



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 17, 2020 – 03:09 pm GMT

PDB ID : 6ZWB
Title : Z-SBTub3 photoswitch bound to tubulin-DARPin D1 complex
Authors : Wranik, M.; Weinert, T.; Olieric, N.; Gao, L.; Kraus, Y.C.M.; Bingham, R.;
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Deposited on : 2020-07-28
Resolution : 1.75 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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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 : 2.15.1
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) : 2.15.1

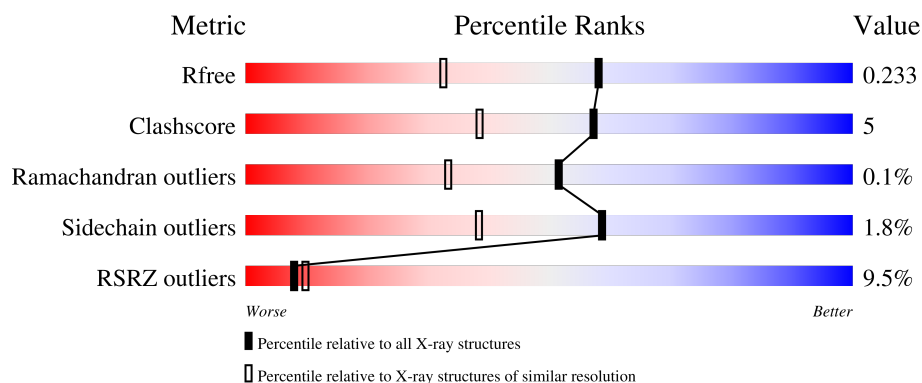
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

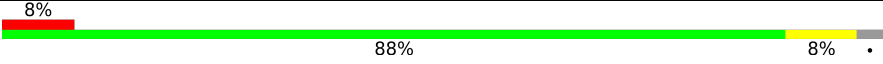
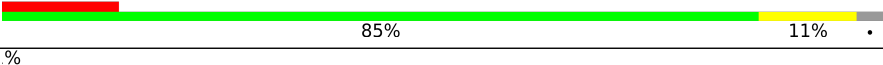
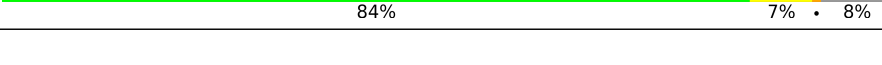
The reported resolution of this entry is 1.75 Å.

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	3764 (1.76-1.72)
Clashscore	141614	3923 (1.76-1.72)
Ramachandran outliers	138981	3878 (1.76-1.72)
Sidechain outliers	138945	3878 (1.76-1.72)
RSRZ outliers	127900	3705 (1.76-1.72)

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 ≥ 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	
2	B	445	
3	F	169	

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 16412 atoms, of which 7729 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	H	N	O	S	1	8	0
			6748	2169	3324	581	650	24			

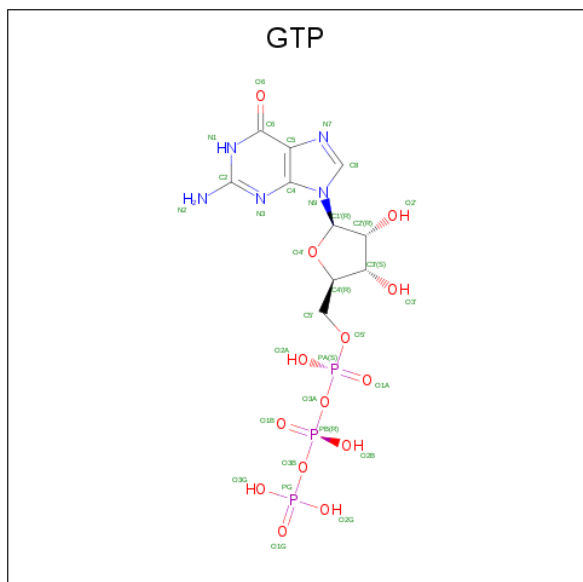
- Molecule 2 is a protein called Tubulin beta-2B chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	431	Total	C	H	N	O	S	0	3	0
			6569	2110	3215	569	647	28			

- Molecule 3 is a protein called Designed Ankyrin Repeat Protein (DARPIN) D1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	F	155	Total	C	H	N	O	S	0	2	0
			2317	731	1158	196	229	3			

- Molecule 4 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).

