



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:32 PM UTC

PDB ID : 6N47 / pdb_00006n47
Title : The structure of SB-2-204-tubulin complex
Authors : Arnst, K.; Banerjee, S.; Wang, Y.; Li, W.; Miller, D.; Li, W.
Deposited on : 2018-11-17
Resolution : 2.60 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:

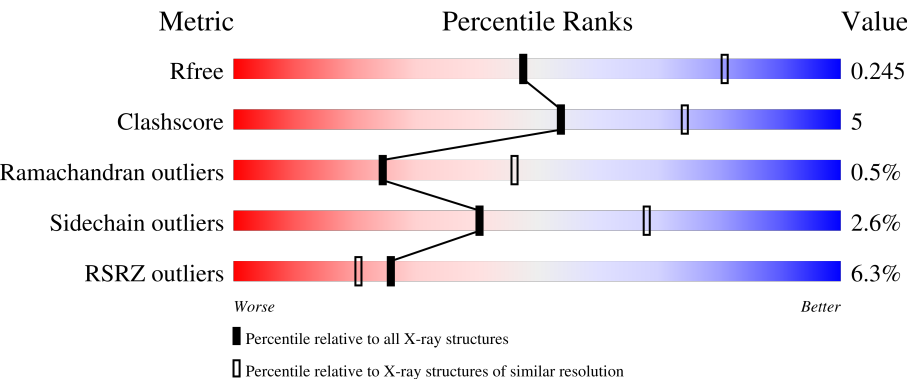
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal 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 i

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

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	450	2% 86% 11%
1	C	450	2% 84% 14%
2	B	445	3% 84% 12%
2	D	445	6% 79% 16% 5%
3	E	143	5% 73% 13% 13%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	F	384	20% 80% 10% 9%

2 Entry composition [i](#)

There are 13 unique types of molecules in this entry. The entry contains 17917 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	441	Total	C	N	O	S	0	1	0
			3446	2180	585	659	22			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	428	Total	C	N	O	S	0	1	0
			3372	2117	577	651	27			
2	D	421	Total	C	N	O	S	0	1	0
			3309	2080	562	640	27			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	124	Total	C	N	O	S	0	1	0
			1036	641	187	202	6			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	3	MET	-	expression tag	UNP P63043
E	4	ALA	-	expression tag	UNP P63043

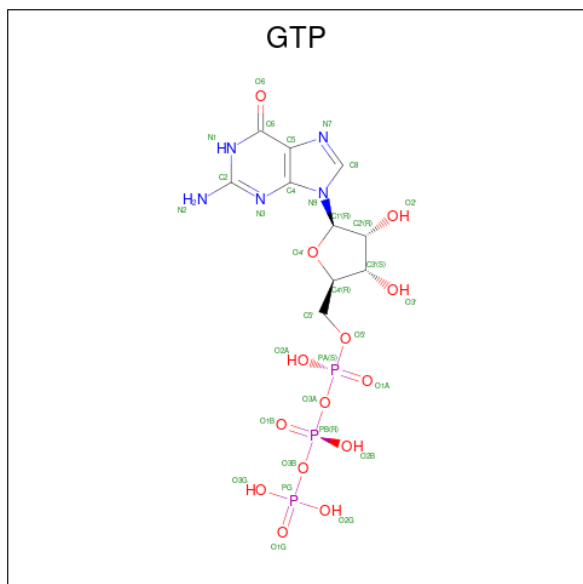
- Molecule 4 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	350	Total	C	N	O	S	0	0	0
			2873	1839	496	524	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 (CCD ID: 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		
5	C	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
5	D	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

- Molecule 6 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	E	1	Total	Ca	0	0
			1	1		

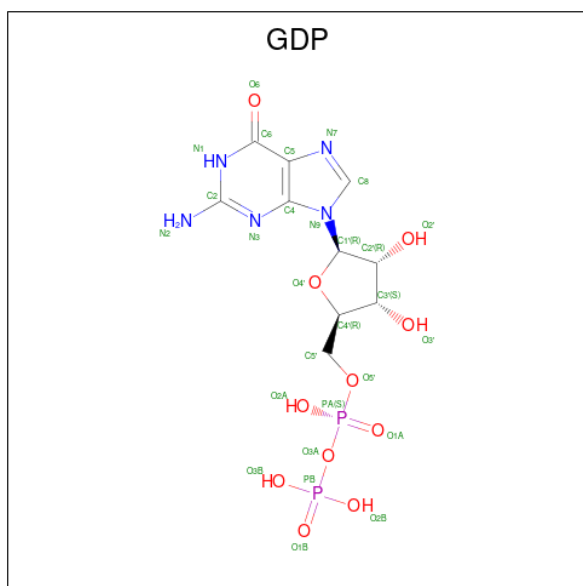
- Molecule 7 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Cl	0	0
			1	1		

- Molecule 8 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

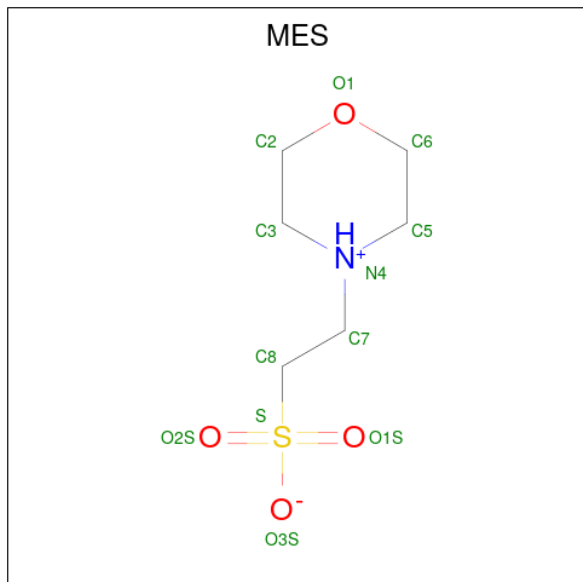
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total	Mg	0	0
			1	1		
8	B	1	Total	Mg	0	0
			1	1		
8	C	1	Total	Mg	0	0
			1	1		
8	D	1	Total	Mg	0	0
			1	1		

- Molecule 9 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



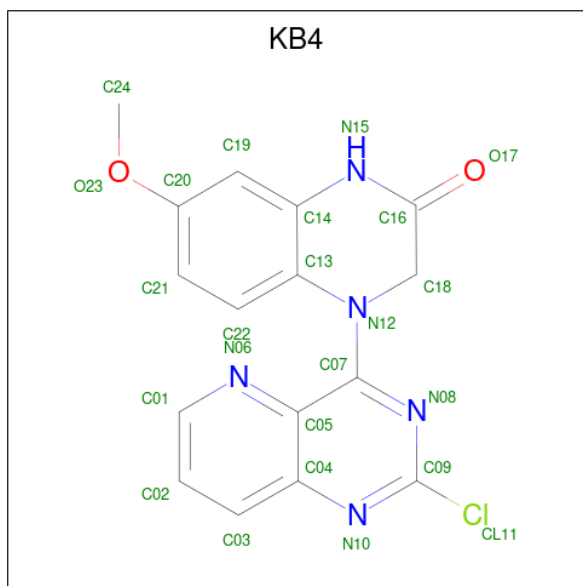
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	B	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- Molecule 10 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: $C_6H_{13}NO_4S$).



