Full wwPDB X-ray Structure Validation Report (i)

Mar 3, 2024 – 10:54 PM EST

PDB ID	:	6O5N
Title	:	Tubulin-RB3_SLD-TTL in complex with compound 10ab
Authors	:	Kumar, G.; Wang, Y.; Li, W.; White, S.W.
Deposited on	:	2019-03-04
Resolution	:	3.00 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

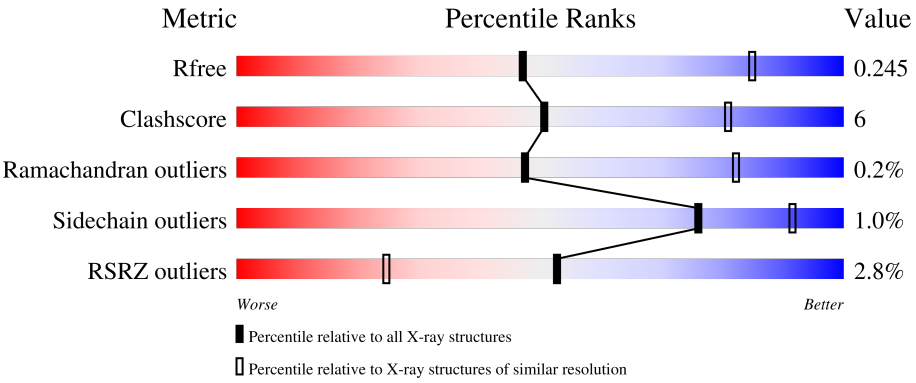
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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	450	83% 14% .
1	C	450	85% 12% .
2	B	445	% 84% 12% .
2	D	445	% 79% 15% 5%
3	E	143	73% 11% 15%

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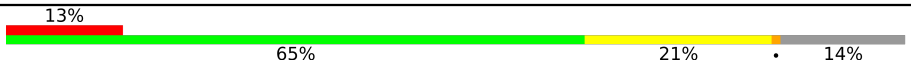
Mol	Chain	Length	Quality of chain
4	F	384	

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 17476 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	437	Total	C	N	O	S	0	0	0
			3416	2163	581	650	22			
1	C	440	Total	C	N	O	S	0	0	0
			3437	2175	584	656	22			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	427	Total	C	N	O	S	0	0	0
			3361	2110	576	649	26			
2	D	421	Total	C	N	O	S	0	0	0
			3309	2080	562	640	27			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	121	Total	C	N	O	S	0	0	0
			1000	617	181	197	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	3	MET	-	expression tag	UNP Q9H169
E	4	ALA	-	expression tag	UNP Q9H169

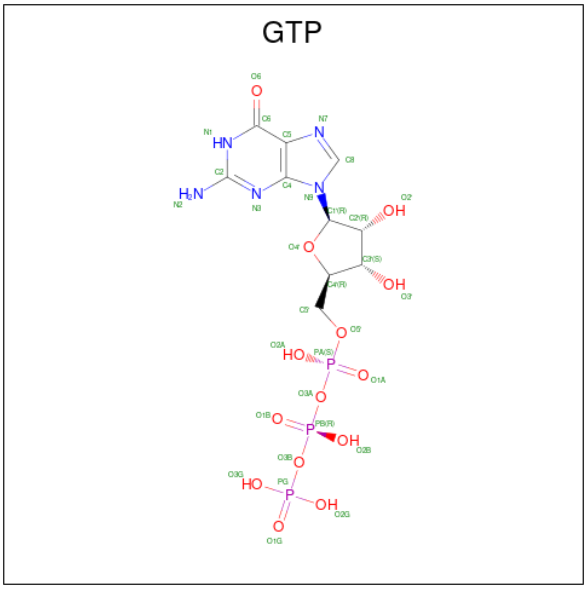
- Molecule 4 is a protein called Tubulin Tyrosine Ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	332	Total	C	N	O	S	0	0	0
			2705	1736	464	491	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 32 10 5 14 3	0	0
5	C	1	Total C N O P 32 10 5 14 3	0	0

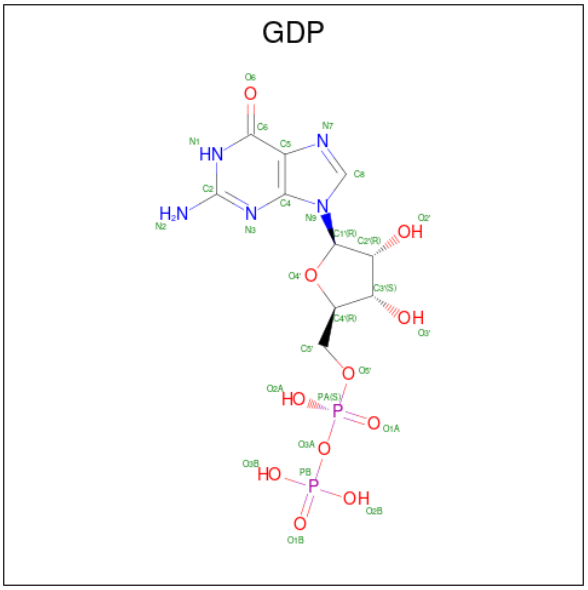
- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

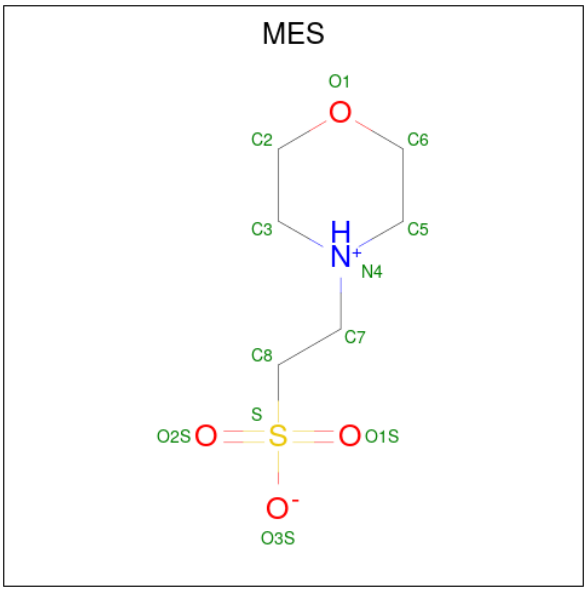
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total Ca 1 1	0	0
7	C	1	Total Ca 1 1	0	0

- Molecule 8 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



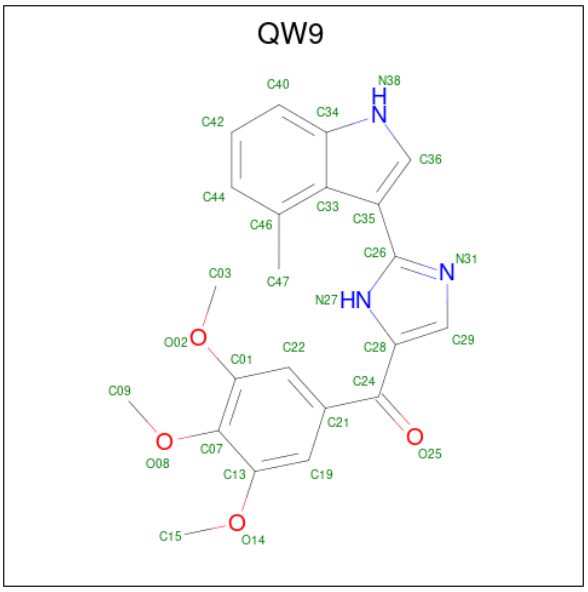
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	1	Total C N O P 28 10 5 11 2	0	0
8	D	1	Total C N O P 28 10 5 11 2	0	0

- Molecule 9 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



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

- Molecule 10 is [2-(4-methyl-1H-indol-3-yl)-1H-imidazol-5-yl](3,4,5-trimethoxyphenyl)methanone (three-letter code: QW9) (formula: $C_{22}H_{21}N_3O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	B	1	Total	C	N	O	0	0
			29	22	3	4		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	D	1	Total	C	N	O	0	0
			29	22	3	4		

- Molecule 11 is water.

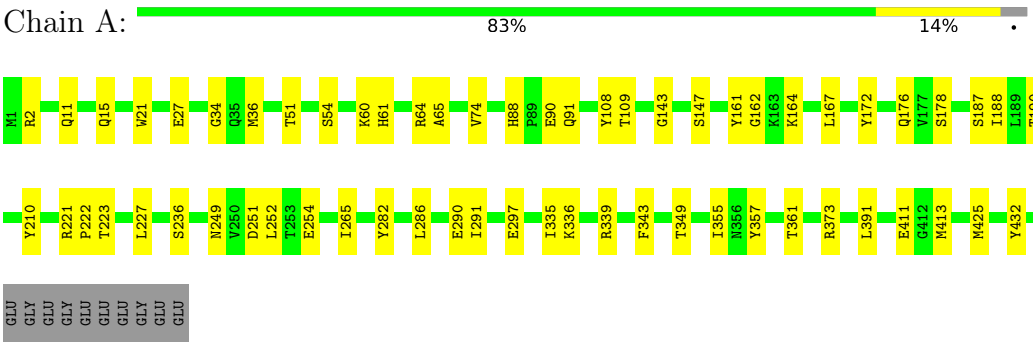
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	14	Total	O	0	0
			14	14		
11	B	7	Total	O	0	0
			7	7		
11	C	13	Total	O	0	0
			13	13		
11	D	3	Total	O	0	0
			3	3		
11	E	1	Total	O	0	0
			1	1		
11	F	3	Total	O	0	0
			3	3		

3 Residue-property plots (i)

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

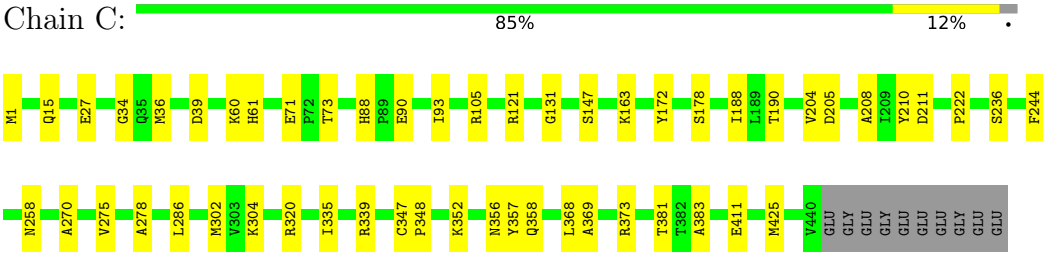
• Molecule 1: Tubulin alpha-1B chain

Chain A:



