



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 06:46 PM UTC

PDB ID : 8CLC / pdb_00008clc
Title : Tubulin (T2R-TTL) complex
Authors : Wranik, M.; Bertrand, Q.; Kepa, M.W.; Weinert, T.; Steinmetz, M.; Standfuss, J.
Deposited on : 2023-02-16
Resolution : 2.70 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

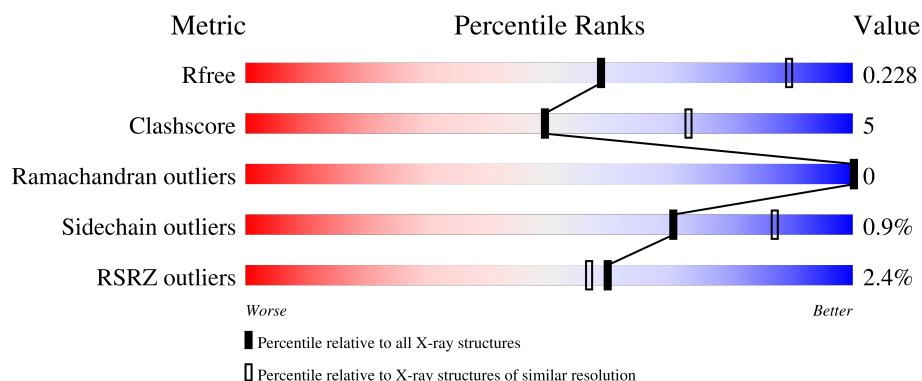
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	440	2% 89% 11%
1	C	440	2% 90% 10%
2	B	430	0% 85% 13% .
2	D	430	3% 84% 15% .
3	E	123	4% 95% 5%

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Mol	Chain	Length	Quality of chain
4	F	332	5% 83% 16%

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 17569 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	439	Total	C	N	O	S	0	1	0
			3436	2173	584	656	23			
1	C	440	Total	C	N	O	S	0	1	0
			3440	2177	584	656	23			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	425	Total	C	N	O	S	2	2	0
			3360	2111	574	649	26			
2	D	427	Total	C	N	O	S	2	1	0
			3358	2107	574	651	26			

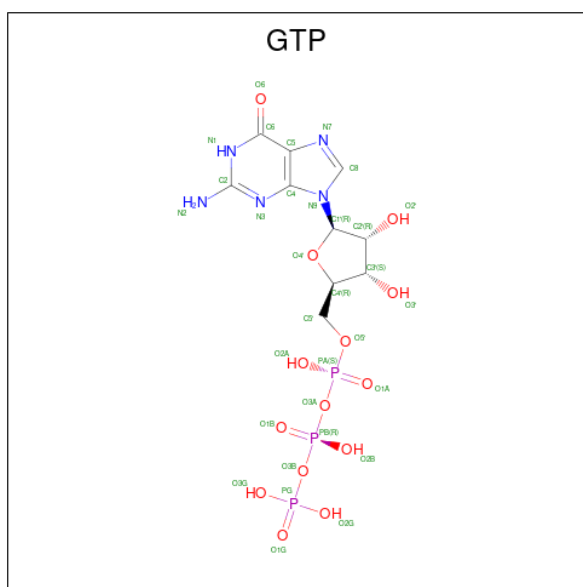
- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	123	Total	C	N	O	S	0	0	0
			1014	625	183	201	5			

- 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	1	0
			2714	1740	464	495	15			

- Molecule 5 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).



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

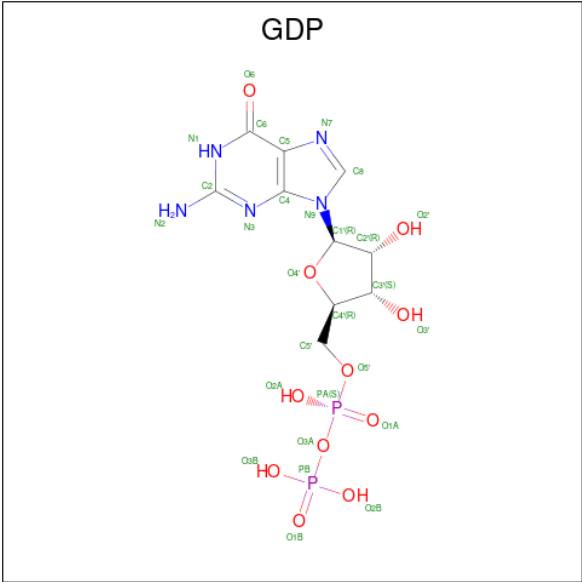
- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 7 is CALCIUM ION (CCD ID: CA) (formula: Ca).

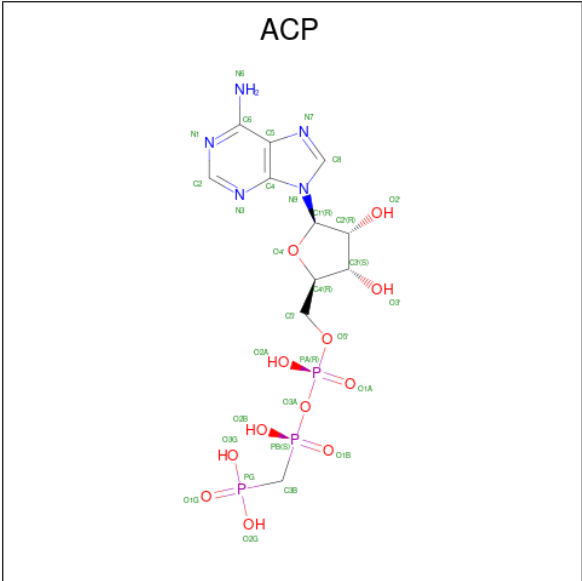
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Ca	0	0
			1	1		
7	C	1	Total	Ca	0	0
			1	1		

- Molecule 8 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



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

- Molecule 9 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (CCD ID: ACP) (formula: C₁₁H₁₈N₅O₁₂P₃).



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

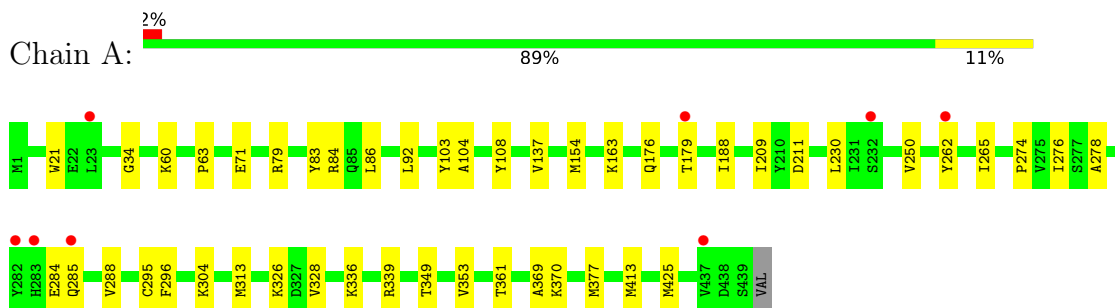
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	15	Total 15	O 15	0	0
10	B	21	Total 21	O 21	0	0
10	C	38	Total 38	O 38	0	0
10	D	3	Total 3	O 3	0	0
10	E	2	Total 2	O 2	0	0
10	F	12	Total 12	O 12	0	0

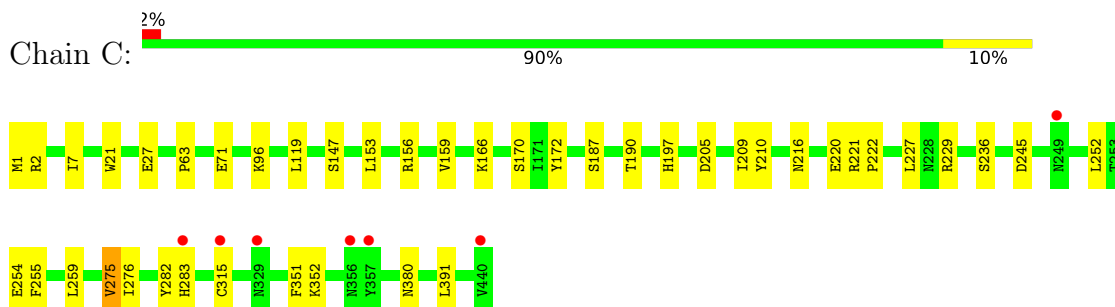
3 Residue-property plots

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.

