
			1020	629	184	202	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	316	Total	C	N	O	S	0	0	0
			2592	1665	445	468	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	B	1	Total	Mg	0	0
			1	1		
6	A	1	Total	Mg	0	0
			1	1		
6	D	1	Total	Mg	0	0
			1	1		
6	C	1	Total	Mg	0	0
			1	1		

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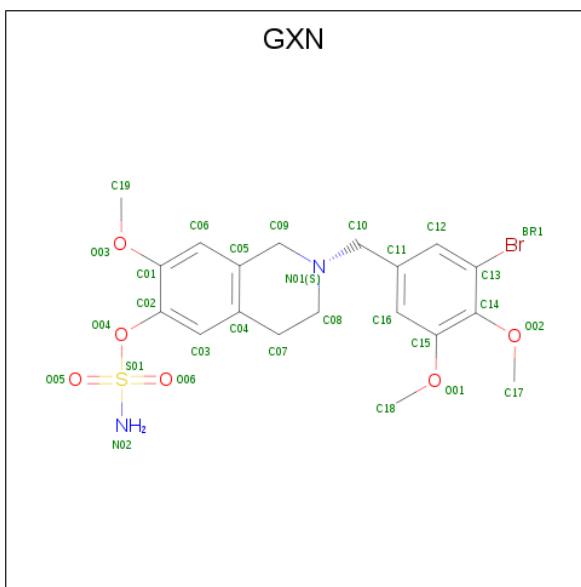
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	F	1	Total Mg 1 1	0	0

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

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- The image displays the chemical structure of Guanosine Diphosphate (GDP). It consists of a guanine base (a purine derivative) linked to a ribose sugar, which is in turn linked to two phosphate groups. The guanine base is shown with its characteristic fused ring system, including the amino group at the 2-position. The ribose sugar is a five-membered ring with hydroxyl groups at the 2' and 3' positions. The two phosphate groups are connected by a pyrophosphate linkage, with the second phosphate group having two hydroxyl groups. The structure is labeled with various atoms and bonds, including the 5' and 3' carbons of the ribose sugar and the phosphate groups.

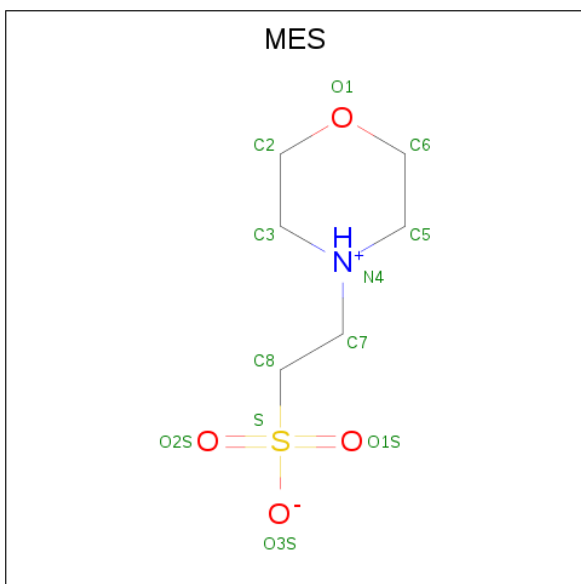
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	B	1	Total 28	C 10	N 5	O 11	P 2	0	0
8	D	1	Total 28	C 10	N 5	O 11	P 2	0	0

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- WORLD WIDE  
PDB  
PROTEIN DATA BANK



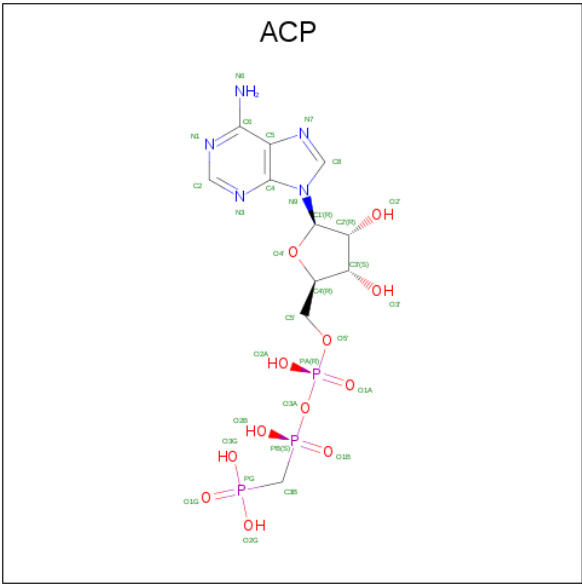
Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
9	B	1	Total	Br	C	H	N	O	S	0	0
			52	1	19	23	2	6	1		
9	D	1	Total	Br	C	H	N	O	S	0	0
			52	1	19	23	2	6	1		

- Molecule 10 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula:  $C_6H_{13}NO_4S$ ).



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

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



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

- Molecule 12 is water.

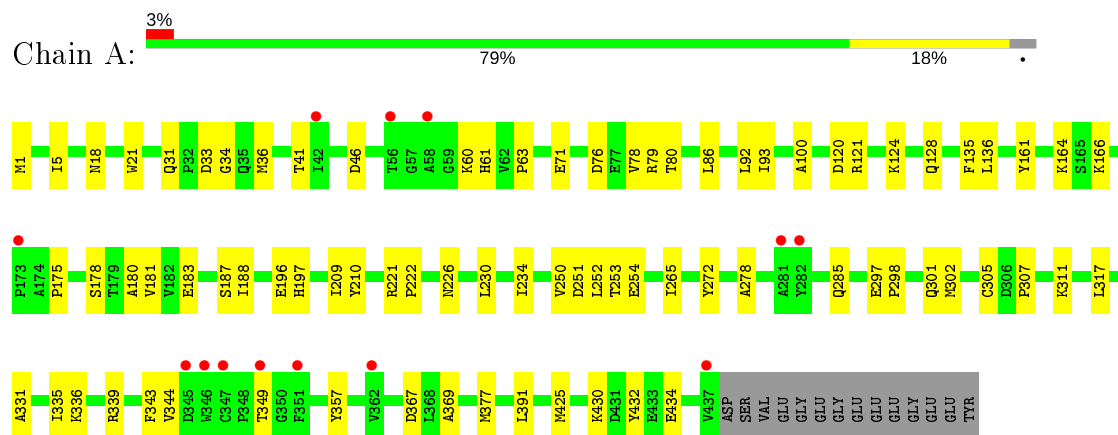
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	55	Total	O	0	0
			55	55		
12	B	56	Total	O	0	0
			56	56		
12	C	124	Total	O	0	0
			124	124		
12	D	30	Total	O	0	0
			30	30		
12	E	21	Total	O	0	0
			21	21		
12	F	17	Total	O	0	0
			17	17		



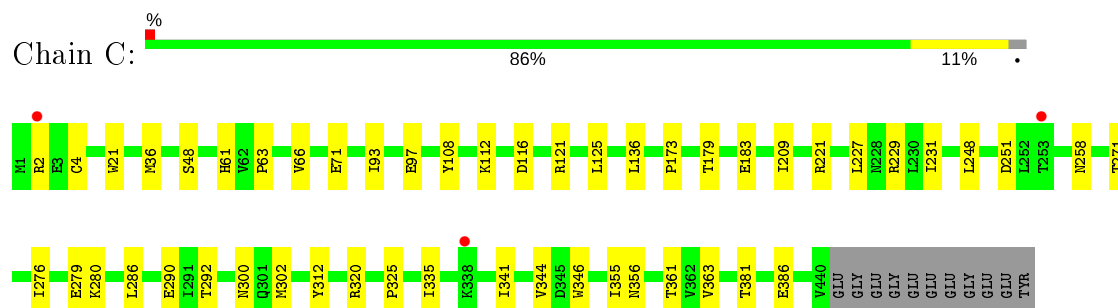
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