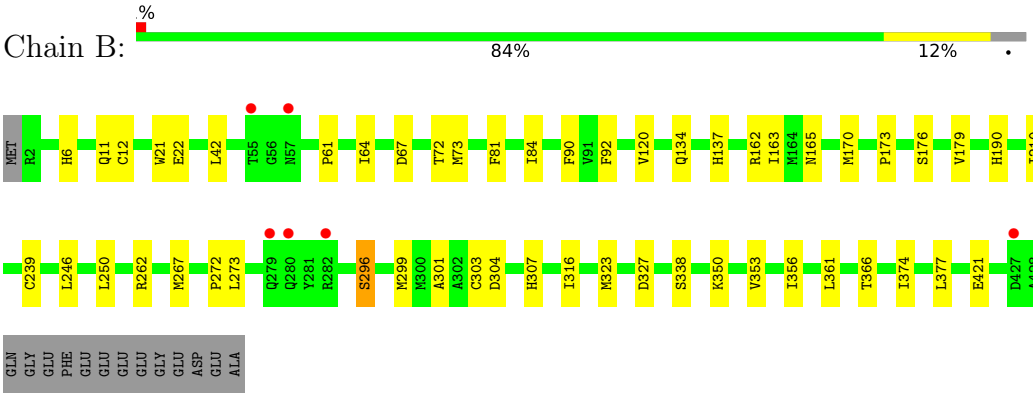
• Molecule 1: Tubulin alpha-1B chain

Chain C:



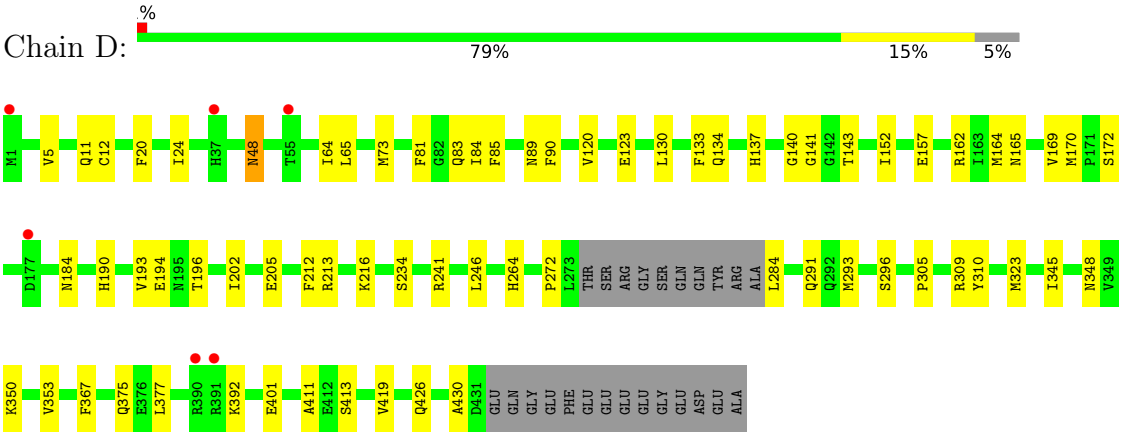
• Molecule 2: Tubulin beta-2B chain

Chain B:



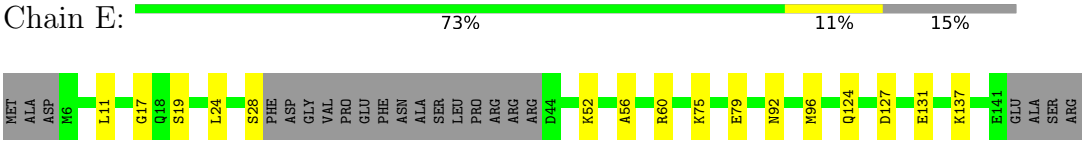
• Molecule 2: Tubulin beta-2B chain

Chain D:



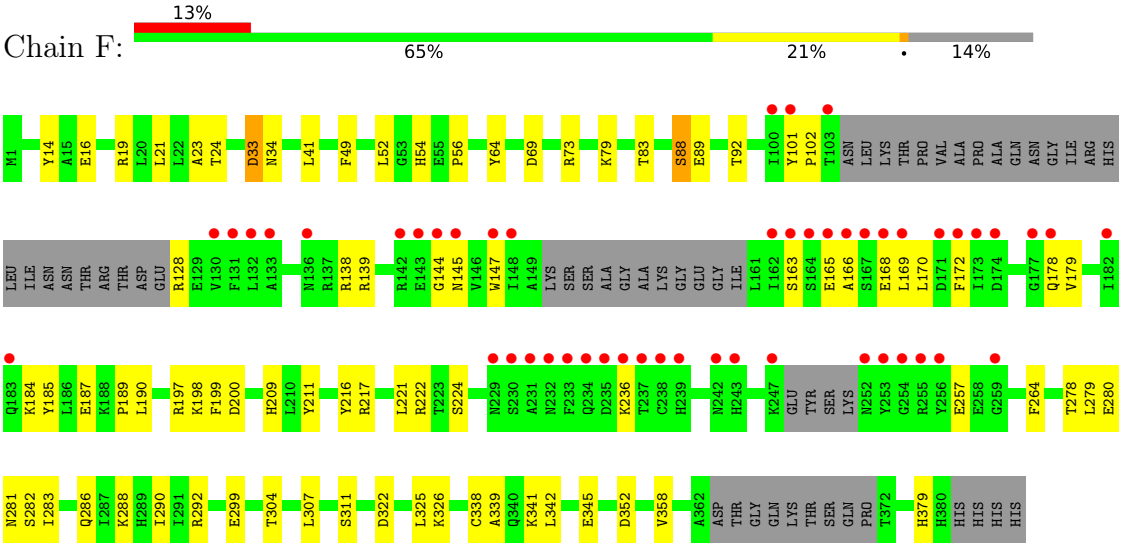
• Molecule 3: Stathmin-4

Chain E:



• Molecule 4: Tubulin Tyrosine Ligase

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	105.30Å 157.76Å 182.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.78 – 3.00 41.78 – 3.00	Depositor EDS
% Data completeness (in resolution range)	96.2 (41.78-3.00) 96.2 (41.78-3.00)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.00 (at 3.01Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.202 , 0.245 0.202 , 0.245	Depositor DCC
R_{free} test set	2941 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	57.3	Xtriage
Anisotropy	0.053	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 39.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	17476	wwPDB-VP
Average B, all atoms (Å^2)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.58% 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: GTP, CA, QW9, MES, MG, GDP

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	0.26	0/3494	0.47	0/4743
1	C	0.28	0/3515	0.48	0/4772
2	B	0.27	0/3436	0.47	0/4654
2	D	0.26	0/3382	0.45	0/4581
3	E	0.24	0/1008	0.39	0/1337
4	F	0.25	0/2765	0.45	0/3737
All	All	0.26	0/17600	0.46	0/23824

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	3416	0	3330	41	0
1	C	3437	0	3348	33	0
2	B	3361	0	3238	34	0
2	D	3309	0	3189	40	0
3	E	1000	0	1018	11	0
4	F	2705	0	2666	47	0
5	A	32	0	12	2	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
7	A	1	0	0	0	0
7	C	1	0	0	0	0
8	B	28	0	12	1	0
8	D	28	0	12	4	0
9	B	24	0	24	2	0
10	B	29	0	0	1	0
10	D	29	0	0	1	0
11	A	14	0	0	1	0
11	B	7	0	0	0	0
11	C	13	0	0	0	0
11	D	3	0	0	0	0
11	E	1	0	0	0	0
11	F	3	0	0	0	0
All	All	17476	0	16861	194	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 6.