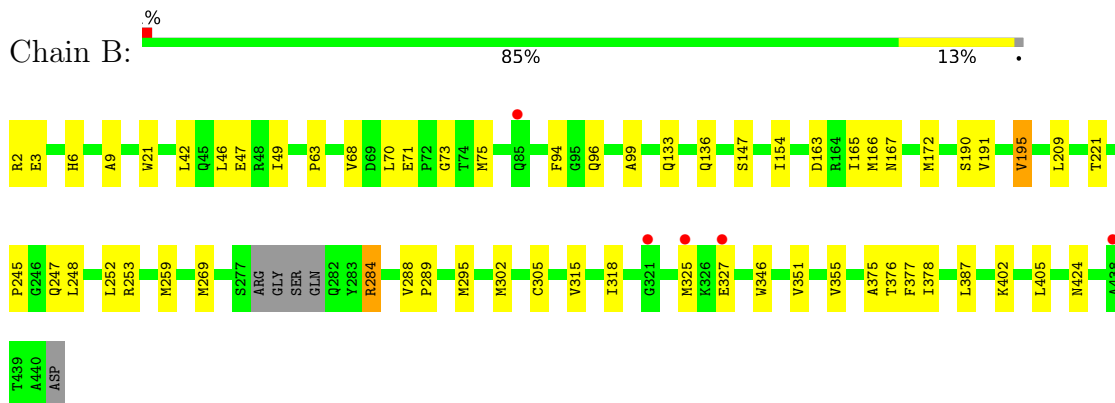
- Molecule 1: Tubulin alpha-1B chain



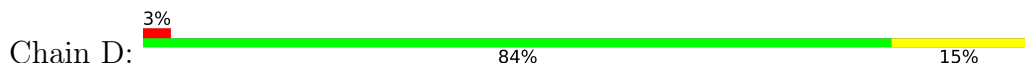
- Molecule 1: Tubulin alpha-1B chain

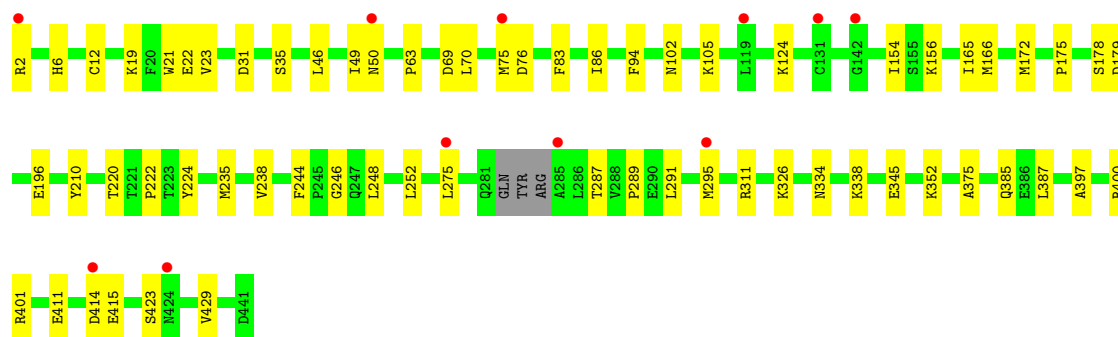


- Molecule 2: Tubulin beta-2B chain

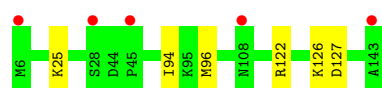


- Molecule 2: Tubulin beta-2B chain

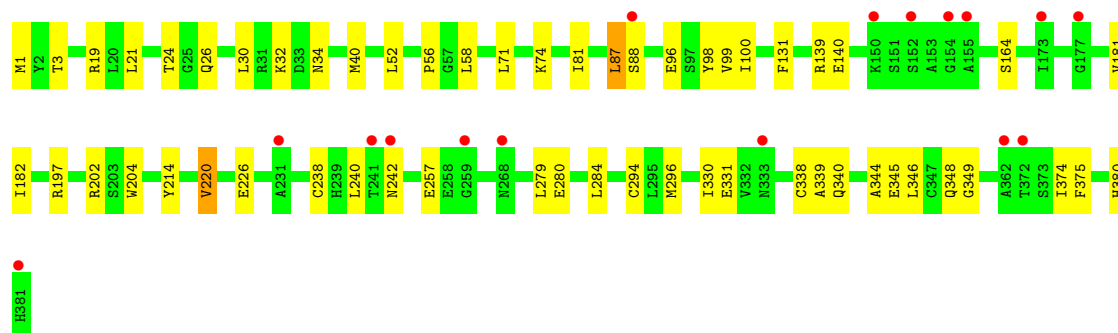
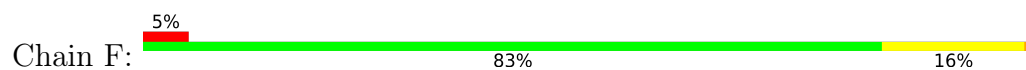




● Molecule 3: Stathmin-4



● Molecule 4: Tubulin-Tyrosine Ligase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	106.53Å 160.48Å 181.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.20 – 2.70 15.20 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.9 (15.20-2.70) 99.3 (15.20-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.27 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.20_4487	Depositor
R, R_{free}	0.186 , 0.234 0.188 , 0.228	Depositor DCC
R_{free} test set	2000 reflections (0.73%)	wwPDB-VP
Wilson B-factor (Å ²)	66.6	Xtriage
Anisotropy	0.008	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.43 , 115.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	17569	wwPDB-VP
Average B, all atoms (Å ²)	78.0	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.*

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: GTP, ACP, MG, CA, 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	0.30	0/3514	0.47	0/4770
1	C	0.18	0/3521	0.34	0/4780
2	B	0.24	0/3437	0.38	0/4655
2	D	0.20	0/3431	0.35	0/4645
3	E	0.06	0/1022	0.17	0/1356
4	F	0.19	0/2777	0.32	0/3750
All	All	0.22	0/17702	0.37	0/23956

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1
2	B	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	284	ARG	Sidechain
1	C	221	ARG	Sidechain