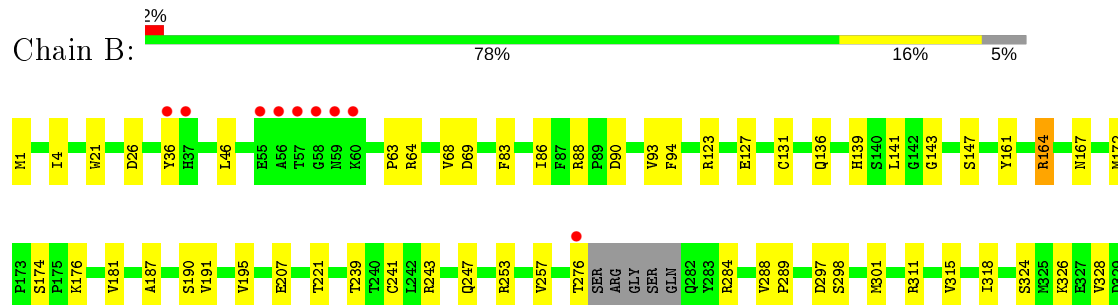
- Molecule 1: Tubulin alpha-1B chain



- Molecule 1: Tubulin alpha-1B chain

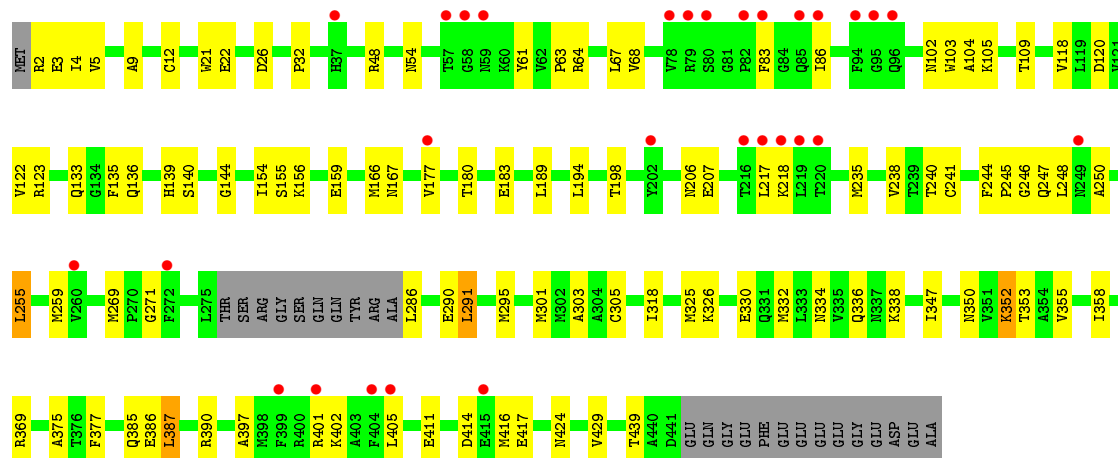


- Molecule 2: Tubulin beta-2B chain

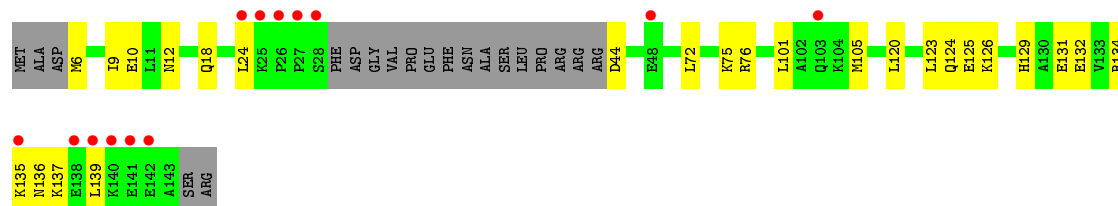




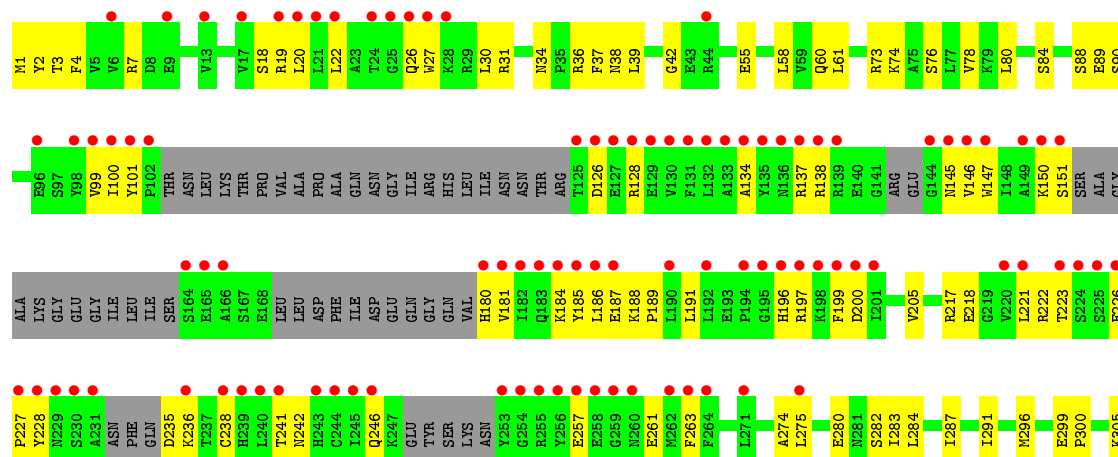
• Molecule 2: Tubulin beta-2B chain



• 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, $\alpha$ , $\beta$ , $\gamma$	105.67Å 159.92Å 181.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.34 – 2.40 48.35 – 2.40	Depositor EDS
% Data completeness (in resolution range)	96.1 (48.34-2.40) 96.1 (48.35-2.40)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.15 (at 2.39Å)	Xtriage
Refinement program	PHENIX (1.13 _2998: ???)	Depositor
R, $R_{free}$	0.195 , 0.240 0.197 , 0.241	Depositor DCC
$R_{free}$ test set	5742 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	63.9	Xtriage
Anisotropy	0.254	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 68.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	17785	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	91.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.64% 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, MG, CA, GTP, ACP, MES, GXN

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	0/3529	0.43	0/4790
1	C	0.30	0/3572	0.43	0/4851
2	B	0.26	0/3452	0.42	0/4672
2	D	0.25	0/3379	0.41	0/4578
3	E	0.25	0/1031	0.36	0/1368
4	F	0.24	0/2649	0.40	0/3573
All	All	0.26	0/17612	0.42	0/23832