All (194) 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:170:MET:HG3	2:B:377:LEU:HD11	1.70	0.72
4:F:14:TYR:HB3	4:F:41:LEU:HD13	1.73	0.70
4:F:64:TYR:O	4:F:311:SER:OG	2.11	0.68
4:F:169:LEU:HA	4:F:172:PHE:HB3	1.76	0.68
1:C:71:GLU:OE2	1:C:73:THR:OG1	2.08	0.67
4:F:101:TYR:O	4:F:128:ARG:NH2	2.28	0.67
2:B:296:SER:N	9:B:504:MES:O3S	2.25	0.65
2:D:157:GLU:OE2	3:E:124:GLN:NE2	2.30	0.64
4:F:280:GLU:OE2	4:F:288:LYS:NZ	2.25	0.62
2:B:323:MET:HG2	2:B:353:VAL:HG21	1.81	0.61
4:F:165:GLU:HB2	4:F:168:GLU:HG3	1.83	0.60
2:D:309:ARG:NH2	2:D:426:GLN:O	2.31	0.60
2:D:375:GLN:HB2	2:D:419:VAL:HG13	1.83	0.60
2:D:401:GLU:HA	3:E:137:LYS:HG3	1.83	0.60
2:B:246:LEU:HD21	2:B:350:LYS:HE2	1.84	0.58
4:F:185:TYR:OH	4:F:198:LYS:NZ	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:278:THR:OG1	4:F:281:ASN:OD1	2.22	0.58
1:A:178:SER:O	2:B:350:LYS:NZ	2.36	0.57
2:B:179:VAL:HG12	1:C:348:PRO:HG2	1.85	0.57
1:A:251:ASP:OD1	1:A:254:GLU:HB2	2.05	0.57
1:C:147:SER:HB2	1:C:190:THR:OG1	2.04	0.57
1:C:105:ARG:NH1	1:C:411:GLU:OE1	2.38	0.56
1:A:54:SER:HB3	1:A:64:ARG:NH1	2.20	0.56
1:C:211:ASP:OD2	1:C:304:LYS:NZ	2.36	0.56
2:D:143:THR:HB	8:D:501:GDP:O1B	2.05	0.56
4:F:278:THR:O	4:F:282:SER:OG	2.21	0.56
1:A:343:PHE:CD1	1:A:349:THR:HG23	2.41	0.55
2:D:140:GLY:O	2:D:184:ASN:ND2	2.38	0.55
2:D:64:ILE:HD13	2:D:120:VAL:HG22	1.89	0.55
2:D:141:GLY:HA3	8:D:501:GDP:O3A	2.06	0.55
1:A:221:ARG:NH1	2:B:327:ASP:OD2	2.31	0.55
2:B:73:MET:HE3	2:B:90:PHE:HD2	1.72	0.54
4:F:88:SER:OG	4:F:89:GLU:HA	2.08	0.54
4:F:138:ARG:NH1	4:F:144:GLY:O	2.41	0.54
3:E:75:LYS:O	3:E:79:GLU:HG3	2.08	0.54
1:C:286:LEU:O	1:C:373:ARG:NH1	2.39	0.53
4:F:338:CYS:SG	4:F:339:ALA:N	2.80	0.53
1:A:2:ARG:O	1:A:51:THR:HG23	2.09	0.53
4:F:79:LYS:O	4:F:83:THR:OG1	2.24	0.53
4:F:21:LEU:O	4:F:24:THR:OG1	2.21	0.53
2:B:12:CYS:HB2	8:B:501:GDP:C8	2.43	0.53
2:D:89:ASN:ND2	2:D:123:GLU:OE2	2.35	0.53
4:F:217:ARG:NH2	4:F:345:GLU:OE2	2.42	0.53
4:F:49:PHE:HA	4:F:52:LEU:HD12	1.91	0.53
1:A:286:LEU:HD12	1:A:290:GLU:HB3	1.90	0.52
2:D:130:LEU:O	2:D:162:ARG:NH1	2.43	0.52
4:F:304:THR:HG21	4:F:311:SER:HB2	1.92	0.52
1:C:210:TYR:CZ	1:C:222:PRO:HD2	2.45	0.51
2:B:316:ILE:HG23	2:B:366:THR:HB	1.93	0.51
1:C:172:TYR:HB3	1:C:205:ASP:HA	1.93	0.51
2:B:173:PRO:HA	2:B:176:SER:HB2	1.92	0.51
2:B:239:CYS:SG	2:B:316:ILE:HD13	2.51	0.50
1:A:164:LYS:NZ	11:A:602:HOH:O	2.45	0.50
1:A:291:ILE:HD13	1:A:373:ARG:HG3	1.93	0.50
1:C:278:ALA:HA	1:C:369:ALA:HB2	1.94	0.50
2:B:267:MET:HG2	2:B:374:ILE:HD13	1.94	0.50
1:C:88:HIS:HE1	1:C:90:GLU:HG3	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:270:ALA:HB3	1:C:302:MET:HE2	1.94	0.49
2:D:170:MET:HG3	2:D:377:LEU:HD11	1.93	0.49
2:B:22:GLU:HG2	2:B:81:PHE:CD1	2.48	0.49
2:D:234:SER:O	2:D:241:ARG:NH2	2.43	0.49
1:A:88:HIS:CD2	1:A:90:GLU:HB2	2.48	0.49
2:B:134:GLN:HA	2:B:165:ASN:O	2.13	0.49
2:B:210:ILE:HG23	2:B:273:LEU:HD13	1.94	0.49
4:F:197:ARG:NH1	4:F:257:GLU:OE2	2.30	0.49
2:D:193:VAL:HG13	2:D:194:GLU:HG2	1.95	0.49
1:C:178:SER:O	2:D:350:LYS:NZ	2.30	0.48
4:F:69:ASP:O	4:F:73:ARG:N	2.43	0.48
2:B:67:ASP:O	2:B:92:PHE:HA	2.13	0.48
1:A:187:SER:HB3	1:A:391:LEU:HD21	1.94	0.48
2:D:196:THR:OG1	2:D:264:HIS:NE2	2.45	0.48
1:A:172:TYR:HB3	1:A:205:ASP:HA	1.95	0.48
1:C:163:LYS:HA	1:C:163:LYS:HD2	1.58	0.48
1:A:265:ILE:HG23	1:A:432:TYR:CZ	2.48	0.48
1:A:335:ILE:HG23	1:A:339:ARG:HD2	1.96	0.48
2:D:73:MET:HE3	2:D:90:PHE:HD2	1.78	0.48
4:F:102:PRO:HD3	4:F:179:VAL:HG22	1.96	0.47
1:C:320:ARG:HA	1:C:356:ASN:O	2.14	0.47
1:C:335:ILE:HG23	1:C:339:ARG:HG3	1.96	0.47
2:D:345:ILE:HG22	2:D:348:ASN:HB3	1.96	0.47
1:A:108:TYR:CE2	1:A:413:MET:HG3	2.49	0.47
1:A:297:GLU:OE2	1:A:339:ARG:NH2	2.40	0.47
1:A:223:THR:O	1:A:227:LEU:HG	2.15	0.47
3:E:56:ALA:O	3:E:60:ARG:NH1	2.48	0.47
1:A:143:GLY:HA3	5:A:501:GTP:O3A	2.15	0.47
1:C:249:ASN:OD1	1:C:356:ASN:ND2	2.47	0.47
2:D:190:HIS:ND1	2:D:411:ALA:HA	2.29	0.47
1:A:109:THR:OG1	1:A:411:GLU:OE2	2.22	0.47
1:C:93:ILE:HD11	1:C:121:ARG:HG3	1.96	0.47
1:C:36:MET:HB3	1:C:61:HIS:CE1	2.50	0.47
4:F:178:GLN:N	4:F:178:GLN:OE1	2.48	0.47
1:A:15:GLN:NE2	5:A:501:GTP:O6	2.44	0.46
1:A:88:HIS:NE2	1:A:90:GLU:HB2	2.29	0.46
1:C:244:PHE:CD1	1:C:358:GLN:HG3	2.49	0.46
1:A:88:HIS:N	1:A:91:GLN:OE1	2.43	0.46
3:E:127:ASP:O	3:E:131:GLU:HG2	2.15	0.46
1:C:188:ILE:HG13	1:C:425:MET:HG3	1.97	0.46
1:A:336:LYS:HG2	3:E:24:LEU:HD13	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:21:TRP:CZ3	2:B:61:PRO:HB3	2.50	0.46
2:D:293:MET:HE2	2:D:367:PHE:HB2	1.97	0.46
2:D:296:SER:HB3	2:D:305:PRO:HD2	1.98	0.46
4:F:145:ASN:OD1	4:F:147:TRP:NE1	2.47	0.46
2:D:172:SER:OG	2:D:205:GLU:OE1	2.22	0.46
1:A:147:SER:HB2	1:A:190:THR:HB	1.98	0.46
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.35	0.45
1:C:1:MET:HG3	1:C:131:GLY:HA3	1.98	0.45
1:C:15:GLN:NE2	5:C:501:GTP:O6	2.44	0.45
2:D:392:LYS:HB2	2:D:392:LYS:HE2	1.76	0.45
9:B:504:MES:H51	9:B:504:MES:H81	1.69	0.45
1:C:88:HIS:CE1	1:C:90:GLU:HG3	2.52	0.45
2:B:296:SER:HA	2:B:299:MET:HG2	1.99	0.45
2:D:81:PHE:O	2:D:84:ILE:HG22	2.16	0.45
2:D:246:LEU:HD23	2:D:350:LYS:HE2	1.99	0.45
1:A:36:MET:HB3	1:A:61:HIS:CE1	2.52	0.45
1:C:275:VAL:HG13	1:C:368:LEU:HD21	1.99	0.44
4:F:307:LEU:HD23	4:F:307:LEU:HA	1.81	0.44
1:C:27:GLU:OE1	1:C:236:SER:OG	2.29	0.44
1:A:27:GLU:OE1	1:A:236:SER:OG	2.25	0.44
2:B:64:ILE:HD13	2:B:120:VAL:HG22	1.99	0.44
2:D:350:LYS:HB2	10:D:502:QW9:C34	2.48	0.44
4:F:16:GLU:OE1	4:F:19:ARG:NE	2.45	0.44
2:D:134:GLN:HA	2:D:165:ASN:O	2.18	0.44
4:F:33:ASP:OD1	4:F:33:ASP:N	2.50	0.43
4:F:163:SER:OG	4:F:168:GLU:OE1	2.24	0.43
1:A:27:GLU:HG2	1:A:361:THR:OG1	2.19	0.43
2:D:212:PHE:O	2:D:216:LYS:HA	2.18	0.43
1:A:11:GLN:HG3	1:A:74:VAL:HG21	2.01	0.43
1:A:207:GLU:OE2	4:F:54:HIS:ND1	2.35	0.43
2:D:5:VAL:HB	2:D:133:PHE:CD1	2.53	0.43
1:C:250:VAL:HG11	1:C:352:LYS:HE3	2.01	0.43
1:A:34:GLY:HA3	1:A:60:LYS:HG3	2.01	0.43
4:F:341:LYS:O	4:F:341:LYS:HD3	2.19	0.42
4:F:211:TYR:CE1	4:F:299:GLU:HG3	2.54	0.42
1:A:210:TYR:CZ	1:A:222:PRO:HD2	2.54	0.42
2:B:262:ARG:NE	2:B:421:GLU:OE2	2.52	0.42
2:B:272:PRO:HD2	2:B:361:LEU:HD13	2.01	0.42
1:C:34:GLY:HA3	1:C:60:LYS:HG3	2.00	0.42
2:D:20:PHE:O	2:D:24:ILE:HG12	2.19	0.42
4:F:279:LEU:HD12	4:F:283:ILE:HB	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:138:ARG:HB2	4:F:145:ASN:ND2	2.34	0.42
1:A:355:ILE:O	3:E:17:GLY:HA3	2.19	0.42
2:B:179:VAL:HG22	1:C:258:ASN:OD1	2.19	0.42
3:E:28:SER:O	3:E:28:SER:OG	2.32	0.42
1:A:357:TYR:CE2	3:E:17:GLY:HA2	2.55	0.42
2:B:221:THR:O	2:B:225:LEU:HD13	2.20	0.42
1:C:39:ASP:OD2	1:C:61:HIS:NE2	2.33	0.42
2:D:310:TYR:CE1	2:D:367:PHE:HZ	2.38	0.42
2:D:323:MET:SD	2:D:353:VAL:HG11	2.59	0.42
4:F:92:THR:O	4:F:326:LYS:HE2	2.20	0.42
4:F:292:ARG:NE	4:F:379:HIS:O	2.50	0.42
1:A:167:LEU:HD22	1:A:252:LEU:HD22	2.02	0.42
1:A:249:ASN:HA	1:A:254:GLU:HB3	2.02	0.42
2:D:272:PRO:HB3	2:D:284:LEU:HD11	2.01	0.42
4:F:138:ARG:HB2	4:F:145:ASN:CG	2.40	0.42
1:A:88:HIS:ND1	1:A:91:GLN:OE1	2.51	0.42
2:D:11:GLN:HB3	8:D:501:GDP:O1A	2.20	0.42
2:D:65:LEU:HD11	2:D:85:PHE:CD2	2.55	0.42
2:D:83:GLN:H	2:D:83:GLN:HG2	1.45	0.42
2:D:169:VAL:HA	2:D:202:ILE:O	2.20	0.42
4:F:166:ALA:O	4:F:170:LEU:HG	2.20	0.42
2:B:42:LEU:HD23	2:B:356:ILE:HD11	2.01	0.41
2:D:12:CYS:HB2	8:D:501:GDP:C8	2.54	0.41
2:B:163:ILE:HG21	2:B:250:LEU:HB3	2.02	0.41
4:F:209:HIS:CE1	4:F:358:VAL:HG22	2.55	0.41
4:F:286:GLN:O	4:F:290:ILE:HG13	2.20	0.41
2:B:301:ALA:O	2:B:303:CYS:N	2.50	0.41
1:C:248:LEU:HD12	1:C:357:TYR:OH	2.20	0.41
1:C:381:THR:HG22	1:C:383:ALA:H	1.85	0.41
4:F:338:CYS:SG	4:F:342:LEU:HB2	2.60	0.41
2:B:11:GLN:HG3	2:B:72:THR:OG1	2.21	0.41
4:F:199:PHE:CD2	4:F:221:LEU:HD23	2.56	0.41
2:B:338:SER:HB2	4:F:34:ASN:HD21	1.85	0.41
1:A:161:TYR:HB3	1:A:164:LYS:HG2	2.02	0.41
1:A:188:ILE:HG13	1:A:425:MET:HG3	2.02	0.41
4:F:211:TYR:CD1	4:F:299:GLU:HG3	2.56	0.41
1:A:176:GLN:NE2	4:F:56:PRO:HB3	2.35	0.41
2:B:81:PHE:O	2:B:84:ILE:HG22	2.21	0.41
2:D:48:ASN:OD1	2:D:48:ASN:N	2.54	0.41
2:D:130:LEU:HD21	2:D:133:PHE:CZ	2.56	0.41
3:E:92:ASN:ND2	3:E:96:MET:SD	2.94	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:216:TYR:OH	4:F:345:GLU:OE1	2.27	0.41
4:F:187:GLU:C	4:F:189:PRO:HD3	2.42	0.40
2:B:350:LYS:HB2	10:B:505:QW9:C34	2.51	0.40
4:F:200:ASP:OD1	4:F:222:ARG:HB2	2.22	0.40
4:F:325:LEU:HD23	4:F:325:LEU:HA	1.82	0.40
1:A:21:TRP:CZ2	1:A:65:ALA:HB2	2.57	0.40
2:B:316:ILE:CG2	2:B:366:THR:HB	2.52	0.40
1:C:208:ALA:HB2	1:C:304:LYS:HG2	2.03	0.40
1:A:54:SER:HB3	1:A:64:ARG:CZ	2.51	0.40
2:B:304:ASP:HB3	2:B:307:HIS:ND1	2.37	0.40
2:D:152:ILE:HG23	2:D:164:MET:HG2	2.03	0.40
1:C:204:VAL:HG22	1:C:302:MET:HE1	2.04	0.40
3:E:11:LEU:HD12	3:E:19:SER:O	2.22	0.40
4:F:190:LEU:HB2	4:F:322:ASP:O	2.22	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	435/450 (97%)	420 (97%)	14 (3%)	1 (0%)	47 82
1	C	438/450 (97%)	424 (97%)	14 (3%)	0	100 100
2	B	425/445 (96%)	412 (97%)	13 (3%)	0	100 100
2	D	417/445 (94%)	405 (97%)	11 (3%)	1 (0%)	47 82
3	E	117/143 (82%)	115 (98%)	2 (2%)	0	100 100
4	F	322/384 (84%)	294 (91%)	26 (8%)	2 (1%)	25 64
All	All	2154/2317 (93%)	2070 (96%)	80 (4%)	4 (0%)	47 82