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	3436	0	3343	36	0
1	C	3440	0	3353	26	0
2	B	3360	0	3238	53	0
2	D	3358	0	3232	41	0
3	E	1014	0	1029	6	0
4	F	2714	0	2682	37	0
5	A	32	0	12	0	0
5	C	32	0	12	0	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	0	0
8	D	28	0	12	1	0
9	F	31	0	14	2	0
10	A	15	0	0	0	0
10	B	21	0	0	0	0
10	C	38	0	0	1	0
10	D	3	0	0	0	0
10	E	2	0	0	0	0
10	F	12	0	0	0	0
All	All	17569	0	16939	185	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 (185) 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:D:295:MET:SD	2:D:375:ALA:HB1	1.84	1.15
2:B:295:MET:CE	2:B:375:ALA:HB1	1.80	1.11
2:B:209:LEU:HD21	2:B:302:MET:HE1	1.39	1.02
2:B:295:MET:HE3	2:B:375:ALA:HB1	1.36	1.01
1:A:176:GLN:NE2	4:F:56:PRO:HG3	1.78	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:269:MET:HE1	2:B:305:CYS:HB2	1.47	0.94
2:D:295:MET:SD	2:D:375:ALA:CB	2.60	0.89
2:B:209:LEU:HD21	2:B:302:MET:CE	2.04	0.86
2:B:269:MET:HE1	2:B:305:CYS:CB	2.07	0.84
2:B:209:LEU:CD2	2:B:302:MET:HE1	2.07	0.83
2:B:269:MET:CE	2:B:305:CYS:HB2	2.11	0.80
2:D:291:LEU:O	2:D:295:MET:HG3	1.81	0.80
2:B:295:MET:HE3	2:B:375:ALA:CB	2.19	0.72
2:B:315:VAL:HB	2:B:351:VAL:HG22	1.71	0.72
1:A:179:THR:HG23	2:B:248:LEU:HA	1.74	0.68
2:D:295:MET:CE	2:D:375:ALA:HB1	2.25	0.67
2:B:195:VAL:HG21	2:B:424:ASN:HD21	1.60	0.65
1:A:179:THR:HG21	2:B:247:GLN:O	1.98	0.63
1:A:265:ILE:HG21	1:A:313:MET:HE1	1.81	0.62
2:B:269:MET:CE	2:B:305:CYS:SG	2.87	0.62
1:C:315:CYS:SG	1:C:351:PHE:CD2	2.94	0.60
1:C:209:ILE:HG22	1:C:227:LEU:HD22	1.84	0.59
2:B:165:ILE:HG21	2:B:252:LEU:HB3	1.84	0.58
2:D:400:ARG:HG3	2:D:401:ARG:HG3	1.85	0.58
4:F:30:LEU:HB3	4:F:34:ASN:HD22	1.69	0.57
4:F:197:ARG:NH1	4:F:257:GLU:OE2	2.33	0.57
2:D:414:ASP:OD2	2:D:415:GLU:N	2.37	0.57
1:A:176:GLN:NE2	4:F:56:PRO:CG	2.61	0.57
2:B:295:MET:CG	2:B:377:PHE:HB2	2.35	0.57
2:B:269:MET:HE2	2:B:305:CYS:SG	2.45	0.56
2:B:191:VAL:O	2:B:195:VAL:HG13	2.04	0.56
2:B:295:MET:HG3	2:B:377:PHE:HB2	1.87	0.56
2:D:175:PRO:HA	2:D:178:SER:HB3	1.86	0.56
4:F:214:TYR:HB3	4:F:375:PHE:HB3	1.88	0.56
1:C:282:TYR:O	1:C:283:HIS:ND1	2.39	0.56
1:C:245:ASP:N	1:C:245:ASP:OD1	2.39	0.56
4:F:338:CYS:SG	4:F:339:ALA:N	2.80	0.55
1:C:259:LEU:O	1:C:380:ASN:ND2	2.31	0.55
1:C:220:GLU:HB2	2:D:326:LYS:HE3	1.88	0.55
2:B:147:SER:OG	2:B:190:SER:OG	2.23	0.54
1:C:119:LEU:HD11	1:C:156:ARG:HB3	1.87	0.54
2:B:195:VAL:CG2	2:B:424:ASN:HD21	2.21	0.54
2:B:163:ASP:O	2:B:253[A]:ARG:NH2	2.39	0.54
1:A:336:LYS:HD2	1:A:336:LYS:C	2.33	0.54
1:A:179:THR:CG2	2:B:247:GLN:O	2.56	0.53
2:B:269:MET:CE	2:B:305:CYS:CB	2.78	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:165:ILE:HG21	2:D:252:LEU:HB3	1.90	0.53
4:F:202:ARG:HB3	4:F:220:VAL:HG12	1.91	0.53
4:F:344:ALA:O	4:F:346:LEU:N	2.38	0.53
4:F:280:GLU:HA	4:F:284:LEU:HB2	1.90	0.53
2:D:63:PRO:HD3	2:D:86:ILE:HG12	1.92	0.52
1:C:96:LYS:O	2:D:2[C]:ARG:NH2	2.43	0.52
1:C:210:TYR:CZ	1:C:222:PRO:HD2	2.44	0.52
1:A:104:ALA:HB2	1:A:413:MET:HE3	1.90	0.52
2:D:46:LEU:HA	2:D:49:ILE:HB	1.92	0.52
2:B:46:LEU:HA	2:B:49:ILE:HB	1.91	0.52
2:B:75:MET:HE2	2:B:94:PHE:HB3	1.92	0.52
2:B:47:GLU:HG2	2:B:245:PRO:HG3	1.91	0.51
2:B:70:LEU:HD12	2:B:99:ALA:HB2	1.92	0.51
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.29	0.51
2:D:196:GLU:OE1	3:E:122:ARG:NH1	2.44	0.51
1:A:83:TYR:HD2	1:A:86:LEU:HD22	1.74	0.51
1:A:108:TYR:HE2	1:A:413:MET:HE2	1.75	0.50
1:A:211:ASP:OD2	1:A:304:LYS:NZ	2.35	0.50
2:B:295:MET:HE1	2:B:375:ALA:HB1	1.81	0.50
1:C:187:SER:HB3	1:C:391:LEU:HD21	1.92	0.50
2:B:259:MET:HE2	2:B:378:ILE:HG22	1.93	0.50
9:F:401:ACP:H8	9:F:401:ACP:O5'	2.12	0.49
1:A:176:GLN:HE21	4:F:56:PRO:CB	2.25	0.49
2:B:2:ARG:C	2:B:133:GLN:HE21	2.19	0.48
1:C:229:ARG:NH1	10:C:603:HOH:O	2.38	0.48
2:D:75:MET:HE2	2:D:94:PHE:HD2	1.77	0.48
2:D:124:LYS:HB3	2:D:124:LYS:HE2	1.63	0.48
2:D:76:ASP:O	2:D:76:ASP:OD1	2.32	0.48
1:A:328:VAL:HG11	1:A:353:VAL:HG11	1.96	0.48
1:A:188:ILE:HG23	1:A:425:MET:HG3	1.94	0.48
2:D:172:MET:HG3	2:D:387:LEU:HD11	1.96	0.47
4:F:139:ARG:HH11	4:F:140:GLU:HG3	1.79	0.47
2:B:221:THR:HG23	2:B:221:THR:O	2.13	0.47
1:A:209:ILE:HG23	1:A:230:LEU:HD23	1.95	0.47
2:B:136:GLN:HA	2:B:167:ASN:O	2.14	0.47
2:D:102:ASN:HB3	2:D:105:LYS:HB2	1.96	0.47
2:D:220:THR:O	2:D:222:PRO:HD3	2.14	0.47
1:C:254:GLU:HG2	1:C:352:LYS:HE2	1.97	0.47
2:D:12:CYS:HB2	8:D:501:GDP:C8	2.49	0.47
2:B:289:PRO:HD3	2:B:327:GLU:OE2	2.14	0.47
2:D:235:MET:HA	2:D:238:VAL:HG22	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:385:GLN:HB2	2:D:429:VAL:HG13	1.97	0.47
2:B:2:ARG:O	2:B:133:GLN:NE2	2.44	0.46
4:F:240:LEU:HD22	9:F:401:ACP:O4'	2.15	0.46
1:A:295:CYS:HB3	1:A:377:MET:SD	2.55	0.46
1:C:2:ARG:HH11	1:C:2:ARG:HG3	1.80	0.46
2:D:6:HIS:CD2	2:D:21:TRP:HE1	2.34	0.46
2:D:154:ILE:HG23	2:D:166:MET:HG2	1.98	0.46
2:D:210:TYR:CE1	2:D:222:PRO:HG2	2.51	0.46
1:A:179:THR:HG22	1:A:179:THR:O	2.16	0.46
1:A:349:THR:HB	3:E:25:LYS:HB3	1.97	0.45
2:B:269:MET:HE1	2:B:305:CYS:SG	2.54	0.45
1:C:315:CYS:SG	1:C:351:PHE:CE2	3.00	0.45
1:C:172:TYR:HB3	1:C:205:ASP:HA	1.98	0.45
4:F:21:LEU:O	4:F:24:THR:OG1	2.34	0.45
2:D:397:ALA:HA	2:D:400:ARG:HH11	1.81	0.45
4:F:19:ARG:HH11	4:F:19:ARG:HG2	1.82	0.45
1:A:176:GLN:HE21	4:F:56:PRO:HB3	1.82	0.45
1:C:147:SER:HB2	1:C:190:THR:HB	1.98	0.45
4:F:81:ILE:HA	4:F:87:LEU:HD23	1.99	0.45
1:C:252:LEU:HA	1:C:255:PHE:HD2	1.82	0.45
1:C:21:TRP:CZ3	1:C:63:PRO:HB3	2.52	0.44
1:C:27:GLU:OE2	1:C:236:SER:OG	2.27	0.44
1:A:188:ILE:HD12	1:A:425:MET:HG3	2.00	0.44
4:F:279:LEU:HG	4:F:284:LEU:HD23	1.99	0.44
4:F:345:GLU:O	4:F:349:GLY:N	2.41	0.44
1:A:103:TYR:HD1	1:A:413:MET:HE1	1.82	0.44
1:A:284:GLU:O	1:A:285:GLN:NE2	2.51	0.44
2:B:209:LEU:CD2	2:B:302:MET:CE	2.83	0.44
2:B:21:TRP:CZ3	2:B:63:PRO:HB3	2.53	0.44
1:A:274:PRO:HB2	1:A:276:ILE:HD13	2.00	0.43
2:D:19:LYS:O	2:D:23:VAL:HG23	2.17	0.43
4:F:226:GLU:HB2	4:F:238:CYS:HB3	1.99	0.43
1:A:84:ARG:HH11	1:A:84:ARG:HG2	1.84	0.43
2:B:288:VAL:HB	2:B:327:GLU:CD	2.44	0.43
1:A:21:TRP:CZ3	1:A:63:PRO:HB3	2.54	0.43
2:B:154:ILE:HG23	2:B:166:MET:HG2	2.00	0.43
1:A:276:ILE:HG22	1:A:369:ALA:HB3	2.00	0.43
2:B:318:ILE:HG23	2:B:376:THR:HB	2.00	0.43
1:A:326:LYS:HB3	1:A:326:LYS:HE2	1.75	0.43
2:D:31:ASP:OD1	2:D:35:SER:N	2.52	0.43
3:E:96:MET:HA	3:E:96:MET:HE2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:340:GLN:H	4:F:340:GLN:CD	2.27	0.43
4:F:348:GLN:O	4:F:348:GLN:NE2	2.52	0.43
2:B:96:GLN:HB3	1:C:1:MET:SD	2.59	0.43
3:E:126:LYS:HE3	3:E:126:LYS:HB3	1.80	0.43
4:F:349:GLY:HA3	4:F:374:ILE:HD11	2.01	0.43
2:D:244:PHE:O	2:D:246:GLY:N	2.48	0.42
1:A:137:VAL:HG21	1:A:154:MET:SD	2.58	0.42
4:F:96:GLU:OE2	4:F:98:TYR:OH	2.33	0.42
1:A:34:GLY:HA3	1:A:60:LYS:HG3	2.01	0.42
1:A:278:ALA:HA	1:A:369:ALA:HB2	2.01	0.42
2:B:288:VAL:HG11	2:B:327:GLU:HG2	2.02	0.42
2:D:2[A]:ARG:HD2	2:D:50:ASN:HD21	1.84	0.42
4:F:1:MET:HE2	4:F:26:GLN:HA	2.00	0.42
2:B:325:MET:SD	2:B:355:VAL:HG21	2.59	0.42
4:F:71:LEU:HD11	4:F:294:CYS:HB3	2.02	0.42
4:F:87:LEU:HD12	4:F:87:LEU:HA	1.80	0.42
1:A:361:THR:HA	1:A:370:LYS:NZ	2.33	0.42
1:C:315:CYS:HG	1:C:351:PHE:HD2	1.54	0.42
4:F:3:THR:HB	4:F:30:LEU:HD11	2.01	0.42
4:F:74:LYS:HB3	4:F:181:VAL:HG21	2.00	0.42
2:D:105:LYS:NZ	2:D:411:GLU:OE2	2.42	0.42
1:C:315:CYS:HG	1:C:351:PHE:HE2	1.53	0.42
2:D:19:LYS:HD3	2:D:19:LYS:HA	1.73	0.42
2:D:22:GLU:HG2	2:D:83:PHE:CD2	2.54	0.42
2:D:156:LYS:NZ	3:E:127:ASP:OD2	2.51	0.42
4:F:40:MET:SD	4:F:52:LEU:HD21	2.60	0.42
4:F:204:TRP:CZ2	4:F:338:CYS:HA	2.54	0.42
2:B:402:LYS:HG3	2:B:405:LEU:HD22	2.01	0.42
1:C:159:VAL:HA	3:E:94:ILE:HG23	2.00	0.42
1:A:163:LYS:HA	1:A:163:LYS:HD3	1.86	0.41
2:B:2:ARG:NH1	2:B:3:GLU:OE2	2.51	0.41
2:D:69:ASP:OD1	2:D:70:LEU:N	2.51	0.41
1:A:79:ARG:HG3	1:A:92:LEU:HD12	2.02	0.41
2:B:42:LEU:HD22	2:B:245:PRO:HG2	2.02	0.41
2:B:71:GLU:HG3	2:B:73:GLY:H	1.85	0.41
2:B:295:MET:CE	2:B:375:ALA:CB	2.73	0.41
4:F:330:ILE:HG22	4:F:331:GLU:HG2	2.01	0.41
4:F:58:LEU:HD12	4:F:58:LEU:HA	1.81	0.41
1:C:7:ILE:HG21	1:C:153:LEU:HD21	2.03	0.41
2:D:248:LEU:HD21	2:D:352:LYS:HB3	2.02	0.41
4:F:296[A]:MET:SD	4:F:380:HIS:ND1	2.92	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:172:MET:HG3	2:B:387:LEU:HD11	2.01	0.41
2:B:325:MET:SD	2:B:355:VAL:HG11	2.59	0.41
1:A:296:PHE:HB2	1:A:339:ARG:HE	1.85	0.41
1:A:176:GLN:HE21	4:F:56:PRO:CG	2.34	0.41
2:D:311:ARG:NH2	2:D:345:GLU:OE2	2.53	0.41
2:D:275:LEU:HD23	2:D:275:LEU:HA	1.92	0.41
2:D:287:THR:HB	2:D:289:PRO:HD2	2.03	0.41
4:F:131:PHE:CE2	4:F:182:ILE:HG21	2.55	0.41
1:C:166:LYS:HE2	1:C:197:HIS:O	2.21	0.40
2:D:179:ASP:OD1	2:D:224:TYR:OH	2.37	0.40
2:D:334:ASN:O	2:D:338:LYS:HD3	2.20	0.40
2:B:9:ALA:HA	2:B:68:VAL:O	2.21	0.40
1:A:361:THR:HA	1:A:370:LYS:HZ1	1.87	0.40
1:C:216:ASN:HB3	1:C:275:VAL:O	2.20	0.40
4:F:32:LYS:HB2	4:F:32:LYS:HE3	1.97	0.40
4:F:99:VAL:O	4:F:100:ILE:HD13	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	438/440 (100%)	423 (97%)	15 (3%)	0	100	100
1	C	439/440 (100%)	425 (97%)	14 (3%)	0	100	100
2	B	423/430 (98%)	409 (97%)	14 (3%)	0	100	100
2	D	423/430 (98%)	406 (96%)	17 (4%)	0	100	100
3	E	119/123 (97%)	117 (98%)	2 (2%)	0	100	100
4	F	321/332 (97%)	302 (94%)	19 (6%)	0	100	100
All	All	2163/2195 (98%)	2082 (96%)	81 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	371/371 (100%)	367 (99%)	4 (1%)	65	85
1	C	372/371 (100%)	368 (99%)	4 (1%)	65	85
2	B	369/371 (100%)	366 (99%)	3 (1%)	73	88
2	D	367/371 (99%)	366 (100%)	1 (0%)	86	94
3	E	110/110 (100%)	110 (100%)	0	100	100
4	F	298/297 (100%)	293 (98%)	5 (2%)	53	79
All	All	1887/1891 (100%)	1870 (99%)	17 (1%)	70	87

