Full wwPDB X-ray Structure Validation Report (i)

Apr 5, 2022 – 01:25 pm BST

PDB ID	:	7Z0F
Title	:	CPAP:S-TUBULIN:IIH5 ALPHAREP COMPLEX
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Deposited on	:	2022-02-22
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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

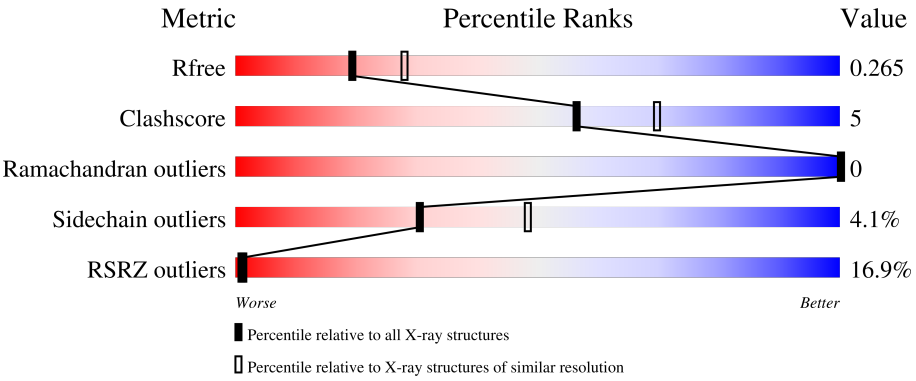
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.27
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.27

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 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 <=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% 82% 14%
2	B	445	30% 85% 10% 5%
3	C	170	9% 75% 16% 8%
4	P	79	25% 46% 54%

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 8066 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 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	438	Total	C	N	O	S	0	0	0
			3386	2143	573	648	22			

- Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	424	Total	C	N	O	S	0	0	0
			3048	1904	521	604	19			

- Molecule 3 is a protein called IIH5 ALPHAREP.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	157	Total	C	N	O	S	0	0	0
			1192	748	212	230	2			

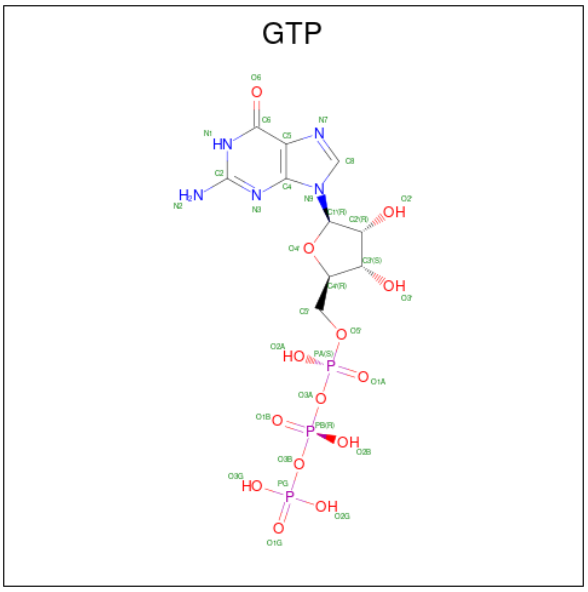
- Molecule 4 is a protein called Centromere protein J.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	P	36	Total	C	N	O	0	0	0
			214	134	36	44			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	319	MET	-	initiating methionine	UNP Q9HC77
P	320	VAL	ALA	engineered mutation	UNP Q9HC77

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

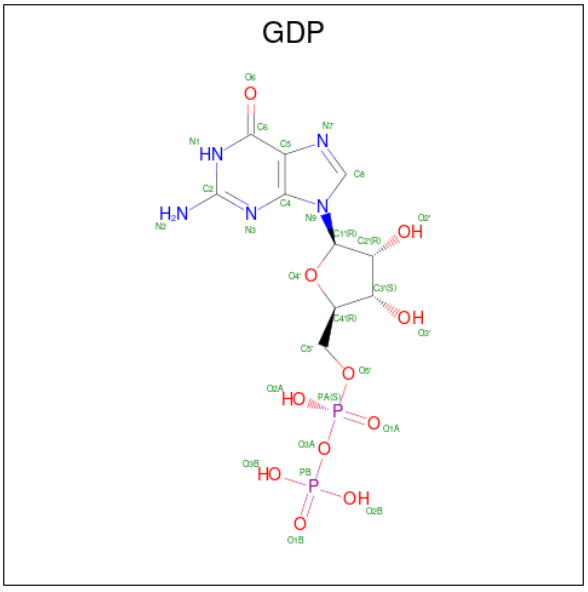


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

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

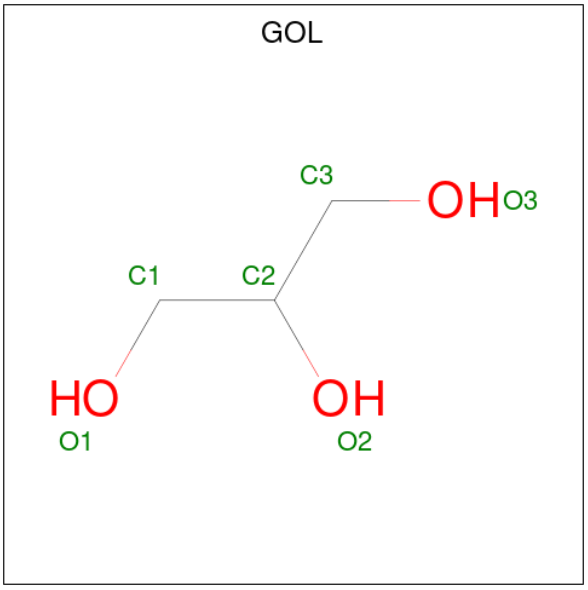
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Mg	0	0
			1	1		

- Molecule 7 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



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

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	C	1	Total	C	O	0	0
			6	3	3		

- Molecule 9 is water.