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	3445	0	3362	50	0
1	C	3476	0	3391	38	0
2	B	3372	0	3258	47	0
2	D	3303	0	3182	79	0
3	E	1020	0	1037	20	0
4	F	2592	0	2565	75	0
5	A	32	0	12	0	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	1	0	0	0	0
7	C	1	0	0	0	0
8	B	28	0	12	0	0
8	D	28	0	12	2	0
9	B	29	23	0	5	0
9	D	29	23	0	4	0
10	B	12	0	12	0	0
11	F	31	0	14	3	0
12	A	55	0	0	1	0
12	B	56	0	0	4	0
12	C	124	0	0	6	0
12	D	30	0	0	4	0
12	E	21	0	0	3	0
12	F	17	0	0	2	0
All	All	17739	46	16869	301	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (301) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:B:502:GXN:BR1	12:B:637:HOH:O	2.05	1.26
9:D:503:GXN:BR1	9:D:503:GXN:C17	2.52	1.12
2:D:385:GLN:HB2	2:D:429:VAL:HG13	1.60	0.84
2:D:295:MET:HE2	2:D:377:PHE:HB2	1.60	0.83
3:E:120:LEU:O	3:E:124:GLN:HG2	1.82	0.80
3:E:44:ASP:N	12:E:201:HOH:O	2.15	0.80
2:D:352:LYS:HE2	2:D:352:LYS:HA	1.65	0.79
9:B:502:GXN:BR1	12:B:631:HOH:O	2.56	0.77
4:F:150:LYS:NZ	12:F:501:HOH:O	2.16	0.77
4:F:73:ARG:HB2	4:F:76:SER:OG	1.87	0.75
4:F:186:LEU:HD12	4:F:320:MET:HG2	1.73	0.70
4:F:134:ALA:HA	4:F:137:ARG:HE	1.56	0.69
2:B:172:MET:HG3	2:B:387:LEU:HD11	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:397:ALA:O	2:D:401:ARG:NH1	2.28	0.67
11:F:401:ACP:O1A	11:F:401:ACP:O3G	2.11	0.67
2:D:83:PHE:O	2:D:86:ILE:HG22	1.94	0.67
2:D:144:GLY:N	8:D:501:GDP:O3B	2.26	0.67
2:B:345:GLU:OE2	4:F:31:ARG:NH1	2.28	0.67
1:C:271:THR:HG23	1:C:300:ASN:O	1.95	0.67
4:F:280:GLU:HA	4:F:284:LEU:HB2	1.78	0.65
2:B:26:ASP:OD2	2:B:369:ARG:HD2	1.97	0.65
2:B:176:LYS:HD3	2:B:207:GLU:HG3	1.79	0.65
1:C:21:TRP:CZ3	1:C:63:PRO:HB3	2.32	0.65
2:D:238:VAL:O	9:D:503:GXN:BR1	2.69	0.65
1:A:21:TRP:CZ3	1:A:63:PRO:HB3	2.32	0.65
2:D:241:CYS:SG	2:D:318:ILE:HD12	2.37	0.65
1:C:271:THR:HA	1:C:302:MET:HE2	1.79	0.64
1:C:279:GLU:O	12:C:601:HOH:O	2.15	0.63
2:B:354:ALA:HB3	9:B:502:GXN:C18	2.29	0.63
2:D:2:ARG:N	12:D:602:HOH:O	2.31	0.63
2:D:118:VAL:O	2:D:122:VAL:HG23	1.99	0.62
1:A:343:PHE:CD1	1:A:349:THR:HG23	2.34	0.62
2:D:155:SER:OG	3:E:126:LYS:NZ	2.30	0.62
4:F:241:THR:OG1	11:F:401:ACP:O3'	2.16	0.61
2:B:136:GLN:HA	2:B:167:ASN:O	2.01	0.61
4:F:205:VAL:HG21	4:F:291:ILE:HD13	1.83	0.60
4:F:188:LYS:HE2	4:F:323:GLU:OE2	2.02	0.60
1:A:226:ASN:ND2	1:A:367:ASP:OD2	2.34	0.60
4:F:185:TYR:HE2	4:F:228:TYR:HH	1.50	0.60
1:A:120:ASP:O	1:A:124:LYS:HG2	2.02	0.60
1:A:430:LYS:HE2	1:A:434:GLU:OE2	2.02	0.60
4:F:1:MET:HB3	4:F:26:GLN:O	2.02	0.59
1:C:386:GLU:OE2	12:C:602:HOH:O	2.16	0.59
4:F:150:LYS:HD3	4:F:151:SER:N	2.18	0.59
1:C:209:ILE:HG22	1:C:227:LEU:HD22	1.85	0.58
4:F:151:SER:HB2	4:F:180:HIS:CD2	2.38	0.58
1:A:278:ALA:HA	1:A:369:ALA:HB2	1.85	0.58
1:C:229:ARG:HD2	1:C:363:VAL:HG21	1.86	0.57
2:B:297:ASP:OD1	2:B:298:SER:N	2.37	0.57
1:A:76:ASP:O	1:A:80:THR:HG22	2.04	0.57
2:B:187:ALA:O	2:B:191:VAL:HG23	2.04	0.57
4:F:145:ASN:HA	4:F:184:LYS:HZ1	1.69	0.57
1:C:248:LEU:HD13	1:C:355:ILE:HD12	1.87	0.57
2:D:402:LYS:HB3	2:D:405:LEU:HD12	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:99:VAL:O	4:F:100:ILE:HD13	2.04	0.57
2:D:295:MET:CE	2:D:377:PHE:HB2	2.35	0.56
4:F:200:ASP:OD1	4:F:222:ARG:HB2	2.04	0.56
3:E:6:MET:N	12:E:203:HOH:O	2.39	0.56
4:F:150:LYS:HD3	4:F:151:SER:H	1.69	0.56
4:F:191:LEU:HD12	4:F:196:HIS:CE1	2.40	0.56
1:A:18:ASN:HD21	1:A:78:VAL:HG22	1.69	0.56
1:A:93:ILE:HD11	1:A:121:ARG:HG3	1.88	0.55
2:D:26:ASP:OD2	2:D:369:ARG:HD2	2.06	0.55
1:A:251:ASP:OD2	1:A:253:THR:OG1	2.25	0.55
1:A:210:TYR:CE1	1:A:222:PRO:HD2	2.42	0.55
2:D:439:THR:HG22	12:D:616:HOH:O	2.07	0.55
4:F:340:GLN:OE1	4:F:340:GLN:N	2.39	0.55
2:D:352:LYS:HD3	2:D:353:THR:H	1.72	0.55
2:B:161:TYR:HB3	2:B:164:ARG:HG3	1.89	0.54
2:D:291:LEU:HD22	2:D:375:ALA:HB3	1.88	0.54
1:A:209:ILE:HG23	1:A:230:LEU:HD23	1.87	0.54
2:B:21:TRP:CZ3	2:B:63:PRO:HB3	2.42	0.54
2:D:21:TRP:CZ3	2:D:63:PRO:HB3	2.43	0.54
1:A:221:ARG:O	1:A:221:ARG:HD3	2.07	0.54
1:C:97:GLU:HG3	2:D:2:ARG:HH12	1.73	0.54
2:D:136:GLN:HA	2:D:167:ASN:O	2.07	0.54
2:D:352:LYS:HD3	2:D:353:THR:N	2.23	0.54
4:F:100:ILE:HD12	4:F:128:ARG:HA	1.90	0.54
1:A:31:GLN:HB2	1:A:33:ASP:OD1	2.08	0.54
4:F:74:LYS:HE3	4:F:331:GLU:OE1	2.08	0.53
2:D:103:TRP:CE3	2:D:189:LEU:HD13	2.42	0.53
1:C:320:ARG:HA	1:C:356:ASN:O	2.07	0.53
2:D:244:PHE:O	2:D:246:GLY:N	2.40	0.53
4:F:3:THR:HG21	4:F:30:LEU:HD11	1.90	0.53
2:D:336:GLN:NE2	12:D:603:HOH:O	2.40	0.53
2:D:387:LEU:HD12	2:D:387:LEU:O	2.09	0.53
2:D:3:GLU:O	2:D:133:GLN:HG2	2.09	0.53
2:D:22:GLU:HG2	2:D:83:PHE:CD1	2.43	0.53
1:A:181[B]:VAL:HG13	9:B:502:GXN:O04	2.09	0.53
2:B:332:MET:O	2:B:335:VAL:HG12	2.08	0.53
2:B:221:THR:HG21	1:C:325:PRO:HB2	1.91	0.53
2:B:69:ASP:O	2:B:94:PHE:HA	2.09	0.53
4:F:340:GLN:HA	4:F:343:TYR:HD2	1.74	0.52
1:C:93:ILE:HD11	1:C:121:ARG:HG3	1.91	0.52
2:D:352:LYS:CE	2:D:352:LYS:HA	2.35	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:83:PHE:O	2:B:86:ILE:HG22	2.09	0.52
2:D:411:GLU:HA	3:E:137:LYS:HD2	1.91	0.52
4:F:221:LEU:O	4:F:261:GLU:HA	2.09	0.52
3:E:125:GLU:HA	3:E:125:GLU:OE1	2.10	0.52
2:D:416:MET:CE	2:D:416:MET:HA	2.39	0.52
11:F:401:ACP:O1B	12:F:501:HOH:O	2.19	0.52
4:F:126:ASP:OD2	4:F:128:ARG:HB2	2.10	0.52
1:A:166:LYS:HE2	1:A:197:HIS:O	2.10	0.51
4:F:7:ARG:HB2	4:F:42:GLY:HA2	1.93	0.51
1:A:188:ILE:HG13	1:A:425:MET:HG3	1.92	0.51
1:A:196:GLU:O	1:A:196:GLU:HG2	2.11	0.51
2:D:109:THR:HG21	2:D:411:GLU:OE1	2.11	0.51
1:A:311:LYS:HE2	1:A:344:VAL:HG12	1.91	0.51
2:D:48:ARG:HD2	2:D:245:PRO:HA	1.92	0.51
4:F:205:VAL:CG2	4:F:291:ILE:HD13	2.40	0.51
2:D:301:MET:HA	2:D:301:MET:HE2	1.92	0.51
1:C:2:ARG:NH2	1:C:251:ASP:OD1	2.43	0.51
2:D:240:THR:HB	2:D:318:ILE:HD13	1.93	0.51
3:E:131:GLU:O	3:E:132:GLU:HB2	2.11	0.51
1:C:276:ILE:HD11	1:C:280:LYS:CB	2.41	0.50
3:E:135:LYS:O	3:E:139:LEU:HG	2.11	0.50
4:F:296:MET:SD	4:F:380:HIS:HB2	2.51	0.50
1:A:250:VAL:HG22	1:A:254:GLU:OE2	2.11	0.50
4:F:223:THR:OG1	4:F:257:GLU:OE2	2.25	0.50
1:A:298:PRO:O	1:A:301:GLN:HG2	2.10	0.50
2:B:1:MET:N	2:B:131:CYS:SG	2.82	0.50
1:A:161:TYR:HB3	1:A:164:LYS:CG	2.42	0.50
2:B:141:LEU:HD12	2:B:172:MET:SD	2.51	0.50
2:D:105:LYS:HA	2:D:109:THR:OG1	2.12	0.50
2:D:156:LYS:HA	2:D:156:LYS:HE2	1.94	0.50
1:A:79:ARG:HG2	1:A:92:LEU:HD12	1.94	0.49
4:F:101:TYR:N	4:F:126:ASP:OD1	2.42	0.49
1:A:265:ILE:HG23	1:A:432:TYR:CZ	2.47	0.49
2:B:143:GLY:O	2:B:147[B]:SER:OG	2.27	0.49
4:F:138:ARG:HB3	4:F:145:ASN:OD1	2.12	0.49
2:B:326:LYS:O	2:B:330:GLU:HG3	2.12	0.49
3:E:6:MET:HB2	12:E:210:HOH:O	2.12	0.49
2:D:286:LEU:HD12	2:D:290:GLU:OE1	2.13	0.49
1:A:336:LYS:HG3	3:E:24:LEU:HD13	1.95	0.49
2:D:102:ASN:OD1	2:D:104:ALA:N	2.46	0.49
12:B:625:HOH:O	3:E:75:LYS:HD2	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:385:GLN:OE1	2:B:389:LYS:HE3	2.13	0.49
2:D:120:ASP:OD1	2:D:123:ARG:NH1	2.45	0.49
3:E:9:ILE:HG12	3:E:10:GLU:HG3	1.95	0.49
4:F:138:ARG:HD2	4:F:145:ASN:HB3	1.95	0.49
4:F:3:THR:CG2	4:F:30:LEU:HD11	2.42	0.49
1:C:36:MET:HB3	1:C:61:HIS:CE1	2.48	0.49
2:D:326:LYS:O	2:D:330:GLU:HG3	2.13	0.49
3:E:132:GLU:O	3:E:136:ASN:N	2.45	0.48
4:F:283:ILE:HG23	4:F:327:VAL:HG22	1.93	0.48
1:A:100:ALA:HB2	2:B:253[A]:ARG:HD2	1.95	0.48
2:B:315:VAL:HG13	2:B:377:PHE:CE1	2.48	0.48
4:F:137:ARG:H	4:F:137:ARG:HD3	1.78	0.48
1:A:317:LEU:HD23	1:A:377:MET:HG3	1.96	0.48
1:A:63:PRO:HD3	1:A:86:LEU:HG	1.96	0.48
2:B:301:MET:CE	2:B:301:MET:HA	2.43	0.48
2:B:36:TYR:CD1	2:B:46:LEU:HD21	2.49	0.48
2:D:12:CYS:HB2	8:D:501:GDP:C8	2.49	0.48
2:D:325:MET:CE	2:D:355:VAL:HG21	2.44	0.48
4:F:242:ASN:O	4:F:246:GLN:HG2	2.13	0.48
4:F:341:LYS:O	4:F:342:LEU:HD23	2.13	0.48
4:F:88:SER:O	4:F:89:GLU:HB3	2.13	0.48
4:F:196:HIS:O	4:F:227:PRO:HA	2.13	0.48
1:C:116:ASP:HB2	12:C:647:HOH:O	2.14	0.48
1:A:234:ILE:HD12	1:A:272:TYR:HB2	1.96	0.47
2:B:396:THR:O	2:B:400[A]:ARG:HG2	2.15	0.47
2:D:291:LEU:HD22	2:D:375:ALA:CB	2.43	0.47
4:F:88:SER:O	4:F:90:SER:N	2.47	0.47
4:F:226:GLU:HB2	4:F:238:CYS:HB3	1.96	0.47
3:E:72:LEU:O	3:E:76:ARG:HG2	2.13	0.47
1:A:36:MET:HB3	1:A:61:HIS:CE1	2.50	0.47
2:D:154:ILE:HG23	2:D:166:MET:HG2	1.97	0.47
2:D:417:GLU:OE2	3:E:129:HIS:NE2	2.44	0.47
4:F:217:ARG:HG3	4:F:218:GLU:HG2	1.97	0.47
1:C:4[A]:CYS:SG	1:C:136:LEU:HG	2.54	0.47
2:D:54:ASN:O	2:D:61:TYR:HA	2.15	0.47
1:A:285:GLN:HA	12:A:617:HOH:O	2.15	0.47
2:B:311:ARG:NH2	2:B:345:GLU:OE1	2.46	0.47
3:E:12:ASN:O	3:E:18:GLN:HA	2.14	0.47
1:A:21:TRP:CH2	1:A:63:PRO:HB3	2.50	0.46
4:F:146:VAL:N	4:F:187:GLU:OE2	2.48	0.46
1:C:108:TYR:O	1:C:112:LYS:HG2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:ALA:O	1:A:183:GLU:HG3	2.16	0.46
1:C:361:THR:HG23	12:C:685:HOH:O	2.16	0.46
4:F:18:SER:O	4:F:22:LEU:HG	2.16	0.46
2:B:181:VAL:HG13	1:C:258:ASN:ND2	2.31	0.46
2:D:217:LEU:O	2:D:218:LYS:HB2	2.15	0.46
4:F:4:PHE:HA	4:F:39:LEU:O	2.15	0.46
4:F:37:PHE:O	4:F:60:GLN:HG2	2.16	0.46
1:A:298:PRO:HA	1:A:301:GLN:NE2	2.31	0.46
1:C:97:GLU:HG3	2:D:2:ARG:NH1	2.30	0.46
2:B:88:ARG:NH1	2:B:90:ASP:HB2	2.31	0.46
3:E:131:GLU:HG3	3:E:134:ARG:HH21	1.81	0.46
4:F:126:ASP:OD2	4:F:128:ARG:N	2.42	0.46
2:B:284:ARG:O	2:B:284:ARG:HG3	2.17	0.45
2:B:181:VAL:HG13	1:C:258:ASN:CG	2.36	0.45
4:F:19:ARG:C	4:F:19:ARG:HD2	2.37	0.45
1:C:179:THR:HG23	5:C:501:GTP:H3'	1.98	0.45
4:F:145:ASN:CA	4:F:184:LYS:HZ1	2.28	0.45
4:F:80:LEU:O	4:F:84:SER:OG	2.25	0.45
2:B:191:VAL:O	2:B:195:VAL:HG23	2.16	0.45
2:B:241:CYS:SG	2:B:318:ILE:HD13	2.56	0.45
3:E:101:LEU:O	3:E:105:MET:HG2	2.16	0.45
2:B:4:ILE:O	2:B:64:ARG:HD2	2.17	0.45
2:D:9:ALA:HA	2:D:68:VAL:O	2.16	0.45
1:C:173:PRO:HB3	1:C:183:GLU:OE1	2.17	0.45
1:A:301:GLN:H	1:A:301:GLN:HG2	1.63	0.45
1:A:305:CYS:O	1:A:307:PRO:HD3	2.16	0.45
2:D:334:ASN:OD1	2:D:338:LYS:HE3	2.17	0.45
1:A:18:ASN:ND2	1:A:78:VAL:HG22	2.32	0.45
1:C:227:LEU:O	1:C:231:ILE:HG13	2.17	0.45
4:F:145:ASN:ND2	4:F:147:TRP:HE1	2.15	0.45
4:F:84:SER:O	4:F:88:SER:N	2.41	0.45
2:D:180:THR:HB	2:D:183:GLU:HG3	1.99	0.44
1:A:331:ALA:O	1:A:335:ILE:HG12	2.17	0.44
1:C:312:TYR:CD1	1:C:341:ILE:HG23	2.52	0.44
1:C:66:VAL:HG23	1:C:125:LEU:CD1	2.47	0.44
2:D:4:ILE:O	2:D:64:ARG:HD2	2.17	0.44
2:B:288:VAL:N	2:B:289:PRO:HD2	2.32	0.44
2:B:324:SER:O	2:B:328:VAL:HG23	2.18	0.44
2:B:414:ASP:OD1	2:B:415:GLU:N	2.50	0.44
2:D:194:LEU:HD22	2:D:198:THR:HG21	2.00	0.44
2:D:271:GLY:HA3	2:D:301:MET:HE2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:347:ILE:HG22	2:D:350:ASN:HB3	2.00	0.44
2:B:123:ARG:O	2:B:127:GLU:HG3	2.17	0.44
2:D:67:LEU:N	2:D:67:LEU:HD12	2.32	0.44
1:C:344:VAL:HG21	1:C:346:TRP:CE2	2.53	0.44
2:D:424:ASN:ND2	12:D:605:HOH:O	2.51	0.44
2:D:48:ARG:HH22	2:D:250:ALA:HB1	1.83	0.44
4:F:88:SER:C	4:F:90:SER:H	2.19	0.44
2:B:176:LYS:CD	2:B:207:GLU:HG3	2.45	0.43
4:F:274:ALA:O	4:F:275:LEU:HD23	2.18	0.43
4:F:39:LEU:HA	4:F:61:LEU:O	2.18	0.43
2:B:68:VAL:HA	2:B:93:VAL:O	2.18	0.43
1:C:276:ILE:HD11	1:C:280:LYS:HB3	2.00	0.43
4:F:299:GLU:HB3	4:F:300:PRO:HD3	1.99	0.43
1:C:229:ARG:CD	1:C:363:VAL:HG21	2.49	0.43
2:D:269[B]:MET:CE	2:D:305:CYS:HB2	2.48	0.43
2:D:248:LEU:HD12	2:D:248:LEU:C	2.39	0.43
4:F:199:PHE:HB3	4:F:223:THR:HG22	1.99	0.43
4:F:341:LYS:O	4:F:341:LYS:HG2	2.18	0.43
9:B:502:GXN:BR1	9:B:502:GXN:C17	3.21	0.43
4:F:235:ASP:OD1	4:F:236:LYS:N	2.52	0.43
2:D:244:PHE:CE1	2:D:358:ILE:HD12	2.54	0.43
4:F:263:PHE:CZ	4:F:341:LYS:HE2	2.54	0.43
2:B:174:SER:HB2	2:B:207:GLU:HB2	2.01	0.43
2:D:305:CYS:HA	2:D:386:GLU:OE1	2.19	0.43
4:F:305:LYS:HE3	4:F:305:LYS:HB2	1.84	0.43
1:A:128:GLN:O	1:A:128:GLN:HG2	2.19	0.43
1:A:175:PRO:HA	1:A:178:SER:HB2	2.00	0.43
1:A:209:ILE:HD11	1:A:302[A]:MET:SD	2.59	0.43
1:C:286:LEU:HA	1:C:290:GLU:OE1	2.19	0.43
1:A:5:ILE:O	1:A:135:PHE:HA	2.19	0.42
2:B:395:PHE:CE1	2:B:422:GLU:HB2	2.54	0.42
1:A:187:SER:HB3	1:A:391:LEU:HD21	2.00	0.42
2:B:247:GLN:NE2	12:B:605:HOH:O	2.52	0.42
2:B:337:ASN:OD1	4:F:36:ARG:NE	2.45	0.42
4:F:30:LEU:HD13	4:F:34:ASN:ND2	2.35	0.42
1:A:18:ASN:OD1	1:A:78:VAL:HG22	2.19	0.42
2:B:239:THR:O	2:B:243:ARG:HG3	2.20	0.42
2:B:276:THR:HG22	2:B:276:THR:O	2.20	0.42
2:D:332:MET:HG2	2:D:353:THR:OG1	2.20	0.42
4:F:150:LYS:CD	4:F:151:SER:H	2.30	0.42
1:C:312:TYR:CE1	1:C:341:ILE:HG23	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:255:LEU:HG	9:D:503:GXN:C12	2.49	0.42
2:D:5:VAL:HB	2:D:135:PHE:CD2	2.54	0.42
2:B:174:SER:CB	2:B:207:GLU:HB2	2.50	0.42
4:F:78:VAL:HG21	4:F:181:VAL:HG11	2.02	0.42
4:F:38:ASN:O	4:F:60:GLN:HA	2.20	0.42
1:A:136:LEU:HD21	1:A:252:LEU:HD21	2.02	0.41
4:F:191:LEU:HA	4:F:197:ARG:O	2.20	0.41
4:F:283:ILE:HG23	4:F:327:VAL:CG2	2.50	0.41
2:D:255:LEU:HD23	2:D:259:MET:HG3	2.02	0.41
2:D:32:PRO:O	2:D:86:ILE:HB	2.20	0.41
1:A:297:GLU:OE2	1:A:339:ARG:NH2	2.52	0.41
1:C:21:TRP:CE3	1:C:63:PRO:HB3	2.55	0.41
2:D:4:ILE:HG13	2:D:133:GLN:NE2	2.34	0.41
2:D:177:VAL:HG21	2:D:206:ASN:HB3	2.02	0.41
2:D:21:TRP:CE3	2:D:63:PRO:HB3	2.56	0.41
4:F:189:PRO:HG2	4:F:191:LEU:HD21	2.03	0.41
4:F:282:SER:HB2	4:F:325:LEU:HD13	2.03	0.41
2:D:235:MET:HE2	2:D:235:MET:HB3	1.90	0.41
2:D:301:MET:CE	2:D:301:MET:HA	2.51	0.41
2:D:207:GLU:HB3	2:D:390:ARG:HH12	1.86	0.41
1:A:1:MET:HB2	1:A:46:ASP:HB2	2.02	0.41
4:F:100:ILE:HD12	4:F:128:ARG:CA	2.49	0.41
4:F:2:TYR:HB2	4:F:27:TRP:CD2	2.56	0.41
1:A:34:GLY:HA3	1:A:60:LYS:HG3	2.02	0.41
2:D:255:LEU:CD2	2:D:259:MET:HG3	2.50	0.41
1:C:292:THR:HG22	1:C:335:ILE:CD1	2.50	0.41
1:C:66:VAL:HG23	1:C:125:LEU:HD11	2.02	0.41
2:B:147[B]:SER:HB2	2:B:190:SER:HG	1.86	0.41
2:D:414:ASP:N	2:D:414:ASP:OD1	2.54	0.41
1:C:276:ILE:CG1	1:C:280:LYS:HB2	2.51	0.40
1:C:48:SER:HB2	12:C:644:HOH:O	2.21	0.40
2:D:303:ALA:O	2:D:305:CYS:N	2.51	0.40
1:C:2:ARG:HG2	12:C:713:HOH:O	2.21	0.40
2:D:159:GLU:HG3	3:E:123:LEU:HD13	2.03	0.40
1:A:251:ASP:OD1	1:A:254:GLU:HG3	2.21	0.40
4:F:287:ILE:HG23	4:F:319:PHE:CE2	2.55	0.40
1:A:357:TYR:OH	3:E:18:GLN:NE2	2.53	0.40
2:D:12:CYS:HB3	2:D:140:SER:HB3	2.02	0.40
2:D:352:LYS:HG2	9:D:503:GXN:N02	2.36	0.40
4:F:185:TYR:HE2	4:F:228:TYR:OH	2.02	0.40
4:F:55:GLU:HB3	4:F:58:LEU:HD12	2.04	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	440/451 (98%)	425 (97%)	15 (3%)	0	100	100
1	C	446/451 (99%)	436 (98%)	10 (2%)	0	100	100
2	B	424/445 (95%)	414 (98%)	10 (2%)	0	100	100
2	D	417/445 (94%)	405 (97%)	12 (3%)	0	100	100
3	E	120/143 (84%)	117 (98%)	3 (2%)	0	100	100
4	F	300/384 (78%)	289 (96%)	11 (4%)	0	100	100
All	All	2147/2319 (93%)	2086 (97%)	61 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	373/379 (98%)	371 (100%)	2 (0%)	88	95
1	C	379/379 (100%)	376 (99%)	3 (1%)	81	91
2	B	371/383 (97%)	369 (100%)	2 (0%)	88	95
2	D	363/383 (95%)	357 (98%)	6 (2%)	60	78
3	E	111/127 (87%)	111 (100%)	0	100	100
4	F	284/342 (83%)	283 (100%)	1 (0%)	91	96

