



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 02:08 PM UTC

PDB ID : 6ZWC / pdb_00006zwc
Title : Z-SBTub2 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 : 2.04 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 types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

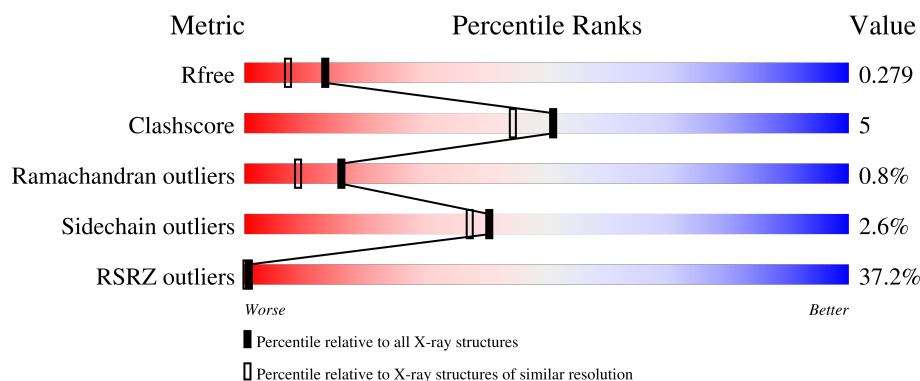
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.04 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}	180053	2260 (2.04-2.04)
Clashscore	190562	2333 (2.04-2.04)
Ramachandran outliers	187476	2318 (2.04-2.04)
Sidechain outliers	187428	2318 (2.04-2.04)
RSRZ outliers	180081	2260 (2.04-2.04)

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 8235 atoms, of which 0 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	436	Total	C	N	O	S	1	6	0
			3398	2154	580	641	23			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	431	Total	C	N	O	S	0	4	0
			3362	2116	570	648	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	N	O	S	0	2	0
			1158	731	195	229	3			

- Molecule 4 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).

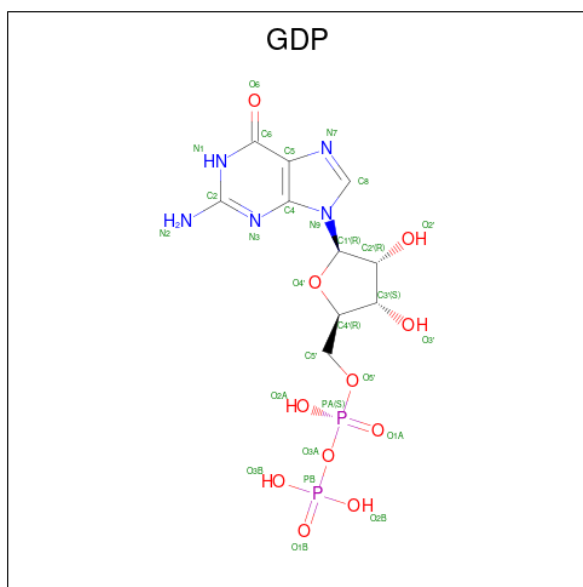


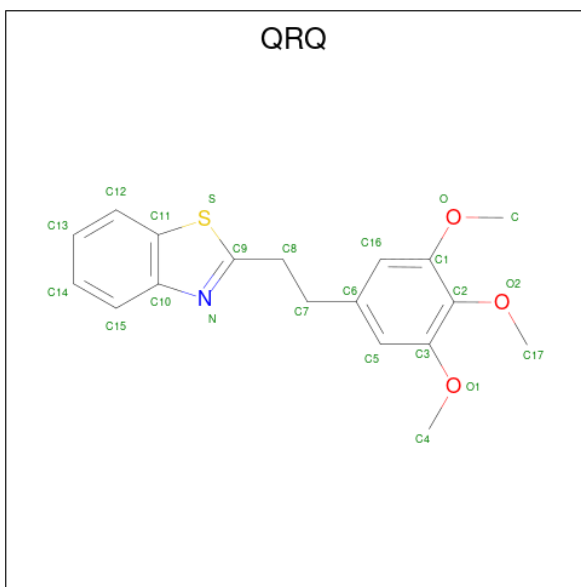
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

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





Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	B	1	Total	C	N	O	S	0	1
			23	18	1	3	1		

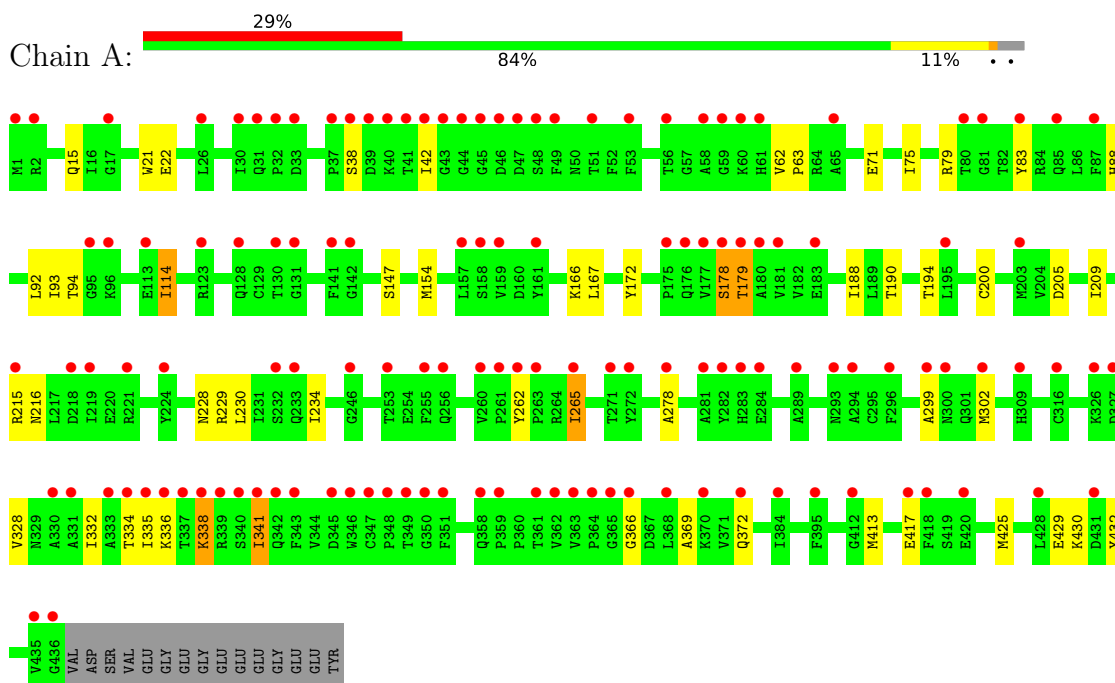
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	109	Total	O	0	0
			109	109		
8	B	83	Total	O	0	0
			83	83		
8	F	41	Total	O	0	0
			41	41		