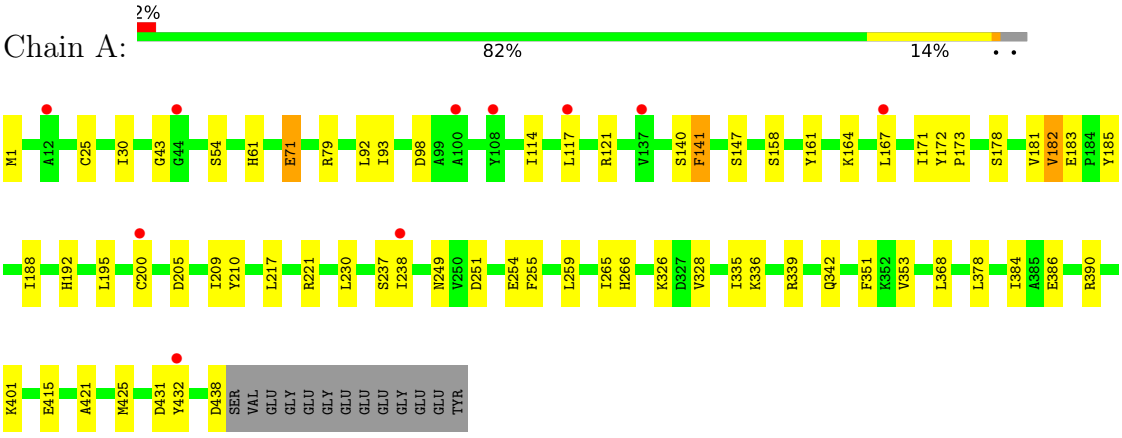
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	114	Total	O	0	0
			114	114		
9	C	44	Total	O	0	0
			44	44		
9	P	1	Total	O	0	0
			1	1		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

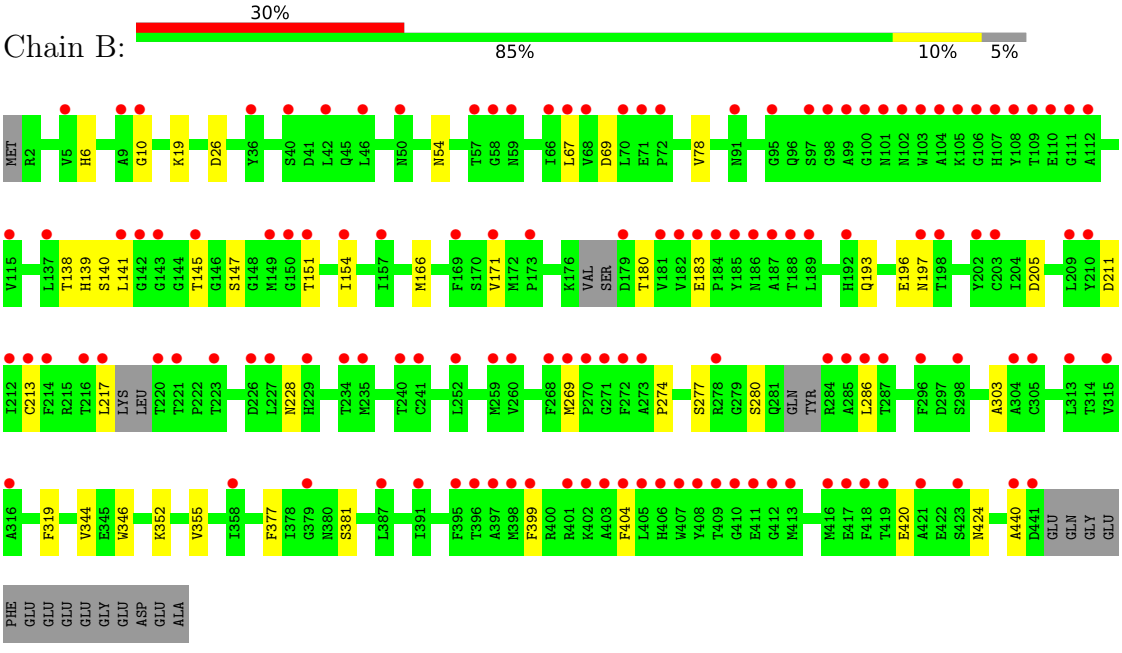
• Molecule 1: Tubulin alpha chain

Chain A:



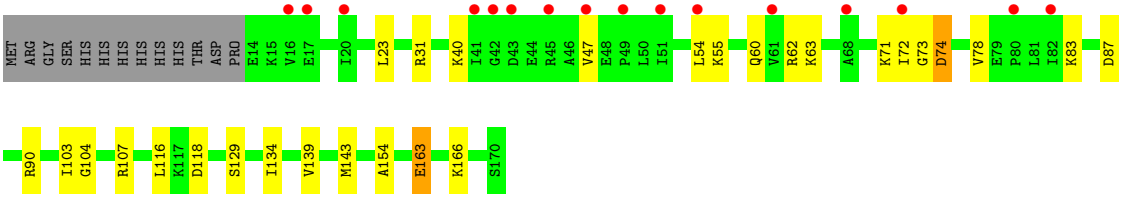
• Molecule 2: Tubulin beta chain

Chain B:

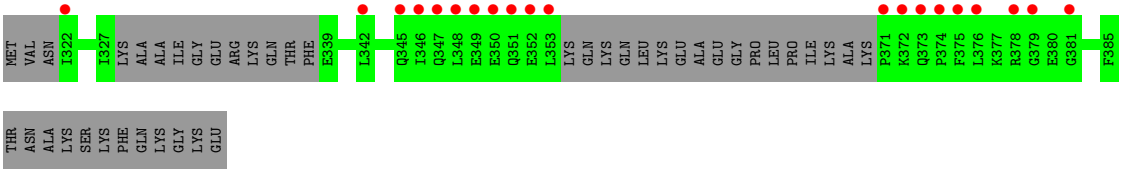


• Molecule 3: IIH5 ALPHAREP

Chain C:



• Molecule 4: Centromere protein J



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	54.28Å 86.71Å 137.61Å 90.00° 96.61° 90.00°	Depositor
Resolution (Å)	45.79 – 2.40 45.79 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.2 (45.79-2.40) 99.2 (45.79-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.34 (at 2.39Å)	Xtriage
Refinement program	BUSTER 2.10.4	Depositor
R, R_{free}	0.222 , 0.273 0.221 , 0.265	Depositor DCC
R_{free} test set	2481 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	67.5	Xtriage
Anisotropy	0.375	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	8066	wwPDB-VP
Average B, all atoms (Å^2)	99.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.01% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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, GOL, GDP, 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	0.50	0/3464	0.69	0/4712
2	B	0.31	0/3108	0.48	0/4245
3	C	0.48	0/1206	0.62	0/1627
4	P	0.32	0/216	0.40	0/294
All	All	0.43	0/7994	0.60	0/10878