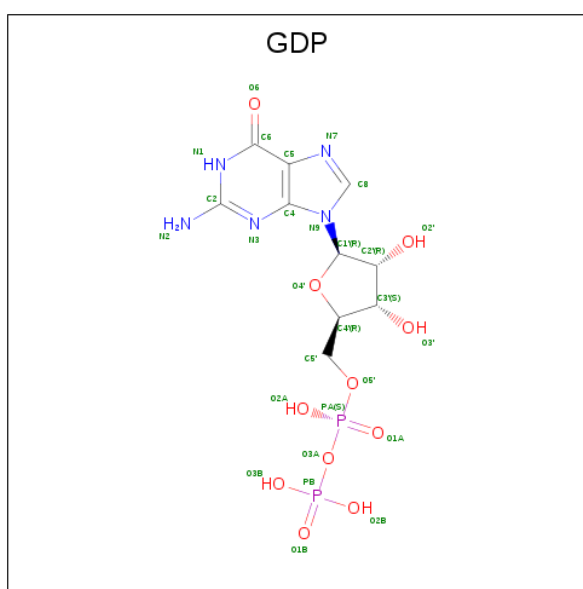


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	H	N	O	P	
			41	10	9	5	14	3	

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

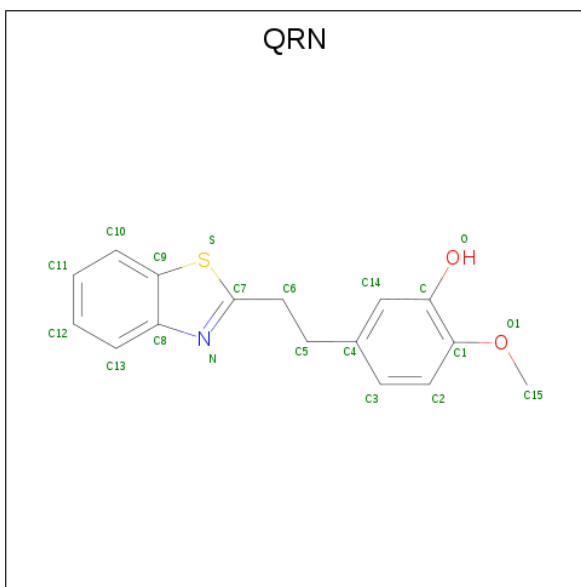
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Mg	0	0
			1	1		

- Molecule 6 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	B	1	Total	C	H	N	O	P	
			38	10	10	5	11	2	

- Molecule 7 is 5-[2-(1,3-benzothiazol-2-yl)ethyl]-2-methoxy-phenol (three-letter code: QRN) (formula: $C_{16}H_{15}NO_2S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	B	1	Total	C	H	N	O	S	
			33	16	13	1	2	1	
									0
									0


- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	310	Total	O		
			310	310	0	0
8	B	219	Total	O		
			219	219	0	0
8	F	136	Total	O		
			136	136	0	0

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.

- Chain A:
-
- 88% 8%
- 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28 29 30 31 32 33 34 35 36 37 38 39 40 41 42 43 44 45 46 47 48 49 50 51 52 53 54 55 56 57 58 59 60 61 62 63 64 65 66 67 68 69 70 71 72 73 74 75 76 77 78 79 80 81 82 83 84 85 86 87 88 89 90 91 92 93 94 95 96 97 98 99 100 101 102 103 104 105 106 107 108 109 110 111 112 113 114 115 116 117 118 119 120 121 122 123 124 125 126 127 128 129 130 131 132 133 134 135 136 137 138 139 140 141 142 143 144 145 146 147 148 149 150 151 152 153 154 155 156 157 158 159 160 161 162 163 164 165 166 167 168 169 170 171 172 173 174 175 176 177 178 179 180 181 182 183 184 185 186 187 188 189 190 191 192 193 194 195 196 197 198 199 200 201 202 203 204 205 206 207 208 209 210 211 212 213 214 215 216 217 218 219 220 221 222 223 224 225 226 227 228 229 230 231 232 233 234 235 236 237 238 239 240 241 242 243 244 245 246 247 248 249 250 251 252 253 254 255 256 257 258 259 260 261 262 263 264 265 266 267 268 269 270 271 272 273 274 275 276 277 278 279 280 281 282 283 284 285 286 287 288 289 290 291 292 293 294 295 296 297 298 299 300

- Chain B:
-
- 13% 85% 11%
- M1 Q11 Y195 E200 T204 E207 R241 K246 T240 P245 Q246 Q247 L248 M249 A250 D251 L252 R253 K254 L255 R264 F272 P273 P274 S277 R278 G279 S280 G281 Q282 Y283 R284 A285 L286 T287 Y288 P289 R295 R322 M325 K326 E327 V328 L333 V337 V338
- Y36 E37 G38 S40 D41 L42 Q45 L46 E47 A56 T57 G58 M59 M60 Y61 D69 T74 M75 D76 S77 V78 F82 F94 S97 R123 E127 D130 Q136 H139 K156 E159 I165 M166 M167 V171 M172 D179 V191
- V355 G356 D357 I358 F377 I378 L387 S392 T396 R400 H401 K402 L405 A406 H407 Y408 T409 G410 E411 G412 M413 D414 E415 M416 T439 A440 D441 G1U G1N G1Y PHE G1U G1U G1U G1U G1Y G1U ASP G1U ALA

- Chain F: 

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	73.87Å 91.72Å 83.01Å 90.00° 97.06° 90.00°	Depositor
Resolution (Å)	45.04 – 1.75 45.04 – 1.75	Depositor EDS
% Data completeness (in resolution range)	61.2 (45.04-1.75) 61.2 (45.04-1.75)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.15 (at 1.75Å)	Xtriage
Refinement program	PHENIX 1.18	Depositor
R, R_{free}	0.185 , 0.234 0.185 , 0.233	Depositor DCC
R_{free} test set	2000 reflections (2.93%)	wwPDB-VP
Wilson B-factor (Å ²)	23.2	Xtriage
Anisotropy	0.020	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 43.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	16412	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.59% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GDP, GTP, MG, QRN

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	0.27	0/3529	0.45	0/4793
2	B	0.27	0/3440	0.45	0/4663
3	F	0.24	0/1181	0.43	0/1606
All	All	0.26	0/8150	0.45	0/11062

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3424	3324	3309	27	0
2	B	3354	3215	3215	38	0
3	F	1159	1158	1157	14	0
4	A	32	9	12	0	0
5	A	1	0	0	0	0
6	B	28	10	12	0	0
7	B	20	13	0	2	0
8	A	310	0	0	13	0
8	B	219	0	0	15	0
8	F	136	0	0	8	0
All	All	8683	7729	7705	77	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 5.