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	162	GLY
4	F	236	LYS
2	D	430	ALA
4	F	23	ALA

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	368/378 (97%)	367 (100%)	1 (0%)	92	97
1	C	371/378 (98%)	370 (100%)	1 (0%)	92	97
2	B	369/383 (96%)	365 (99%)	4 (1%)	73	90
2	D	364/383 (95%)	359 (99%)	5 (1%)	67	88
3	E	109/127 (86%)	108 (99%)	1 (1%)	78	92
4	F	294/342 (86%)	287 (98%)	7 (2%)	49	79
All	All	1875/1991 (94%)	1856 (99%)	19 (1%)	76	91

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

Mol	Chain	Res	Type
1	A	282	TYR
2	B	137	HIS
2	B	162	ARG
2	B	190	HIS
2	B	296	SER
1	C	347	CYS
2	D	48	ASN
2	D	137	HIS
2	D	213	ARG
2	D	291	GLN
2	D	413	SER
3	E	52	LYS
4	F	33	ASP
4	F	88	SER
4	F	139	ARG

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Mol	Chain	Res	Type
4	F	184	LYS
4	F	224	SER
4	F	264	PHE
4	F	352	ASP

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

Mol	Chain	Res	Type
1	A	301	GLN
2	B	426	GLN
4	F	183	GLN

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 13 ligands modelled in this entry, 5 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	$\#\|Z\| > 2$
8	GDP	D	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.29	5 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
9	MES	B	503	-	12,12,12	2.24	1 (8%)	14,16,16	2.04	5 (35%)
5	GTP	A	501	6	26,34,34	1.16	2 (7%)	32,54,54	1.46	7 (21%)
9	MES	B	504	-	12,12,12	2.30	1 (8%)	14,16,16	1.91	5 (35%)
8	GDP	B	501	6	24,30,30	0.98	1 (4%)	30,47,47	1.11	3 (10%)
5	GTP	C	501	6	26,34,34	1.15	2 (7%)	32,54,54	1.51	7 (21%)
10	QW9	B	505	-	30,32,32	1.24	5 (16%)	34,46,46	1.59	9 (26%)
10	QW9	D	502	-	30,32,32	1.26	5 (16%)	34,46,46	1.62	9 (26%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	GDP	D	501	-	-	4/12/32/32	0/3/3/3
9	MES	B	503	-	-	5/6/14/14	0/1/1/1
5	GTP	A	501	6	-	8/18/38/38	0/3/3/3
9	MES	B	504	-	-	4/6/14/14	0/1/1/1
8	GDP	B	501	6	-	3/12/32/32	0/3/3/3
5	GTP	C	501	6	-	3/18/38/38	0/3/3/3
10	QW9	B	505	-	-	2/10/18/18	0/4/4/4
10	QW9	D	502	-	-	2/10/18/18	0/4/4/4

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	504	MES	C8-S	-7.73	1.66	1.77
9	B	503	MES	C8-S	-7.50	1.66	1.77
5	C	501	GTP	C5-C6	-4.11	1.39	1.47
5	A	501	GTP	C5-C6	-4.08	1.39	1.47
10	D	502	QW9	C29-N31	-2.93	1.31	1.36
10	B	505	QW9	C29-N31	-2.90	1.31	1.36
8	B	501	GDP	C6-N1	-2.43	1.34	1.37
10	B	505	QW9	C21-C24	2.34	1.53	1.49
8	D	501	GDP	C6-N1	-2.29	1.34	1.37
10	D	502	QW9	C21-C24	2.29	1.53	1.49
10	D	502	QW9	O25-C24	-2.28	1.18	1.22
10	B	505	QW9	O25-C24	-2.19	1.18	1.22
10	D	502	QW9	C35-C26	2.16	1.54	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	505	QW9	C35-C26	2.15	1.53	1.48
5	A	501	GTP	C2-N3	2.12	1.38	1.33
5	C	501	GTP	C2-N3	2.05	1.38	1.33
10	B	505	QW9	O14-C13	2.03	1.40	1.37
10	D	502	QW9	O14-C13	2.02	1.40	1.37

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	B	505	QW9	C35-C26-N27	4.54	129.46	123.67
10	D	502	QW9	C35-C26-N27	4.20	129.03	123.67
9	B	504	MES	C5-N4-C3	3.96	117.74	108.83
9	B	503	MES	C6-C5-N4	-3.67	104.54	110.10
9	B	503	MES	C5-N4-C3	3.42	116.53	108.83
5	C	501	GTP	C5-C6-N1	3.27	119.73	113.95
5	A	501	GTP	C5-C6-N1	3.23	119.65	113.95
10	B	505	QW9	C46-C33-C34	-3.14	117.66	122.70
10	D	502	QW9	C46-C33-C34	-3.12	117.69	122.70
5	C	501	GTP	PA-O3A-PB	-3.07	122.30	132.83
10	D	502	QW9	O02-C01-C07	3.05	120.52	115.16
9	B	503	MES	C7-N4-C5	2.97	118.83	111.23
10	D	502	QW9	C03-O02-C01	-2.96	113.07	117.53
8	D	501	GDP	C3'-C2'-C1'	2.94	105.41	100.98
10	D	502	QW9	O02-C01-C22	-2.93	119.08	124.12
5	C	501	GTP	PB-O3B-PG	-2.90	122.86	132.83
5	C	501	GTP	C8-N7-C5	2.86	108.43	102.99
5	C	501	GTP	C2-N1-C6	-2.81	119.92	125.10
8	B	501	GDP	PA-O3A-PB	-2.78	123.27	132.83
5	A	501	GTP	C2-N1-C6	-2.78	119.98	125.10
5	A	501	GTP	C8-N7-C5	2.77	108.27	102.99
9	B	503	MES	O3S-S-C8	2.77	110.24	105.77
9	B	504	MES	C6-C5-N4	-2.73	105.97	110.10
10	D	502	QW9	O14-C13-C07	2.73	119.95	115.16
5	A	501	GTP	PA-O3A-PB	-2.72	123.50	132.83
10	B	505	QW9	O02-C01-C07	2.68	119.87	115.16
5	A	501	GTP	PB-O3B-PG	-2.68	123.64	132.83
9	B	504	MES	O2S-S-C8	2.64	110.09	106.92
10	B	505	QW9	C03-O02-C01	-2.58	113.63	117.53
10	D	502	QW9	C44-C46-C33	2.58	120.59	118.49
10	B	505	QW9	O14-C13-C07	2.55	119.65	115.16
10	B	505	QW9	C15-O14-C13	-2.54	113.69	117.53
10	B	505	QW9	O02-C01-C22	-2.45	119.91	124.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	B	505	QW9	C44-C46-C33	2.44	120.47	118.49
10	D	502	QW9	O14-C13-C19	-2.40	119.99	124.12
8	D	501	GDP	C8-N7-C5	2.32	107.40	102.99
8	B	501	GDP	C5-C6-N1	2.31	118.03	113.95
8	D	501	GDP	C5-C6-N1	2.30	118.01	113.95
8	B	501	GDP	C8-N7-C5	2.25	107.27	102.99
10	D	502	QW9	C15-O14-C13	-2.20	114.21	117.53
5	A	501	GTP	O6-C6-C5	-2.19	120.09	124.37
9	B	504	MES	C7-N4-C5	2.17	116.79	111.23
10	B	505	QW9	O14-C13-C19	-2.16	120.40	124.12
5	C	501	GTP	C3'-C2'-C1'	2.15	104.22	100.98
9	B	504	MES	O1S-S-C8	2.15	109.50	106.92
8	D	501	GDP	O2B-PB-O3A	2.14	111.81	104.64
8	D	501	GDP	C2'-C3'-C4'	2.12	106.76	102.64
5	A	501	GTP	C3'-C2'-C1'	2.12	104.17	100.98
5	C	501	GTP	O6-C6-C5	-2.07	120.32	124.37
9	B	503	MES	O1S-S-C8	2.06	109.40	106.92