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	3386	0	3255	39	0
2	B	3048	0	2729	30	0
3	C	1192	0	1199	16	0
4	P	214	0	127	0	0
5	A	32	0	12	0	0
6	A	1	0	0	0	0
7	B	28	0	12	0	0
8	C	6	0	8	0	0
9	A	114	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	C	44	0	0	1	0
9	P	1	0	0	0	0
All	All	8066	0	7342	76	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 (76) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:GLY:H	3:C:40:LYS:NZ	1.61	0.97
1:A:43:GLY:H	3:C:40:LYS:HZ3	1.26	0.80
1:A:401:LYS:NZ	2:B:440:ALA:HA	1.99	0.76
3:C:72:ILE:HD12	3:C:74:ASP:H	1.55	0.70
2:B:140:SER:HA	2:B:171:VAL:HB	1.74	0.70
1:A:43:GLY:H	3:C:40:LYS:HZ2	1.41	0.69
1:A:79:ARG:HG2	1:A:92:LEU:HD23	1.76	0.66
2:B:180:THR:HB	2:B:183:GLU:HG2	1.79	0.65
1:A:401:LYS:HZ3	2:B:440:ALA:HA	1.59	0.64
3:C:62:ARG:NH1	3:C:87:ASP:OD2	2.30	0.64
3:C:47:VAL:HG22	3:C:72:ILE:HD13	1.81	0.62
1:A:188:ILE:HG23	1:A:425:MET:HG3	1.82	0.61
2:B:205:ASP:HB3	2:B:303:ALA:HA	1.83	0.60
1:A:161:TYR:HB3	1:A:164:LYS:HD2	1.83	0.60
1:A:195:LEU:HD12	1:A:266:HIS:HE1	1.67	0.59
2:B:319:PHE:HB2	2:B:355:VAL:HG22	1.83	0.59
1:A:336:LYS:HZ3	1:A:351:PHE:HE1	1.48	0.58
1:A:255:PHE:O	1:A:259:LEU:HB2	2.03	0.57
1:A:265:ILE:HD11	1:A:431:ASP:HB3	1.87	0.56
1:A:217:LEU:HD21	1:A:368:LEU:HD23	1.89	0.55
1:A:43:GLY:N	3:C:40:LYS:HZ3	2.03	0.55
2:B:274:PRO:HB3	2:B:286:LEU:HD22	1.88	0.55
2:B:180:THR:HB	2:B:183:GLU:CG	2.37	0.54
1:A:43:GLY:N	3:C:40:LYS:NZ	2.45	0.54
2:B:67:LEU:HD22	2:B:78:VAL:HG11	1.89	0.54
3:C:78:VAL:HB	3:C:107:ARG:HH21	1.73	0.53
2:B:154:ILE:HG23	2:B:166:MET:HG2	1.89	0.53
1:A:173:PRO:HB3	1:A:183:GLU:OE2	2.09	0.53
2:B:6:HIS:HE1	2:B:138:THR:CG2	2.22	0.53
1:A:265:ILE:HG23	1:A:432:TYR:CE2	2.44	0.53
2:B:269:MET:HE3	2:B:381:SER:HB3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:386:GLU:O	1:A:390:ARG:HG3	2.09	0.52
2:B:141:LEU:HA	2:B:147:SER:HB3	1.90	0.52
1:A:54:SER:O	1:A:61:HIS:HA	2.10	0.51
1:A:167:LEU:HD12	1:A:200:CYS:HB3	1.92	0.50
2:B:196:GLU:OE2	2:B:424:ASN:ND2	2.43	0.50
2:B:19:LYS:HD3	2:B:228:ASN:HB3	1.93	0.50
2:B:69:ASP:HA	2:B:145:THR:HG21	1.93	0.50
2:B:277:SER:OG	2:B:280:SER:OG	2.31	0.49
1:A:401:LYS:HZ1	2:B:440:ALA:HA	1.74	0.49
2:B:6:HIS:HE1	2:B:138:THR:HG23	1.77	0.49
1:A:249:ASN:HA	1:A:254:GLU:HB3	1.95	0.48
3:C:73:GLY:HA2	3:C:103:ILE:HG12	1.94	0.48
1:A:209:ILE:HG23	1:A:230:LEU:HD23	1.94	0.48
2:B:344:VAL:HG13	2:B:346:TRP:NE1	2.29	0.48
3:C:116:LEU:HD13	3:C:154:ALA:HA	1.96	0.48
2:B:344:VAL:HG13	2:B:346:TRP:CD1	2.48	0.48
2:B:6:HIS:CE1	2:B:138:THR:HG23	2.48	0.48
1:A:140:SER:HA	1:A:171:ILE:HB	1.96	0.47
1:A:172:TYR:HB3	1:A:205:ASP:HA	1.96	0.47
1:A:336:LYS:NZ	1:A:351:PHE:CE1	2.79	0.47
3:C:23:LEU:O	3:C:31:ARG:HG2	2.13	0.47
1:A:192:HIS:CG	1:A:421:ALA:HA	2.50	0.46
2:B:213:CYS:HA	2:B:217:LEU:HB2	1.97	0.46
2:B:344:VAL:HG13	2:B:346:TRP:CE2	2.51	0.46
3:C:163:GLU:HG3	9:C:642:HOH:O	2.16	0.45
1:A:328:VAL:HG11	1:A:353:VAL:HG11	1.99	0.45
1:A:71:GLU:HB2	1:A:98:ASP:HB3	1.98	0.45
1:A:335:ILE:O	1:A:339:ARG:HB2	2.18	0.44
3:C:104:GLY:HA2	3:C:134:ILE:HG12	1.99	0.44
1:A:117:LEU:O	1:A:121:ARG:HG2	2.18	0.43
1:A:336:LYS:NZ	1:A:351:PHE:HE1	2.13	0.43
2:B:154:ILE:HG22	2:B:197:ASN:HB3	2.00	0.43
1:A:238:ILE:HG12	1:A:378:LEU:HD21	1.99	0.43
2:B:344:VAL:CG1	2:B:346:TRP:CE2	3.02	0.43
1:A:141:PHE:O	1:A:147:SER:HB3	2.19	0.42
1:A:182:VAL:O	1:A:185:TYR:HB2	2.19	0.42
2:B:151:THR:HB	2:B:193:GLN:HG3	2.02	0.42
3:C:139:VAL:O	3:C:143:MET:HG2	2.19	0.42
2:B:10:GLY:HA2	2:B:145:THR:HB	2.01	0.41
2:B:205:ASP:CB	2:B:303:ALA:HA	2.51	0.41
1:A:25:CYS:HB3	1:A:30:ILE:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:54:LEU:HD12	3:C:54:LEU:HA	1.97	0.41
1:A:210:TYR:HE2	1:A:221:ARG:NH1	2.19	0.41
1:A:93:ILE:HG22	1:A:114:ILE:HD11	2.03	0.40
1:A:181:VAL:HG22	2:B:352:LYS:HE2	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	436/451 (97%)	421 (97%)	15 (3%)	0	100	100
2	B	416/445 (94%)	404 (97%)	12 (3%)	0	100	100
3	C	155/170 (91%)	152 (98%)	3 (2%)	0	100	100
4	P	30/79 (38%)	29 (97%)	1 (3%)	0	100	100
All	All	1037/1145 (91%)	1006 (97%)	31 (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	360/379 (95%)	347 (96%)	13 (4%)	35	54
2	B	301/383 (79%)	293 (97%)	8 (3%)	44	65

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	C	117/135 (87%)	106 (91%)	11 (9%)	8 13
4	P	10/68 (15%)	10 (100%)	0	100 100
All	All	788/965 (82%)	756 (96%)	32 (4%)	30 48

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	71	GLU
1	A	141	PHE
1	A	158	SER
1	A	178	SER
1	A	182	VAL
1	A	237	SER
1	A	251	ASP
1	A	326	LYS
1	A	342	GLN
1	A	384	ILE
1	A	415	GLU
1	A	438	ASP
2	B	26	ASP
2	B	54	ASN
2	B	139	HIS
2	B	211	ASP
2	B	377	PHE
2	B	399	PHE
2	B	404	PHE
2	B	420	GLU
3	C	55	LYS
3	C	60	GLN
3	C	63	LYS
3	C	71	LYS
3	C	74	ASP
3	C	83	LYS
3	C	90	ARG
3	C	118	ASP
3	C	129	SER
3	C	163	GLU
3	C	166	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 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	$\#\|Z\| > 2$
8	GOL	C	500	-	5,5,5	0.19	0	5,5,5	0.53	0
7	GDP	B	600	-	24,30,30	1.04	1 (4%)	31,47,47	2.09	6 (19%)
5	GTP	A	600	6	26,34,34	0.90	1 (3%)	33,54,54	2.10	6 (18%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	GOL	C	500	-	-	2/4/4/4	-
7	GDP	B	600	-	-	4/12/32/32	0/3/3/3
5	GTP	A	600	6	-	4/18/38/38	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	600	GDP	C6-N1	3.20	1.38	1.33
5	A	600	GTP	C6-N1	3.06	1.38	1.33