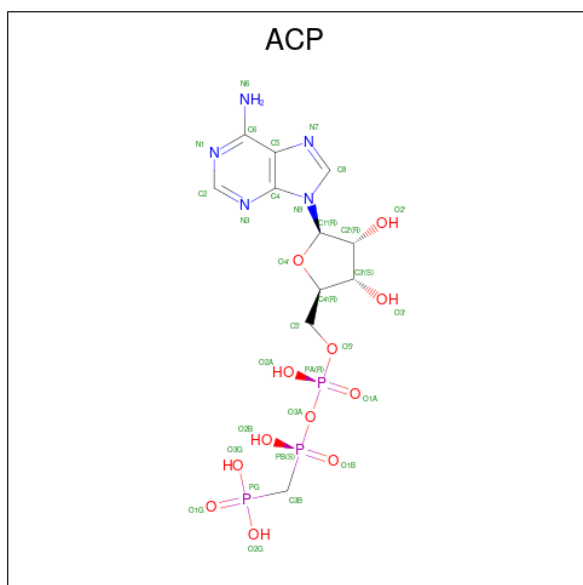
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
10	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 11 is 4-(2-chloropyrido[3,2-d]pyrimidin-4-yl)-7-methoxy-3,4-dihydroquinoxalin-2(1H)-one (CCD ID: KB4) (formula: $C_{16}H_{12}ClN_5O_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	B	1	Total	C	Cl	N	O	0	0
			24	16	1	5	2		
11	D	1	Total	C	Cl	N	O	0	0
			24	16	1	5	2		

- Molecule 12 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (CCD ID: ACP) (formula: $C_{11}H_{18}N_5O_{12}P_3$).



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

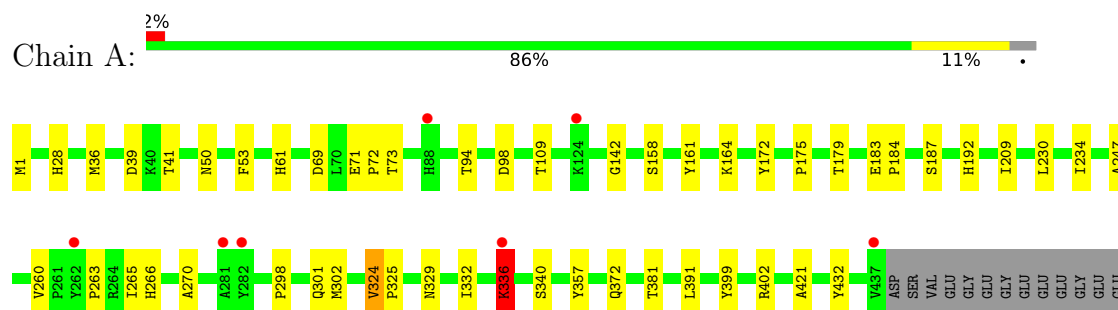
- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	52	Total	O	0	0
			52	52		
13	B	46	Total	O	0	0
			46	46		
13	C	94	Total	O	0	0
			94	94		
13	D	15	Total	O	0	0
			15	15		
13	E	11	Total	O	0	0
			11	11		
13	F	11	Total	O	0	0
			11	11		

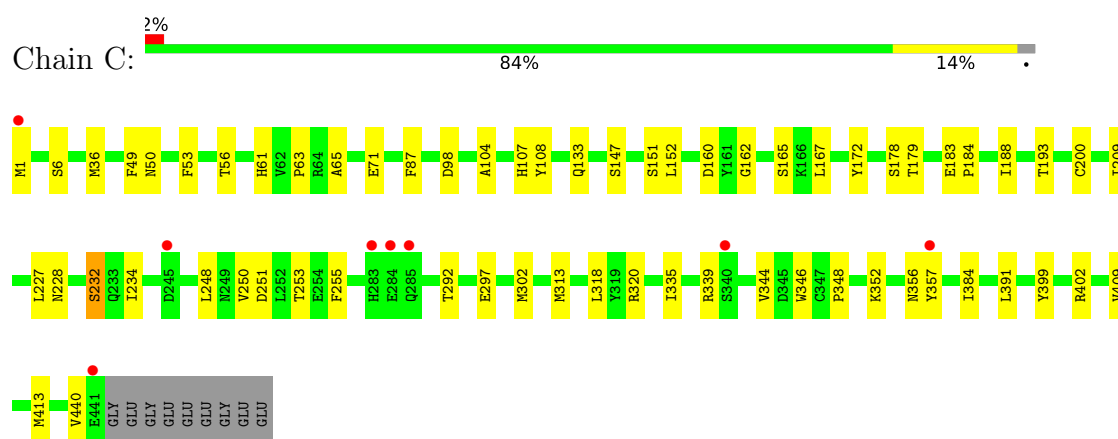
3 Residue-property plots [i](#)

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.