All (77) 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)
2:B:325:MET:SD	2:B:355:VAL:HG11	2.07	0.94
2:B:264:ARG:NH1	8:B:601:HOH:O	2.05	0.90
1:A:326:LYS:NZ	8:A:601:HOH:O	2.11	0.82
1:A:221:ARG:NE	8:A:604:HOH:O	2.15	0.78
3:F:94:GLU:OE1	8:F:201:HOH:O	2.03	0.76
2:B:248:LEU:HD23	2:B:250:ALA:HB2	1.68	0.75
2:B:200:GLU:OE1	8:B:602:HOH:O	2.06	0.72
1:A:437:VAL:HG12	8:A:652:HOH:O	1.91	0.70
2:B:255:LEU:HD21	8:B:758:HOH:O	1.91	0.70
2:B:278:ARG:NH2	8:B:604:HOH:O	2.24	0.69
2:B:392:SER:OG	8:B:603:HOH:O	2.13	0.66
3:F:144:LYS:NZ	8:F:205:HOH:O	2.27	0.66
1:A:431:ASP:OD1	8:A:603:HOH:O	2.14	0.66
1:A:239:THR:OG1	8:A:602:HOH:O	2.13	0.66
1:A:332:ILE:HG22	1:A:336:LYS:HE2	1.78	0.66
1:A:243:ARG:NE	8:A:602:HOH:O	2.27	0.65
1:A:1:MET:HE3	8:A:873:HOH:O	1.96	0.65
2:B:252:LEU:HD22	8:B:602:HOH:O	1.97	0.65
3:F:156[B]:ASN:ND2	8:F:206:HOH:O	2.29	0.65
3:F:36:ASN:O	8:F:202:HOH:O	2.14	0.65
1:A:214:ARG:NH2	8:A:611:HOH:O	2.34	0.61
1:A:234:ILE:HD13	1:A:302:MET:SD	2.41	0.61
1:A:362:VAL:HG23	8:A:835:HOH:O	1.99	0.60
3:F:121:ALA:HB1	3:F:161:LEU:HD21	1.82	0.60
2:B:171:VAL:HA	2:B:204:ILE:O	2.03	0.59
2:B:295:MET:HG2	2:B:377:PHE:HB2	1.85	0.58
3:F:166:GLN:NE2	8:F:209:HOH:O	2.36	0.57
3:F:156[A]:ASN:ND2	8:F:207:HOH:O	2.32	0.56
1:A:209:ILE:HG23	1:A:230:LEU:HD23	1.88	0.56
3:F:64[A]:GLU:OE2	8:F:203:HOH:O	2.18	0.55
2:B:255:LEU:HD11	8:B:758:HOH:O	2.06	0.55
3:F:160:ASP:OD2	8:F:204:HOH:O	2.18	0.55
3:F:130:GLU:O	3:F:134:LYS:HG2	2.09	0.53
8:A:604:HOH:O	2:B:325:MET:HE3	2.08	0.53
2:B:75:MET:HG3	2:B:94:PHE:CD2	2.44	0.53
2:B:191:VAL:O	2:B:195:VAL:HG13	2.10	0.51
2:B:11:GLN:HA	2:B:74:THR:HG21	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:278:ARG:NH1	8:B:610:HOH:O	2.41	0.50
3:F:144:LYS:H	3:F:144:LYS:HD2	1.76	0.49
2:B:165:ILE:HG21	2:B:252:LEU:HB3	1.93	0.49
1:A:275:VAL:HG13	1:A:368:LEU:HD21	1.95	0.49
3:F:112:TRP:O	3:F:144:LYS:HD2	2.12	0.49
2:B:396:THR:O	2:B:400:ARG:HG3	2.14	0.47
1:A:97:GLU:HG3	2:B:1:MET:HG3	1.96	0.47
1:A:341:ILE:HD12	1:A:341:ILE:O	2.15	0.46
1:A:123[B]:ARG:NH1	8:A:631:HOH:O	2.49	0.45
1:A:188:ILE:HG23	1:A:425:MET:HG3	1.98	0.45
2:B:69:ASP:HB3	2:B:94:PHE:CD2	2.51	0.45
2:B:240:THR:HG23	8:B:609:HOH:O	2.17	0.44
1:A:210:TYR:CZ	1:A:214:ARG:HD3	2.53	0.44
2:B:248:LEU:HD12	8:B:641:HOH:O	2.18	0.44
2:B:172:MET:HG3	2:B:387:LEU:HD21	1.99	0.43
2:B:402:LYS:HG3	2:B:405:LEU:HD22	1.99	0.43
2:B:195:VAL:HB	8:B:601:HOH:O	2.17	0.43
2:B:255:LEU:HD13	7:B:502:QRN:C8	2.48	0.43
2:B:39:ASP:OD2	2:B:39:ASP:N	2.51	0.43
1:A:2:ARG:O	1:A:133:GLN:NE2	2.48	0.43
2:B:123:ARG:O	2:B:127:GLU:HG2	2.19	0.43
2:B:248:LEU:HD21	7:B:502:QRN:S	2.58	0.43
1:A:328:VAL:O	1:A:332:ILE:HG12	2.19	0.43
2:B:47:GLU:HB3	8:B:759:HOH:O	2.19	0.42
2:B:195:VAL:CG2	8:B:601:HOH:O	2.67	0.42
1:A:26:LEU:HD12	1:A:363:VAL:HG22	2.01	0.42
1:A:1:MET:HG3	1:A:2:ARG:H	1.83	0.42
1:A:62:VAL:HG11	1:A:88:HIS:CE1	2.55	0.42
2:B:378:ILE:HG21	8:B:758:HOH:O	2.20	0.42
2:B:274:PRO:HB3	2:B:286:LEU:CD2	2.50	0.41
2:B:136:GLN:HA	2:B:167:ASN:O	2.21	0.41
2:B:400:ARG:HD2	3:F:112:TRP:NE1	2.35	0.41
1:A:71:GLU:HG2	1:A:98:ASP:HB3	2.03	0.41
2:B:245:PRO:HB3	8:B:759:HOH:O	2.20	0.41
3:F:144:LYS:HD3	3:F:145:PHE:HD1	1.87	0.40
1:A:406:HIS:HD2	8:A:887:HOH:O	2.04	0.40
2:B:156:LYS:O	2:B:159:GLU:HG2	2.21	0.40
1:A:317:LEU:HD13	1:A:332:ILE:HD11	2.04	0.40
1:A:341:ILE:HB	8:A:614:HOH:O	2.20	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	443/451 (98%)	431 (97%)	12 (3%)	0	100	100
2	B	432/445 (97%)	416 (96%)	15 (4%)	1 (0%)	47	29
3	F	155/169 (92%)	154 (99%)	1 (1%)	0	100	100
All	All	1030/1065 (97%)	1001 (97%)	28 (3%)	1 (0%)	51	33