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	B	600	GDP	C5-C6-N1	-8.34	112.03	123.43
5	A	600	GTP	C5-C6-N1	-8.20	112.22	123.43
5	A	600	GTP	C2-N1-C6	6.11	125.63	115.93
7	B	600	GDP	C2-N1-C6	5.86	125.25	115.93
5	A	600	GTP	C4-C5-C6	-3.33	117.61	120.80
5	A	600	GTP	N3-C2-N1	-2.86	123.41	127.22
7	B	600	GDP	N3-C2-N1	-2.79	123.50	127.22
7	B	600	GDP	C4-C5-C6	-2.62	118.30	120.80
5	A	600	GTP	O5'-PA-O1A	2.38	118.38	109.07
7	B	600	GDP	C2-N3-C4	-2.24	112.80	115.36
5	A	600	GTP	C2-N3-C4	-2.10	112.96	115.36
7	B	600	GDP	O3B-PB-O3A	2.06	111.54	104.64

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	600	GTP	C5'-O5'-PA-O1A
5	A	600	GTP	C5'-O5'-PA-O2A
7	B	600	GDP	C5'-O5'-PA-O1A
7	B	600	GDP	C5'-O5'-PA-O2A
8	C	500	GOL	C1-C2-C3-O3
8	C	500	GOL	O2-C2-C3-O3
7	B	600	GDP	C5'-O5'-PA-O3A
7	B	600	GDP	PB-O3A-PA-O2A
5	A	600	GTP	PB-O3B-PG-O3G
5	A	600	GTP	C5'-O5'-PA-O3A

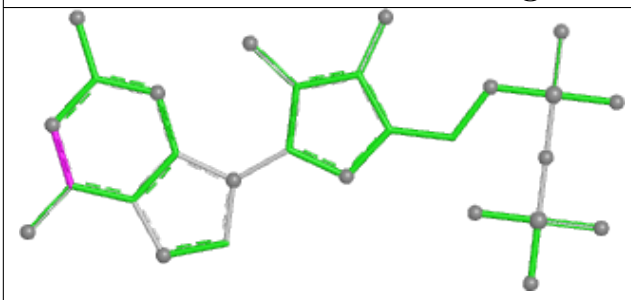
There are no ring outliers.

No monomer is involved in short contacts.

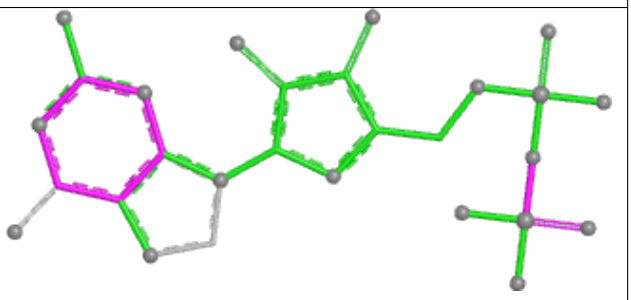
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