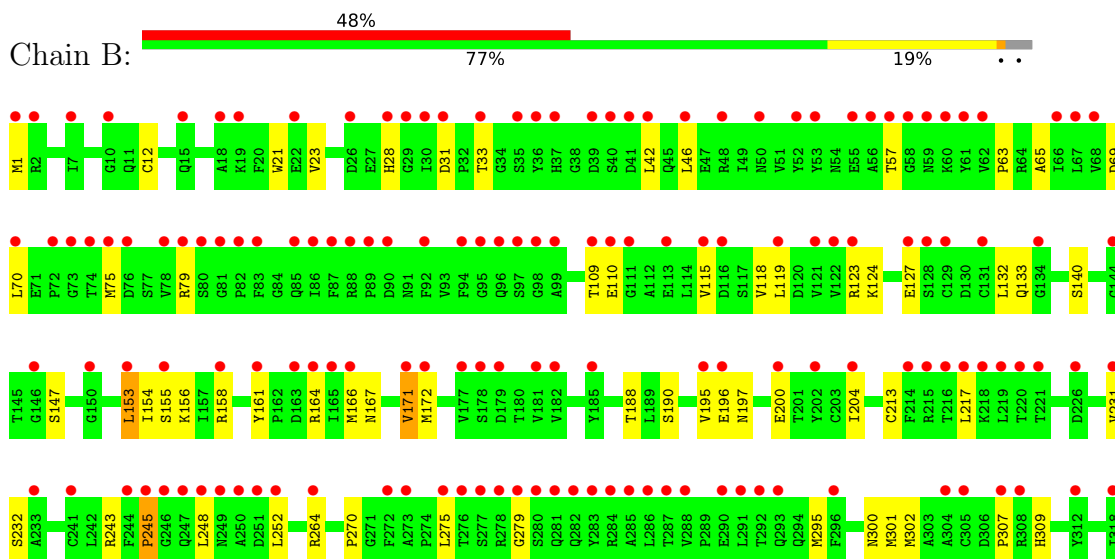
3 Residue-property plots

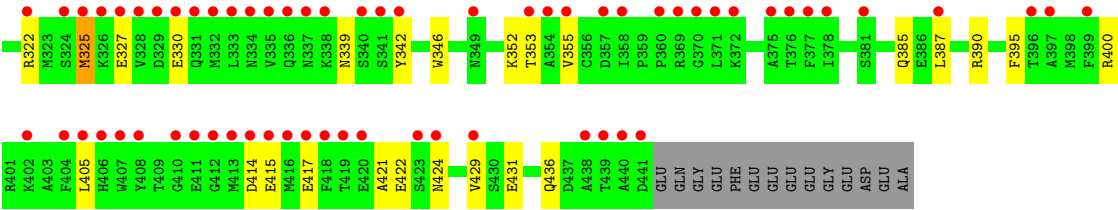
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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

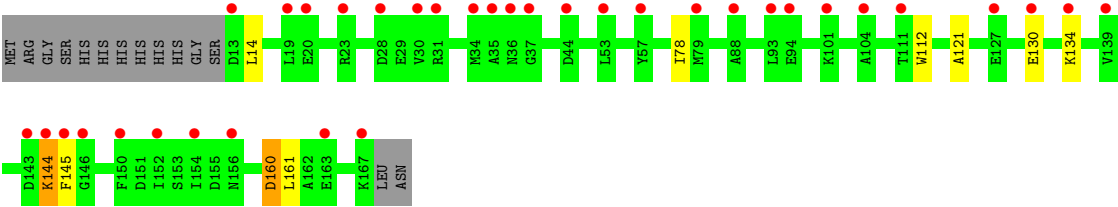
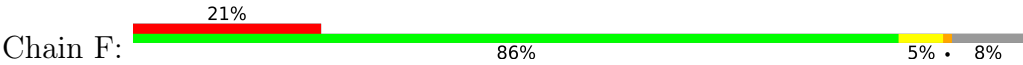


• Molecule 2: Tubulin beta-2B chain





● Molecule 3: Designed Ankyrin Repeat Protein (DARPIN) D1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	73.90Å 91.85Å 82.81Å 90.00° 96.58° 90.00°	Depositor
Resolution (Å)	45.19 – 2.04 45.19 – 2.04	Depositor EDS
% Data completeness (in resolution range)	58.4 (45.19-2.04) 58.6 (45.19-2.04)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.57 (at 2.05Å)	Xtriage
Refinement program	PHENIX 1.18	Depositor
R, R_{free}	0.225 , 0.281 0.226 , 0.279	Depositor DCC
R_{free} test set	1207 reflections (1.59%)	wwPDB-VP
Wilson B-factor (Å ²)	26.7	Xtriage
Anisotropy	0.063	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 30.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	8235	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.48% 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: MG, GDP, QRQ, GTP

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	0.10	0/3491	0.27	0/4744
2	B	0.09	0/3448	0.27	0/4674
3	F	0.08	0/1180	0.22	0/1604
All	All	0.09	0/8119	0.26	0/11022