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	GLU
1	A	250	VAL
1	A	262	TYR
1	A	288	VAL
2	B	195	VAL
2	B	284	ARG
2	B	346	TRP
1	C	71	GLU
1	C	170	SER
1	C	275	VAL
1	C	276	ILE
2	D	423	SER
4	F	87	LEU
4	F	88	SER
4	F	164	SER
4	F	220	VAL
4	F	242	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	GLN
1	A	101	ASN
1	A	192	HIS
1	A	256	GLN
1	A	285	GLN
1	A	300	ASN
1	A	309	HIS
1	A	393	HIS
2	B	37	HIS
2	B	331	GLN
2	B	385	GLN
2	B	406	HIS
2	B	424	ASN
2	B	436	GLN
1	C	133	GLN
1	C	256	GLN
1	C	300	ASN
1	C	301	GLN
2	D	50	ASN
2	D	101	ASN
2	D	167	ASN
2	D	331	GLN
2	D	349	ASN
3	E	51	GLN
3	E	91	ASN
4	F	333	ASN
4	F	348	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 10 ligands modelled in this entry, 5 are monoatomic - leaving 5 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	-	29,30,30	0.52	0	45,47,47	0.46	0
5	GTP	A	501	6	33,34,34	0.60	0	50,54,54	0.48	0
9	ACP	F	401	-	31,33,33	0.73	1 (3%)	47,52,52	0.59	1 (2%)
5	GTP	C	501	6	33,34,34	0.61	0	50,54,54	0.48	0
8	GDP	B	501	6	29,30,30	0.55	0	45,47,47	0.42	0

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	-	-	2/16/32/32	0/3/3/3
5	GTP	A	501	6	-	5/22/38/38	0/3/3/3
9	ACP	F	401	-	-	3/19/38/38	0/3/3/3
5	GTP	C	501	6	-	6/22/38/38	0/3/3/3
8	GDP	B	501	6	-	3/16/32/32	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	F	401	ACP	PB-O2B	-2.37	1.50	1.56

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	F	401	ACP	O1G-PG-C3B	-2.15	106.69	111.37

There are no chirality outliers.