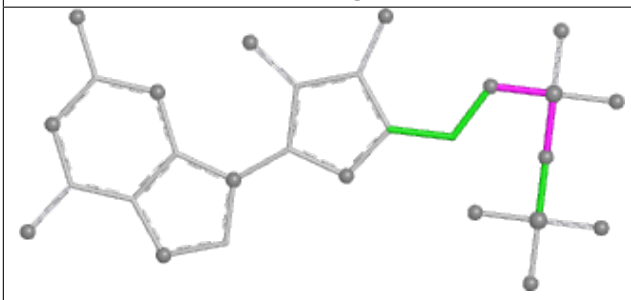
Ligand GDP B 600



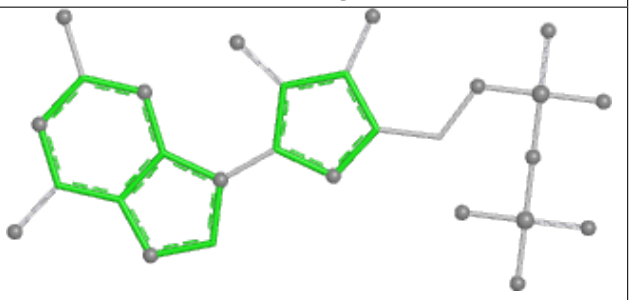
Bond lengths



Bond angles

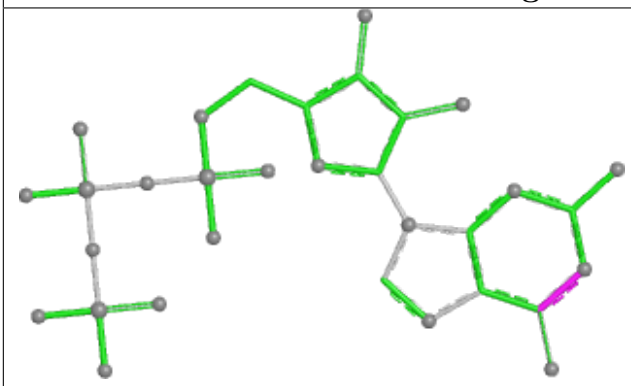


Torsions

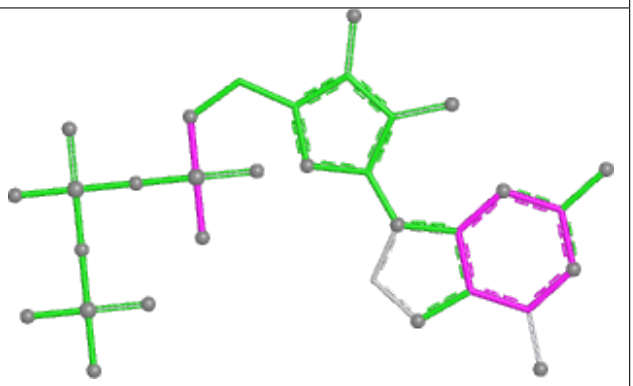


Rings

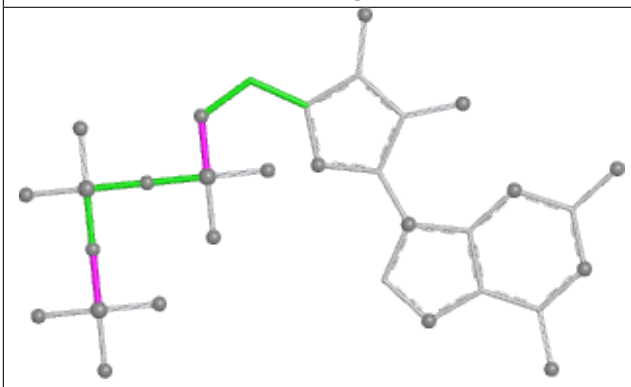
Ligand GTP A 600



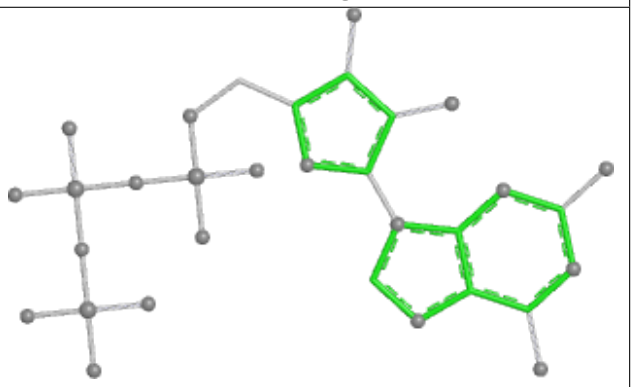
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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^{th} 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	438/451 (97%)	0.71	10 (2%) 60 58	53, 76, 100, 113	1 (0%)
2	B	424/445 (95%)	1.67	132 (31%) 0 0	90, 128, 166, 179	0
3	C	157/170 (92%)	0.75	16 (10%) 6 6	61, 82, 107, 114	0
4	P	36/79 (45%)	3.02	20 (55%) 0 0	141, 154, 205, 209	0
All	All	1055/1145 (92%)	1.18	178 (16%) 1 1	53, 94, 156, 209	1 (0%)

All (178) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	416	MET	10.4
2	B	70	LEU	10.1
4	P	351	GLN	9.8
2	B	410	GLY	9.5
2	B	408	TYR	9.5
2	B	108	TYR	9.3
2	B	182	VAL	8.9
2	B	413	MET	8.8
2	B	403	ALA	8.7
2	B	409	THR	8.3
2	B	111	GLY	8.2
2	B	99	ALA	8.0
2	B	418	PHE	8.0
4	P	353	LEU	7.9
4	P	376	LEU	7.9
2	B	142	GLY	7.8
4	P	346	ILE	7.7
2	B	109	THR	7.5
2	B	104	ALA	7.4
4	P	348	LEU	6.7
3	C	16	VAL	6.0

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Mol	Chain	Res	Type	RSRZ
2	B	421	ALA	6.0
2	B	107	HIS	6.0
2	B	406	HIS	5.8
4	P	347	GLN	5.7
4	P	379	GLY	5.7
2	B	210	TYR	5.7
2	B	419	THR	5.6
2	B	285	ALA	5.6
2	B	304	ALA	5.6
2	B	59	ASN	5.4
2	B	440	ALA	5.4
2	B	411	GLU	5.4
2	B	405	LEU	5.4
2	B	106	GLY	5.4
4	P	350	GLU	5.3
2	B	404	PHE	5.2
2	B	401	ARG	5.1
2	B	100	GLY	5.1
2	B	212	ILE	4.8
2	B	417	GLU	4.8
4	P	349	GLU	4.7
2	B	441	ASP	4.5
4	P	371	PRO	4.4
2	B	36	TYR	4.3
3	C	45	ARG	4.3
2	B	396	THR	4.3
2	B	103	TRP	4.2
2	B	398	MET	4.2
2	B	272	PHE	4.2
2	B	399	PHE	4.1
2	B	145	THR	4.1
2	B	72	PRO	4.0
2	B	95	GLY	4.0
4	P	375	PHE	4.0
2	B	387	LEU	3.9
2	B	98	GLY	3.9
2	B	284	ARG	3.9
4	P	342	LEU	3.9
4	P	374	PRO	3.8
4	P	352	GLU	3.7
2	B	9	ALA	3.7
2	B	184	PRO	3.7