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	3398	0	3291	29	0
2	B	3362	0	3225	46	0
3	F	1158	0	1156	8	0
4	A	32	0	12	2	0
5	A	1	0	0	0	0
6	B	28	0	12	1	0
7	B	23	0	0	1	0
8	A	109	0	0	2	0
8	B	83	0	0	2	0
8	F	41	0	0	0	0
All	All	8235	0	7696	82	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 (82) 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:1:MET:HB3	2:B:133:GLN:HB3	1.68	0.76
1:A:172:TYR:HB3	1:A:205:ASP:HA	1.76	0.66
1:A:336:LYS:HA	1:A:341:ILE:HD11	1.79	0.65
2:B:195:VAL:HG21	2:B:424:ASN:HD21	1.62	0.65
2:B:132:LEU:O	2:B:164:ARG:NH1	2.33	0.61
1:A:215:ARG:NH1	1:A:216:ASN:OD1	2.35	0.60
1:A:372:GLN:NE2	8:A:604:HOH:O	2.34	0.59
2:B:158[B]:ARG:NH2	8:B:608:HOH:O	2.38	0.57
2:B:115:VAL:HG23	2:B:153[B]:LEU:HD23	1.88	0.55
3:F:112:TRP:HB3	3:F:144:LYS:HZ1	1.71	0.55
2:B:301:MET:HE3	2:B:307:PRO:HG2	1.89	0.54
1:A:15:GLN:NE2	4:A:501:GTP:O6	2.41	0.54
2:B:264:ARG:NE	2:B:431:GLU:OE2	2.40	0.54
2:B:390:ARG:NH1	8:B:603:HOH:O	2.32	0.53
2:B:195:VAL:HG23	2:B:196:GLU:HG2	1.89	0.53
1:A:278:ALA:HA	1:A:369:ALA:HB2	1.90	0.53
2:B:42:LEU:HG	2:B:245:PRO:HG3	1.90	0.53
2:B:75:MET:HE2	2:B:79:ARG:HH22	1.75	0.51
3:F:144:LYS:HD2	3:F:144:LYS:H	1.75	0.51
1:A:154:MET:HE1	1:A:166:LYS:HB3	1.93	0.51
3:F:121:ALA:HB1	3:F:161:LEU:HD21	1.91	0.50
3:F:160:ASP:OD1	3:F:160:ASP:N	2.43	0.50
1:A:413:MET:HE3	1:A:417:GLU:HB3	1.94	0.50
3:F:144:LYS:HD3	3:F:145:PHE:CD2	2.48	0.49
2:B:188:THR:HG22	2:B:421:ALA:HB1	1.95	0.48
2:B:118:VAL:HG11	2:B:153[A]:LEU:HD11	1.95	0.48
1:A:167:LEU:HG	1:A:200:CYS:HB3	1.96	0.48
2:B:213:CYS:HA	2:B:217:LEU:HB2	1.95	0.47
2:B:400:ARG:HD2	3:F:112:TRP:NE1	2.29	0.47
2:B:414:ASP:OD1	2:B:415:GLU:N	2.46	0.47
2:B:21:TRP:CZ2	2:B:65:ALA:HB2	2.50	0.47
3:F:130:GLU:O	3:F:134:LYS:HG2	2.15	0.47
2:B:270:PRO:HG2	2:B:302:MET:HB2	1.97	0.47
2:B:154:ILE:HG23	2:B:166:MET:HG2	1.97	0.47
1:A:228:ASN:OD1	4:A:501:GTP:N1	2.34	0.46
2:B:325:MET:HG2	2:B:355:VAL:HG11	1.98	0.46
1:A:262:TYR:HB2	1:A:265:ILE:HD11	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:TRP:CZ3	1:A:63:PRO:HB3	2.51	0.45
2:B:12:CYS:HB2	6:B:501:GDP:C8	2.52	0.45
2:B:109:THR:OG1	2:B:110:GLU:N	2.49	0.45
1:A:188:ILE:HD12	1:A:425:MET:HG3	1.99	0.45
2:B:28:HIS:CE1	2:B:243:ARG:HB3	2.52	0.45
2:B:309:HIS:O	2:B:436:GLN:NE2	2.50	0.44
2:B:31:ASP:OD1	2:B:33:THR:OG1	2.27	0.44
2:B:395:PHE:CE1	2:B:422:GLU:HB2	2.52	0.44
1:A:265:ILE:HG22	1:A:432:TYR:CZ	2.53	0.44
2:B:155:SER:OG	2:B:197:ASN:ND2	2.50	0.44
2:B:161:TYR:HB3	2:B:164:ARG:HG3	2.00	0.43
1:A:178:SER:O	1:A:179:THR:OG1	2.35	0.43
2:B:123:ARG:O	2:B:127:GLU:HG2	2.19	0.43
2:B:140:SER:HA	2:B:171:VAL:HG13	2.00	0.43
2:B:21:TRP:CZ3	2:B:63:PRO:HB3	2.53	0.43
2:B:385:GLN:HB2	2:B:429:VAL:HG13	2.00	0.43
2:B:119:LEU:HD11	2:B:156:LYS:HB3	1.99	0.43
1:A:93:ILE:HG22	1:A:114:ILE:HD11	2.00	0.43
1:A:22:GLU:HG3	1:A:83:TYR:OH	2.19	0.43
1:A:338:LYS:HE3	1:A:338:LYS:HB3	1.77	0.43
2:B:172:MET:HG3	2:B:387:LEU:HD21	2.01	0.43
2:B:167:ASN:ND2	2:B:200:GLU:OE1	2.50	0.43
1:A:234:ILE:HD13	1:A:302:MET:SD	2.59	0.42
1:A:147:SER:HB2	1:A:190:THR:HB	2.00	0.42
1:A:429:GLU:HG2	8:A:602:HOH:O	2.19	0.42
2:B:23:VAL:HG21	2:B:232:SER:HB2	2.01	0.42
1:A:430:LYS:HE3	1:A:430:LYS:HB3	1.82	0.42
2:B:339:ASN:HB3	2:B:342:TYR:HD2	1.84	0.42
2:B:352:LYS:HB2	7:B:502[B]:QRQ:C15	2.49	0.42
2:B:133:GLN:NE2	2:B:252:LEU:H	2.17	0.42
3:F:112:TRP:HB3	3:F:144:LYS:NZ	2.35	0.42
2:B:275:LEU:HD11	2:B:300:ASN:HA	2.02	0.41
1:A:229[A]:ARG:NE	1:A:366:GLY:HA2	2.35	0.41
2:B:346:TRP:CD1	2:B:346:TRP:H	2.36	0.41
2:B:147:SER:HB2	2:B:190:SER:OG	2.21	0.41
1:A:75:ILE:HD12	1:A:94:THR:HG22	2.02	0.41
2:B:204:ILE:HD13	2:B:231:VAL:HG13	2.03	0.41
1:A:79:ARG:HG2	1:A:92:LEU:HD13	2.02	0.41
1:A:328:VAL:O	1:A:332:ILE:HG12	2.21	0.41
2:B:75:MET:HE2	2:B:79:ARG:NH2	2.36	0.41
2:B:327:GLU:HA	2:B:330:GLU:HG2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:VAL:HG11	1:A:88:HIS:CE1	2.56	0.40
1:A:209:ILE:HG23	1:A:230:LEU:HD23	2.02	0.40
2:B:69:ASP:OD1	2:B:70:LEU:N	2.54	0.40
1:A:215:ARG:CZ	1:A:299:ALA:HB1	2.51	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%)	416 (94%)	19 (4%)	5 (1%)	11	5
2	B	433/445 (97%)	411 (95%)	19 (4%)	3 (1%)	18	10
3	F	155/169 (92%)	150 (97%)	5 (3%)	0	100	100
All	All	1028/1065 (96%)	977 (95%)	43 (4%)	8 (1%)	16	9

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	57	THR
1	A	38	SER
2	B	245	PRO
1	A	178	SER
1	A	179	THR
2	B	279	GLY
1	A	114	ILE
1	A	42	ILE

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	361/379 (95%)	354 (98%)	7 (2%)	50	50
2	B	365/383 (95%)	353 (97%)	12 (3%)	33	28
3	F	120/132 (91%)	116 (97%)	4 (3%)	33	28
All	All	846/894 (95%)	823 (97%)	23 (3%)	40	36