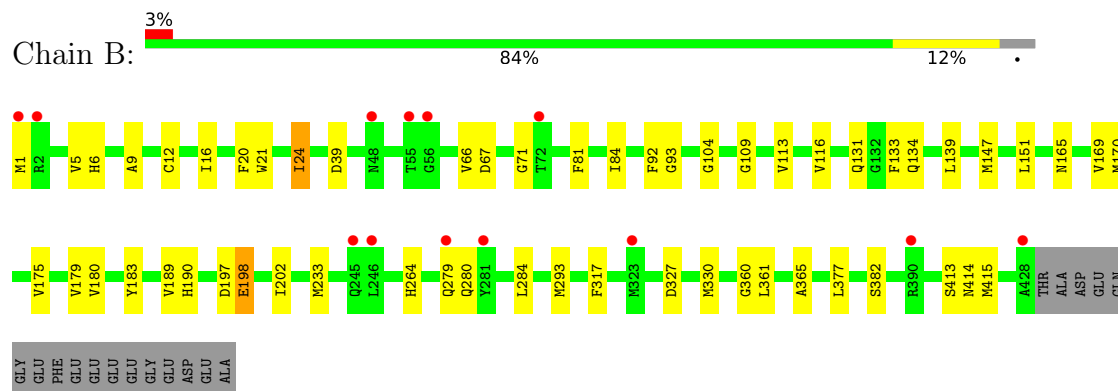
• Molecule 1: Tubulin alpha-1B chain



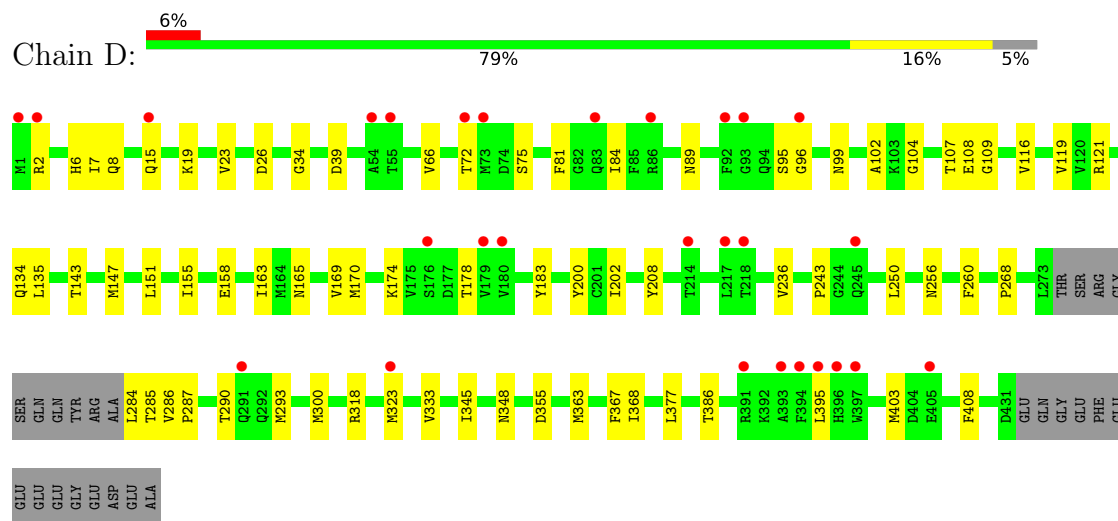
• Molecule 1: Tubulin alpha-1B chain



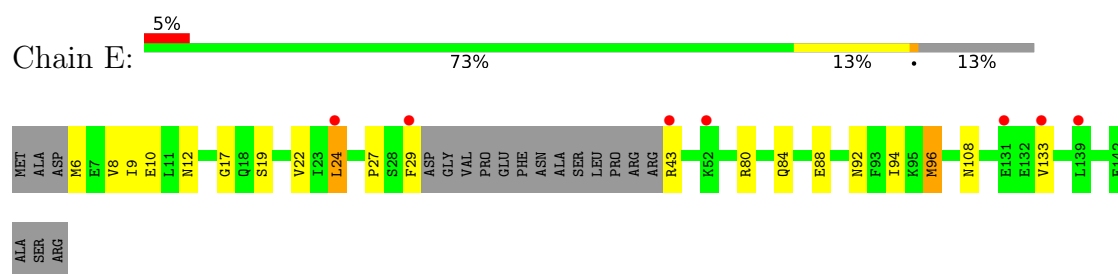
• Molecule 2: Tubulin beta-2B chain



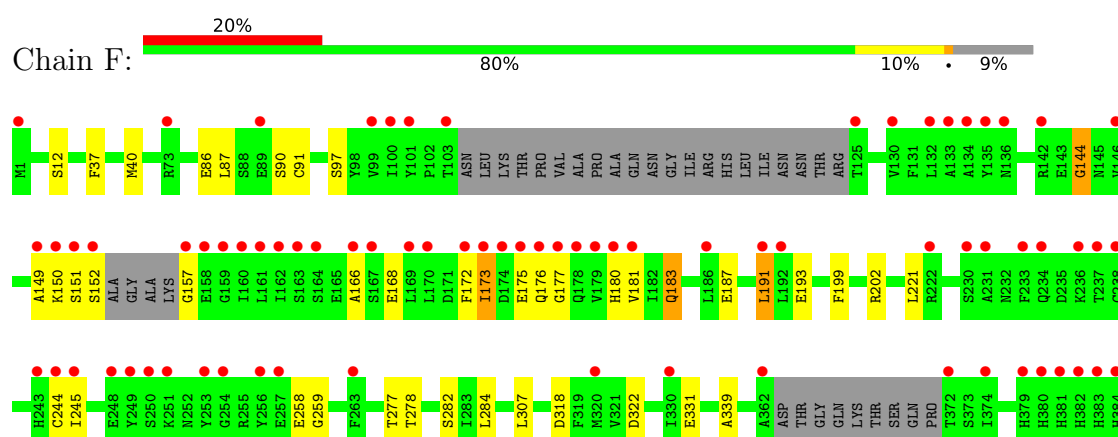
- Molecule 2: Tubulin beta-2B chain



- Molecule 3: Stathmin-4



- Molecule 4: Uncharacterized protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	105.30Å 157.84Å 182.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.60 50.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.8 (50.00-2.60) 99.5 (50.00-2.60)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.40 (at 2.58Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.201 , 0.246 0.205 , 0.245	Depositor DCC
R_{free} test set	4729 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	39.8	Xtriage
Anisotropy	0.039	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 39.5	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	0.93	EDS
Total number of atoms	17917	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.59% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MES, GDP, MG, KB4, CL, ACP, CA, 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	1.01	0/3494	1.46	3/4743 (0.1%)
1	C	1.01	0/3524	1.41	7/4784 (0.1%)
2	B	1.02	0/3450	1.42	2/4672 (0.0%)
2	D	1.03	0/3382	1.48	4/4581 (0.1%)
3	E	0.99	0/1048	1.61	0/1389
4	F	1.04	0/2941	1.38	2/3973 (0.1%)
All	All	1.02	0/17839	1.44	18/24142 (0.1%)

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	96	GLY	CA-C-O	-6.98	117.42	122.45
1	A	142	GLY	CA-C-N	5.95	125.76	120.10
1	A	142	GLY	C-N-CA	5.95	125.76	120.10
2	B	327	ASP	CA-CB-CG	5.74	118.34	112.60
2	D	285	THR	CA-C-N	5.66	124.86	120.33
2	D	285	THR	C-N-CA	5.66	124.86	120.33
1	C	160	ASP	CA-CB-CG	5.58	118.18	112.60
2	D	260	PHE	CB-CA-C	5.50	118.27	110.02
1	A	336	LYS	CB-CA-C	-5.49	101.67	110.79
1	C	56	THR	CA-C-N	5.22	125.87	120.03
1	C	56	THR	C-N-CA	5.22	125.87	120.03
4	F	339	ALA	CA-C-N	5.10	127.42	120.54
4	F	339	ALA	C-N-CA	5.10	127.42	120.54
1	C	297	GLU	CB-CA-C	5.08	115.20	110.17
2	B	93	GLY	CA-C-O	-5.07	117.21	122.28
1	C	147	SER	CA-C-N	5.06	125.56	119.94
1	C	147	SER	C-N-CA	5.06	125.56	119.94
1	C	313	MET	N-CA-C	-5.00	107.14	114.39