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	501	GTP	PB-O3B-PG-O2G
5	A	501	GTP	C5'-O5'-PA-O2A
5	C	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O2A
8	B	501	GDP	C5'-O5'-PA-O1A
8	B	501	GDP	C5'-O5'-PA-O2A
8	D	501	GDP	C5'-O5'-PA-O1A
8	D	501	GDP	C5'-O5'-PA-O2A
9	B	503	MES	C8-C7-N4-C5
9	B	503	MES	C7-C8-S-O1S
9	B	503	MES	C7-C8-S-O2S
9	B	503	MES	C7-C8-S-O3S
9	B	504	MES	C8-C7-N4-C5
10	D	502	QW9	C07-C01-O02-C03
10	B	505	QW9	C07-C01-O02-C03
9	B	504	MES	C7-C8-S-O3S
10	D	502	QW9	C22-C01-O02-C03
10	B	505	QW9	C22-C01-O02-C03
5	A	501	GTP	C3'-C4'-C5'-O5'
8	D	501	GDP	PA-O3A-PB-O1B

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Mol	Chain	Res	Type	Atoms
5	A	501	GTP	O4'-C4'-C5'-O5'
9	B	503	MES	C8-C7-N4-C3
5	A	501	GTP	C5'-O5'-PA-O3A
5	C	501	GTP	C5'-O5'-PA-O3A
8	D	501	GDP	C5'-O5'-PA-O3A
5	A	501	GTP	C5'-O5'-PA-O1A
9	B	504	MES	C7-C8-S-O1S
9	B	504	MES	C7-C8-S-O2S
5	A	501	GTP	PB-O3B-PG-O1G
5	A	501	GTP	PB-O3B-PG-O3G
8	B	501	GDP	C5'-O5'-PA-O3A

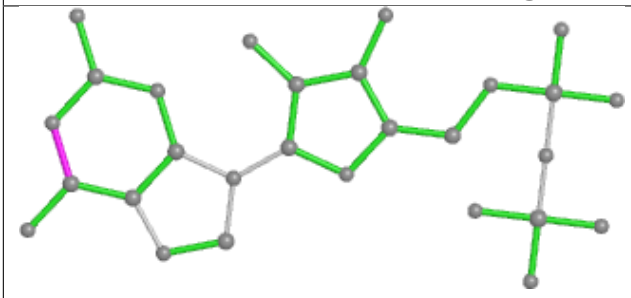
There are no ring outliers.

7 monomers are involved in 12 short contacts:

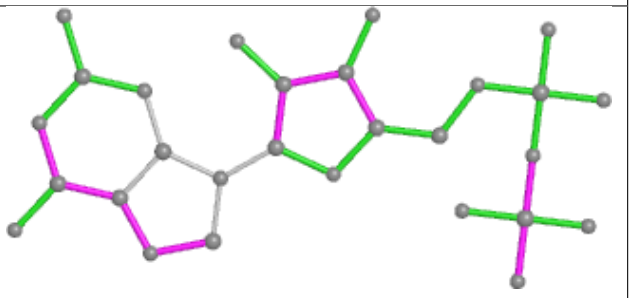
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	D	501	GDP	4	0
5	A	501	GTP	2	0
9	B	504	MES	2	0
8	B	501	GDP	1	0
5	C	501	GTP	1	0
10	B	505	QW9	1	0
10	D	502	QW9	1	0

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 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.