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	GLU
1	A	194	THR
1	A	265	ILE
1	A	334	THR
1	A	335	ILE
1	A	338	LYS
1	A	341	ILE
2	B	46	LEU
2	B	124	LYS
2	B	153[A]	LEU
2	B	153[B]	LEU
2	B	171	VAL
2	B	248	LEU
2	B	295	MET
2	B	322	ARG
2	B	325	MET
2	B	353	THR
2	B	405	LEU
2	B	417	GLU
3	F	14	LEU
3	F	78	ILE
3	F	144	LYS
3	F	160	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	GLN
1	A	18	ASN
1	A	35	GLN
1	A	85	GLN
1	A	197	HIS
1	A	233	GLN
1	A	300	ASN
1	A	406	HIS
2	B	45	GLN
2	B	133	GLN
2	B	197	ASN
2	B	331	GLN
2	B	385	GLN
2	B	424	ASN
2	B	436	GLN
3	F	125	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	33,34,34	0.99	2 (6%)	50,54,54	1.58	8 (16%)
7	QRQ	B	502[B]	-	25,25,25	0.96	1 (4%)	32,34,34	0.73	1 (3%)
6	GDP	B	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.74	6 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GTP	A	501	5	-	5/22/38/38	0/3/3/3
7	QRQ	B	502[B]	-	-	2/11/11/11	0/3/3/3
6	GDP	B	501	-	-	4/16/32/32	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[B]	QRQ	C7-C8	-4.12	1.33	1.52
6	B	501	GDP	C5-C4	3.14	1.47	1.38
6	B	501	GDP	C6-N1	-2.36	1.34	1.38
4	A	501	GTP	C2-N3	2.15	1.38	1.33
6	B	501	GDP	C5-N7	-2.04	1.35	1.39
4	A	501	GTP	PA-O3A	2.04	1.61	1.59

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	501	GDP	C5-C4-N3	-6.07	118.73	128.39
4	A	501	GTP	C5-C4-N3	-5.00	120.44	128.39
6	B	501	GDP	C2-N3-C4	4.98	120.88	112.30
4	A	501	GTP	C2-N3-C4	4.62	120.25	112.30
6	B	501	GDP	N9-C4-N3	4.50	134.95	125.95
7	B	502[B]	QRQ	C8-C7-C6	3.69	125.68	112.70
6	B	501	GDP	C6-C5-N7	3.20	136.12	130.29
4	A	501	GTP	N9-C4-N3	3.18	132.30	125.95
4	A	501	GTP	C2-N1-C6	-2.83	119.97	125.11
4	A	501	GTP	N9-C8-N7	-2.63	108.53	113.40
6	B	501	GDP	C4-C5-N7	-2.55	106.62	110.67
4	A	501	GTP	C8-N7-C5	2.48	108.68	104.26
4	A	501	GTP	C5-C6-N1	2.48	119.57	113.25
4	A	501	GTP	O6-C6-C5	-2.38	120.24	126.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	501	GDP	O6-C6-C5	-2.18	120.78	126.53

There are no chirality outliers.

All (11) torsion outliers are listed below:

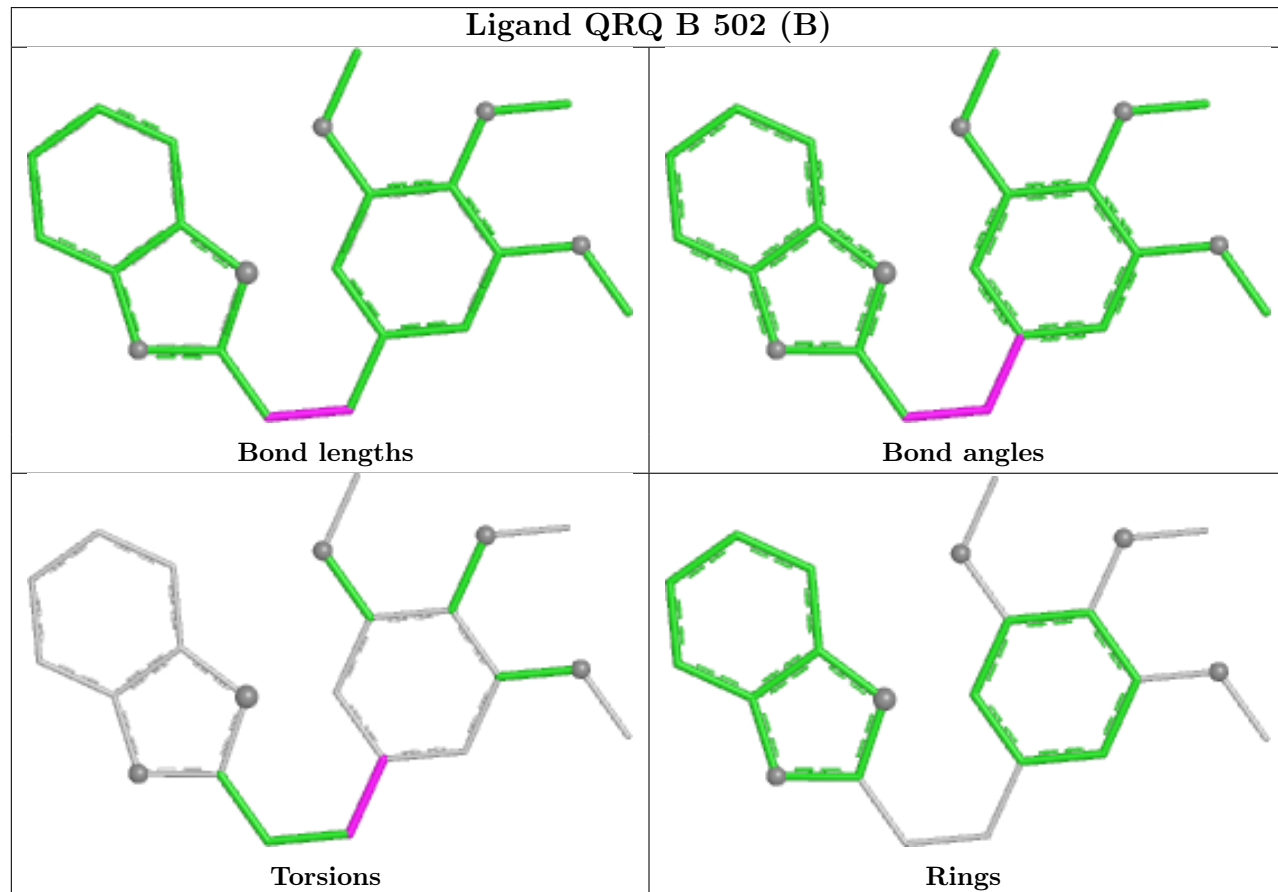
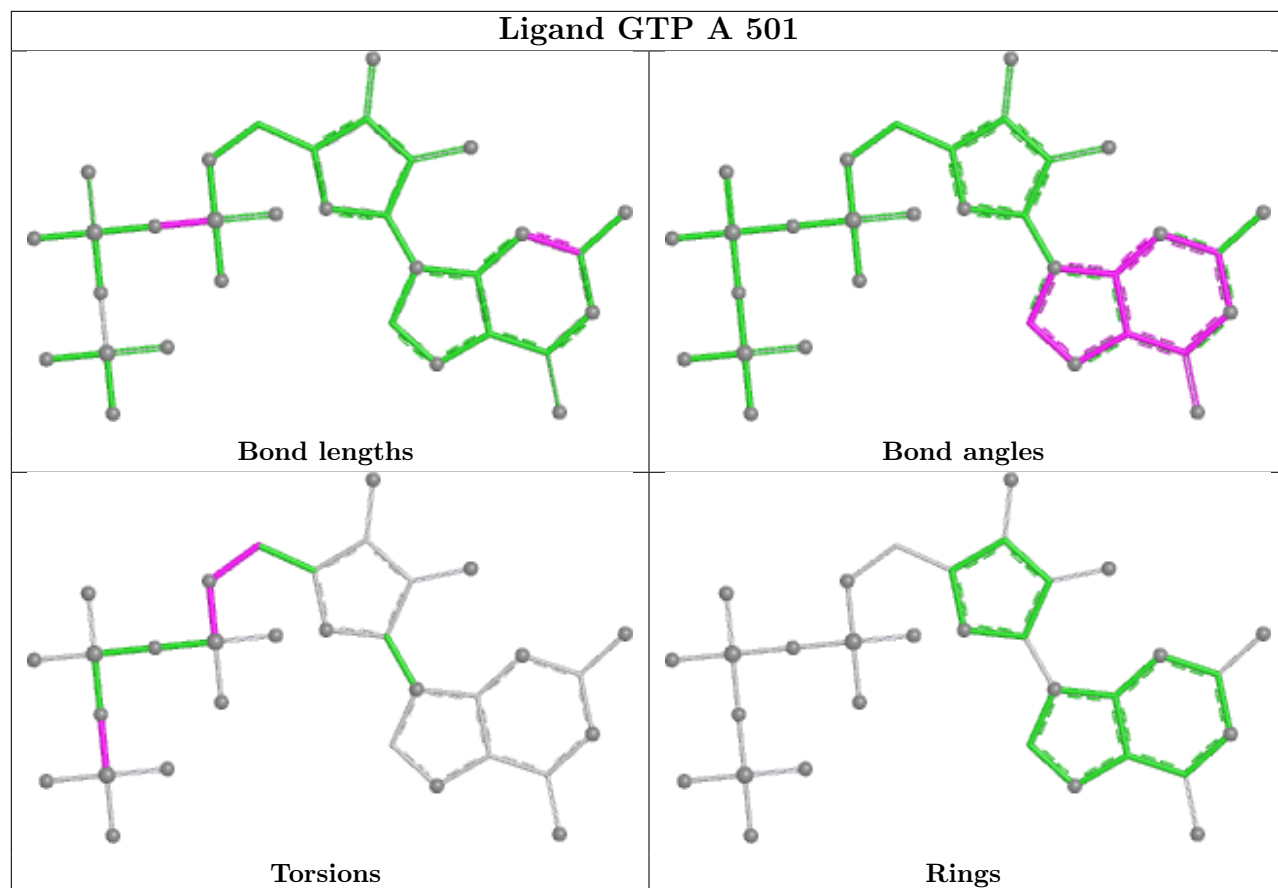
Mol	Chain	Res	Type	Atoms
4	A	501	GTP	PB-O3B-PG-O2G
4	A	501	GTP	C5'-O5'-PA-O3A
4	A	501	GTP	C5'-O5'-PA-O1A
4	A	501	GTP	C5'-O5'-PA-O2A
6	B	501	GDP	C5'-O5'-PA-O3A
6	B	501	GDP	C5'-O5'-PA-O1A
6	B	501	GDP	C5'-O5'-PA-O2A
7	B	502[B]	QRQ	C16-C6-C7-C8
7	B	502[B]	QRQ	C5-C6-C7-C8
4	A	501	GTP	C4'-C5'-O5'-PA
6	B	501	GDP	PB-O3A-PA-O2A