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	3331	32	0
1	C	3446	0	3353	34	0
2	B	3372	0	3255	42	0
2	D	3309	0	3189	37	0
3	E	1036	0	1055	15	0
4	F	2873	0	2824	19	0
5	A	32	0	12	0	0
5	C	32	0	12	0	0
5	D	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
6	E	1	0	0	0	0
7	A	1	0	0	0	0
8	A	1	0	0	0	0
8	B	1	0	0	0	0
8	C	1	0	0	0	0
8	D	1	0	0	0	0
9	B	28	0	12	0	0
10	B	24	0	26	2	0
11	B	24	0	0	0	0
11	D	24	0	0	2	0
12	F	31	0	14	2	0
13	A	52	0	0	0	0
13	B	46	0	0	0	0
13	C	94	0	0	0	0
13	D	15	0	0	0	0
13	E	11	0	0	0	0
13	F	11	0	0	0	0
All	All	17917	0	17095	169	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 (169) 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:20:PHE:CE1	2:B:24:ILE:CD1	2.69	0.76
2:D:134:GLN:HA	2:D:165:ASN:O	1.88	0.74
2:B:170:MET:HG3	2:B:377:LEU:HD21	1.70	0.72
2:B:179:VAL:HG12	1:C:348:PRO:HG2	1.71	0.72
2:B:20:PHE:CE1	2:B:24:ILE:HD12	2.24	0.72
1:C:234:ILE:HD13	1:C:302:MET:SD	2.29	0.71
2:D:99:ASN:HD22	2:D:178:THR:HG21	1.55	0.71
2:B:197:ASP:OD1	10:B:504:MES:H32	1.93	0.69
2:B:165:ASN:HD22	2:B:198:GLU:HG3	1.58	0.68
2:B:139:LEU:HD12	2:B:170:MET:SD	2.34	0.67
1:A:69:ASP:O	1:A:94:THR:HA	1.97	0.65
2:B:317:PHE:CZ	2:B:330:MET:HE3	2.33	0.64
4:F:168:GLU:O	4:F:172:PHE:N	2.30	0.64
1:C:209:ILE:HG22	1:C:227:LEU:HD22	1.80	0.63
2:B:189:VAL:HB	2:B:415:MET:HE3	1.81	0.62
2:B:134:GLN:HA	2:B:165:ASN:O	1.99	0.62
2:B:116:VAL:HG11	2:B:151:LEU:HD21	1.82	0.62
2:D:200:TYR:CZ	2:D:236:VAL:CG1	2.82	0.62
1:C:107:HIS:O	1:C:152:LEU:HD22	1.98	0.61
1:A:336:LYS:NZ	3:E:6:MET:SD	2.74	0.61
1:A:247:ALA:CB	3:E:12:ASN:HD22	2.14	0.60
2:B:317:PHE:CE1	2:B:330:MET:HE3	2.36	0.59
2:B:279:GLN:NE2	2:B:280:GLN:O	2.34	0.59
1:A:247:ALA:HB1	3:E:12:ASN:HD22	1.66	0.59
2:B:20:PHE:CZ	2:B:24:ILE:HD13	2.38	0.59
2:B:189:VAL:HG11	2:B:415:MET:HE2	1.85	0.59
2:D:102:ALA:HB2	2:D:403:MET:HE3	1.85	0.57
2:D:290:THR:HG22	2:D:333:VAL:HG21	1.86	0.57
1:C:248:LEU:HD12	1:C:357:TYR:OH	2.05	0.57
2:D:200:TYR:CZ	2:D:236:VAL:HG13	2.41	0.56
2:D:169:VAL:HA	2:D:202:ILE:O	2.05	0.56
1:A:71:GLU:HB2	1:A:98:ASP:HB3	1.87	0.56
1:A:234:ILE:HD13	1:A:302:MET:SD	2.45	0.55
2:B:104:GLY:O	2:B:109:GLY:HA3	2.06	0.55
3:E:80:ARG:O	3:E:84:GLN:HG3	2.07	0.55
2:B:197:ASP:OD2	10:B:504:MES:H52	2.06	0.55
1:C:71:GLU:HG2	1:C:98:ASP:HB3	1.89	0.54
1:A:332:ILE:HG22	1:A:336:LYS:CE	2.37	0.54
4:F:199:PHE:CD2	4:F:221:LEU:HD23	2.42	0.54
3:E:6:MET:HE3	3:E:22:VAL:HG21	1.89	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.25	0.54
2:D:102:ALA:HB2	2:D:403:MET:CE	2.37	0.54
2:B:165:ASN:ND2	2:B:198:GLU:HG3	2.21	0.54
2:B:189:VAL:HB	2:B:415:MET:CE	2.38	0.53
1:C:172:TYR:CE2	1:C:391:LEU:HD22	2.44	0.53
2:B:113:VAL:HG23	2:B:151:LEU:HD12	1.91	0.52
1:A:357:TYR:CE2	3:E:17:GLY:HA2	2.44	0.52
4:F:278:THR:O	4:F:282:SER:OG	2.21	0.52
1:A:71:GLU:HG2	1:A:72:PRO:HD2	1.92	0.52
2:D:7:ILE:O	2:D:135:LEU:HA	2.11	0.51
1:A:324:VAL:HG22	1:A:325:PRO:HD2	1.92	0.51
2:B:165:ASN:HD22	2:B:198:GLU:CG	2.24	0.51
4:F:173:ILE:HG23	4:F:176:GLN:HB2	1.92	0.51
1:A:329:ASN:ND2	3:E:8:VAL:HG21	2.25	0.51
1:C:6:SER:O	1:C:65:ALA:HA	2.11	0.51
1:C:151:SER:HB3	1:C:193:THR:HG21	1.93	0.50
2:B:20:PHE:CD1	2:B:233:MET:HE2	2.46	0.50
1:A:298:PRO:HA	1:A:301:GLN:CD	2.36	0.50
4:F:151:SER:HB2	4:F:180:HIS:CE1	2.46	0.50
2:B:169:VAL:HA	2:B:202:ILE:O	2.11	0.50
1:A:332:ILE:HG22	1:A:336:LYS:HE3	1.94	0.49
2:B:81:PHE:O	2:B:84:ILE:HG22	2.11	0.49
2:D:200:TYR:CZ	2:D:236:VAL:HG11	2.47	0.49
1:A:187:SER:HB3	1:A:391:LEU:HD21	1.95	0.49
2:D:170:MET:HE2	2:D:377:LEU:HD21	1.95	0.49
2:D:72:THR:O	2:D:75:SER:OG	2.26	0.49
2:D:174:LYS:HD3	2:D:208:TYR:CD2	2.48	0.49
2:B:67:ASP:O	2:B:92:PHE:HA	2.13	0.49
4:F:37:PHE:CZ	4:F:40:MET:HE3	2.48	0.49
1:A:209:ILE:HD11	1:A:302:MET:SD	2.54	0.48
1:C:63:PRO:HG2	1:C:87:PHE:CE1	2.48	0.48
2:D:345:ILE:HG22	2:D:348:ASN:HB3	1.96	0.48
2:B:20:PHE:CZ	2:B:24:ILE:CD1	2.96	0.48
2:D:163:ILE:HG21	2:D:250:LEU:HB3	1.95	0.48
2:D:6:HIS:HE2	2:D:8:GLN:HG2	1.78	0.48
2:D:151:LEU:O	2:D:155:ILE:HG13	2.14	0.48
1:C:234:ILE:CD1	1:C:302:MET:SD	3.02	0.48
1:A:263:PRO:O	1:A:266:HIS:HD2	1.97	0.48
1:C:255:PHE:CZ	1:C:318:LEU:HD22	2.48	0.48
3:E:43:ARG:O	3:E:43:ARG:HG3	2.14	0.48
1:C:167:LEU:HD22	1:C:200:CYS:HB3	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:256:ASN:HB3	11:D:503:KB4:C19	2.45	0.47
4:F:173:ILE:HD13	4:F:180:HIS:CE1	2.49	0.47
1:A:336:LYS:HD3	3:E:24:LEU:HD13	1.97	0.47
1:C:133:GLN:HE21	1:C:253:THR:HG21	1.80	0.47
2:D:104:GLY:O	2:D:109:GLY:HA3	2.15	0.47
2:D:256:ASN:HB3	11:D:503:KB4:C20	2.44	0.47
2:D:89:ASN:HA	2:D:119:VAL:HG21	1.96	0.47
2:D:318:ARG:O	2:D:363:MET:HA	2.14	0.47
1:C:250:VAL:HG11	1:C:352:LYS:HE3	1.96	0.47
4:F:331:GLU:OE2	12:F:401:ACP:O1G	2.33	0.47
1:A:39:ASP:OD2	1:A:61:HIS:HE1	1.98	0.46
4:F:97:SER:OG	4:F:183:GLN:OE1	2.32	0.46
4:F:149:ALA:HA	4:F:181:VAL:O	2.16	0.46
2:B:293:MET:HE3	2:B:365:ALA:HB1	1.98	0.46
1:C:399:TYR:O	1:C:402:ARG:NH2	2.48	0.46
1:C:1:MET:C	1:C:1:MET:SD	2.98	0.46
1:C:292:THR:HG22	1:C:335:ILE:CD1	2.46	0.46
2:B:360:GLY:C	2:B:361:LEU:HD12	2.40	0.46
1:C:104:ALA:HB2	1:C:413:MET:SD	2.56	0.46
4:F:150:LYS:NZ	12:F:401:ACP:O5'	2.48	0.46
4:F:173:ILE:HG21	4:F:180:HIS:NE2	2.31	0.45
1:C:320:ARG:HA	1:C:356:ASN:O	2.16	0.45
4:F:191:LEU:O	4:F:191:LEU:HD12	2.16	0.45
1:A:183:GLU:N	1:A:184:PRO:CD	2.79	0.45
2:B:190:HIS:ND1	2:B:414:ASN:ND2	2.62	0.45
2:D:200:TYR:OH	2:D:236:VAL:HG13	2.16	0.45
1:A:332:ILE:HG22	1:A:336:LYS:NZ	2.32	0.45
2:D:66:VAL:HG12	2:D:147:MET:HE1	1.99	0.45
1:C:133:GLN:HE21	1:C:253:THR:CG2	2.30	0.45
2:B:189:VAL:CB	2:B:415:MET:CE	2.95	0.44
2:D:34:GLY:HA2	2:D:84:ILE:HD11	1.99	0.44
1:C:162:GLY:HA2	3:E:94:ILE:HD11	1.98	0.44
2:D:293:MET:CG	2:D:367:PHE:HB2	2.48	0.44
1:A:28:HIS:O	1:A:36:MET:HE3	2.18	0.44
2:D:121:ARG:NE	2:D:158:GLU:OE2	2.34	0.44
1:A:1:MET:C	1:A:1:MET:SD	3.00	0.44
2:D:268:PRO:HG2	2:D:300:MET:HB2	1.98	0.44
1:C:167:LEU:HA	1:C:200:CYS:O	2.17	0.43
1:C:440:VAL:O	1:C:440:VAL:HG23	2.18	0.43
2:D:81:PHE:O	2:D:84:ILE:HG22	2.18	0.43
3:E:92:ASN:O	3:E:96:MET:HG2	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:9:ALA:HA	2:B:66:VAL:O	2.18	0.43
1:C:183:GLU:N	1:C:184:PRO:CD	2.81	0.43
2:D:116:VAL:O	2:D:119:VAL:HG12	2.19	0.43
2:D:183:TYR:CD1	2:D:408:PHE:HE2	2.36	0.43
2:B:12:CYS:SG	2:B:16:ILE:HD12	2.58	0.43
4:F:157:GLY:CA	4:F:245:ILE:HD11	2.49	0.43
1:C:36:MET:HB3	1:C:61:HIS:CE1	2.54	0.43
1:A:71:GLU:OE1	1:A:73:THR:CB	2.66	0.43
1:A:399:TYR:O	1:A:402:ARG:NH1	2.50	0.43
2:D:236:VAL:HG22	2:D:368:ILE:HG12	2.01	0.43
1:A:50:ASN:HA	1:A:53:PHE:O	2.18	0.42
1:C:50:ASN:HA	1:C:53:PHE:O	2.18	0.42
2:B:317:PHE:HZ	2:B:330:MET:CE	2.32	0.42
2:D:19:LYS:O	2:D:23:VAL:HG23	2.19	0.42
2:B:197:ASP:O	2:B:264:HIS:HB2	2.20	0.42
1:A:265:ILE:HG23	1:A:432:TYR:CE1	2.55	0.42
4:F:322:ASP:OD1	4:F:322:ASP:C	2.62	0.42
3:E:27:PRO:C	3:E:29:PHE:H	2.28	0.42
1:C:335:ILE:HG23	1:C:339:ARG:HG3	2.00	0.42
3:E:88:GLU:HA	3:E:88:GLU:OE1	2.20	0.42
2:B:179:VAL:HG12	1:C:348:PRO:CG	2.46	0.42
4:F:202:ARG:NE	4:F:318:ASP:OD1	2.43	0.42
2:B:147:MET:HE2	2:B:151:LEU:HD11	2.01	0.41
1:A:270:ALA:HB3	1:A:302:MET:CG	2.50	0.41
1:C:36:MET:HE1	1:C:49:PHE:CE2	2.55	0.41
2:D:107:THR:OG1	2:D:108:GLU:N	2.52	0.41
1:A:161:TYR:HB3	1:A:164:LYS:HG2	2.02	0.41
2:D:286:VAL:HB	2:D:287:PRO:HD3	2.02	0.41
1:A:209:ILE:HG23	1:A:230:LEU:HD23	2.02	0.41
2:B:1:MET:SD	2:B:131:GLN:HA	2.61	0.41
1:C:108:TYR:CD1	3:E:108:ASN:CG	2.99	0.41
4:F:144:GLY:HA3	4:F:187:GLU:OE1	2.20	0.41
1:A:260:VAL:HG11	1:A:266:HIS:HB3	2.02	0.41
2:B:180:VAL:O	2:B:183:TYR:HB2	2.21	0.41
2:B:293:MET:CE	2:B:365:ALA:HB1	2.50	0.41
2:B:317:PHE:CZ	2:B:330:MET:CE	3.03	0.41
1:C:344:VAL:HG21	1:C:346:TRP:CE2	2.56	0.41
1:C:409:VAL:HA	1:C:413:MET:O	2.20	0.41
2:D:66:VAL:HG12	2:D:147:MET:CE	2.51	0.41
3:E:9:ILE:HD12	3:E:10:GLU:HG3	2.02	0.41
4:F:307:LEU:HD23	4:F:307:LEU:HA	1.91	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:263:PRO:O	1:A:266:HIS:CD2	2.73	0.41
1:C:228:ASN:O	1:C:232:SER:OG	2.38	0.40
2:D:165:ASN:HB2	2:D:250:LEU:HD22	2.02	0.40
4:F:258:GLU:HA	4:F:259:GLY:HA2	1.81	0.40
1:A:192:HIS:CG	1:A:421:ALA:HA	2.57	0.40
2:B:5:VAL:O	2:B:133:PHE:HA	2.21	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%)	416 (96%)	18 (4%)	1 (0%)	43	66
1	C	439/450 (98%)	422 (96%)	16 (4%)	1 (0%)	43	66
2	B	427/445 (96%)	408 (96%)	17 (4%)	2 (0%)	24	46
2	D	417/445 (94%)	389 (93%)	27 (6%)	1 (0%)	43	66
3	E	121/143 (85%)	115 (95%)	6 (5%)	0	100	100
4	F	342/384 (89%)	320 (94%)	17 (5%)	5 (2%)	8	18
All	All	2181/2317 (94%)	2070 (95%)	101 (5%)	10 (0%)	24	46