All (19) torsion outliers are listed below:

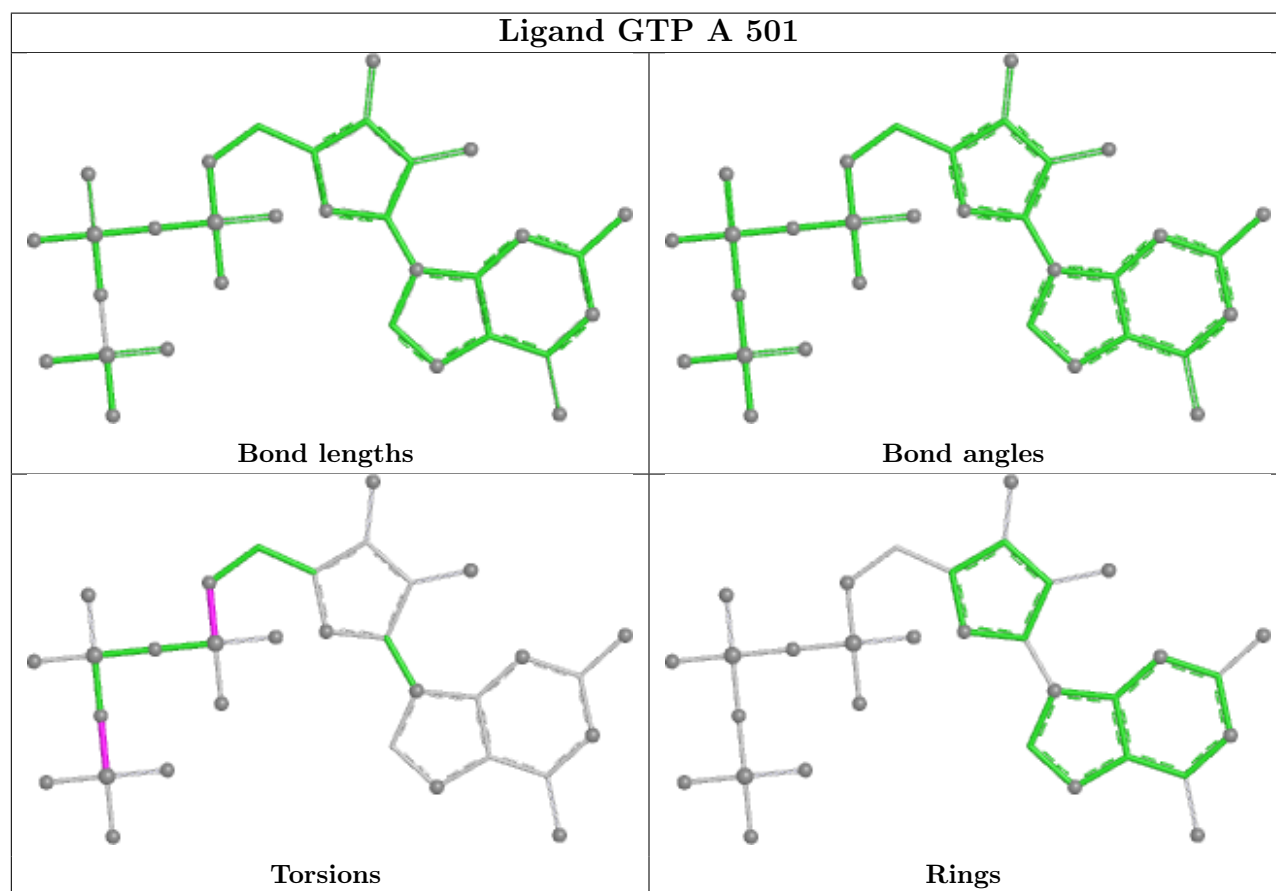
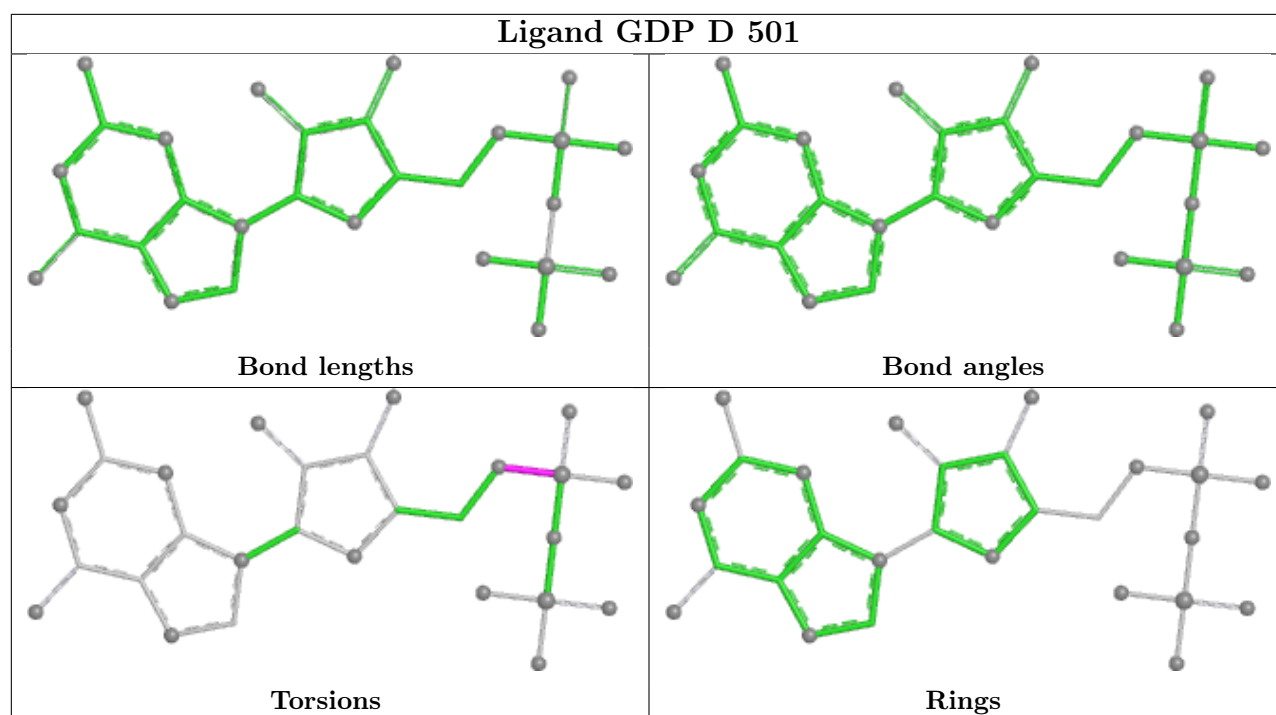
Mol	Chain	Res	Type	Atoms
5	A	501	GTP	C5'-O5'-PA-O3A
5	A	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	PB-O3B-PG-O3G
5	C	501	GTP	C5'-O5'-PA-O3A
5	C	501	GTP	C5'-O5'-PA-O1A
8	B	501	GDP	C5'-O5'-PA-O3A
8	B	501	GDP	C5'-O5'-PA-O1A
8	B	501	GDP	C5'-O5'-PA-O2A
8	D	501	GDP	C5'-O5'-PA-O3A
8	D	501	GDP	C5'-O5'-PA-O2A
9	F	401	ACP	PB-C3B-PG-O1G
5	A	501	GTP	PB-O3B-PG-O2G
5	A	501	GTP	PB-O3B-PG-O3G
5	A	501	GTP	C5'-O5'-PA-O2A
5	C	501	GTP	C5'-O5'-PA-O2A
9	F	401	ACP	PB-C3B-PG-O2G
9	F	401	ACP	C5'-O5'-PA-O1A
5	C	501	GTP	PB-O3A-PA-O1A
5	C	501	GTP	PB-O3A-PA-O2A

There are no ring outliers.