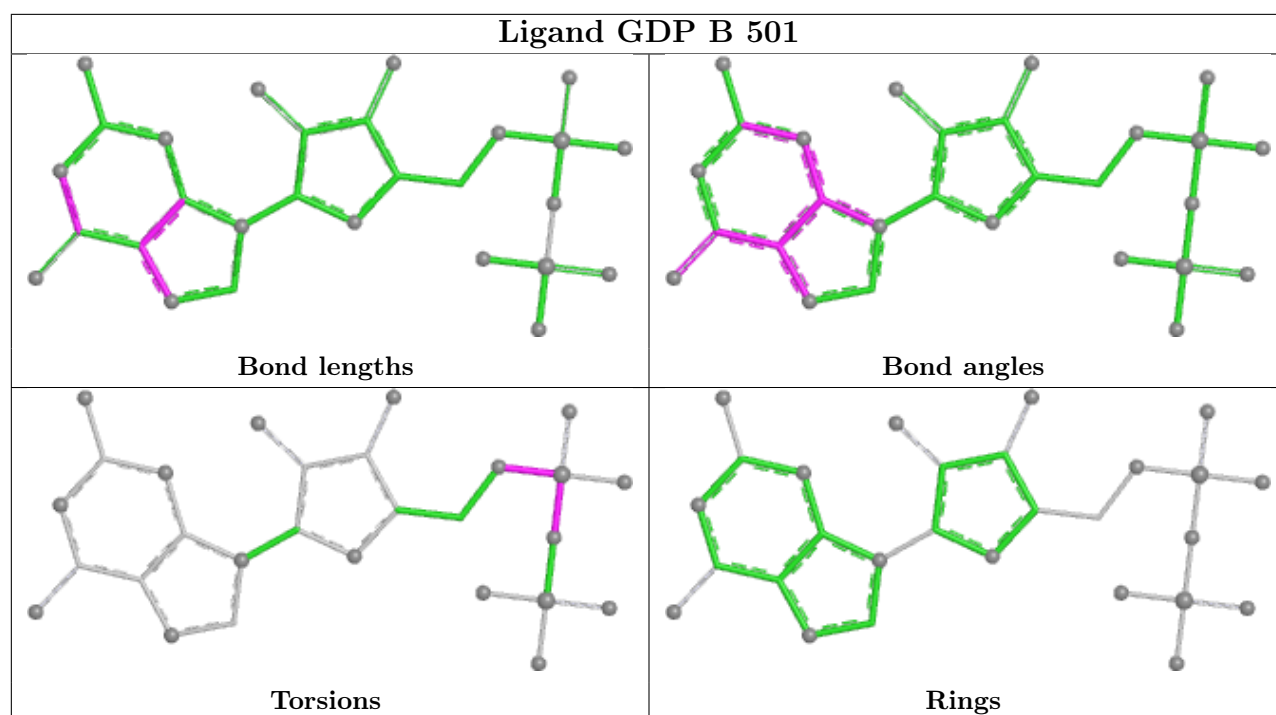
There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	501	GTP	2	0
7	B	502[B]	QRQ	1	0
6	B	501	GDP	1	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	436/451 (96%)	1.63	132 (30%)  	14, 27, 53, 79	8 (1%)
2	B	431/445 (96%)	2.18	213 (49%)  	12, 34, 65, 96	4 (0%)
3	F	155/169 (91%)	1.40	35 (22%)  	15, 26, 46, 62	2 (1%)
All	All	1022/1065 (95%)	1.83	380 (37%)  	12, 29, 60, 96	14 (1%)