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	1881/1993 (94%)	1867 (99%)	14 (1%)	81	92

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	THR
1	A	71	GLU
2	B	139	HIS
2	B	164	ARG
1	C	71	GLU
1	C	221	ARG
1	C	381	THR
2	D	139	HIS
2	D	247	GLN
2	D	255	LEU
2	D	291	LEU
2	D	352	LYS
2	D	387	LEU
4	F	20	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	45	GLN
1	C	11	GLN
2	D	247	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 carbohydrates in this entry.

## 5.6 Ligand geometry

Of 15 ligands modelled in this entry, 7 are monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
9	GXN	D	503	-	31,31,31	4.63	8 (25%)	45,45,45	1.87	7 (15%)
10	MES	B	503	-	12,12,12	2.20	1 (8%)	14,16,16	1.86	4 (28%)
5	GTP	A	501	6	26,34,34	0.96	1 (3%)	33,54,54	1.65	6 (18%)
11	ACP	F	401	6	27,33,33	1.66	6 (22%)	32,52,52	1.43	4 (12%)
9	GXN	B	502	-	31,31,31	4.62	8 (25%)	45,45,45	1.74	8 (17%)
5	GTP	C	501	6	26,34,34	0.98	1 (3%)	33,54,54	1.74	6 (18%)
8	GDP	B	501	6	24,30,30	1.22	2 (8%)	31,47,47	1.92	7 (22%)
8	GDP	D	501	6	24,30,30	1.18	2 (8%)	31,47,47	1.94	8 (25%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	GXN	D	503	-	-	7/15/24/24	0/3/3/3
10	MES	B	503	-	-	1/6/14/14	0/1/1/1
5	GTP	A	501	6	-	8/18/38/38	0/3/3/3
11	ACP	F	401	6	-	5/15/38/38	0/3/3/3
9	GXN	B	502	-	-	4/15/24/24	0/3/3/3
5	GTP	C	501	6	-	8/18/38/38	0/3/3/3
8	GDP	B	501	6	-	3/12/32/32	0/3/3/3
8	GDP	D	501	6	-	7/12/32/32	0/3/3/3

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	D	503	GXN	BR1-C13	-21.33	1.41	1.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	502	GXN	BR1-C13	-21.31	1.41	1.89
9	B	502	GXN	S01-N02	9.93	1.69	1.58
9	D	503	GXN	S01-N02	9.93	1.69	1.58
10	B	503	MES	C8-S	-7.34	1.67	1.77
9	B	502	GXN	O06-S01	5.72	1.47	1.42
9	D	503	GXN	O06-S01	5.66	1.47	1.42
9	D	503	GXN	O05-S01	5.30	1.46	1.42
9	B	502	GXN	O05-S01	4.78	1.46	1.42
8	D	501	GDP	C6-C5	4.19	1.48	1.41
8	B	501	GDP	C6-C5	4.15	1.48	1.41
11	F	401	ACP	PB-O1B	4.15	1.61	1.51
9	D	503	GXN	O02-C14	-3.78	1.31	1.38
9	B	502	GXN	O02-C14	-3.65	1.31	1.38
11	F	401	ACP	PB-O2B	-3.40	1.48	1.56
5	C	501	GTP	C6-N1	3.18	1.38	1.33
9	B	502	GXN	C16-C11	2.92	1.44	1.39
11	F	401	ACP	PG-O2G	2.89	1.61	1.54
5	A	501	GTP	C6-N1	2.85	1.38	1.33
11	F	401	ACP	PG-O3G	2.85	1.61	1.54
11	F	401	ACP	PB-O3A	2.81	1.61	1.58
9	D	503	GXN	C12-C13	2.72	1.44	1.38
9	B	502	GXN	C12-C13	2.65	1.43	1.38
9	B	502	GXN	O04-S01	2.54	1.64	1.61
9	D	503	GXN	O04-S01	2.50	1.64	1.61
11	F	401	ACP	C5-C4	2.49	1.47	1.40
9	D	503	GXN	C16-C11	2.46	1.43	1.39
8	B	501	GDP	C5-C4	2.45	1.47	1.40
8	D	501	GDP	C5-C4	2.42	1.47	1.40