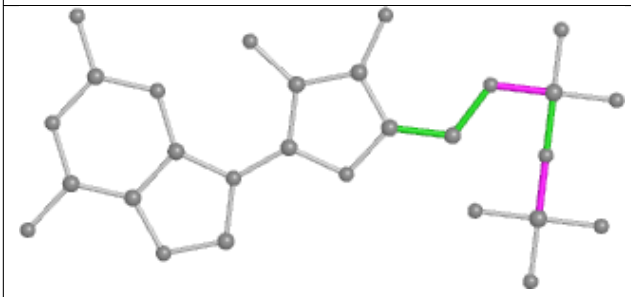
Ligand GDP D 501



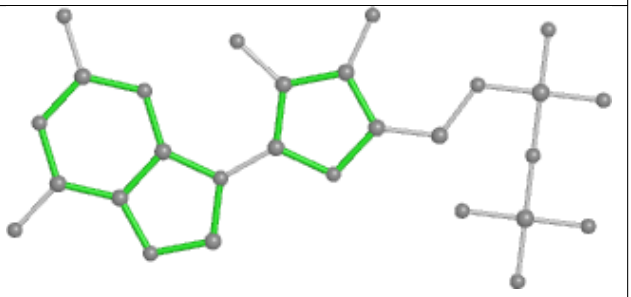
Bond lengths



Bond angles

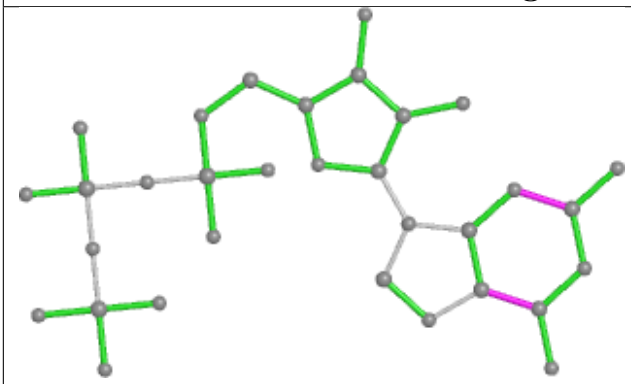


Torsions

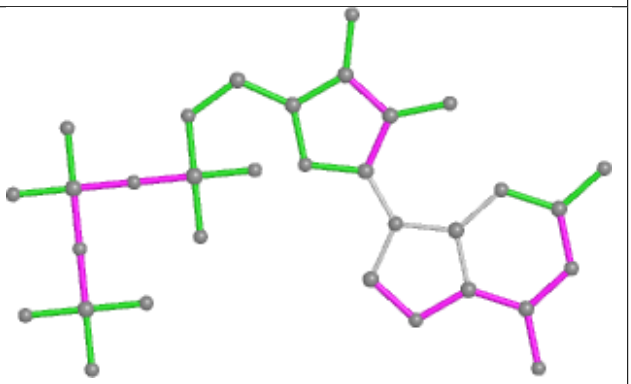


Rings

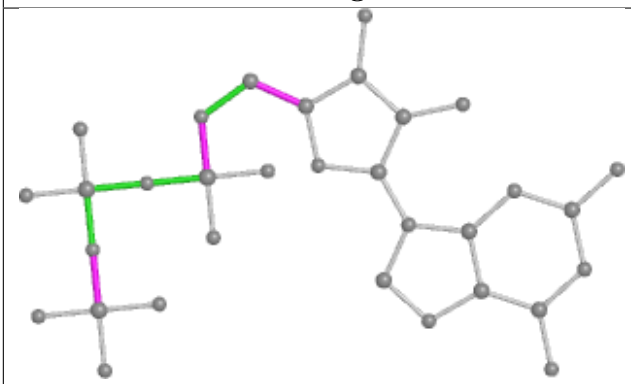
Ligand GTP A 501



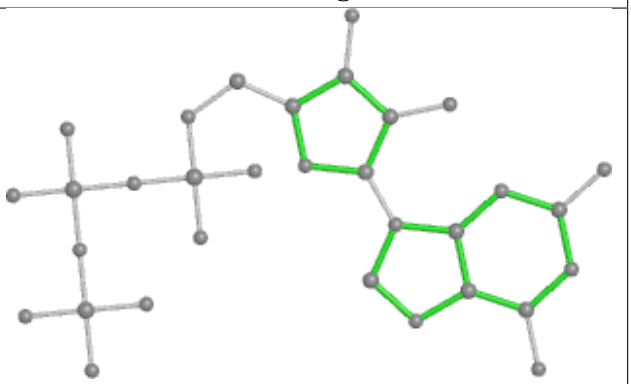
Bond lengths



Bond angles

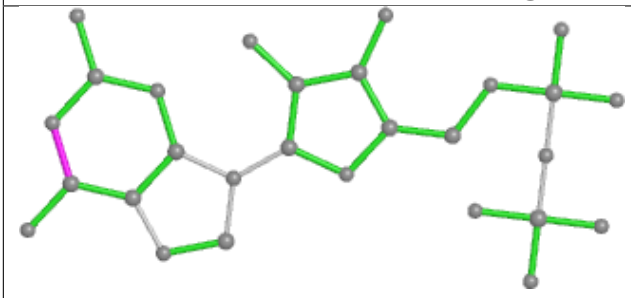


Torsions

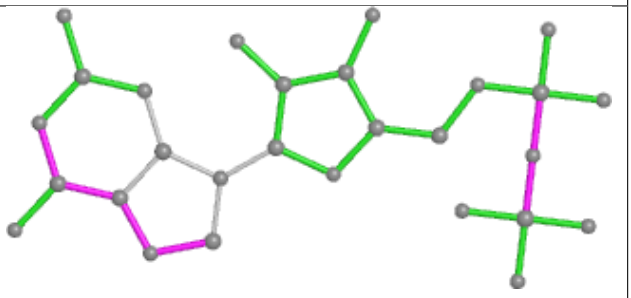


Rings

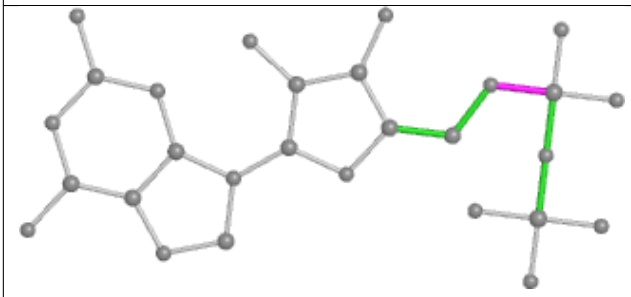
Ligand GDP B 501



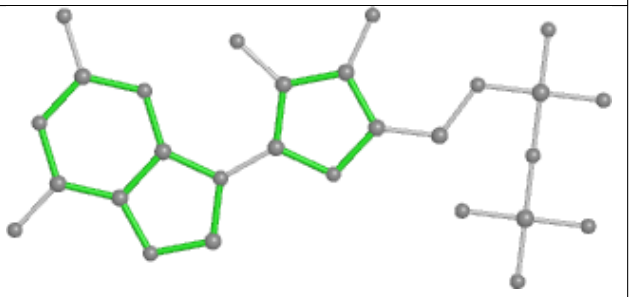
Bond lengths



Bond angles

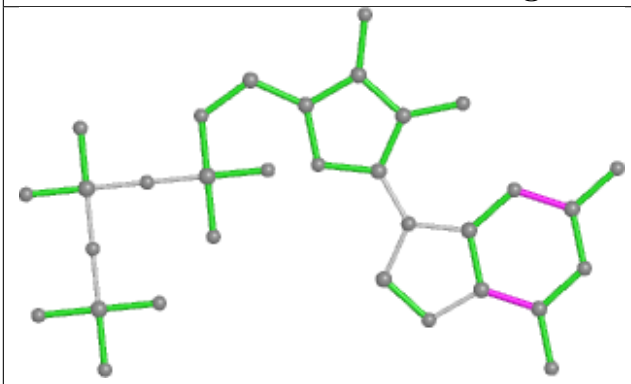


Torsions

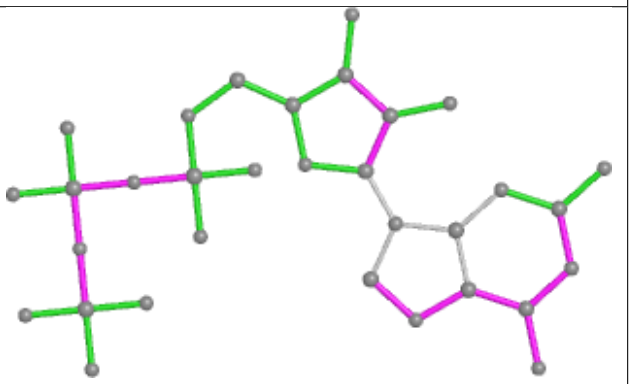


Rings

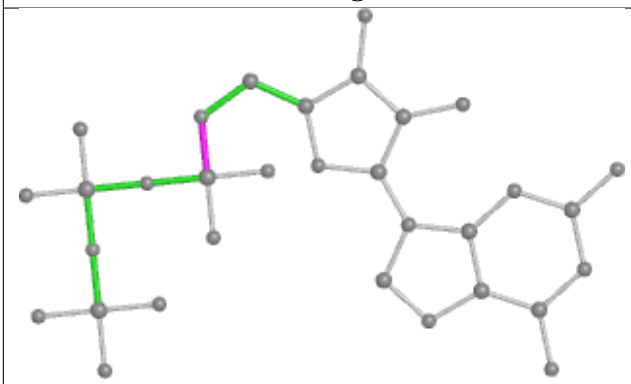
Ligand GTP C 501



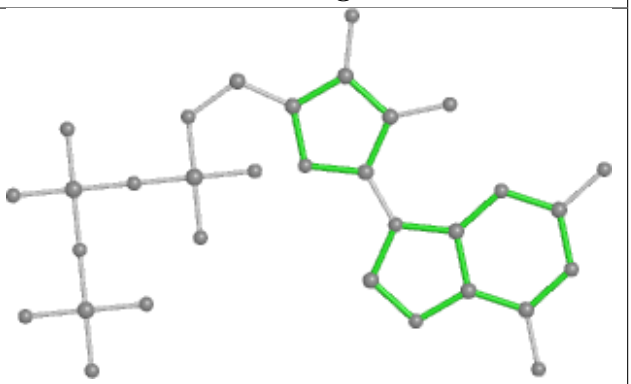
Bond lengths



Bond angles

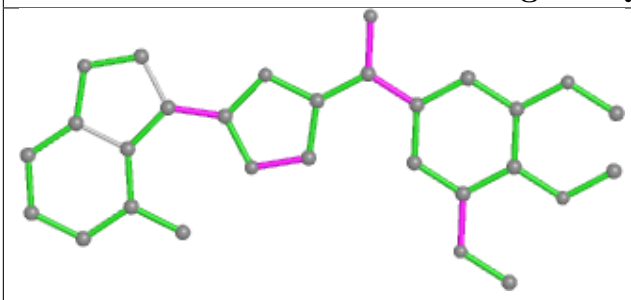


Torsions

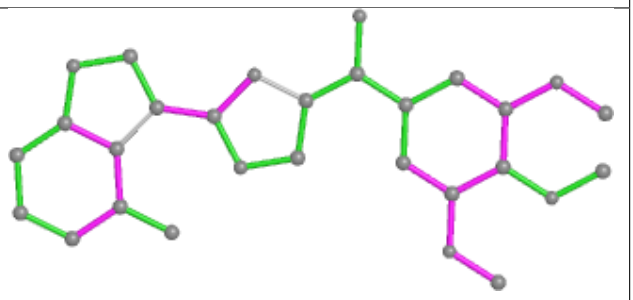


Rings

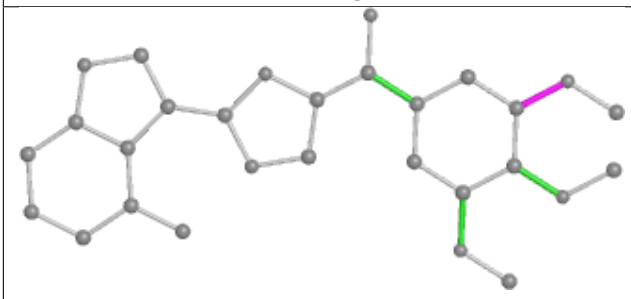
Ligand QW9 B 505



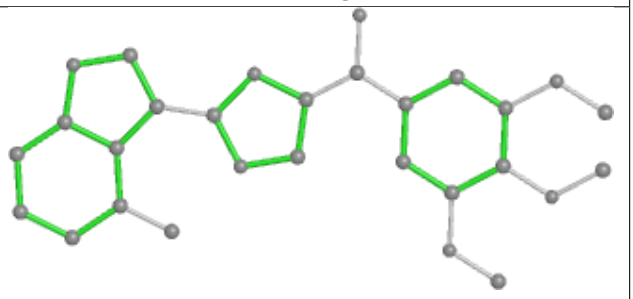
Bond lengths



Bond angles

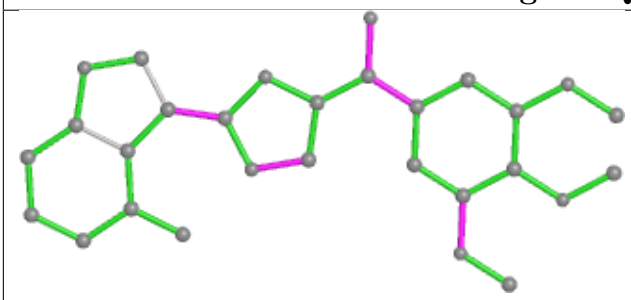


Torsions

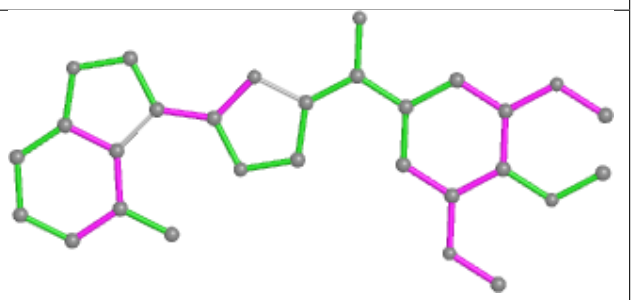


Rings

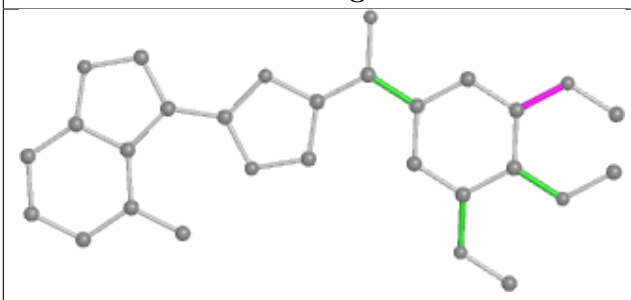
Ligand QW9 D 502



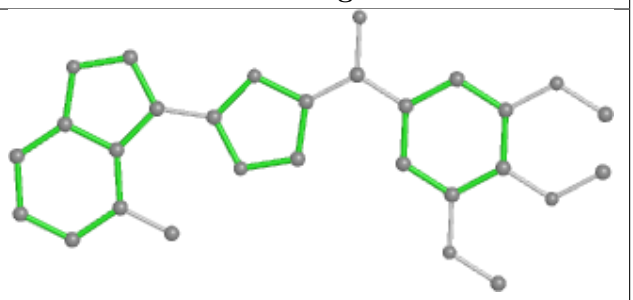
Bond lengths



Bond angles



Torsions



Rings

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^{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	437/450 (97%)	-0.43	0 100 100	33, 56, 88, 149	0
1	C	440/450 (97%)	-0.61	0 100 100	21, 38, 71, 121	0
2	B	427/445 (95%)	-0.37	6 (1%) 75 49	21, 46, 95, 156	0
2	D	421/445 (94%)	-0.05	6 (1%) 75 49	35, 74, 117, 142	0
3	E	121/143 (84%)	-0.15	0 100 100	34, 74, 116, 133	0
4	F	332/384 (86%)	0.44	50 (15%) 2 1	44, 91, 168, 193	0
All	All	2178/2317 (94%)	-0.23	62 (2%) 53 25	21, 59, 127, 193	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	163	SER	6.7
4	F	234	GLN	6.3
4	F	233	PHE	6.2
4	F	232	ASN	5.1
4	F	100	ILE	4.8
4	F	133	ALA	4.6
4	F	254	GLY	4.5
4	F	132	LEU	4.1
4	F	169	LEU	4.0
4	F	173	ILE	4.0
4	F	230	SER	3.9
4	F	164	SER	3.5
4	F	178	GLN	3.4
4	F	168	GLU	3.3
4	F	167	SER	3.2
4	F	256	TYR	3.2
4	F	255	ARG	3.2
4	F	239	HIS	3.1
2	D	37	HIS	3.1