All (380) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	43	GLY	8.8
1	A	262	TYR	8.7
2	B	248	LEU	7.7
1	A	41	THR	7.3
2	B	247	GLN	7.3
2	B	285	ALA	7.2
1	A	44	GLY	7.2
1	A	177	VAL	7.2
2	B	283	TYR	7.1
1	A	365	GLY	7.0
2	B	246	GLY	6.9
1	A	281	ALA	6.8
1	A	42	ILE	6.0
2	B	78	VAL	5.9
2	B	325	MET	5.8
2	B	249	ASN	5.8
2	B	333	LEU	5.8
1	A	1	MET	5.7
2	B	272	PHE	5.5
2	B	1	MET	5.5
2	B	286	LEU	5.3
2	B	338	LYS	5.3
2	B	406	HIS	5.2

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Mol	Chain	Res	Type	RSRZ
2	B	59	ASN	5.2
2	B	282	GLN	5.2
2	B	56	ALA	5.1
2	B	412	GLY	5.1
2	B	324	SER	5.0
2	B	407	TRP	5.0
1	A	363	VAL	5.0
2	B	42	LEU	5.0
2	B	82	PRO	4.9
2	B	355	VAL	4.9
2	B	220	THR	4.8
2	B	281	GLN	4.8
1	A	265	ILE	4.7
1	A	195	LEU	4.7
3	F	144	LYS	4.7
2	B	72	PRO	4.6
2	B	94	PHE	4.6
2	B	73	GLY	4.5
2	B	415	GLU	4.5
2	B	328	VAL	4.5
1	A	178	SER	4.5
2	B	291	LEU	4.4
1	A	282	TYR	4.3
2	B	250	ALA	4.3
2	B	277	SER	4.3
1	A	435	VAL	4.3
2	B	278	ARG	4.3
1	A	47	ASP	4.3
2	B	279	GLY	4.2
2	B	337	ASN	4.2
2	B	245	PRO	4.1
2	B	273	ALA	4.1
1	A	45	GLY	4.1
2	B	37	HIS	4.1
2	B	342	TYR	4.1
2	B	68	VAL	4.1
2	B	41	ASP	4.1
2	B	127	GLU	4.0
2	B	241	CYS	4.0
1	A	59	GLY	4.0
2	B	441	ASP	4.0
1	A	335	ILE	4.0

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Mol	Chain	Res	Type	RSRZ
2	B	358	ILE	4.0
1	A	58	ALA	3.9
3	F	145	PHE	3.9
1	A	40	LYS	3.9
1	A	38	SER	3.9
3	F	35	ALA	3.9
1	A	364	PRO	3.9
2	B	75	MET	3.9
2	B	172	MET	3.9
1	A	56	THR	3.9
1	A	346	TRP	3.8
2	B	280	SER	3.8
2	B	57	THR	3.8
1	A	338	LYS	3.8
2	B	334	ASN	3.8
1	A	348	PRO	3.7
2	B	296	PHE	3.7
2	B	318	ILE	3.7
1	A	60	LYS	3.7
1	A	175	PRO	3.7
2	B	293	GLN	3.7
3	F	146	GLY	3.7
2	B	80	SER	3.7
1	A	337	THR	3.7
2	B	163[A]	ASP	3.7
2	B	329	ASP	3.7
2	B	371	LEU	3.7
1	A	37	PRO	3.7
1	A	345	ASP	3.7
1	A	49	PHE	3.6
2	B	405	LEU	3.6
1	A	349	THR	3.6
1	A	347	CYS	3.6
2	B	81	GLY	3.6
1	A	128	GLN	3.6
2	B	440	ALA	3.5
2	B	60	LYS	3.5
2	B	76	ASP	3.5
2	B	179	ASP	3.5
2	B	61	TYR	3.5
2	B	97	SER	3.5
2	B	113	GLU	3.5

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Mol	Chain	Res	Type	RSRZ
2	B	29	GLY	3.4
2	B	153[A]	LEU	3.4
1	A	362	VAL	3.4
2	B	33	THR	3.4
2	B	416	MET	3.4
1	A	246	GLY	3.4
2	B	161	TYR	3.4
1	A	302	MET	3.4
2	B	79	ARG	3.4
2	B	284	ARG	3.4
1	A	39	ASP	3.4
2	B	111	GLY	3.4
1	A	418	PHE	3.4
2	B	129	CYS	3.3
2	B	414	ASP	3.3
3	F	88	ALA	3.3
2	B	39	ASP	3.3
2	B	74	THR	3.2
1	A	283	HIS	3.2
3	F	167	LYS	3.2
2	B	336	GLN	3.2
3	F	28	ASP	3.2
2	B	335	VAL	3.2
1	A	215	ARG	3.2
2	B	36	TYR	3.2
2	B	252	LEU	3.2
2	B	83	PHE	3.2
1	A	263	PRO	3.2
2	B	372	LYS	3.2
1	A	65	ALA	3.1
2	B	58	GLY	3.1
3	F	139	VAL	3.1
2	B	340	SER	3.1
2	B	404	PHE	3.1
2	B	378	ILE	3.1
2	B	116	ASP	3.1
2	B	88	ARG	3.0
2	B	419	THR	3.0
3	F	34	MET	3.0
1	A	342	GLN	3.0
2	B	341	SER	3.0
2	B	349	ASN	3.0