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	D	503	GXN	O06-S01-O05	-6.13	114.17	119.97
9	D	503	GXN	O03-C01-C02	5.58	123.19	115.41
5	C	501	GTP	N3-C2-N1	-5.46	119.94	127.22
9	B	502	GXN	O06-S01-O05	-5.18	115.07	119.97
5	A	501	GTP	N3-C2-N1	-5.15	120.36	127.22
8	B	501	GDP	C2-N3-C4	5.01	121.08	115.36
8	D	501	GDP	C2-N3-C4	4.76	120.80	115.36
5	C	501	GTP	C2-N3-C4	4.58	120.58	115.36
10	B	503	MES	C5-N4-C3	4.45	118.85	108.83
8	B	501	GDP	C6-C5-C4	-4.21	116.77	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	D	503	GXN	O03-C01-C06	-4.19	116.91	124.12
9	B	502	GXN	O02-C14-C15	4.18	126.15	120.12
9	B	502	GXN	O03-C01-C02	4.18	121.24	115.41
8	B	501	GDP	C6-N1-C2	4.13	122.50	115.93
8	D	501	GDP	C6-N1-C2	4.11	122.46	115.93
8	D	501	GDP	C5-C6-N1	-4.07	117.86	123.43
11	F	401	ACP	PA-O3A-PB	-4.04	119.75	132.56
5	A	501	GTP	C2-N3-C4	3.93	119.84	115.36
9	D	503	GXN	C17-O02-C14	3.91	125.48	114.78
9	D	503	GXN	O02-C14-C15	3.85	125.67	120.12
8	D	501	GDP	C6-C5-C4	-3.78	117.19	120.80
8	B	501	GDP	C5-C6-N1	-3.75	118.30	123.43
9	B	502	GXN	C17-O02-C14	3.71	124.93	114.78
8	B	501	GDP	N3-C2-N1	-3.60	122.42	127.22
8	D	501	GDP	N3-C2-N1	-3.30	122.82	127.22
11	F	401	ACP	C3'-C2'-C1'	3.23	105.84	100.98
11	F	401	ACP	N3-C2-N1	-3.16	123.74	128.68
9	B	502	GXN	O02-C14-C13	-3.12	114.74	120.74
9	B	502	GXN	O03-C01-C06	-3.09	118.80	124.12
8	D	501	GDP	PA-O3A-PB	-2.96	122.68	132.83
8	B	501	GDP	C4-C5-N7	-2.92	106.36	109.40
5	A	501	GTP	C5-C6-N1	-2.89	119.48	123.43
8	D	501	GDP	C4-C5-N7	-2.88	106.40	109.40
5	C	501	GTP	C5-C6-N1	-2.74	119.69	123.43
10	B	503	MES	O3S-S-C8	2.67	110.09	105.77
5	C	501	GTP	PB-O3B-PG	-2.65	123.74	132.83
11	F	401	ACP	C4-C5-N7	-2.63	106.65	109.40
9	B	502	GXN	C07-C08-N01	-2.62	108.22	111.07
5	A	501	GTP	C6-N1-C2	2.62	120.09	115.93
5	A	501	GTP	PB-O3B-PG	-2.60	123.92	132.83
5	C	501	GTP	PA-O3A-PB	-2.59	123.93	132.83
9	D	503	GXN	O02-C14-C13	-2.53	115.87	120.74
5	C	501	GTP	C6-N1-C2	2.50	119.90	115.93
5	A	501	GTP	PA-O3A-PB	-2.35	124.77	132.83
10	B	503	MES	O1S-S-C8	2.26	109.63	106.92
9	D	503	GXN	O01-C15-C14	2.22	119.06	115.16
8	B	501	GDP	O2B-PB-O3A	2.20	112.01	104.64
10	B	503	MES	C7-N4-C5	2.18	116.81	111.23
9	B	502	GXN	O01-C15-C14	2.07	118.80	115.16
8	D	501	GDP	C3'-C2'-C1'	2.04	104.05	100.98

There are no chirality outliers.

All (43) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	D	503	GXN	C13-C14-O02-C17
11	F	401	ACP	PG-C3B-PB-O1B
11	F	401	ACP	PG-C3B-PB-O2B
11	F	401	ACP	PG-C3B-PB-O3A
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	D	503	GXN	C14-C15-O01-C18
11	F	401	ACP	O4'-C4'-C5'-O5'
9	D	503	GXN	C16-C15-O01-C18
9	D	503	GXN	C15-C14-O02-C17
11	F	401	ACP	C3'-C4'-C5'-O5'
9	B	502	GXN	C16-C15-O01-C18
9	B	502	GXN	C14-C15-O01-C18
9	D	503	GXN	C02-C01-O03-C19
9	B	502	GXN	C02-C01-O03-C19
5	C	501	GTP	PB-O3A-PA-O2A
9	D	503	GXN	C06-C01-O03-C19
8	D	501	GDP	PB-O3A-PA-O2A
5	C	501	GTP	C4'-C5'-O5'-PA
9	B	502	GXN	C06-C01-O03-C19
5	A	501	GTP	PB-O3A-PA-O2A
5	A	501	GTP	C4'-C5'-O5'-PA
5	A	501	GTP	PB-O3B-PG-O1G
5	C	501	GTP	PB-O3B-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-O3B
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-O1A
8	D	501	GDP	PB-O3A-PA-O1A
8	D	501	GDP	C4'-C5'-O5'-PA
9	D	503	GXN	C11-C10-N01-C09

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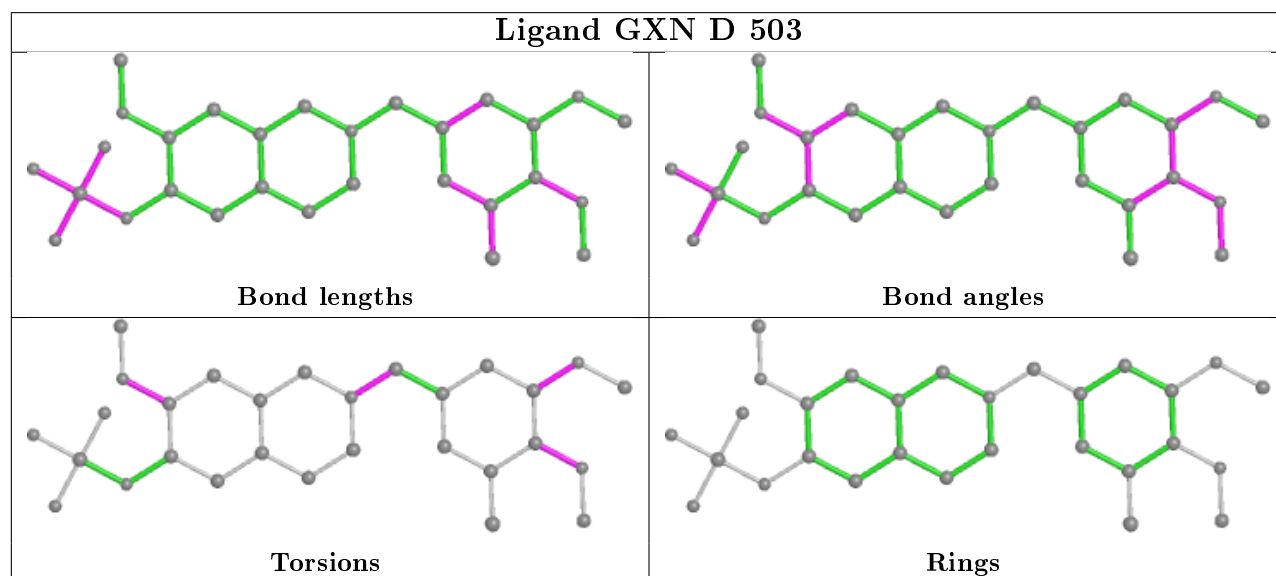
Mol	Chain	Res	Type	Atoms
10	B	503	MES	C8-C7-N4-C3

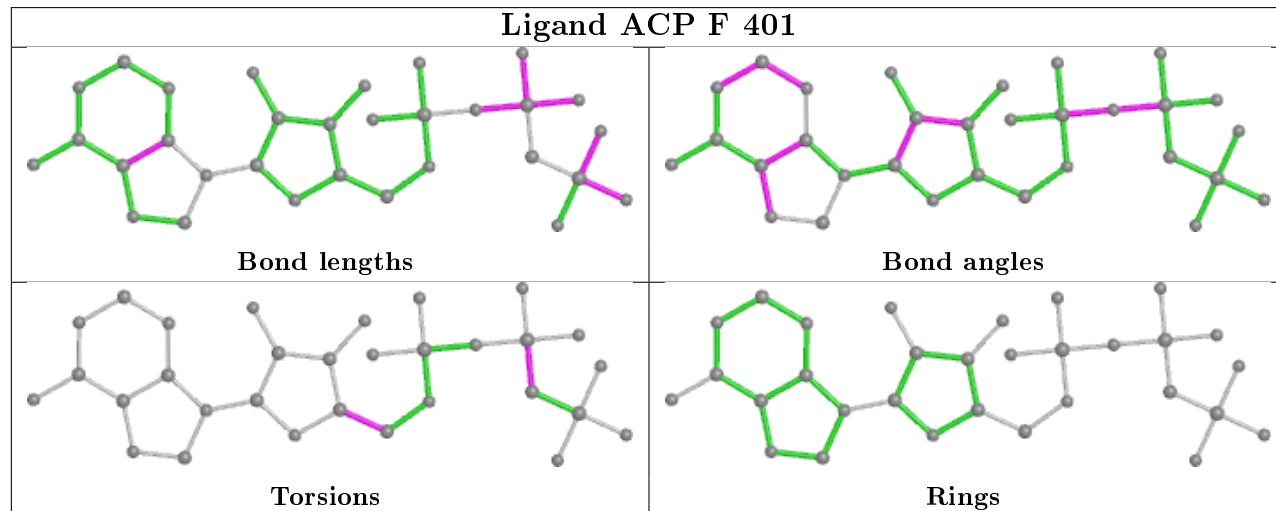
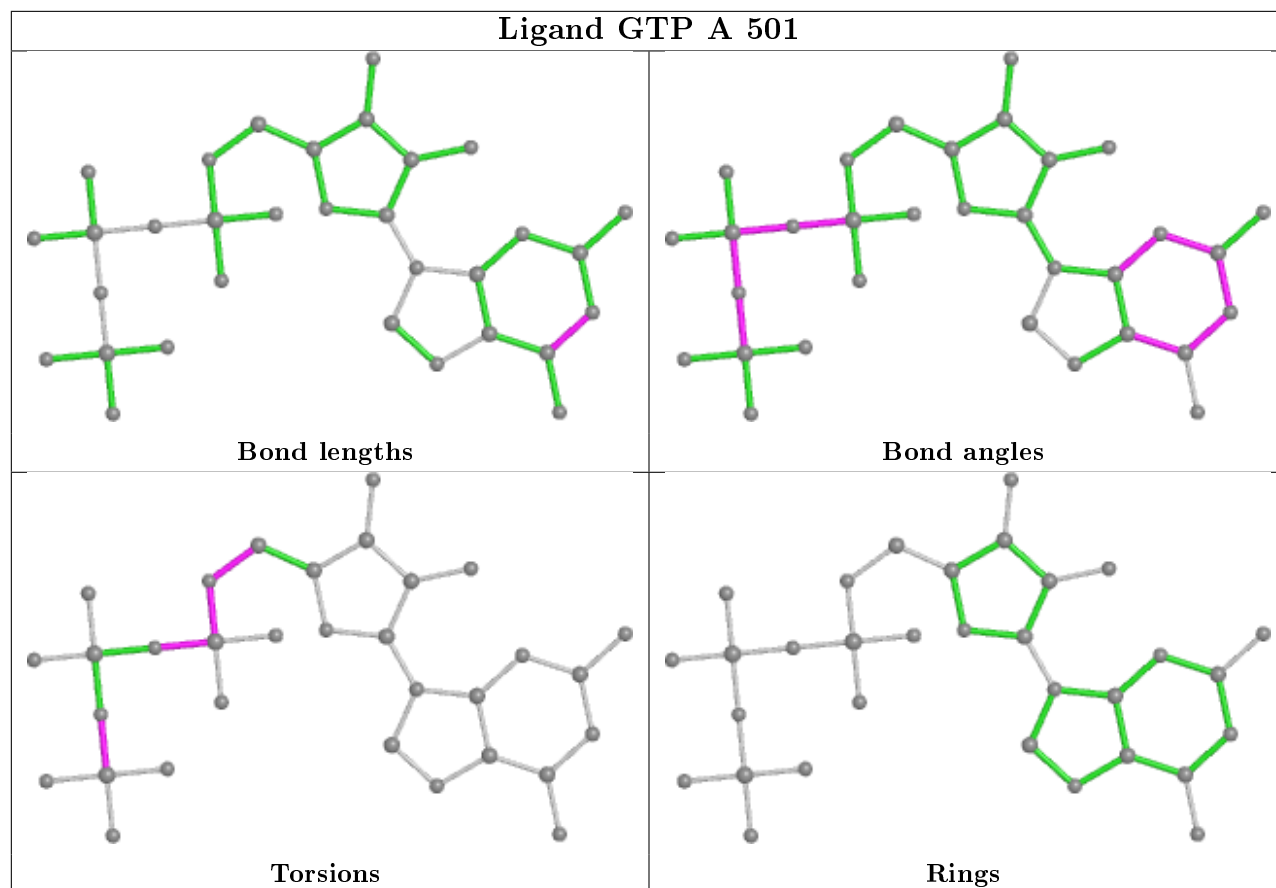
There are no ring outliers.