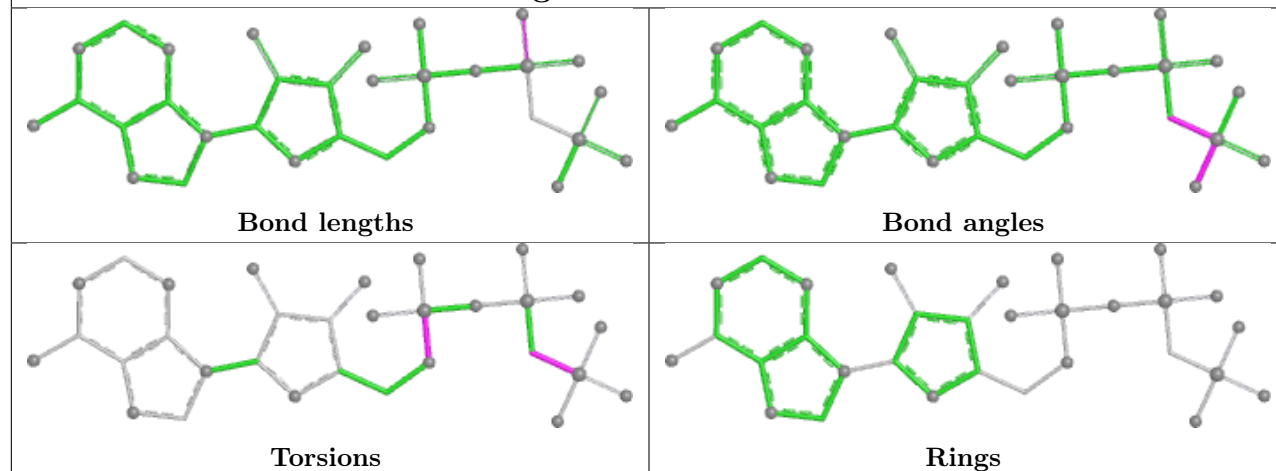
2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	D	501	GDP	1	0
9	F	401	ACP	2	0

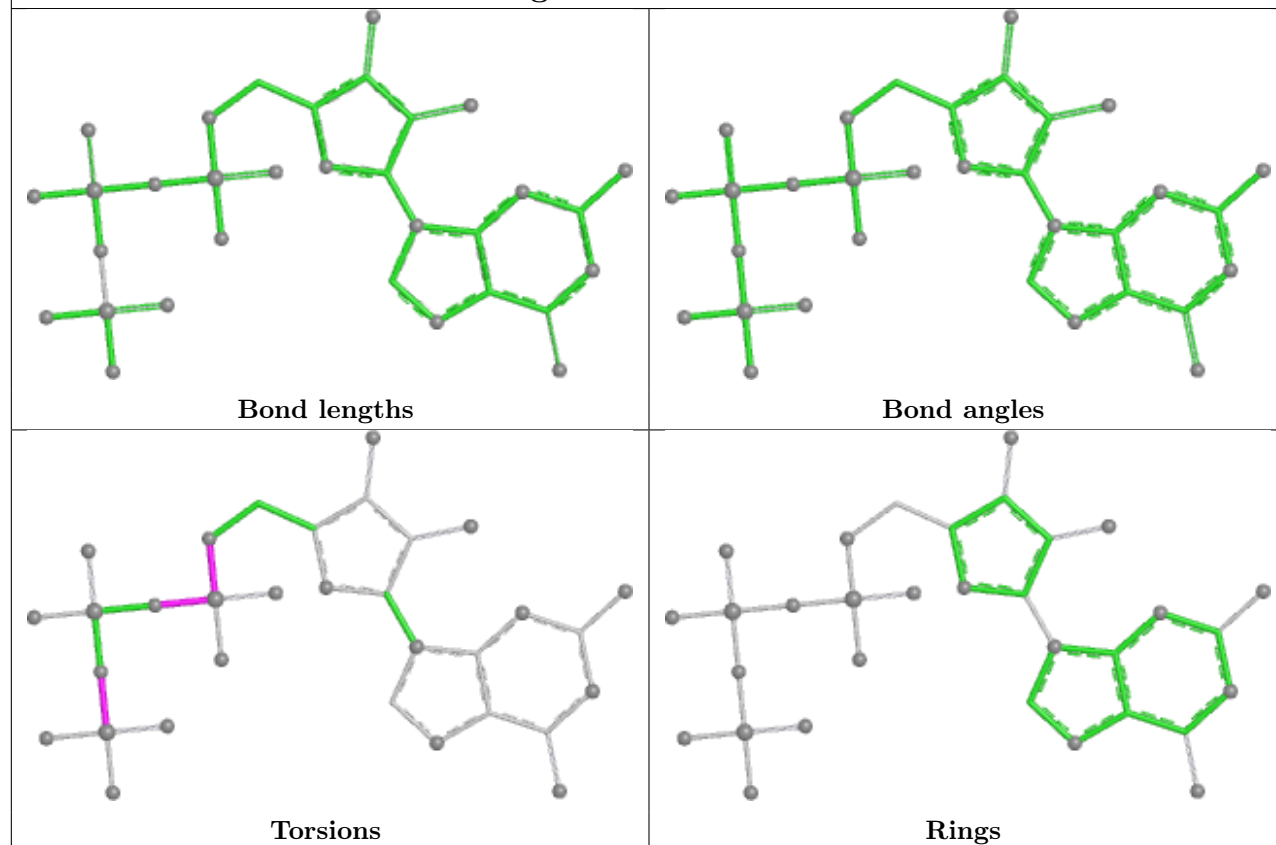
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

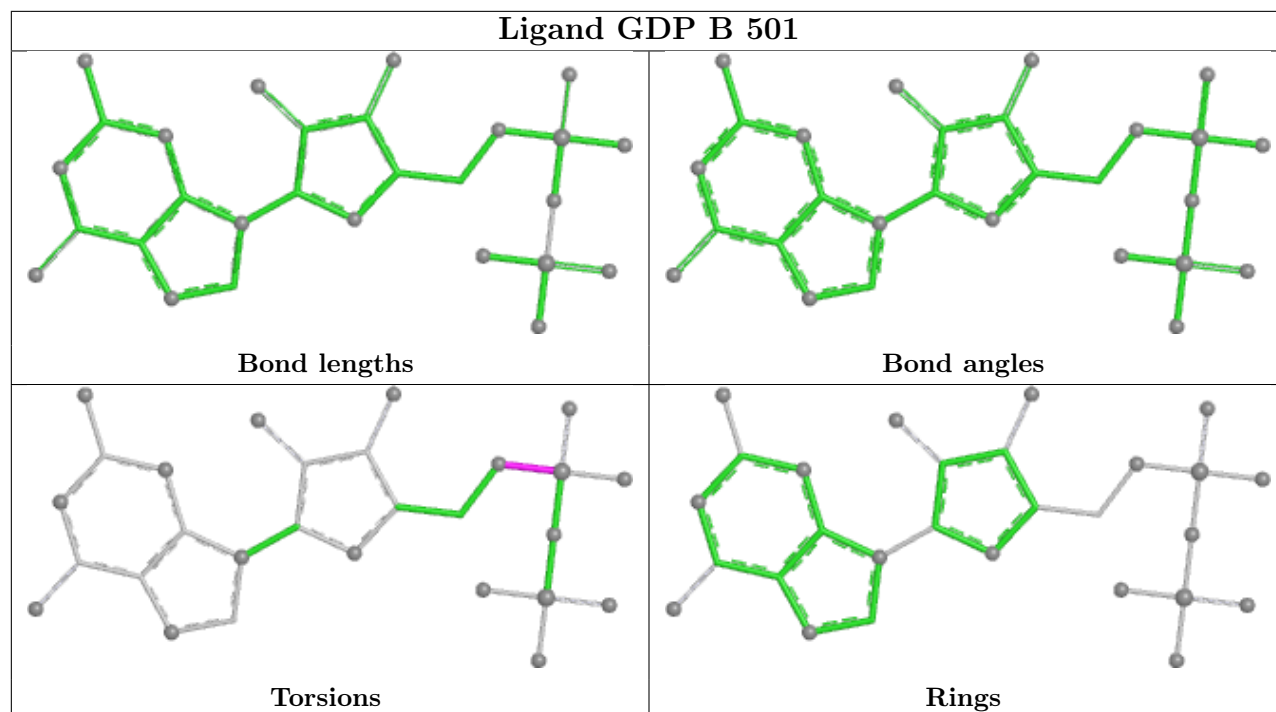


Ligand ACP F 401



Ligand GTP C 501





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
4	F	5
3	E	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	28:SER	C	44:ASP	N	32.44
1	F	362:ALA	C	372:THR	N	16.72
1	F	155:ALA	C	162:ILE	N	13.81
1	F	102:PRO	C	125:THR	N	12.29
1	F	246:GLN	C	256:TYR	N	11.47
1	F	231:ALA	C	235:ASP	N	6.17