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	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	368/379 (97%)	362 (98%)	6 (2%)	62	44
2	B	364/383 (95%)	356 (98%)	8 (2%)	52	29
3	F	121/132 (92%)	120 (99%)	1 (1%)	81	72
All	All	853/894 (95%)	838 (98%)	15 (2%)	59	38

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	THR
1	A	263	PRO

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Mol	Chain	Res	Type
1	A	302	MET
1	A	338	LYS
1	A	362	VAL
1	A	430	LYS
2	B	139	HIS
2	B	207	GLU
2	B	249	ASN
2	B	322	ARG
2	B	326	LYS
2	B	357	ASP
2	B	406	HIS
2	B	441	ASP
3	F	144	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 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
4	GTP	A	501	5	26,34,34	1.03	1 (3%)	33,54,54	1.75	8 (24%)
6	GDP	B	501	-	24,30,30	1.09	3 (12%)	31,47,47	1.94	8 (25%)
7	QRN	B	502	-	20,22,22	1.76	2 (10%)	23,30,30	2.44	4 (17%)

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
4	GTP	A	501	5	-	6/18/38/38	0/3/3/3
6	GDP	B	501	-	-	4/12/32/32	0/3/3/3
7	QRN	B	502	-	-	3/6/7/7	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	502	QRN	C6-C7	-6.79	1.45	1.49
6	B	501	GDP	C6-C5	3.36	1.47	1.41
4	A	501	GTP	C6-N1	3.10	1.38	1.33
7	B	502	QRN	C6-C5	-2.84	1.33	1.53
6	B	501	GDP	C5-C4	2.36	1.47	1.40
6	B	501	GDP	O4'-C1'	2.16	1.44	1.41

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	502	QRN	C5-C6-C7	9.64	128.84	112.67
4	A	501	GTP	N3-C2-N1	-5.47	119.92	127.22
6	B	501	GDP	C6-N1-C2	4.74	123.46	115.93
7	B	502	QRN	C6-C5-C4	4.74	129.93	113.28
6	B	501	GDP	C6-C5-C4	-4.64	116.37	120.80
6	B	501	GDP	C5-C6-N1	-4.28	117.58	123.43
4	A	501	GTP	C2-N3-C4	4.10	120.04	115.36
6	B	501	GDP	C2-N3-C4	3.75	119.64	115.36
6	B	501	GDP	N3-C2-N1	-3.50	122.55	127.22
4	A	501	GTP	PB-O3B-PG	-3.20	121.84	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	502	QRN	C9-C8-N	3.10	115.25	108.04
6	B	501	GDP	PA-O3A-PB	-2.98	122.61	132.83
4	A	501	GTP	C5-C6-N1	-2.71	119.72	123.43
4	A	501	GTP	C6-N1-C2	2.61	120.08	115.93
4	A	501	GTP	PA-O3A-PB	-2.46	124.40	132.83
6	B	501	GDP	C1'-N9-C4	-2.20	122.78	126.64
6	B	501	GDP	C4-C5-N7	-2.16	107.15	109.40
4	A	501	GTP	N2-C2-N1	2.08	120.49	117.25
7	B	502	QRN	C8-C9-S	-2.03	109.16	111.85
4	A	501	GTP	C6-C5-C4	-2.01	118.88	120.80

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	501	GTP	C5'-O5'-PA-O1A
4	A	501	GTP	C5'-O5'-PA-O2A
6	B	501	GDP	C5'-O5'-PA-O1A
6	B	501	GDP	C5'-O5'-PA-O2A
7	B	502	QRN	C5-C6-C7-N
4	A	501	GTP	PB-O3A-PA-O1A
4	A	501	GTP	PB-O3B-PG-O1G
7	B	502	QRN	C3-C4-C5-C6
7	B	502	QRN	C14-C4-C5-C6
4	A	501	GTP	PB-O3B-PG-O3G
4	A	501	GTP	C5'-O5'-PA-O3A
6	B	501	GDP	C5'-O5'-PA-O3A
6	B	501	GDP	PB-O3A-PA-O1A