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Mol	Chain	Res	Type	RSRZ
2	B	280	GLN	3.0
2	B	279	GLN	3.0
4	F	236	LYS	3.0
2	B	55	THR	2.9
4	F	231	ALA	2.9
4	F	130	VAL	2.8
4	F	103	THR	2.8
4	F	238	CYS	2.8
4	F	136	ASN	2.7
4	F	131	PHE	2.7
4	F	253	TYR	2.7
4	F	243	HIS	2.7
2	B	282	ARG	2.7
4	F	147	TRP	2.7
4	F	242	ASN	2.7
4	F	162	ILE	2.6
4	F	177	GLY	2.6
2	D	1	MET	2.5
4	F	183	GLN	2.4
2	B	427	ASP	2.4
4	F	259	GLY	2.4
2	D	55	THR	2.4
4	F	182	ILE	2.4
2	B	57	ASN	2.3
4	F	165	GLU	2.3
4	F	252	ASN	2.3
4	F	172	PHE	2.3
2	D	390	ARG	2.2
4	F	101	TYR	2.2
4	F	145	ASN	2.2
2	D	177	ASP	2.2
4	F	235	ASP	2.2
4	F	171	ASP	2.2
4	F	144	GLY	2.2
4	F	166	ALA	2.2
4	F	247	LYS	2.1
4	F	237	THR	2.1
4	F	174	ASP	2.1
4	F	143	GLU	2.1
4	F	148	ILE	2.1
2	D	391	ARG	2.1
4	F	229	ASN	2.0

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Mol	Chain	Res	Type	RSRZ
4	F	142	ARG	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)

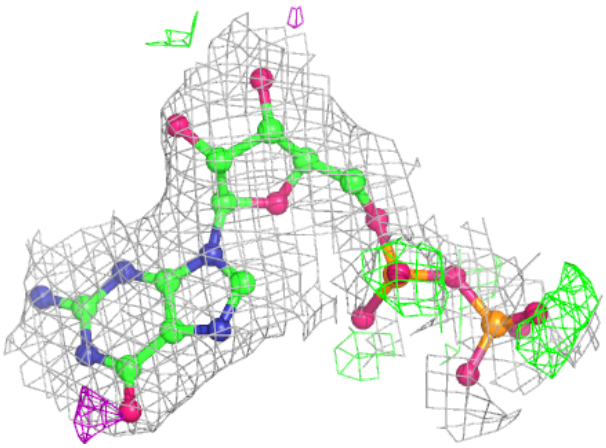
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

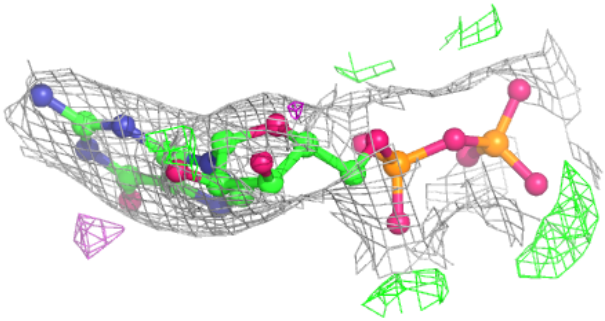
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
8	GDP	D	501	28/28	0.93	0.16	65,74,76,77	0
9	MES	B	504	12/12	0.93	0.22	89,90,97,99	0
9	MES	B	503	12/12	0.94	0.21	51,58,78,79	0
6	MG	A	502	1/1	0.96	0.45	39,39,39,39	0
5	GTP	C	501	32/32	0.96	0.19	27,32,45,46	0
10	QW9	D	502	29/29	0.96	0.19	47,53,58,59	0
6	MG	C	502	1/1	0.97	0.34	28,28,28,28	0
8	GDP	B	501	28/28	0.97	0.15	21,30,34,35	0
5	GTP	A	501	32/32	0.97	0.21	30,35,42,43	0
7	CA	C	503	1/1	0.98	0.05	56,56,56,56	0
6	MG	B	502	1/1	0.98	0.25	24,24,24,24	0
10	QW9	B	505	29/29	0.98	0.22	32,38,46,48	0
7	CA	A	503	1/1	0.98	0.05	85,85,85,85	0

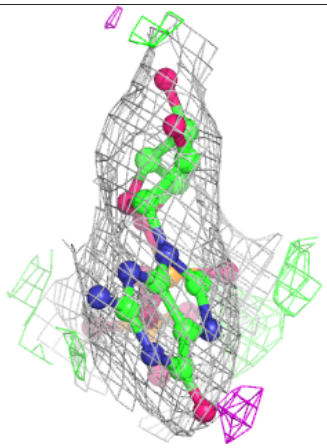
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around GDP 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)