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Mol	Chain	Res	Type	RSRZ
3	F	134	LYS	3.0
2	B	99	ALA	3.0
2	B	171	VAL	3.0
2	B	196	GLU	3.0
1	A	436	GLY	3.0
1	A	343	PHE	3.0
2	B	92	PHE	3.0
2	B	399	PHE	3.0
2	B	46	LEU	2.9
2	B	387	LEU	2.9
2	B	177	VAL	2.9
1	A	95	GLY	2.9
1	A	46	ASP	2.9
2	B	28	HIS	2.9
1	A	123[A]	ARG	2.9
2	B	408	TYR	2.9
3	F	20	GLU	2.9
2	B	109	THR	2.9
1	A	261	PRO	2.9
2	B	87	PHE	2.9
2	B	7	ILE	2.9
1	A	327	ASP	2.8
2	B	332	MET	2.8
2	B	221	THR	2.8
1	A	341	ILE	2.8
1	A	370	LYS	2.8
1	A	358	GLN	2.8
3	F	53	LEU	2.8
2	B	22	GLU	2.8
2	B	292	THR	2.8
2	B	35	SER	2.8
1	A	218	ASP	2.8
1	A	296	PHE	2.8
3	F	150	PHE	2.8
1	A	232[A]	SER	2.8
2	B	155	SER	2.8
2	B	322	ARG	2.8
3	F	130	GLU	2.8
1	A	351	PHE	2.8
1	A	366	GLY	2.8
2	B	244	PHE	2.8
2	B	18	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	51	THR	2.8
1	A	181	VAL	2.8
3	F	30	VAL	2.8
1	A	339	ARG	2.7
2	B	40	SER	2.7
1	A	395	PHE	2.7
1	A	278	ALA	2.7
1	A	368	LEU	2.7
3	F	93	LEU	2.7
1	A	130	THR	2.7
2	B	62	VAL	2.7
2	B	330	GLU	2.7
2	B	119	LEU	2.7
2	B	164	ARG	2.7
2	B	369	ARG	2.7
1	A	372	GLN	2.7
2	B	312	TYR	2.7
3	F	36	ASN	2.7
3	F	143	ASP	2.7
2	B	123	ARG	2.7
3	F	104	ALA	2.7
2	B	185	TYR	2.7
2	B	181	VAL	2.7
2	B	48	ARG	2.7
1	A	333	ALA	2.6
2	B	354	ALA	2.6
1	A	300	ASN	2.6
2	B	275	LEU	2.6
3	F	19	LEU	2.6
1	A	224	TYR	2.6
2	B	53	TYR	2.6
1	A	384	ILE	2.6
2	B	288	VAL	2.6
2	B	158[A]	ARG	2.6
1	A	17	GLY	2.6
2	B	308	ARG	2.6
2	B	98	GLY	2.6
2	B	411	GLU	2.6
3	F	156[A]	ASN	2.6
2	B	2	ARG	2.6
2	B	402	LYS	2.6
1	A	80	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	331	ALA	2.6
1	A	428	LEU	2.6
2	B	15	GLN	2.5
2	B	182	VAL	2.5
2	B	52	TYR	2.5
1	A	33	ASP	2.5
2	B	353	THR	2.5
3	F	13	ASP	2.5
1	A	299	ALA	2.5
1	A	330	ALA	2.5
2	B	360	PRO	2.5
1	A	157	LEU	2.5
2	B	67	LEU	2.5
2	B	144	GLY	2.5
3	F	23	ARG	2.5
1	A	334	THR	2.5
2	B	287	THR	2.5
2	B	217	LEU	2.5
2	B	219	LEU	2.5
2	B	66	ILE	2.5
2	B	115	VAL	2.5
2	B	50	ASN	2.5
1	A	316	CYS	2.5
2	B	131	CYS	2.5
1	A	420	GLU	2.5
2	B	233	ALA	2.5
2	B	438	ALA	2.5
2	B	166	MET	2.5
1	A	336	LYS	2.5
1	A	2	ARG	2.5
3	F	154	ILE	2.5
2	B	55	GLU	2.4
2	B	357	ASP	2.4
2	B	381	SER	2.4
2	B	89	PRO	2.4
3	F	79	MET	2.4
1	A	131	GLY	2.4
2	B	424	ASN	2.4
2	B	327	GLU	2.4
1	A	48	SER	2.4
2	B	396	THR	2.4
2	B	19	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
3	F	31	ARG	2.4
1	A	309	HIS	2.4
2	B	70	LEU	2.4
2	B	214	PHE	2.4
1	A	158	SER	2.4
2	B	178	SER	2.4
1	A	361	THR	2.4
2	B	304	ALA	2.4
1	A	256	GLN	2.4
2	B	90	ASP	2.4
1	A	260	VAL	2.4
2	B	165	ILE	2.4
2	B	326	LYS	2.4
2	B	202	TYR	2.3
1	A	113	GLU	2.3
1	A	233	GLN	2.3
2	B	251	ASP	2.3
1	A	219	ILE	2.3
1	A	271	THR	2.3
1	A	284	GLU	2.3
2	B	200	GLU	2.3
2	B	96	GLN	2.3
2	B	375	ALA	2.3
2	B	95	GLY	2.3
1	A	255	PHE	2.3
1	A	340	SER	2.3
2	B	30	ILE	2.3
1	A	31[A]	GLN	2.3
1	A	83	TYR	2.3
2	B	215	ARG	2.3
2	B	418	PHE	2.3
3	F	94	GLU	2.3
2	B	231	VAL	2.3
1	A	96	LYS	2.3
2	B	31	ASP	2.3
1	A	142	GLY	2.3
1	A	183	GLU	2.2
2	B	195	VAL	2.2
2	B	429	VAL	2.2
1	A	221	ARG	2.2
2	B	218	LYS	2.2
1	A	81	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	410	GLY	2.2
1	A	417	GLU	2.2
2	B	420	GLU	2.2
2	B	204	ILE	2.2
3	F	152	ILE	2.2
1	A	431	ASP	2.2
3	F	44	ASP	2.2
3	F	127	GLU	2.2
1	A	203	MET	2.2
2	B	86	ILE	2.2
2	B	121	VAL	2.2
2	B	10	GLY	2.2
2	B	150	GLY	2.2
2	B	290	GLU	2.2
2	B	85	GLN	2.2
2	B	397	ALA	2.2
2	B	439	THR	2.2
1	A	87	PHE	2.1
3	F	163	GLU	2.1
1	A	180	ALA	2.1
2	B	128	SER	2.1
3	F	101	LYS	2.1
1	A	161	TYR	2.1
1	A	293	ASN	2.1
2	B	276	THR	2.1
2	B	376	THR	2.1
1	A	61	HIS	2.1
2	B	134	GLY	2.1
2	B	423	SER	2.1
2	B	413	MET	2.1
2	B	110	GLU	2.1
3	F	57	TYR	2.1
1	A	32	PRO	2.1
1	A	176	GLN	2.1
1	A	179	THR	2.1
1	A	253	THR	2.1
1	A	359	PRO	2.1
2	B	216	THR	2.1
2	B	307	PRO	2.1
1	A	30	ILE	2.1
1	A	350	GLY	2.1
2	B	264	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	159	VAL	2.1
2	B	305[A]	CYS	2.1
2	B	26	ASP	2.1
2	B	370	GLY	2.1
1	A	53	PHE	2.1
1	A	141	PHE	2.1
2	B	417	GLU	2.0
1	A	26	LEU	2.0
1	A	85	GLN	2.0
2	B	331	GLN	2.0
1	A	272	TYR	2.0
1	A	326	LYS	2.0
2	B	146	GLY	2.0
2	B	122	VAL	2.0
2	B	377	PHE	2.0
1	A	289	ALA	2.0
1	A	294	ALA	2.0
2	B	226	ASP	2.0
3	F	111	THR	2.0
1	A	412	GLY	2.0
3	F	37	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 oligosaccharides 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($\text{\AA}^2$)	Q<0.9
7	QRQ	B	502[B]	23/23	0.77	0.21	17,25,32,35	23
6	GDP	B	501	28/28	0.88	0.12	19,27,37,41	0