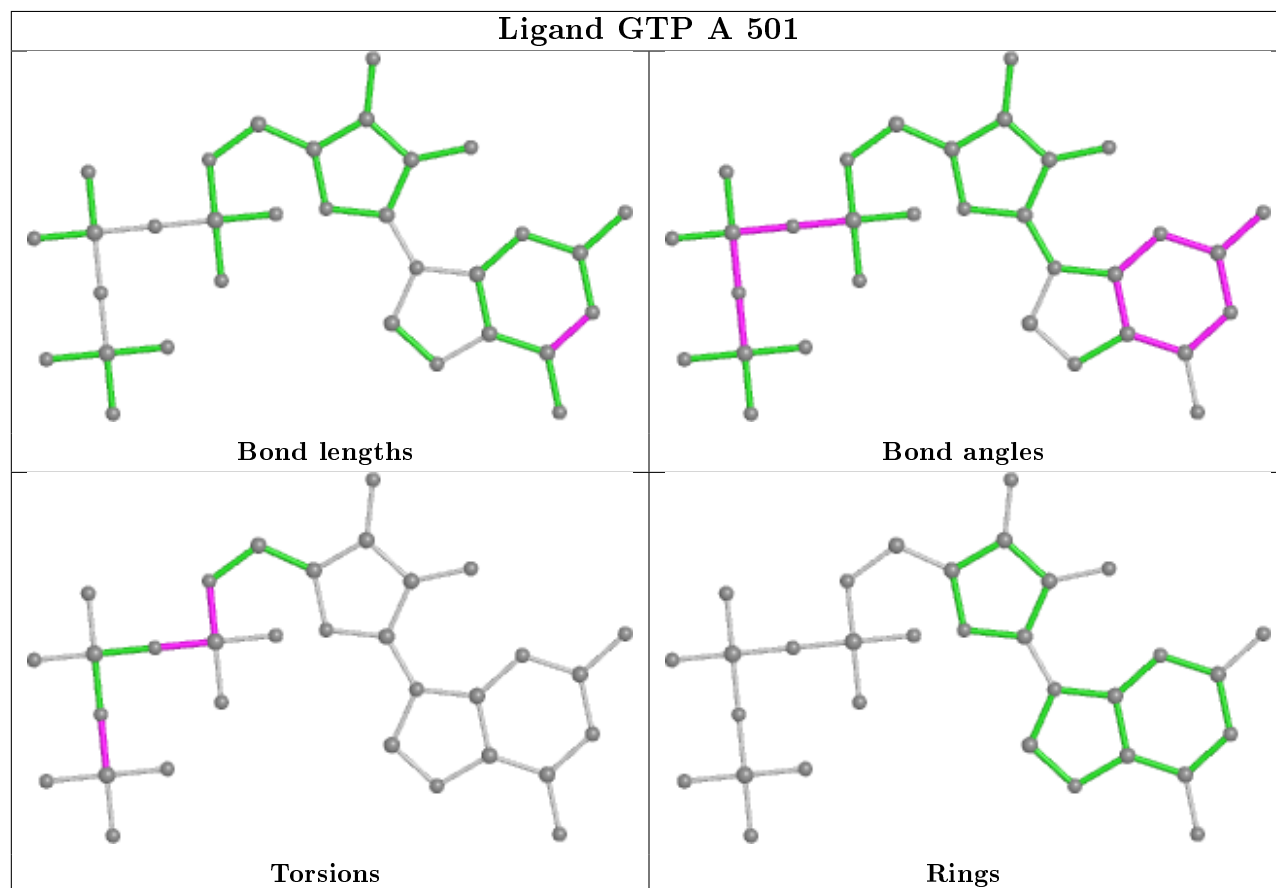
There are no ring outliers.

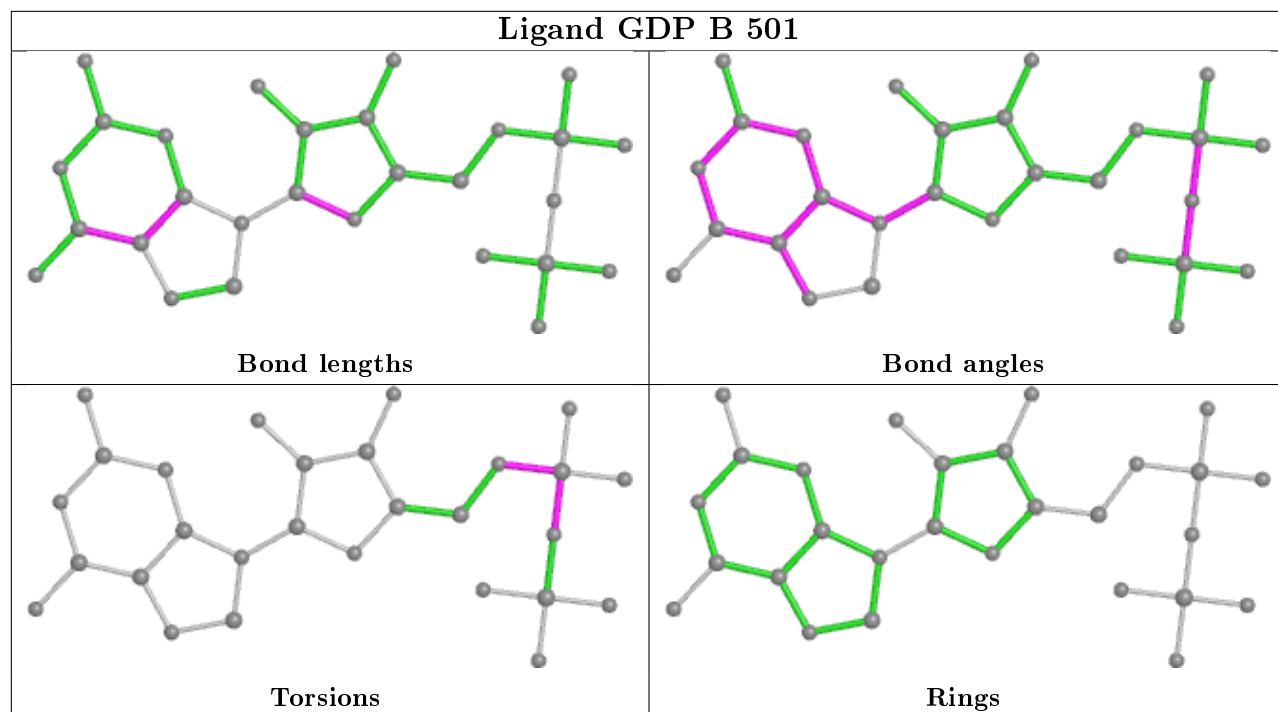
1 monomer is involved in 2 short contacts:

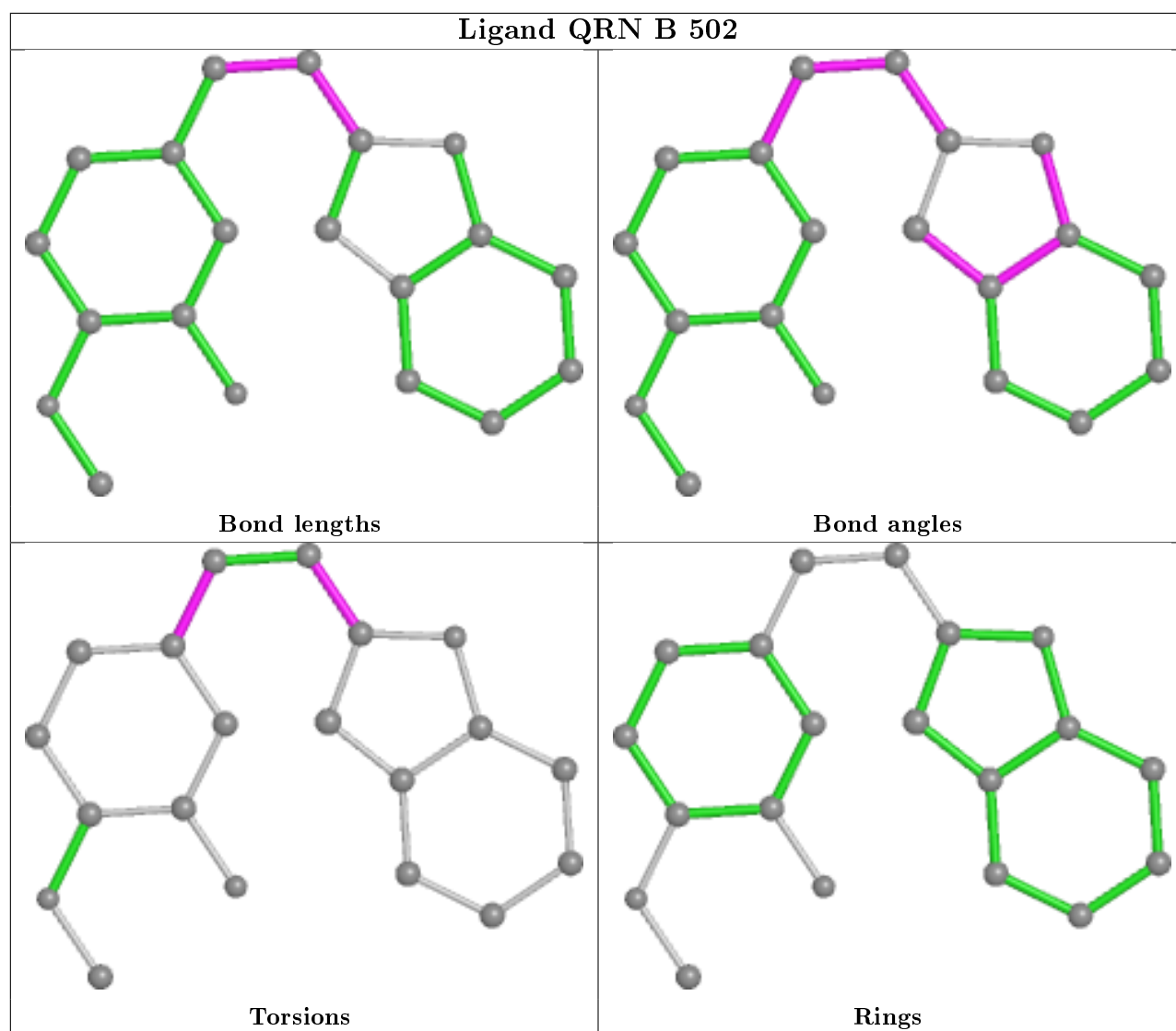
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	502	QRN	2	0