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Mol	Chain	Res	Type	RSRZ
2	B	188	THR	3.7
2	B	214	PHE	3.6
2	B	407	TRP	3.6
2	B	397	ALA	3.6
2	B	40	SER	3.6
2	B	68	VAL	3.5
3	C	72	ILE	3.5
2	B	187	ALA	3.5
2	B	102	ASN	3.4
2	B	423	SER	3.4
2	B	192	HIS	3.4
2	B	391	ILE	3.4
2	B	46	LEU	3.4
2	B	213	CYS	3.3
2	B	197	ASN	3.3
1	A	108	TYR	3.3
2	B	112	ALA	3.3
2	B	189	LEU	3.3
2	B	412	GLY	3.3
2	B	181	VAL	3.3
4	P	372	LYS	3.2
4	P	345	GLN	3.2
2	B	287	THR	3.2
2	B	186	ASN	3.2
2	B	286	LEU	3.2
2	B	183	GLU	3.1
2	B	220	THR	3.0
2	B	313	LEU	3.0
2	B	66	ILE	3.0
3	C	41	ILE	3.0
3	C	49	PRO	3.0
2	B	110	GLU	2.9
2	B	241	CYS	2.9
2	B	150	GLY	2.9
2	B	259	MET	2.9
2	B	169	PHE	2.9
2	B	5	VAL	2.9
1	A	100	ALA	2.8
2	B	273	ALA	2.8
2	B	154	ILE	2.8
2	B	226	ASP	2.7
3	C	47	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
2	B	223	THR	2.7
3	C	82	ILE	2.7
2	B	216	THR	2.7
2	B	151	THR	2.6
2	B	58	GLY	2.6
2	B	203	CYS	2.6
2	B	143	GLY	2.6
2	B	202	TYR	2.6
2	B	235	MET	2.6
2	B	268	PHE	2.6
2	B	298	SER	2.5
2	B	179	ASP	2.5
3	C	54	LEU	2.5
1	A	44	GLY	2.5
2	B	271	GLY	2.5
4	P	378	ARG	2.5
3	C	61	VAL	2.5
2	B	57	THR	2.5
4	P	373	GLN	2.5
4	P	381	GLY	2.5
2	B	42	LEU	2.5
4	P	322	ILE	2.4
2	B	227	LEU	2.4
2	B	305	CYS	2.4
2	B	157	ILE	2.4
1	A	117	LEU	2.4
2	B	270	PRO	2.4
3	C	42	GLY	2.4
2	B	379	GLY	2.4
2	B	105	LYS	2.3
1	A	167	LEU	2.3
3	C	68	ALA	2.3
2	B	269	MET	2.3
2	B	296	PHE	2.3
2	B	185	TYR	2.3
2	B	67	LEU	2.3
2	B	115	VAL	2.3
3	C	20	ILE	2.3
1	A	12	ALA	2.2
2	B	315	VAL	2.2
2	B	71	GLU	2.2
1	A	432	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	402	LYS	2.2
2	B	209	LEU	2.2
2	B	10	GLY	2.2
2	B	278	ARG	2.1
2	B	50	ASN	2.1
2	B	198	THR	2.1
2	B	97	SER	2.1
3	C	17	GLU	2.1
1	A	137	VAL	2.1
2	B	240	THR	2.1
2	B	395	PHE	2.1
3	C	51	ILE	2.1
2	B	221	THR	2.1
1	A	200	CYS	2.1
2	B	173	PRO	2.1
2	B	316	ALA	2.1
2	B	260	VAL	2.1
2	B	217	LEU	2.0
2	B	234	THR	2.0
2	B	171	VAL	2.0
3	C	80	PRO	2.0
2	B	229	HIS	2.0
1	A	238	ILE	2.0
2	B	141	LEU	2.0
2	B	252	LEU	2.0
2	B	358	ILE	2.0
2	B	91	ASN	2.0
2	B	101	ASN	2.0
2	B	137	LEU	2.0
2	B	149	MET	2.0
3	C	43	ASP	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

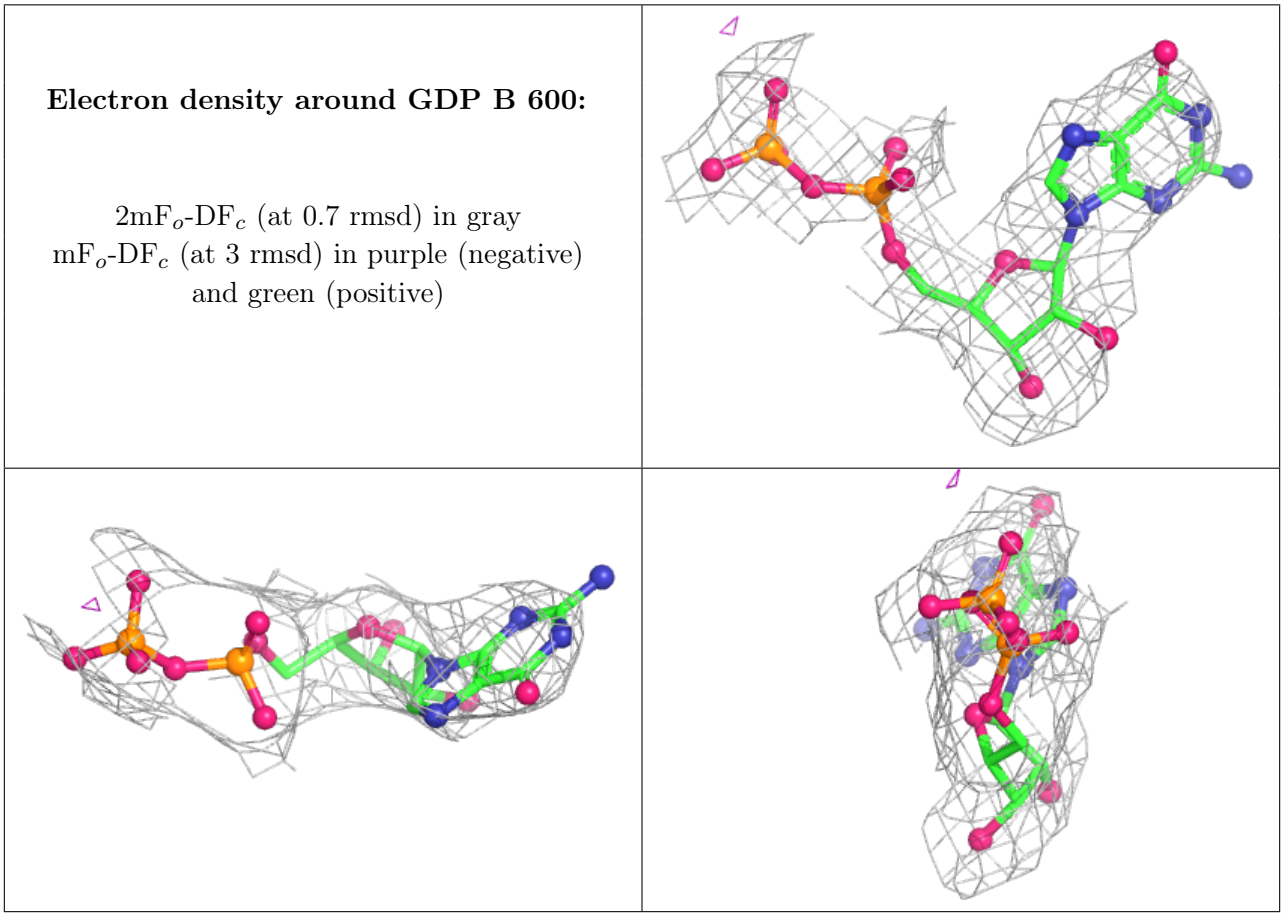
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
8	GOL	C	500	6/6	0.87	0.22	76,77,77,77	0
7	GDP	B	600	28/28	0.91	0.17	156,157,158,158	0
5	GTP	A	600	32/32	0.97	0.17	66,71,73,73	0
6	MG	A	601	1/1	0.97	0.12	72,72,72,72	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.