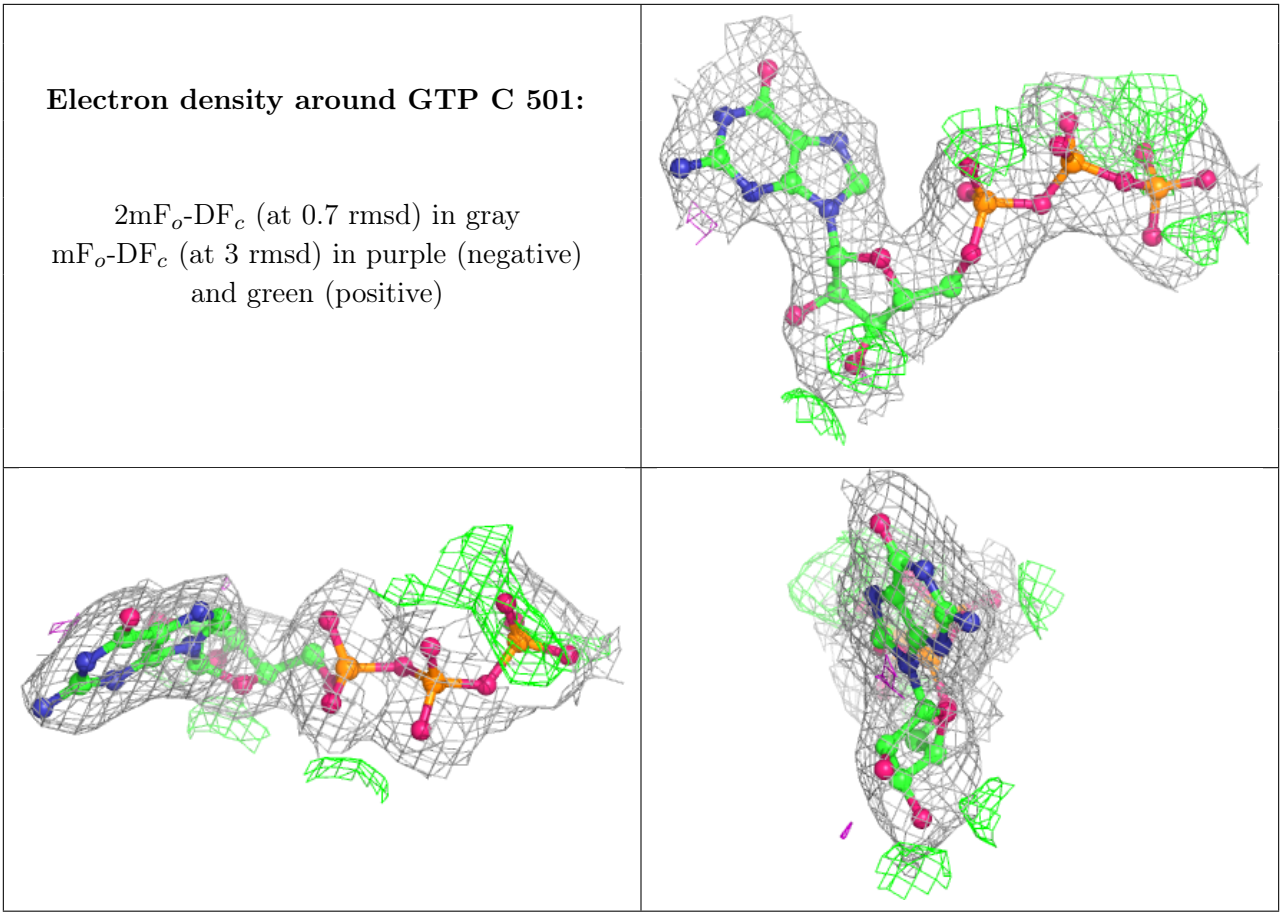






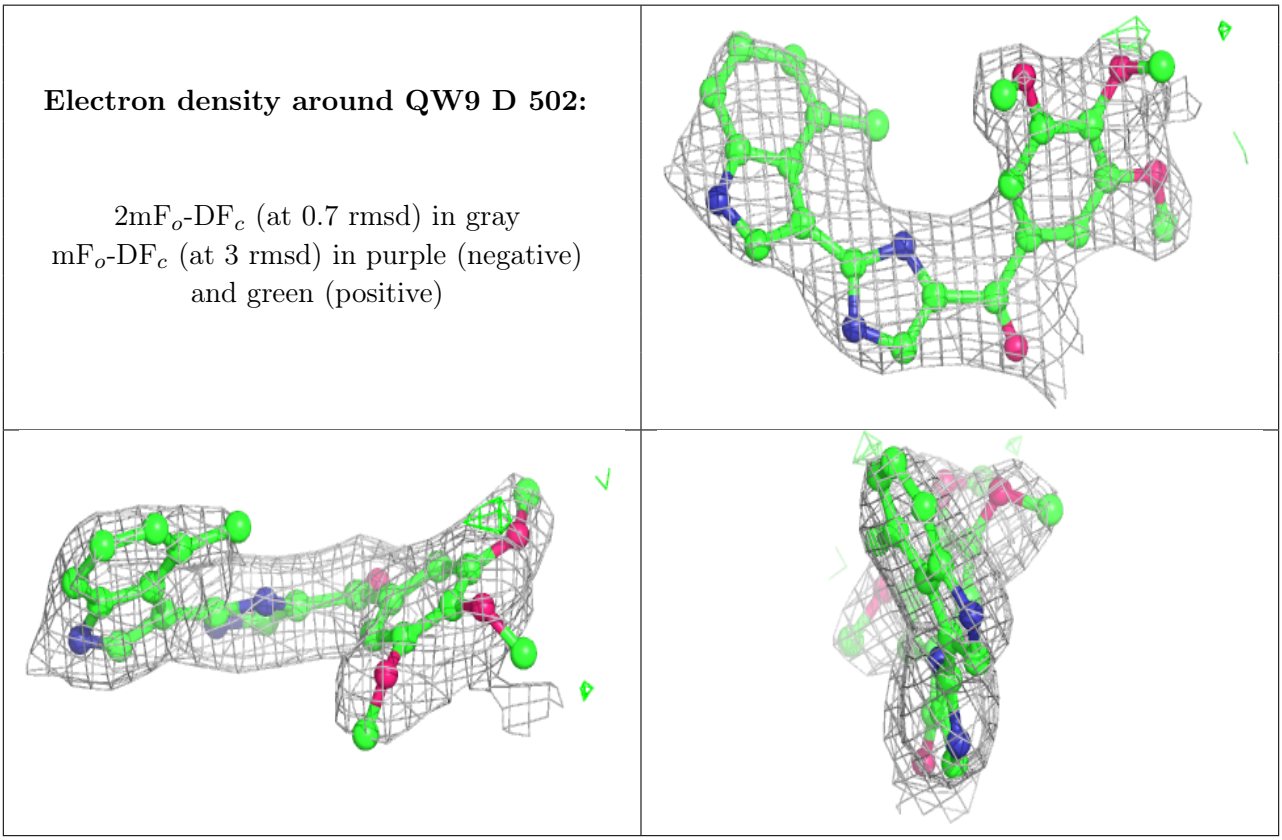
Electron density around GTP C 501:

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



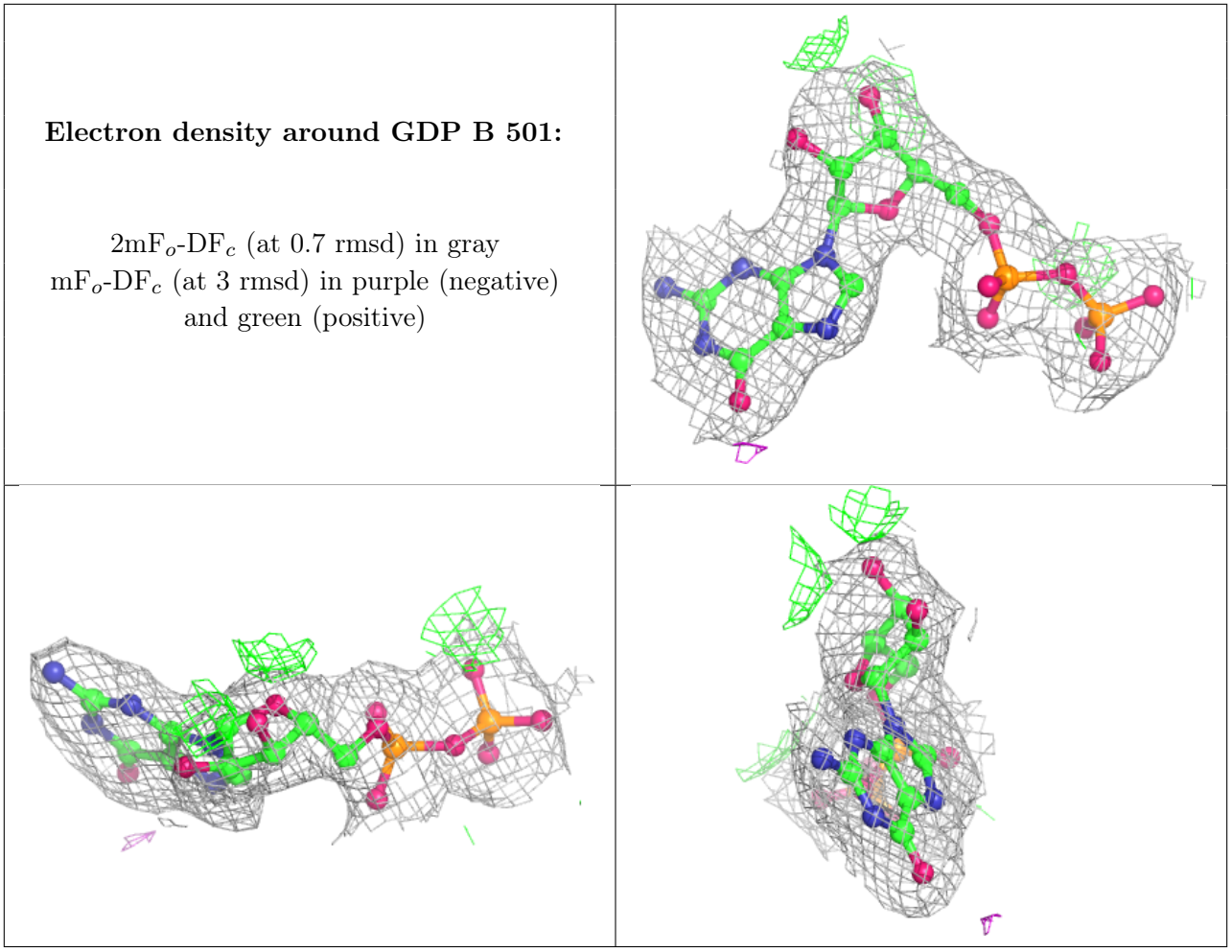
Electron density around QW9 D 502:

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



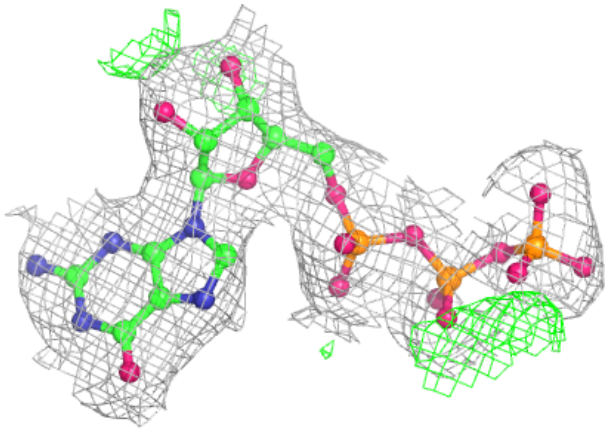
Electron density around GDP B 501:

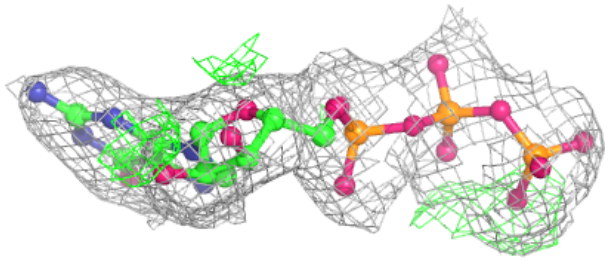
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

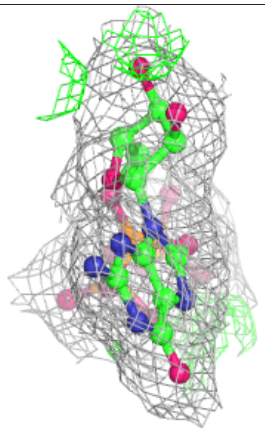


Electron density around GTP A 501:

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

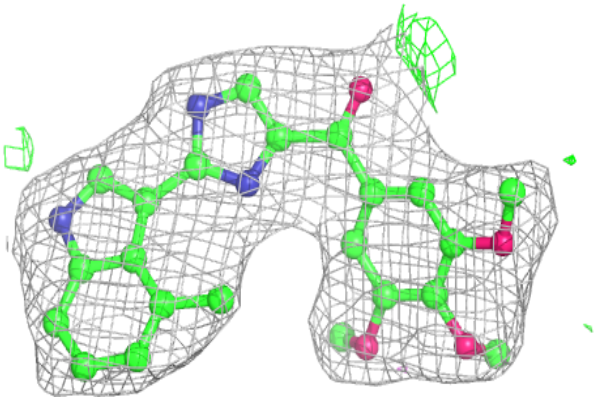


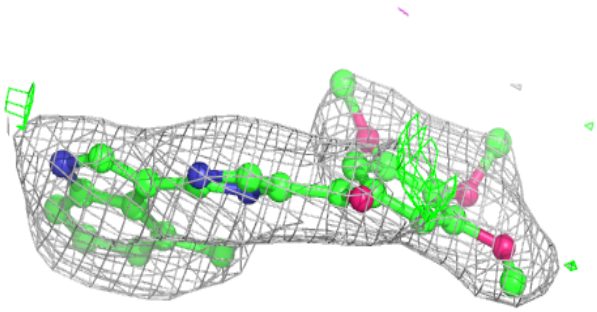


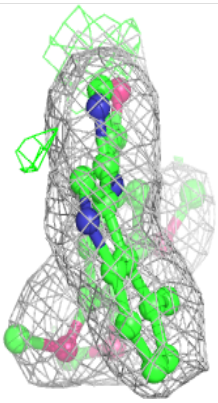


Electron density around QW9 B 505:

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







6.5 Other polymers (i)

There are no such residues in this entry.