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	71	GLY
1	C	178	SER
2	D	243	PRO
4	F	144	GLY
4	F	166	ALA
4	F	175	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	109	THR
4	F	91	CYS
2	B	39	ASP
4	F	177	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	368/378 (97%)	358 (97%)	10 (3%)	39	67
1	C	372/378 (98%)	366 (98%)	6 (2%)	55	79
2	B	371/383 (97%)	365 (98%)	6 (2%)	55	79
2	D	364/383 (95%)	353 (97%)	11 (3%)	36	64
3	E	113/127 (89%)	109 (96%)	4 (4%)	32	59
4	F	315/342 (92%)	303 (96%)	12 (4%)	29	56
All	All	1903/1991 (96%)	1854 (97%)	49 (3%)	40	68

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	THR
1	A	158	SER
1	A	172	TYR
1	A	175	PRO
1	A	179	THR
1	A	324	VAL
1	A	336	LYS
1	A	340	SER
1	A	372	GLN
1	A	381	THR
2	B	24	ILE
2	B	175	VAL
2	B	198	GLU
2	B	284	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	382	SER
2	B	413	SER
1	C	165	SER
1	C	179	THR
1	C	188	ILE
1	C	232	SER
1	C	251	ASP
1	C	384	ILE
2	D	2	ARG
2	D	15	GLN
2	D	26	ASP
2	D	39	ASP
2	D	95	SER
2	D	143	THR
2	D	284	LEU
2	D	323	MET
2	D	355	ASP
2	D	386	THR
2	D	395	LEU
3	E	19	SER
3	E	24	LEU
3	E	96	MET
3	E	133	VAL
4	F	12	SER
4	F	86	GLU
4	F	87	LEU
4	F	90	SER
4	F	152	SER
4	F	173	ILE
4	F	183	GLN
4	F	191	LEU
4	F	193	GLU
4	F	244	CYS
4	F	277	THR
4	F	284	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	50	ASN
1	A	61	HIS
1	A	102	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	266	HIS
1	A	285	GLN
1	A	309	HIS
1	A	393	HIS
1	A	406	HIS
2	B	165	ASN
2	B	347	ASN
1	C	11	GLN
1	C	15	GLN
1	C	85	GLN
1	C	133	GLN
1	C	293	ASN
1	C	356	ASN
2	D	15	GLN
2	D	99	ASN
2	D	134	GLN
2	D	137	HIS
2	D	165	ASN
2	D	195	ASN
2	D	329	GLN
2	D	347	ASN
2	D	426	GLN
3	E	12	ASN
3	E	92	ASN
4	F	136	ASN
4	F	180	HIS
4	F	242	ASN
4	F	333	ASN

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 18 ligands modelled in this entry, 9 are monoatomic - leaving 9 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
5	GTP	A	501	8	33,34,34	0.59	0	50,54,54	0.66	0
5	GTP	C	501	8	33,34,34	0.53	0	50,54,54	0.67	0
11	KB4	B	506	-	27,27,27	2.41	7 (25%)	32,39,39	2.31	9 (28%)
10	MES	B	505	-	12,12,12	0.68	0	15,16,16	0.50	0
9	GDP	B	501	8	29,30,30	1.44	4 (13%)	45,47,47	1.68	8 (17%)
5	GTP	D	501	8	33,34,34	0.53	0	50,54,54	0.71	0
11	KB4	D	503	-	27,27,27	2.33	9 (33%)	32,39,39	2.13	7 (21%)
10	MES	B	504	-	12,12,12	0.78	0	15,16,16	0.72	0
12	ACP	F	401	-	31,33,33	2.30	11 (35%)	47,52,52	1.85	10 (21%)

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
5	GTP	A	501	8	-	6/22/38/38	0/3/3/3
5	GTP	C	501	8	-	6/22/38/38	0/3/3/3
11	KB4	B	506	-	-	3/6/18/18	0/4/4/4
10	MES	B	505	-	-	0/6/14/14	0/1/1/1
9	GDP	B	501	8	-	3/16/32/32	0/3/3/3
5	GTP	D	501	8	-	9/22/38/38	0/3/3/3
11	KB4	D	503	-	-	3/6/18/18	0/4/4/4
10	MES	B	504	-	-	1/6/14/14	0/1/1/1
12	ACP	F	401	-	-	3/19/38/38	0/3/3/3