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	439/440 (99%)	-0.03	8 (1%) 67 65	32, 68, 116, 239	1 (0%)
1	C	440/440 (100%)	-0.21	7 (1%) 70 68	34, 55, 96, 133	1 (0%)
2	B	425/430 (98%)	-0.09	5 (1%) 76 75	27, 63, 111, 163	6 (1%)
2	D	427/430 (99%)	0.10	11 (2%) 57 54	33, 80, 131, 181	4 (0%)
3	E	123/123 (100%)	0.18	5 (4%) 41 37	53, 80, 144, 173	0
4	F	332/332 (100%)	0.34	16 (4%) 35 32	40, 95, 172, 218	1 (0%)
All	All	2186/2195 (99%)	0.01	52 (2%) 59 56	27, 72, 135, 239	13 (0%)

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	295	MET	4.8
4	F	362	ALA	4.2
4	F	372	THR	4.0
2	B	321	GLY	3.7
4	F	259	GLY	3.6
1	A	283	HIS	3.5
4	F	381	HIS	3.4
4	F	152	SER	3.1
1	C	356	ASN	3.1
2	D	2[A]	ARG	3.1
1	A	282	TYR	3.1
4	F	150	LYS	3.1
2	B	325	MET	3.0
3	E	143	ALA	2.8
4	F	155	ALA	2.8
3	E	45	PRO	2.8
4	F	173	ILE	2.7
3	E	108	ASN	2.7
4	F	231	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	23	LEU	2.6
2	B	438	ALA	2.6
1	C	329	ASN	2.6
2	B	85	GLN	2.6
2	D	424	ASN	2.5
2	D	275	LEU	2.5
4	F	268	ASN	2.4
3	E	28	SER	2.4
2	D	119	LEU	2.4
1	C	249	ASN	2.4
4	F	241	THR	2.3
4	F	333	ASN	2.3
2	D	414	ASP	2.3
1	C	283	HIS	2.3
4	F	88	SER	2.3
1	C	357	TYR	2.2
4	F	177	GLY	2.2
2	D	50	ASN	2.2
4	F	154	GLY	2.2
2	D	131	CYS	2.2
1	A	232	SER	2.2
2	D	75	MET	2.2
3	E	6	MET	2.2
1	C	440	VAL	2.1
1	A	285	GLN	2.1
1	C	315	CYS	2.1
4	F	242	ASN	2.1
1	A	262	TYR	2.1
2	B	327	GLU	2.1
2	D	142	GLY	2.1
2	D	285	ALA	2.1
1	A	179	THR	2.0
1	A	437	VAL	2.0

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

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

6.3 Carbohydrates ⓘ

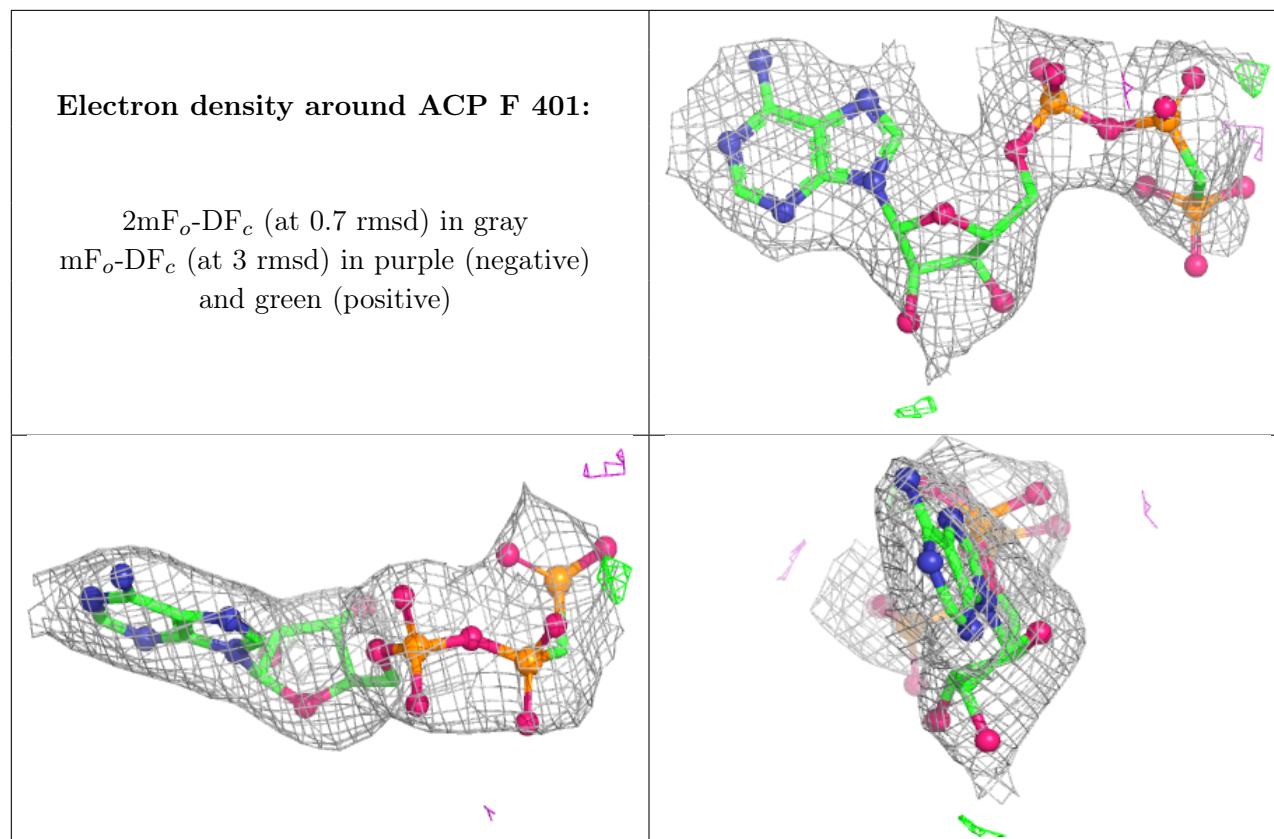
There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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.

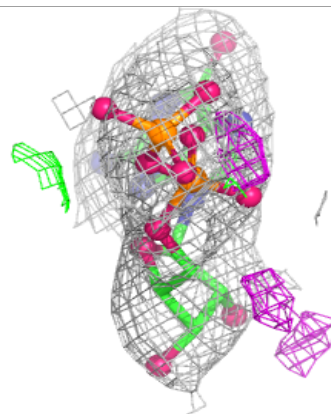
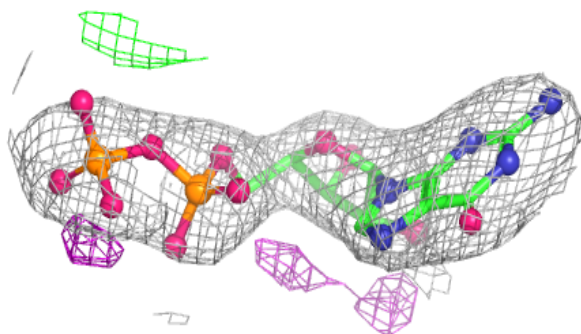
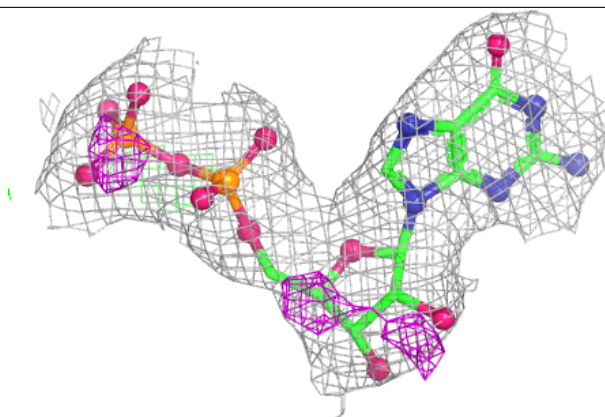
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
9	ACP	F	401	31/31	0.84	0.09	92,115,145,162	0
8	GDP	D	501	28/28	0.93	0.10	66,76,101,113	0
6	MG	B	502	1/1	0.93	0.18	57,57,57,57	0
7	CA	A	503	1/1	0.95	0.05	89,89,89,89	0
5	GTP	A	501	32/32	0.96	0.07	37,50,68,79	0
7	CA	C	503	1/1	0.96	0.05	72,72,72,72	0
8	GDP	B	501	28/28	0.97	0.07	34,50,64,71	0
6	MG	C	502	1/1	0.98	0.03	45,45,45,45	0
6	MG	A	502	1/1	0.98	0.03	44,44,44,44	0
5	GTP	C	501	32/32	0.98	0.06	36,46,62,72	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.