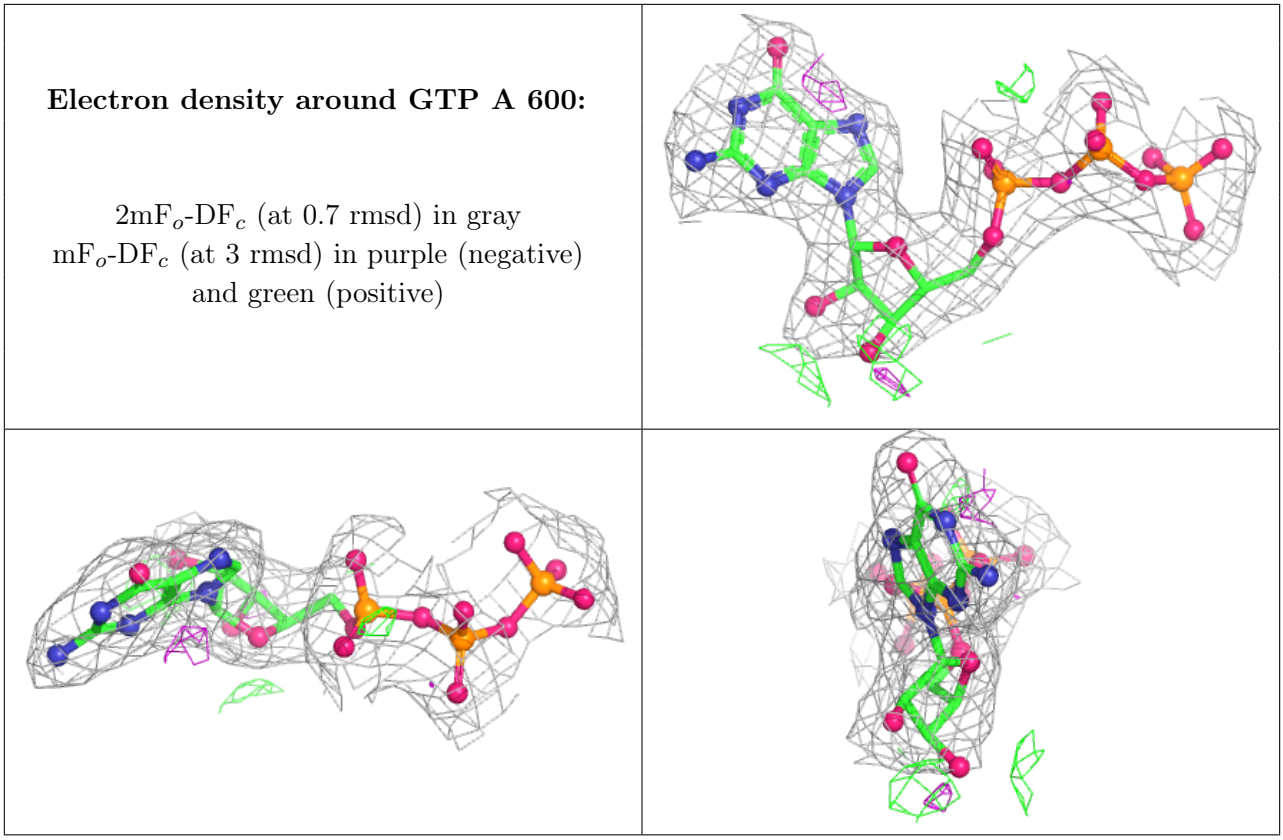
Electron density around GDP B 600:

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



Electron density around GTP A 600:

$2mF_o$-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.