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	D	503	KB4	C16-N15	7.72	1.44	1.35
11	B	506	KB4	C16-N15	7.25	1.43	1.35
12	F	401	ACP	PG-O1G	6.09	1.62	1.50
12	F	401	ACP	C5-C4	5.13	1.48	1.39
12	F	401	ACP	PB-O1B	4.82	1.62	1.51
11	B	506	KB4	C14-N15	4.72	1.47	1.39
9	B	501	GDP	PA-O3A	4.23	1.64	1.59
11	B	506	KB4	C14-C13	-3.96	1.36	1.40
11	B	506	KB4	C05-C04	-3.93	1.35	1.42
11	D	503	KB4	C14-N15	3.91	1.46	1.39
12	F	401	ACP	PB-O3A	3.69	1.62	1.58
12	F	401	ACP	PB-O2B	-3.43	1.48	1.56
11	D	503	KB4	C18-C16	3.38	1.55	1.51
11	D	503	KB4	C13-N12	3.32	1.46	1.40
11	B	506	KB4	C18-C16	3.04	1.55	1.51
9	B	501	GDP	C5-C4	2.90	1.46	1.38
12	F	401	ACP	PG-O3G	2.89	1.61	1.55
11	D	503	KB4	O17-C16	-2.85	1.17	1.23
11	D	503	KB4	C05-C04	-2.77	1.37	1.42
12	F	401	ACP	C5-N7	-2.75	1.34	1.39
9	B	501	GDP	C6-N1	-2.67	1.33	1.38
11	B	506	KB4	O17-C16	-2.64	1.18	1.23
12	F	401	ACP	PA-O3A	2.63	1.62	1.59
12	F	401	ACP	C5-C6	2.59	1.48	1.41
11	D	503	KB4	C14-C13	-2.50	1.37	1.40
11	B	506	KB4	C18-N12	-2.48	1.42	1.46
12	F	401	ACP	PG-O2G	-2.39	1.49	1.55
11	D	503	KB4	C18-N12	-2.27	1.42	1.46
11	D	503	KB4	C07-N12	2.26	1.44	1.39
12	F	401	ACP	C8-N7	2.14	1.35	1.31
9	B	501	GDP	C4-N9	-2.13	1.32	1.38

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	B	506	KB4	N10-C09-N08	-7.94	122.70	130.58
11	D	503	KB4	N10-C09-N08	-6.85	123.78	130.58
12	F	401	ACP	C5-C4-N3	-6.04	118.40	126.72
11	B	506	KB4	CL11-C09-N10	5.87	120.58	115.72
12	F	401	ACP	N3-C4-N9	4.98	135.64	127.17
9	B	501	GDP	C5-C4-N3	-4.87	120.64	128.39
11	D	503	KB4	CL11-C09-N10	4.42	119.37	115.72
11	D	503	KB4	C14-N15-C16	-4.14	119.50	124.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	501	GDP	N9-C4-N3	4.09	134.13	125.95
9	B	501	GDP	C2-N3-C4	3.93	119.07	112.30
11	D	503	KB4	C09-N08-C07	3.73	122.05	111.13
11	D	503	KB4	C13-N12-C07	3.68	126.00	119.21
12	F	401	ACP	C2-N3-C4	3.66	120.76	111.83
12	F	401	ACP	N3-C2-N1	-3.38	123.47	128.58
9	B	501	GDP	O4'-C1'-N9	-3.32	100.84	108.36
9	B	501	GDP	O6-C6-C5	-3.18	118.15	126.53
11	B	506	KB4	C14-N15-C16	-3.17	120.66	124.45
11	B	506	KB4	C09-N08-C07	3.10	120.20	111.13
11	B	506	KB4	C13-N12-C07	3.06	124.85	119.21
11	D	503	KB4	C02-C03-C04	-2.94	116.07	120.09
12	F	401	ACP	C4-C5-N7	-2.89	107.28	110.58
12	F	401	ACP	O1G-PG-C3B	-2.77	105.34	111.37
11	B	506	KB4	C18-N12-C13	2.69	117.72	114.97
12	F	401	ACP	C3'-C2'-C1'	2.66	106.50	101.46
11	B	506	KB4	C01-N06-C05	2.60	120.38	117.31
9	B	501	GDP	C6-C5-N7	2.58	134.99	130.29
11	B	506	KB4	C18-C16-N15	-2.37	113.18	116.13
12	F	401	ACP	PB-O3A-PA	-2.37	124.65	132.37
9	B	501	GDP	O6-C6-N1	2.24	124.32	120.11
11	D	503	KB4	C01-N06-C05	2.24	119.94	117.31
9	B	501	GDP	C8-N9-C4	2.18	110.11	106.03
12	F	401	ACP	C5-N7-C8	2.13	106.80	103.45
11	B	506	KB4	C02-C01-N06	-2.04	120.98	123.97
12	F	401	ACP	C2-N1-C6	2.02	122.04	118.73

There are no chirality outliers.

All (34) 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	A	501	GTP	C5'-O5'-PA-O2A
5	C	501	GTP	PB-O3B-PG-O3G
5	C	501	GTP	C5'-O5'-PA-O3A
5	C	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O2A
5	D	501	GTP	PB-O3B-PG-O2G
5	D	501	GTP	C5'-O5'-PA-O3A
5	D	501	GTP	C5'-O5'-PA-O1A
9	B	501	GDP	C5'-O5'-PA-O3A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	B	501	GDP	C5'-O5'-PA-O1A
10	B	504	MES	C8-C7-N4-C5
11	B	506	KB4	C05-C07-N12-C13
11	D	503	KB4	C05-C07-N12-C13
11	B	506	KB4	N08-C07-N12-C18
12	F	401	ACP	C3'-C4'-C5'-O5'
5	D	501	GTP	PB-O3B-PG-O1G
11	D	503	KB4	N08-C07-N12-C18
12	F	401	ACP	O4'-C4'-C5'-O5'
5	D	501	GTP	C5'-O5'-PA-O2A
9	B	501	GDP	C5'-O5'-PA-O2A
11	D	503	KB4	C05-C07-N12-C18
5	A	501	GTP	PB-O3B-PG-O1G
5	D	501	GTP	PA-O3A-PB-O1B
5	A	501	GTP	PB-O3B-PG-O2G
5	A	501	GTP	PB-O3B-PG-O3G
11	B	506	KB4	C05-C07-N12-C18
12	F	401	ACP	PB-O3A-PA-O2A
5	C	501	GTP	PB-O3A-PA-O1A
5	C	501	GTP	PB-O3A-PA-O2A
5	D	501	GTP	PG-O3B-PB-O2B
5	D	501	GTP	PA-O3A-PB-O2B
5	D	501	GTP	C3'-C4'-C5'-O5'