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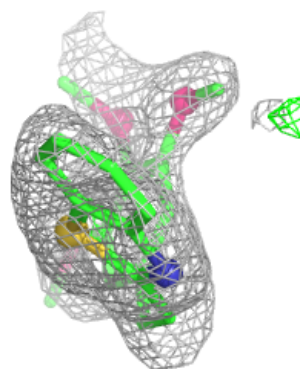
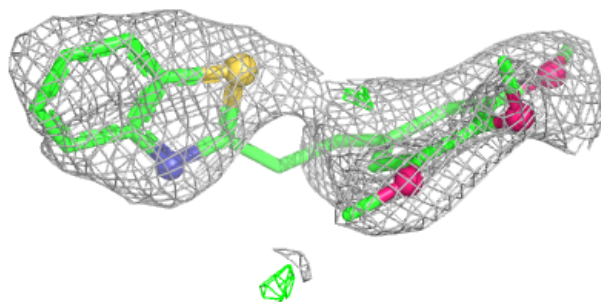
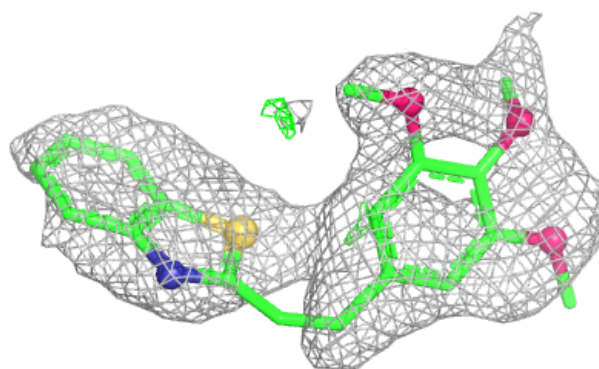
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	GTP	A	501	32/32	0.94	0.09	12,18,26,34	0
5	MG	A	502	1/1	0.96	0.04	20,20,20,20	0

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.

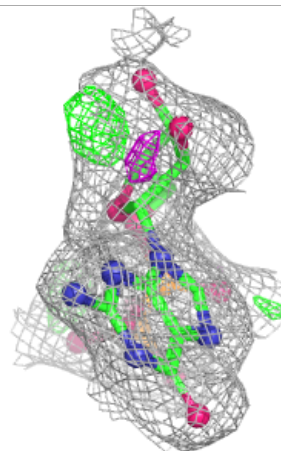
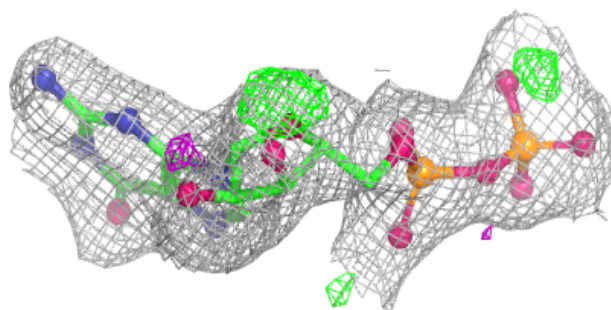
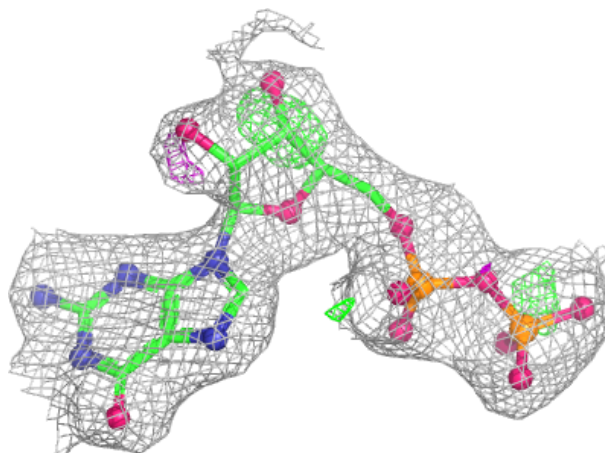
Electron density around QRQ B 502 (B):

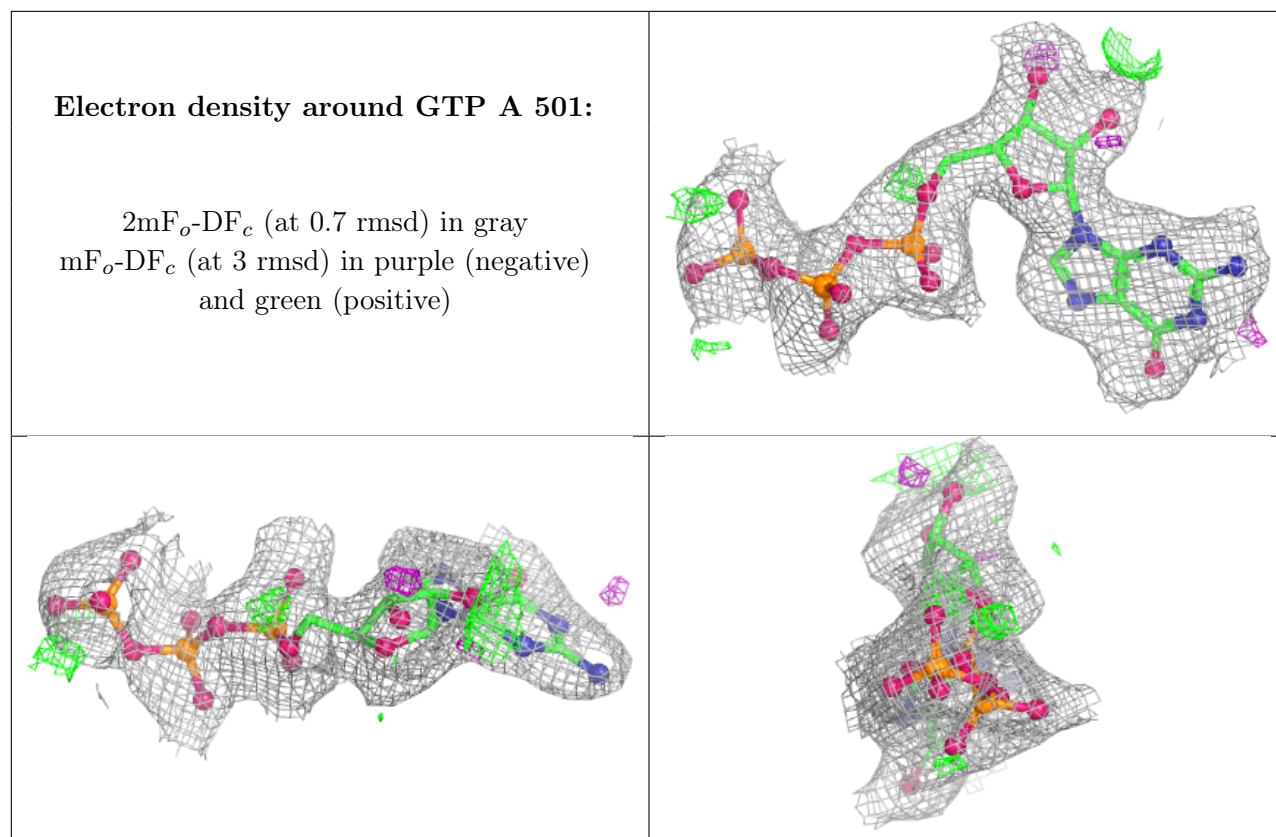
2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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.