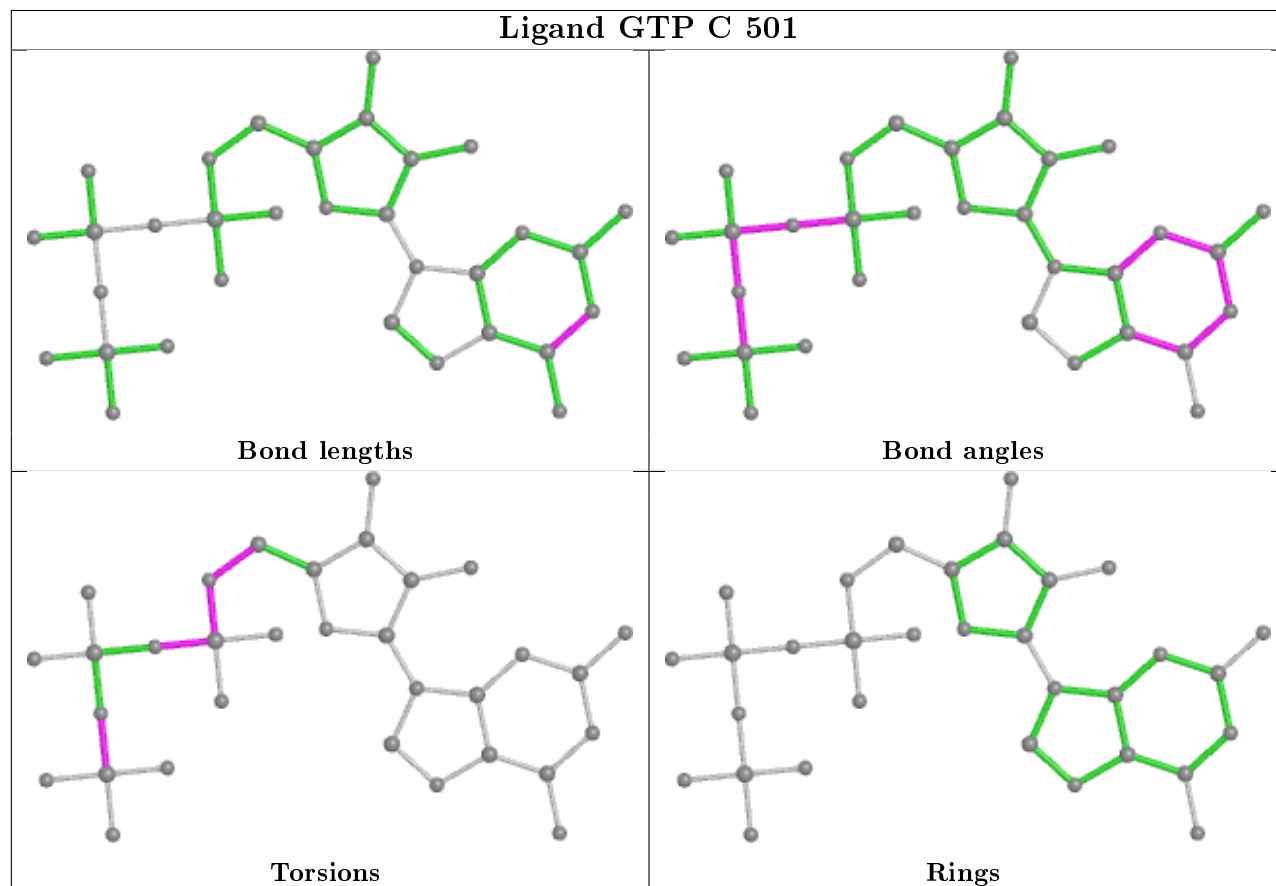
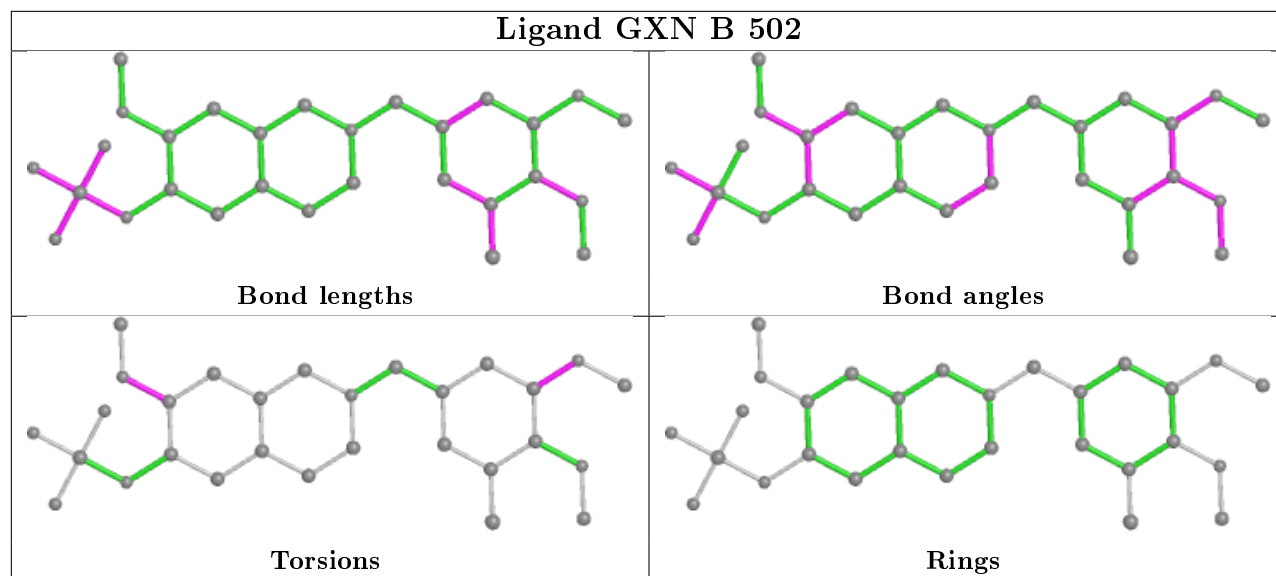
5 monomers are involved in 15 short contacts:

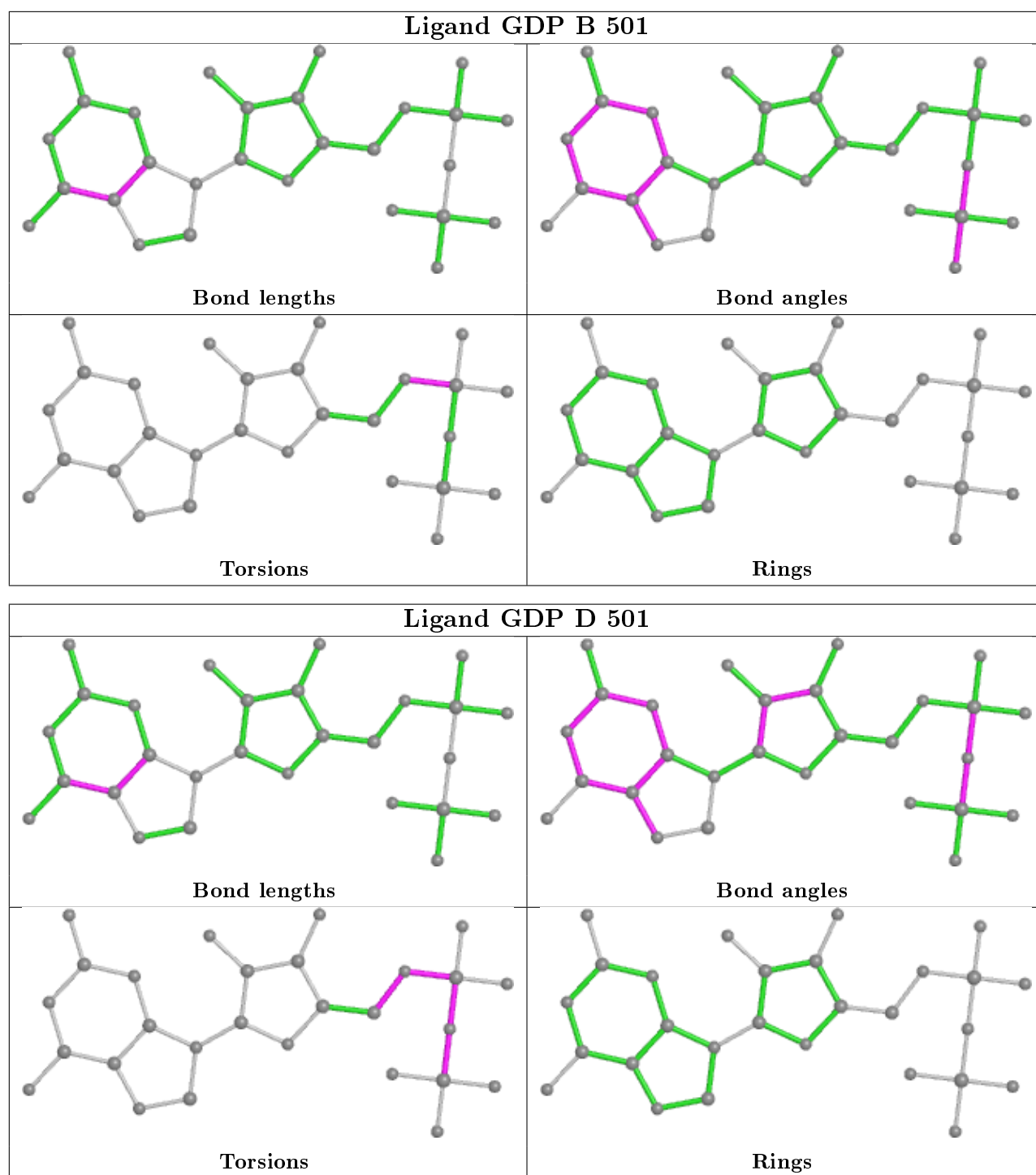
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	D	503	GXN	4	0
11	F	401	ACP	3	0
9	B	502	GXN	5	0
5	C	501	GTP	1	0
8	D	501	GDP	2	0

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.









## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	437/451 (96%)	0.07	13 (2%) 50 49	54, 81, 135, 171	0
1	C	440/451 (97%)	-0.21	3 (0%) 87 86	43, 62, 103, 137	0
2	B	422/445 (94%)	-0.01	10 (2%) 59 57	47, 70, 117, 171	0
2	D	420/445 (94%)	0.26	29 (6%) 16 15	59, 102, 148, 177	0
3	E	123/143 (86%)	0.25	13 (10%) 6 5	58, 100, 154, 185	0
4	F	316/384 (82%)	1.35	105 (33%) 0 0	67, 121, 193, 226	0
All	All	2158/2319 (93%)	0.23	173 (8%) 12 11	43, 85, 154, 226	0

All (173) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	130	VAL	8.8
4	F	132	LEU	8.1
4	F	182	ILE	7.4
4	F	131	PHE	7.3
4	F	138	ARG	7.3
4	F	181	VAL	6.6
4	F	134	ALA	6.5
3	E	141	GLU	6.4
4	F	100	ILE	6.3
4	F	186	LEU	6.2
4	F	166	ALA	5.6
4	F	199	PHE	5.6
4	F	238	CYS	5.5
4	F	225	SER	5.5
4	F	362	ALA	5.2
4	F	346	LEU	5.2
4	F	21	LEU	5.0
4	F	183	GLN	5.0
4	F	231	ALA	4.9

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Mol	Chain	Res	Type	RSRZ
3	E	27	PRO	4.9
1	A	282	TYR	4.9
3	E	24	LEU	4.7
4	F	44	ARG	4.6
4	F	128	ARG	4.6
2	B	59	ASN	4.6
4	F	255	ARG	4.4
3	E	26	PRO	4.4
1	A	437	VAL	4.4
4	F	240	LEU	4.4
4	F	17	VAL	4.3
4	F	254	GLY	4.3
2	D	177	VAL	4.3
4	F	361	LEU	4.2
4	F	164	SER	4.2
4	F	229	ASN	4.2
4	F	220	VAL	4.1
4	F	133	ALA	4.1
4	F	239	HIS	4.1
2	D	219	LEU	4.1
4	F	253	TYR	4.1
2	B	36	TYR	4.1
4	F	259	GLY	4.0
4	F	223	THR	4.0
2	B	57	THR	4.0
4	F	145	ASN	4.0
4	F	230	SER	4.0
4	F	342	LEU	4.0
4	F	101	TYR	3.9
2	D	216	THR	3.8
4	F	372	THR	3.8
2	D	217	LEU	3.8
4	F	20	LEU	3.8
4	F	25	GLY	3.8
4	F	139	ARG	3.8
2	D	57	THR	3.8
4	F	99	VAL	3.8
4	F	264	PHE	3.8
4	F	190	LEU	3.8
4	F	197	ARG	3.7
4	F	127	GLU	3.7
2	D	37	HIS	3.6

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Mol	Chain	Res	Type	RSRZ
4	F	194	PRO	3.6
2	D	58	GLY	3.6
1	A	281	ALA	3.6
2	D	249	ASN	3.6
4	F	147	TRP	3.6
2	B	60	LYS	3.5
4	F	224	SER	3.5
3	E	25	LYS	3.5
4	F	256	TYR	3.5
4	F	192	LEU	3.5
3	E	140	LYS	3.5
4	F	27	TRP	3.4
4	F	198	LYS	3.4
4	F	263	PHE	3.4
1	A	346	TRP	3.4
2	B	58	GLY	3.3
2	D	404	PHE	3.3
2	B	56	ALA	3.3
4	F	226	GLU	3.3
4	F	136	ASN	3.3
2	D	401	ARG	3.3
4	F	137	ARG	3.2
3	E	142	GLU	3.2
4	F	98	TYR	3.1
2	D	96	GLN	3.1
4	F	96	GLU	3.1
4	F	246	GLN	3.1
4	F	228	TYR	3.0
4	F	28	LYS	3.0
2	D	218	LYS	3.0
4	F	26	GLN	3.0
4	F	13	VAL	3.0
4	F	260	ASN	3.0
3	E	28	SER	2.9
1	A	58	ALA	2.9
2	D	405	LEU	2.9
4	F	180	HIS	2.9
1	A	347	CYS	2.8
4	F	196	HIS	2.8
2	B	37	HIS	2.8
4	F	184	LYS	2.8
1	A	345	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
2	D	260	VAL	2.7
2	D	415	GLU	2.7
4	F	241	THR	2.7
4	F	262	MET	2.7
2	D	95	GLY	2.7
4	F	150	LYS	2.7
4	F	258	GLU	2.6
2	D	79	ARG	2.6
4	F	135	TYR	2.6
4	F	144	GLY	2.6
4	F	201	ILE	2.6
3	E	138	GLU	2.6
4	F	243	HIS	2.6
2	D	82	PRO	2.6
1	A	56	THR	2.6
4	F	125	THR	2.6
3	E	135	LYS	2.5
4	F	22	LEU	2.5
4	F	257	GLU	2.5
4	F	323	GLU	2.5
1	C	2	ARG	2.5
1	C	338	LYS	2.5
4	F	195	GLY	2.4
4	F	187	GLU	2.4
1	A	42	ILE	2.4
4	F	129	GLU	2.4
3	E	139	LEU	2.4
2	D	83	PHE	2.4
1	C	253	THR	2.4
2	D	78	VAL	2.4
4	F	9	GLU	2.4
4	F	227	PRO	2.4
2	D	220	THR	2.4
2	B	337	ASN	2.3
2	D	399	PHE	2.3
4	F	343	TYR	2.3
4	F	19	ARG	2.3
2	B	55	GLU	2.3
4	F	338	CYS	2.3
2	D	59	ASN	2.3
4	F	200	ASP	2.3
4	F	151	SER	2.3

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Mol	Chain	Res	Type	RSRZ
4	F	24	THR	2.3
4	F	126	ASP	2.2
1	A	349	THR	2.2
4	F	244	CYS	2.2
4	F	245	ILE	2.2
4	F	6	VAL	2.2
4	F	336	PRO	2.1
2	D	202	TYR	2.1
2	B	276	THR	2.1
2	D	85	GLN	2.1
4	F	146	VAL	2.1
2	D	86	ILE	2.1
1	A	351	PHE	2.1
3	E	48	GLU	2.1
4	F	102	PRO	2.1
4	F	165	GLU	2.1
4	F	271	LEU	2.1
4	F	275	LEU	2.1
2	D	80	SER	2.1
2	D	272	PHE	2.1
4	F	149	ALA	2.1
1	A	362	VAL	2.1
4	F	185	TYR	2.1
2	D	94	PHE	2.1
3	E	103	GLN	2.1
4	F	236	LYS	2.1
4	F	221	LEU	2.0
1	A	173	PRO	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 carbohydrates 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,

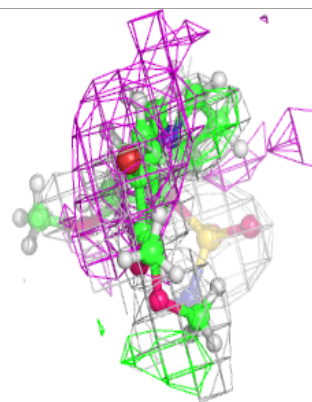
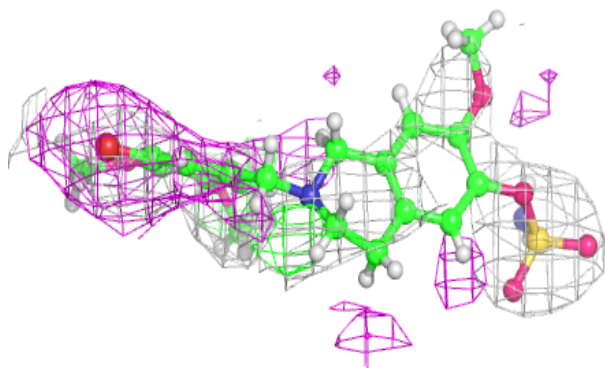
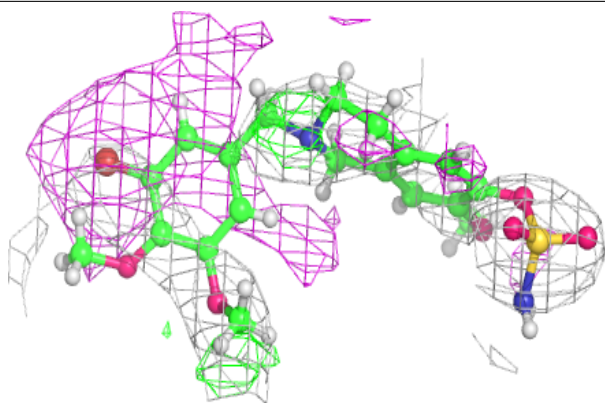
median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
9	GXN	D	503	29/29	0.62	0.44	49,116,142,148	52
9	GXN	B	502	29/29	0.71	0.21	30,66,83,83	0
7	CA	A	503	1/1	0.79	0.23	259,259,259,259	0
11	ACP	F	401	31/31	0.84	0.16	104,123,179,183	0
6	MG	D	502	1/1	0.91	0.07	77,77,77,77	0
7	CA	C	503	1/1	0.92	0.18	118,118,118,118	0
8	GDP	D	501	28/28	0.94	0.14	71,86,110,116	0
6	MG	B	504	1/1	0.95	0.20	50,50,50,50	0
10	MES	B	503	12/12	0.96	0.14	53,79,92,103	0
6	MG	F	402	1/1	0.96	0.09	166,166,166,166	0
6	MG	C	502	1/1	0.96	0.16	58,58,58,58	0
5	GTP	C	501	32/32	0.98	0.18	44,53,64,65	0
8	GDP	B	501	28/28	0.98	0.23	43,52,61,66	0
6	MG	A	502	1/1	0.98	0.18	55,55,55,55	0
5	GTP	A	501	32/32	0.98	0.23	45,56,70,74	0

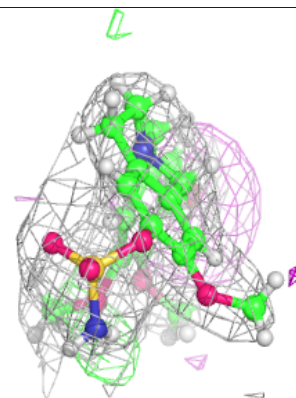
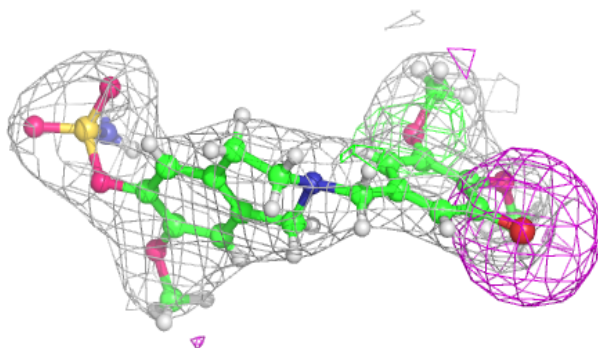
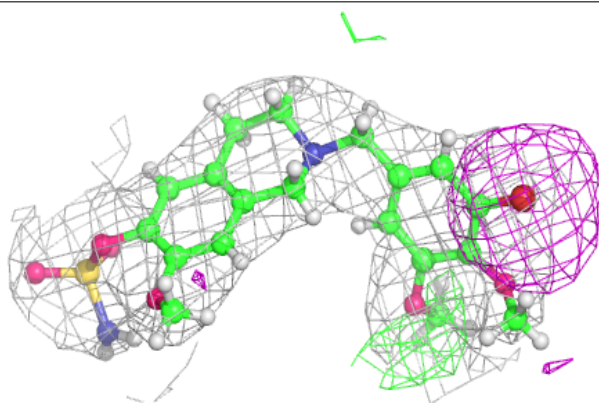
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around GXN 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)