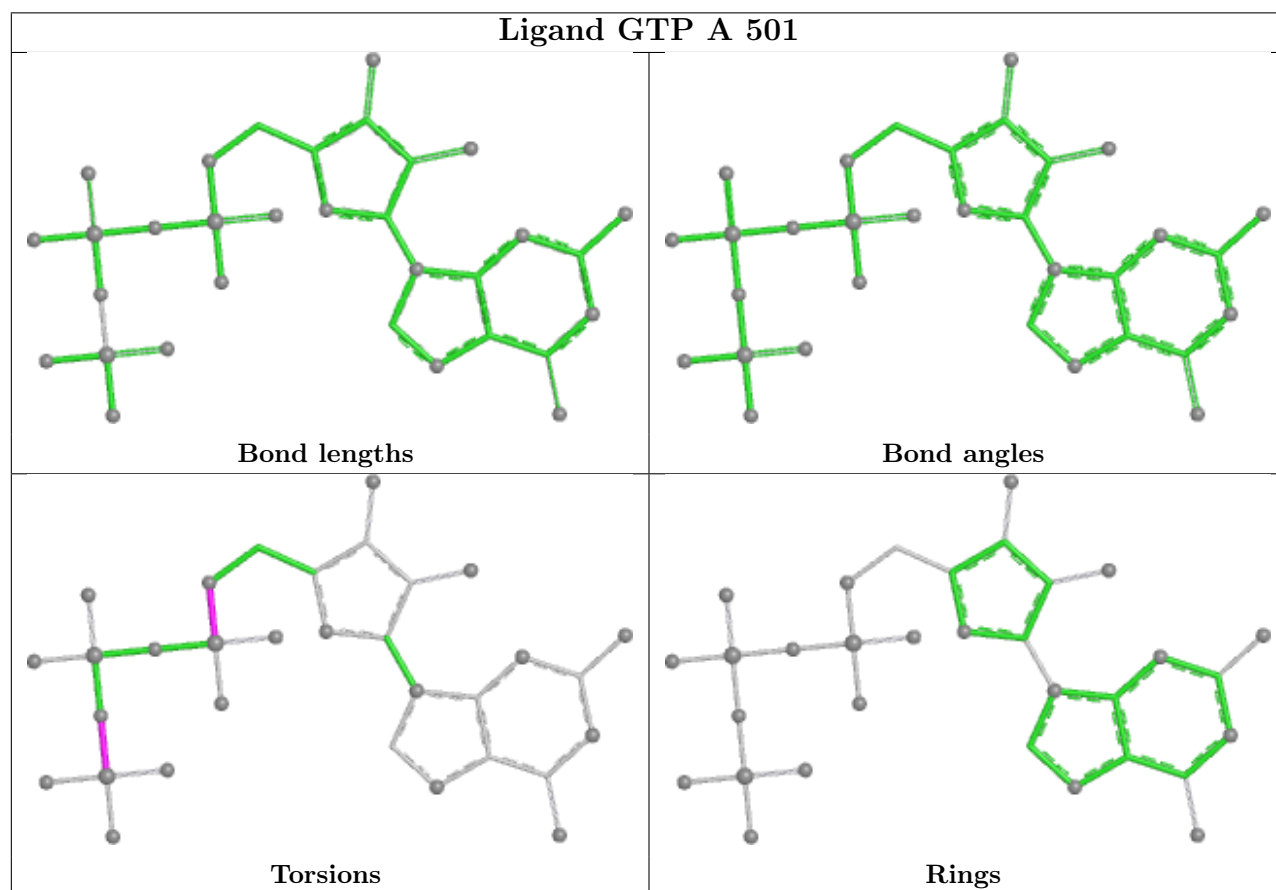
There are no ring outliers.

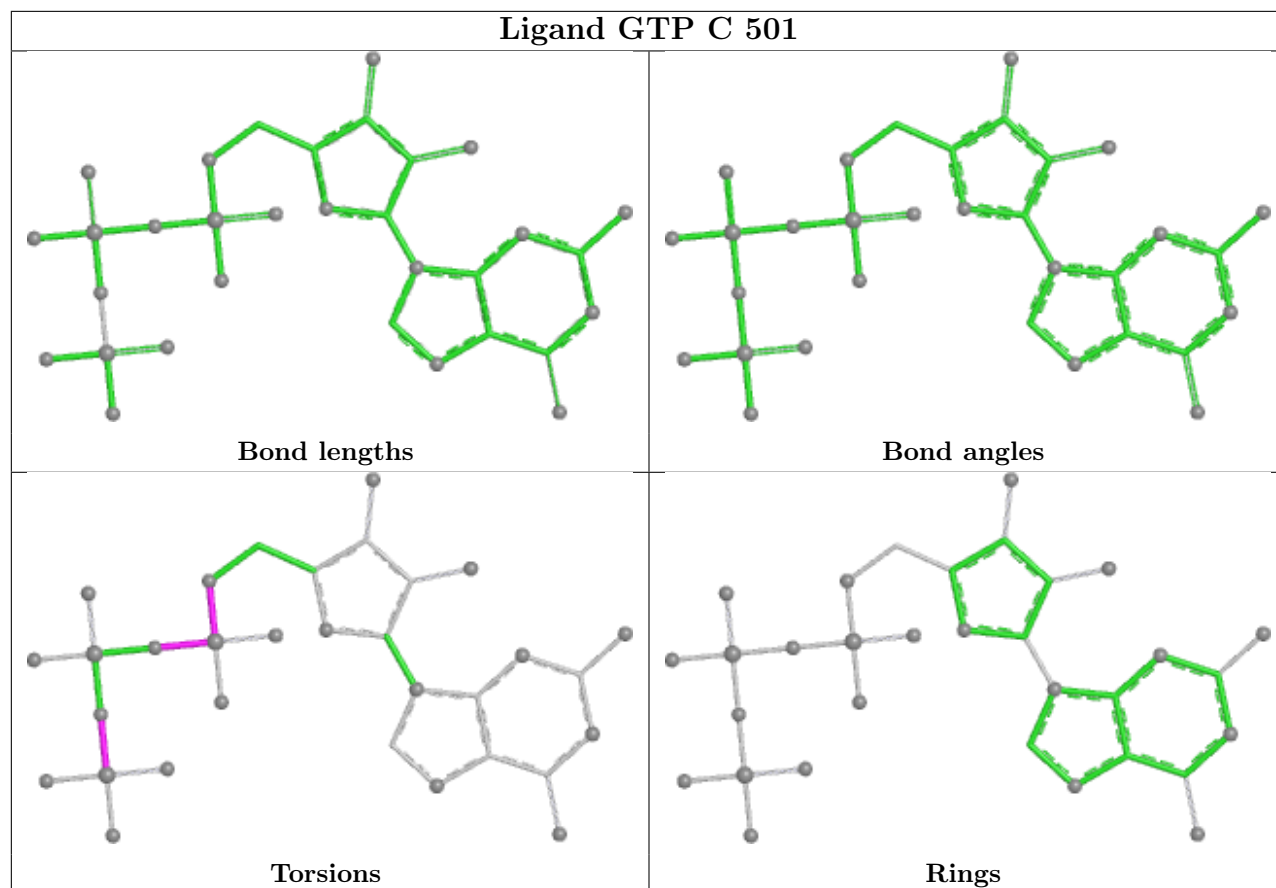
3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	D	503	KB4	2	0
10	B	504	MES	2	0
12	F	401	ACP	2	0

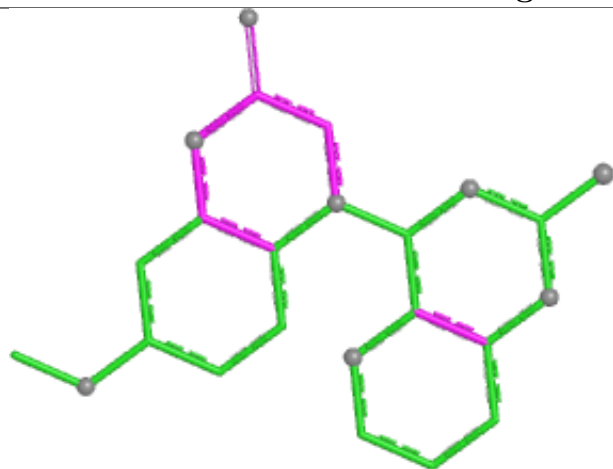
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