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, 95th 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 ²)	Q<0.9
1	A	437/451 (96%)	0.55	36 (8%) 11 15	13, 28, 90, 132	1 (0%)
2	B	431/445 (96%)	0.81	59 (13%) 3 3	15, 36, 95, 155	0
3	F	155/169 (91%)	-0.02	2 (1%) 77 82	15, 24, 59, 112	0
All	All	1023/1065 (96%)	0.58	97 (9%) 8 10	13, 30, 91, 155	1 (0%)

All (97) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	285	ALA	14.2
2	B	283	TYR	13.3
1	A	239	THR	11.7
1	A	437	VAL	10.3
1	A	42	ILE	9.9
2	B	56	ALA	7.8
1	A	177	VAL	6.7
1	A	43	GLY	6.5
2	B	247	GLN	5.9
1	A	38	SER	5.7
1	A	41	THR	5.6
1	A	1	MET	5.4
1	A	349	THR	5.3
2	B	279	GLY	5.2
2	B	59	ASN	5.2
2	B	97	SER	5.1
2	B	57	THR	5.0
2	B	282	GLN	4.9
1	A	45	GLY	4.8
2	B	440	ALA	4.8
1	A	44	GLY	4.6
2	B	441	ASP	4.6
2	B	94	PHE	4.6

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Mol	Chain	Res	Type	RSRZ
2	B	326	LYS	4.5
2	B	1	MET	4.4
2	B	37	HIS	4.4
2	B	286	LEU	4.4
2	B	412	GLY	4.4
2	B	288	VAL	4.3
2	B	42	LEU	4.3
1	A	341	ILE	4.2
2	B	281	GLN	4.1
2	B	58	GLY	4.0
2	B	75	MET	4.0
3	F	167	LYS	4.0
2	B	46	LEU	3.9
2	B	333	LEU	3.9
2	B	41	ASP	3.8
2	B	284	ARG	3.8
2	B	82	PRO	3.8
1	A	309	HIS	3.8
2	B	39	ASP	3.8
1	A	350	GLY	3.7
2	B	407	TRP	3.6
2	B	74	THR	3.5
2	B	439	THR	3.5
1	A	238	ILE	3.5
1	A	46	ASP	3.3
1	A	281	ALA	3.3
2	B	338	LYS	3.3
1	A	40	LYS	3.2
1	A	337	THR	3.2
1	A	363	VAL	3.1
1	A	130	THR	3.1
2	B	246	GLY	3.1
1	A	178	SER	3.0
2	B	36	TYR	2.9
2	B	322	ARG	2.9
1	A	364	PRO	2.8
1	A	80	THR	2.8
2	B	410	GLY	2.7
1	A	348	PRO	2.7
2	B	204	ILE	2.7
1	A	362	VAL	2.7
2	B	179	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	347	CYS	2.6
2	B	278	ARG	2.6
1	A	59	GLY	2.5
2	B	130	ASP	2.5
1	A	282	TYR	2.5
2	B	414	ASP	2.5
1	A	340	SER	2.5
2	B	328	VAL	2.5
2	B	409	THR	2.5
1	A	351	PHE	2.5
2	B	61	TYR	2.4
2	B	218	LYS	2.4
2	B	280	SER	2.4
1	A	179	THR	2.4
2	B	337	ASN	2.4
2	B	358	ILE	2.3
2	B	277	SER	2.3
1	A	262	TYR	2.3
2	B	215	ARG	2.2
2	B	272	PHE	2.2
2	B	287	THR	2.2
2	B	78	VAL	2.1
1	A	335	ILE	2.1
1	A	435	VAL	2.1
2	B	416	MET	2.1
2	B	245	PRO	2.1
2	B	289	PRO	2.1
1	A	338	LYS	2.1
2	B	76	ASP	2.1
2	B	248	LEU	2.1
3	F	13	ASP	2.0
2	B	40	SER	2.0

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

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

6.3 Carbohydrates ⓘ

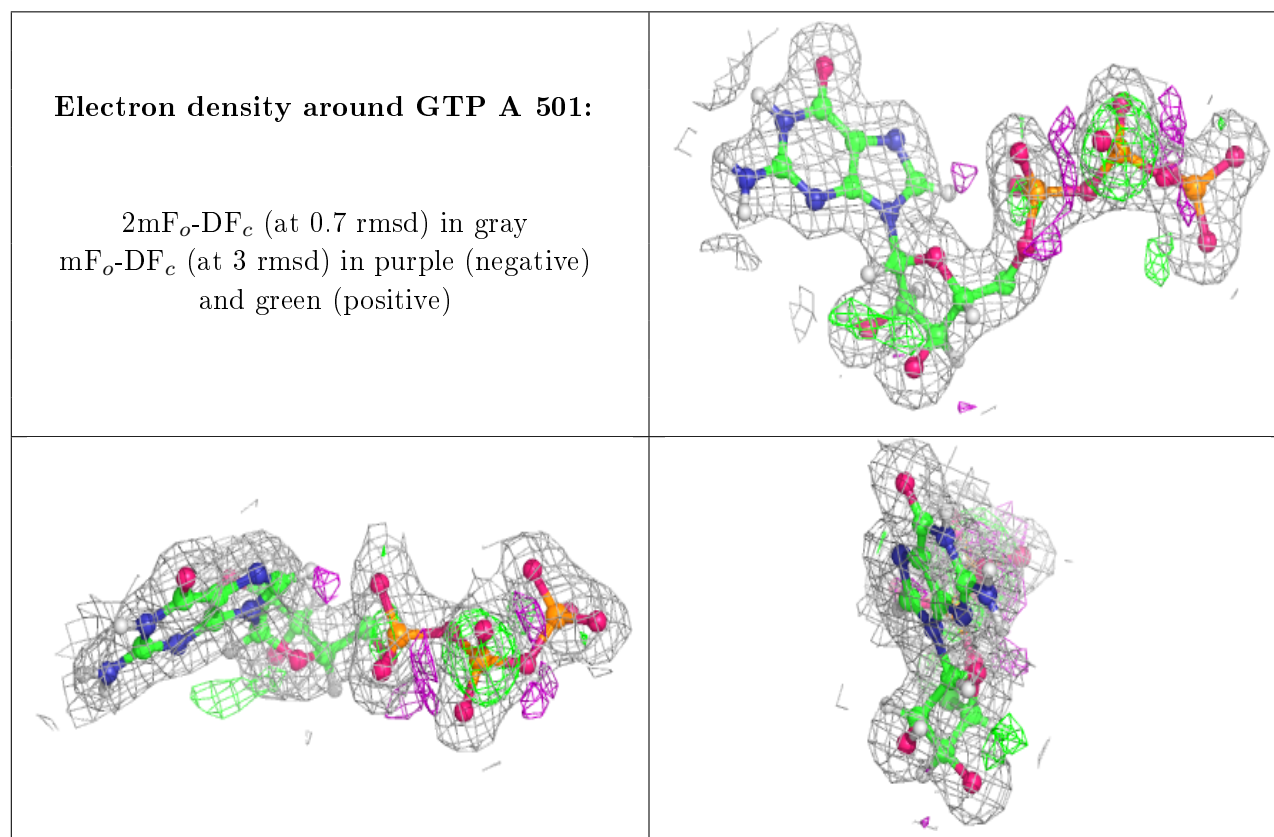
There are no monosaccharides in this entry.