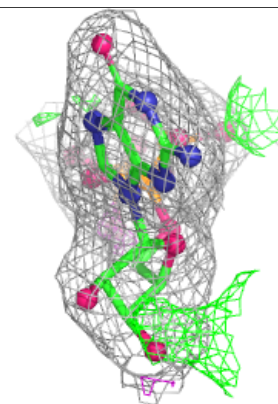
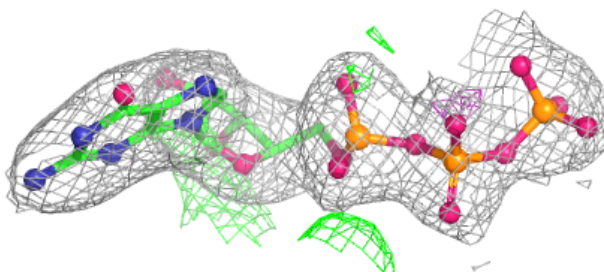
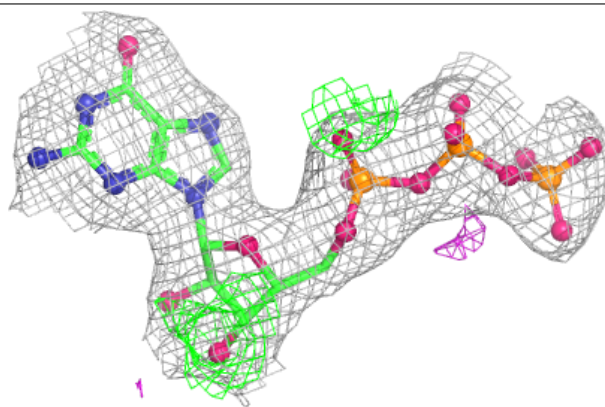


Electron density around GDP D 501:

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

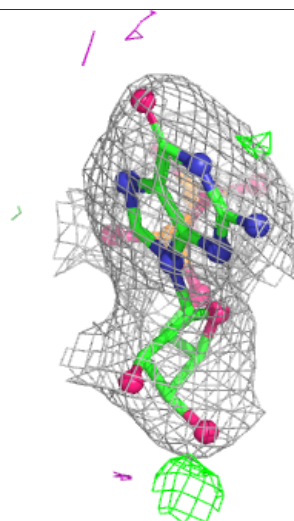
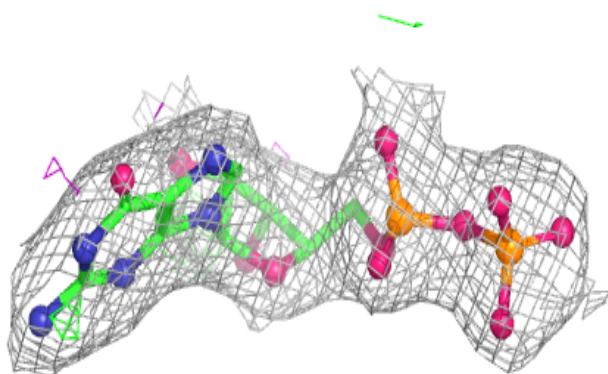
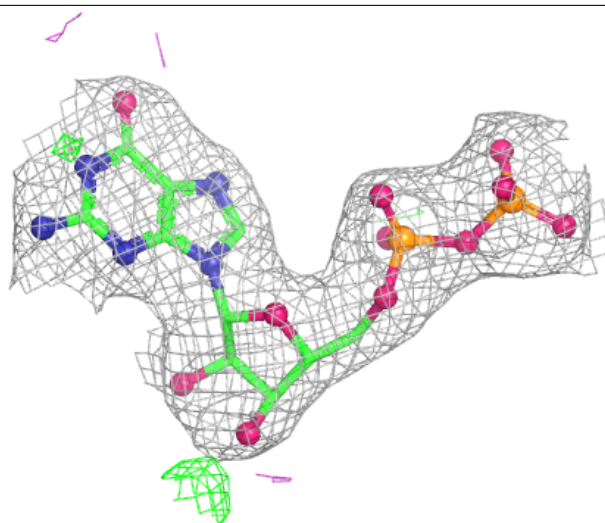
**Electron density around GTP A 501:**

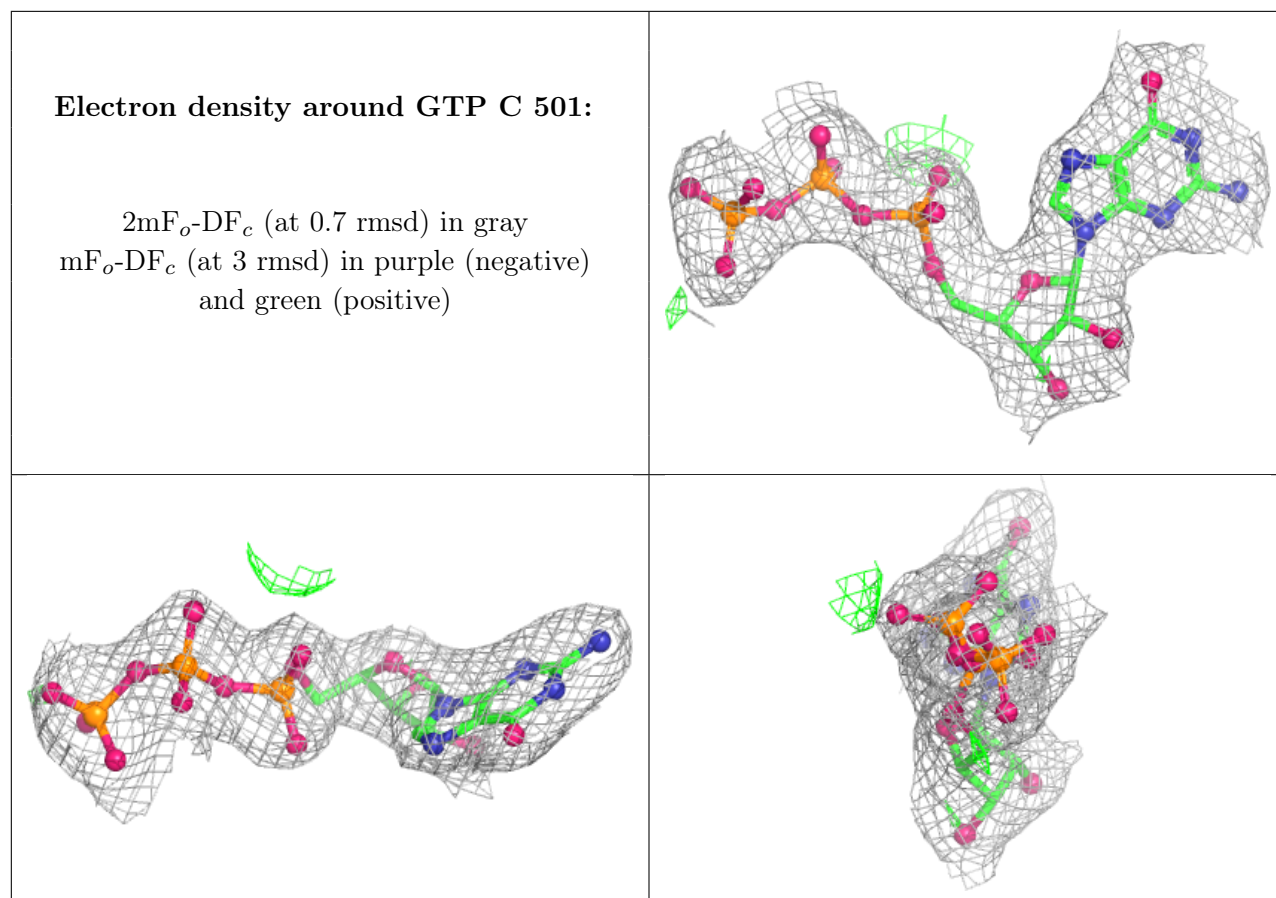
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around GDP B 501:

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





6.5 Other polymers ⓘ

There are no such residues in this entry.