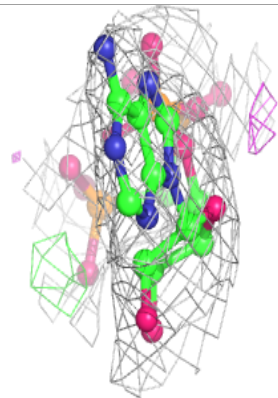
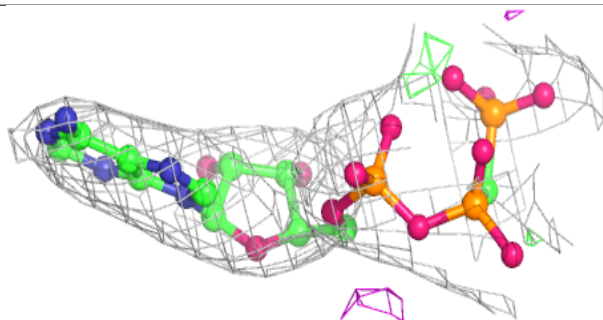
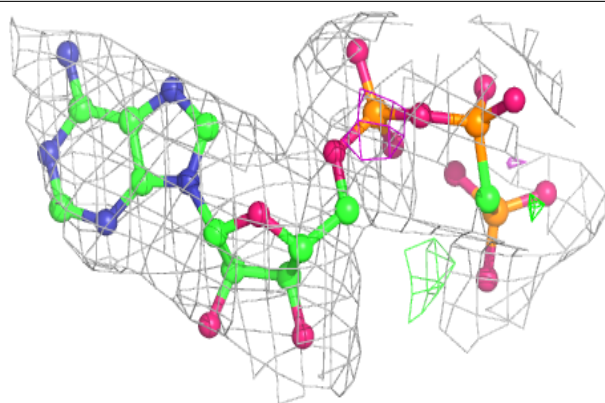
**Electron density around GXN B 502:**

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

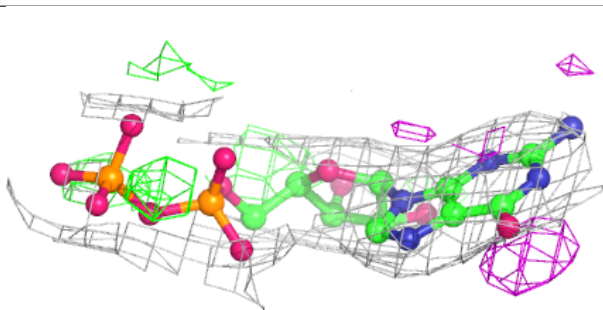
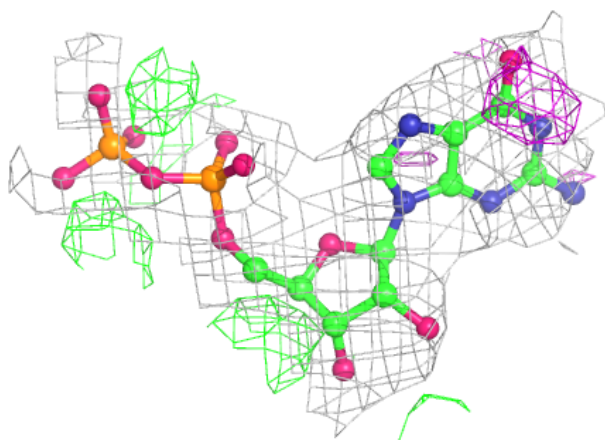


**Electron density around ACP F 401:**

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

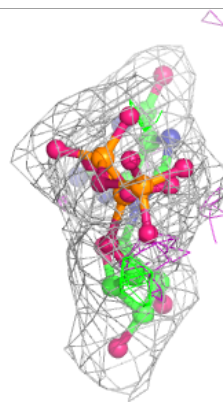
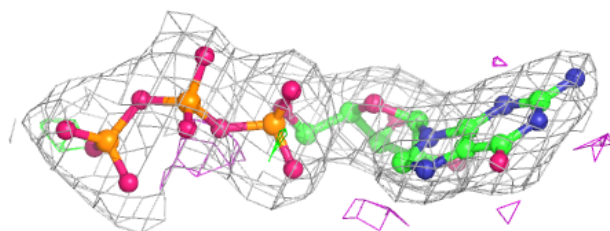
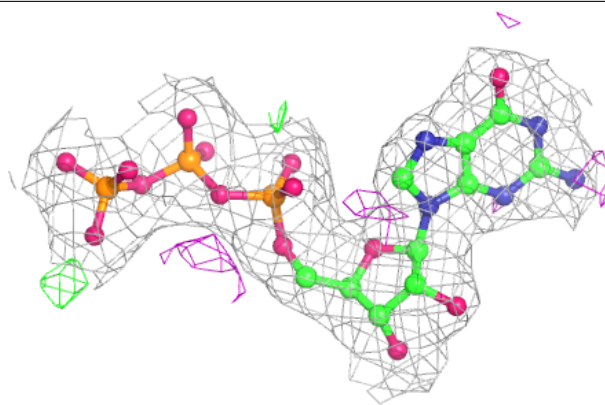
**Electron density around GDP D 501:**

$2mF_o-DF_c$  (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:**

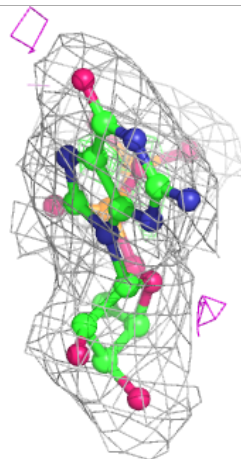
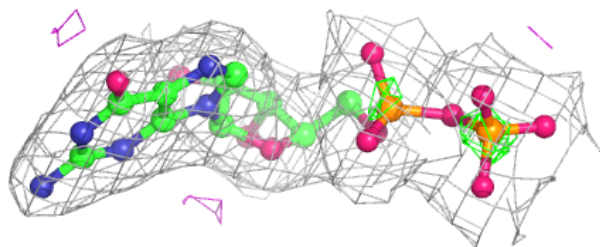
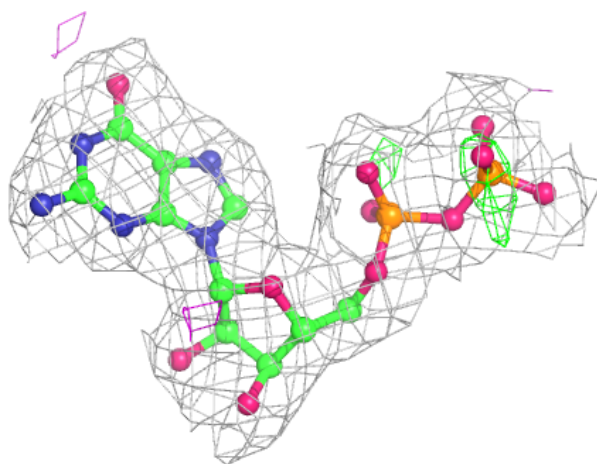
$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

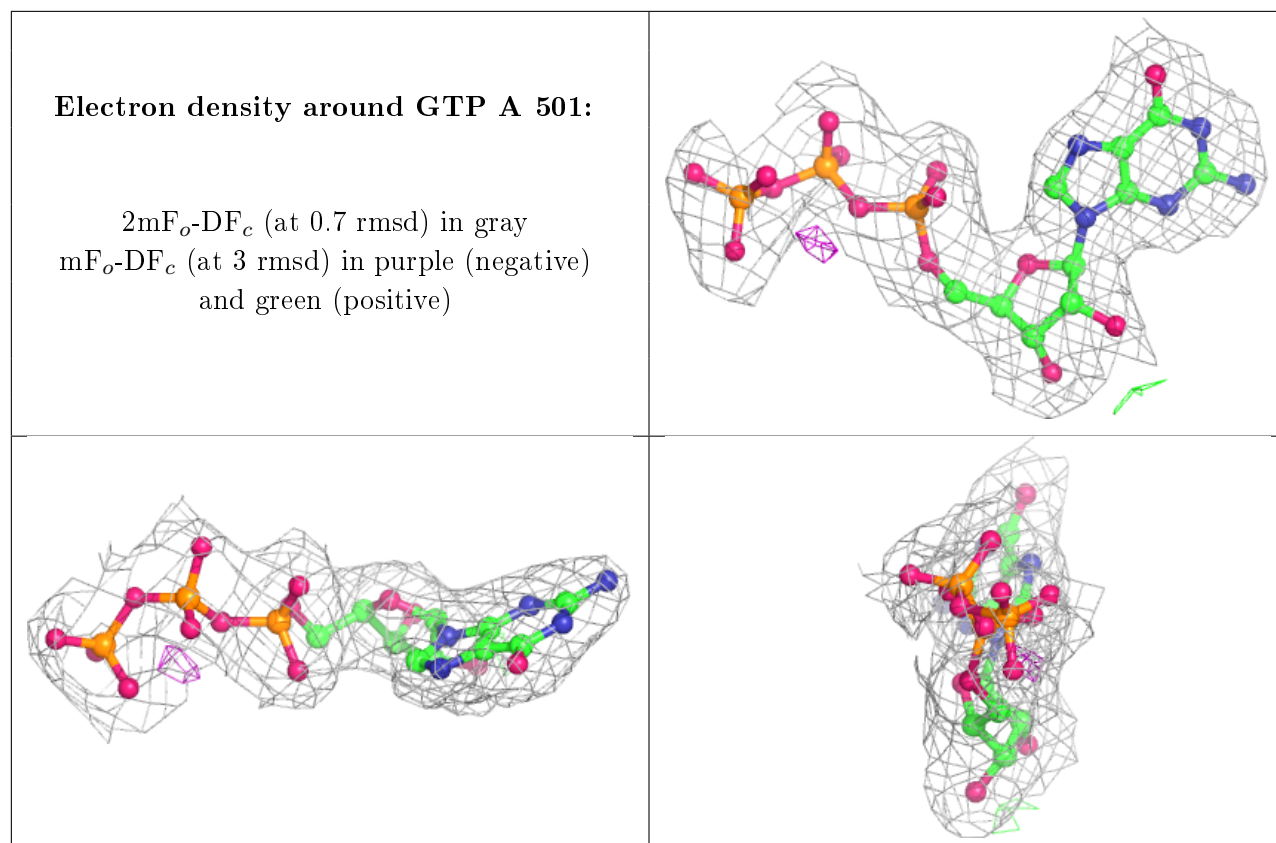




**Electron density around GDP B 501:**

$2mF_o-DF_c$  (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.