6.4 Ligands [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, 95th 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.

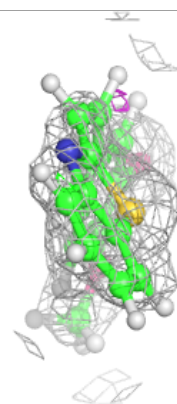
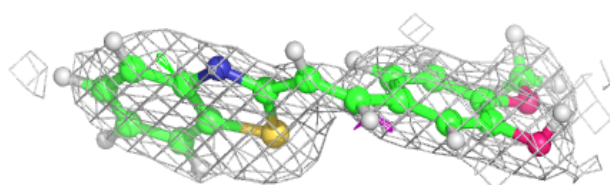
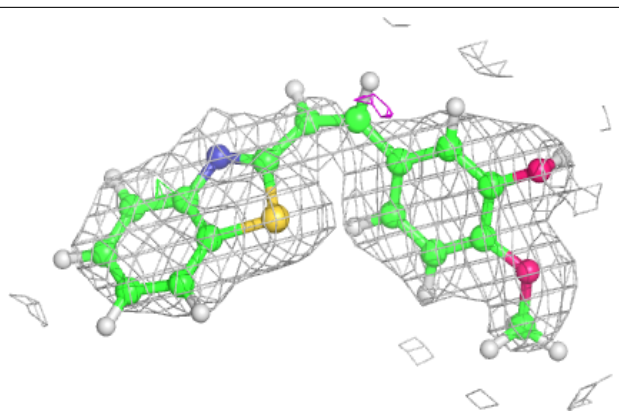
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	GTP	A	501	32/32	0.91	0.15	10,16,30,69	0
7	QRN	B	502	20/20	0.91	0.17	21,49,71,85	0
6	GDP	B	501	28/28	0.96	0.09	15,23,29,30	0
5	MG	A	502	1/1	0.98	0.07	28,28,28,28	0

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.

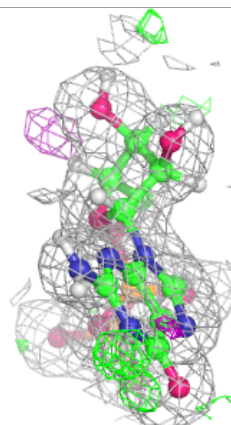
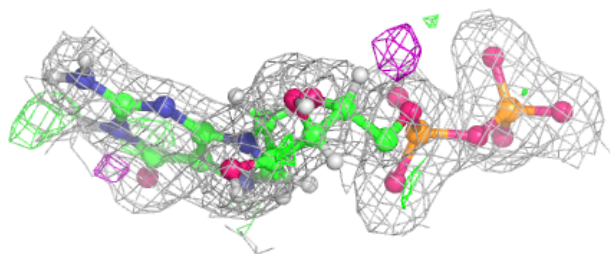
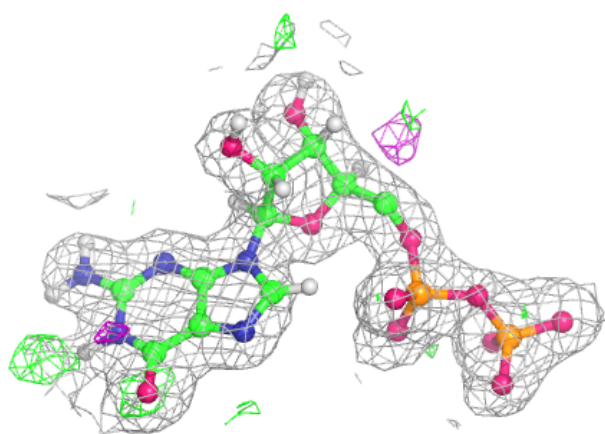


Electron density around QRN B 502:

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

**Electron density around 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

There are no such residues in this entry.