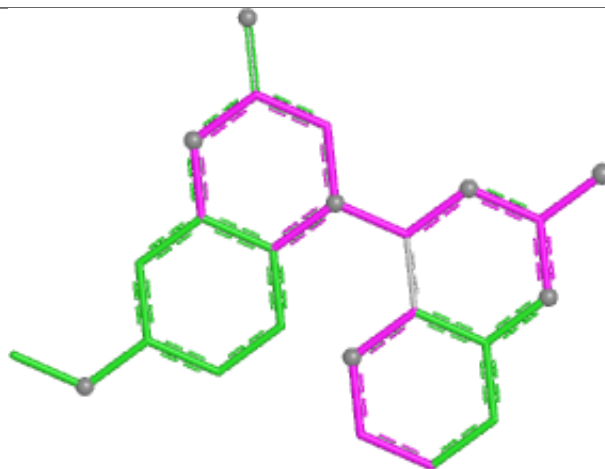




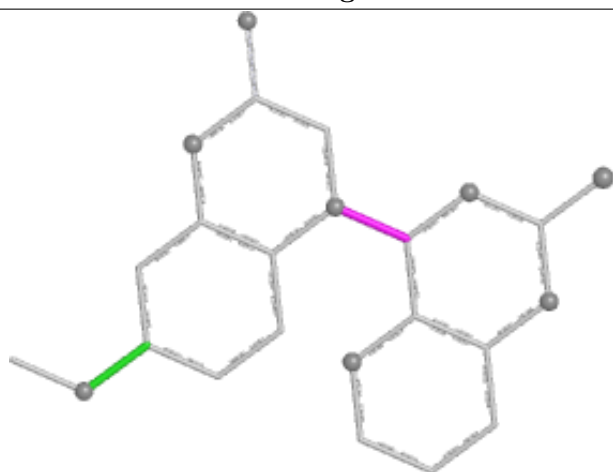
Ligand KB4 B 506



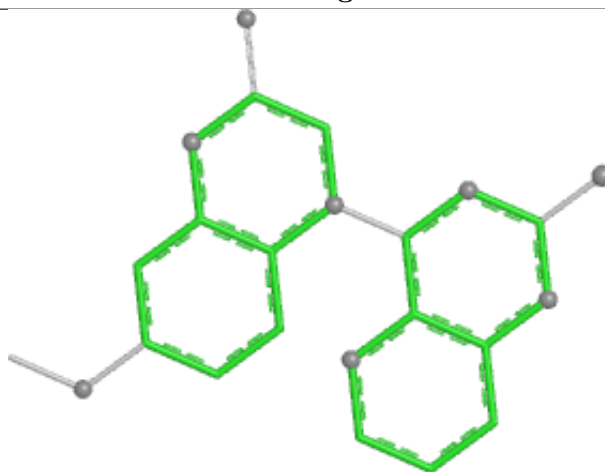
Bond lengths



Bond angles

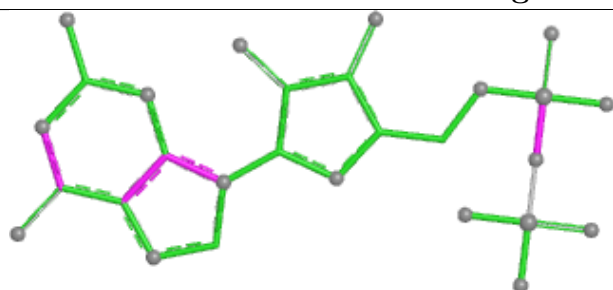


Torsions

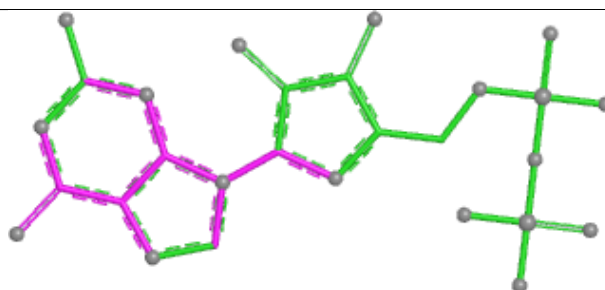


Rings

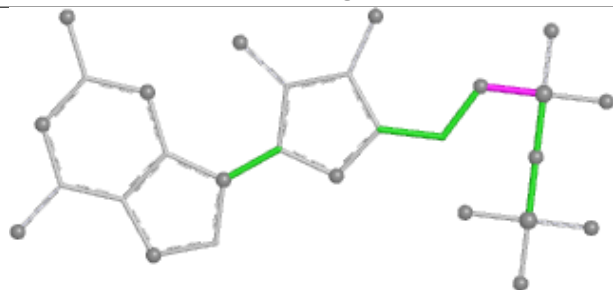
Ligand GDP B 501



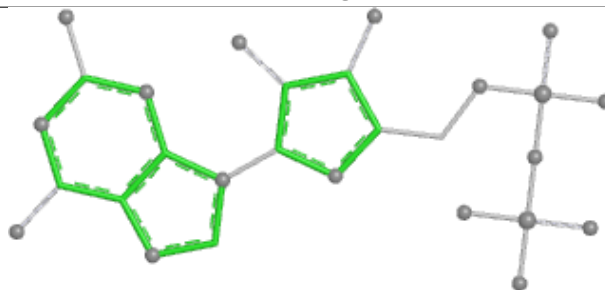
Bond lengths



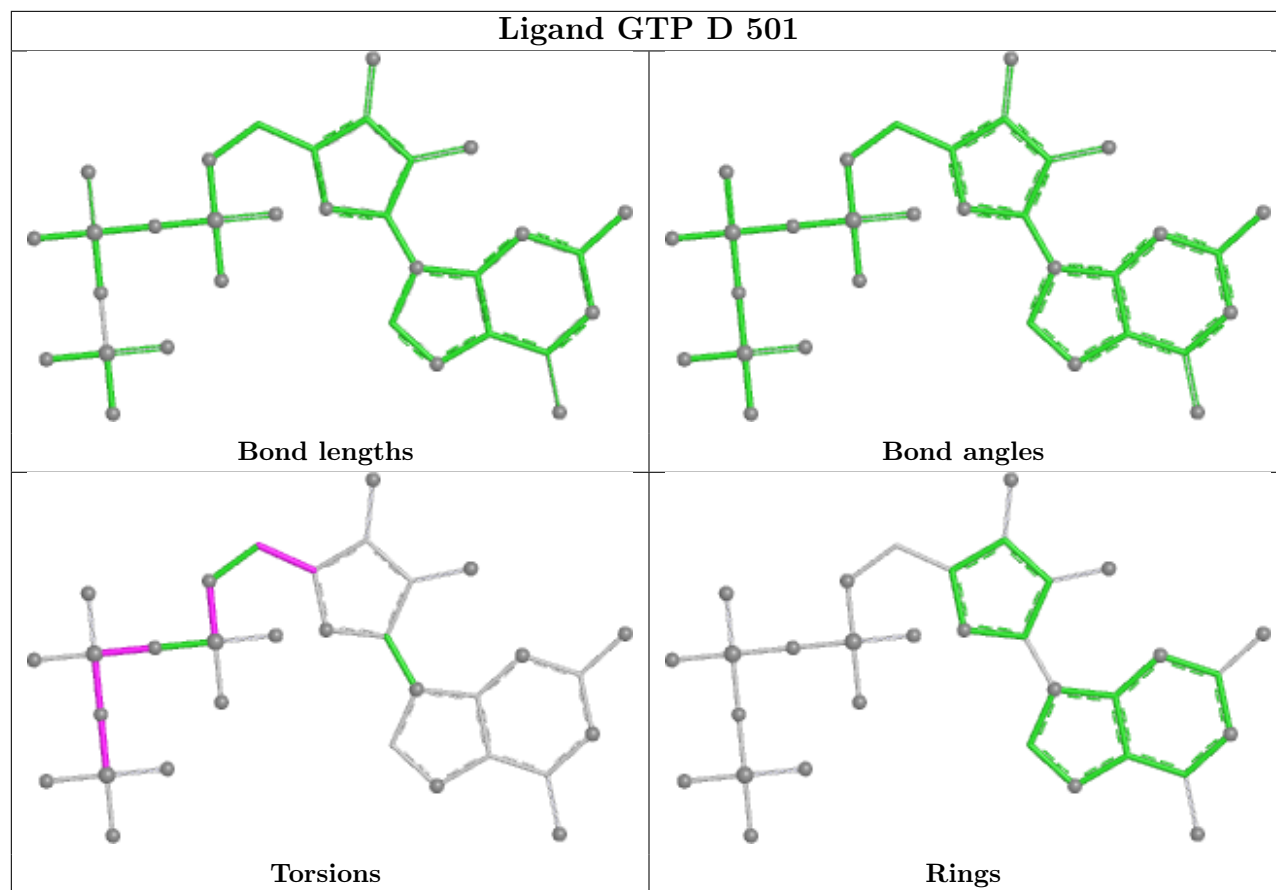
Bond angles

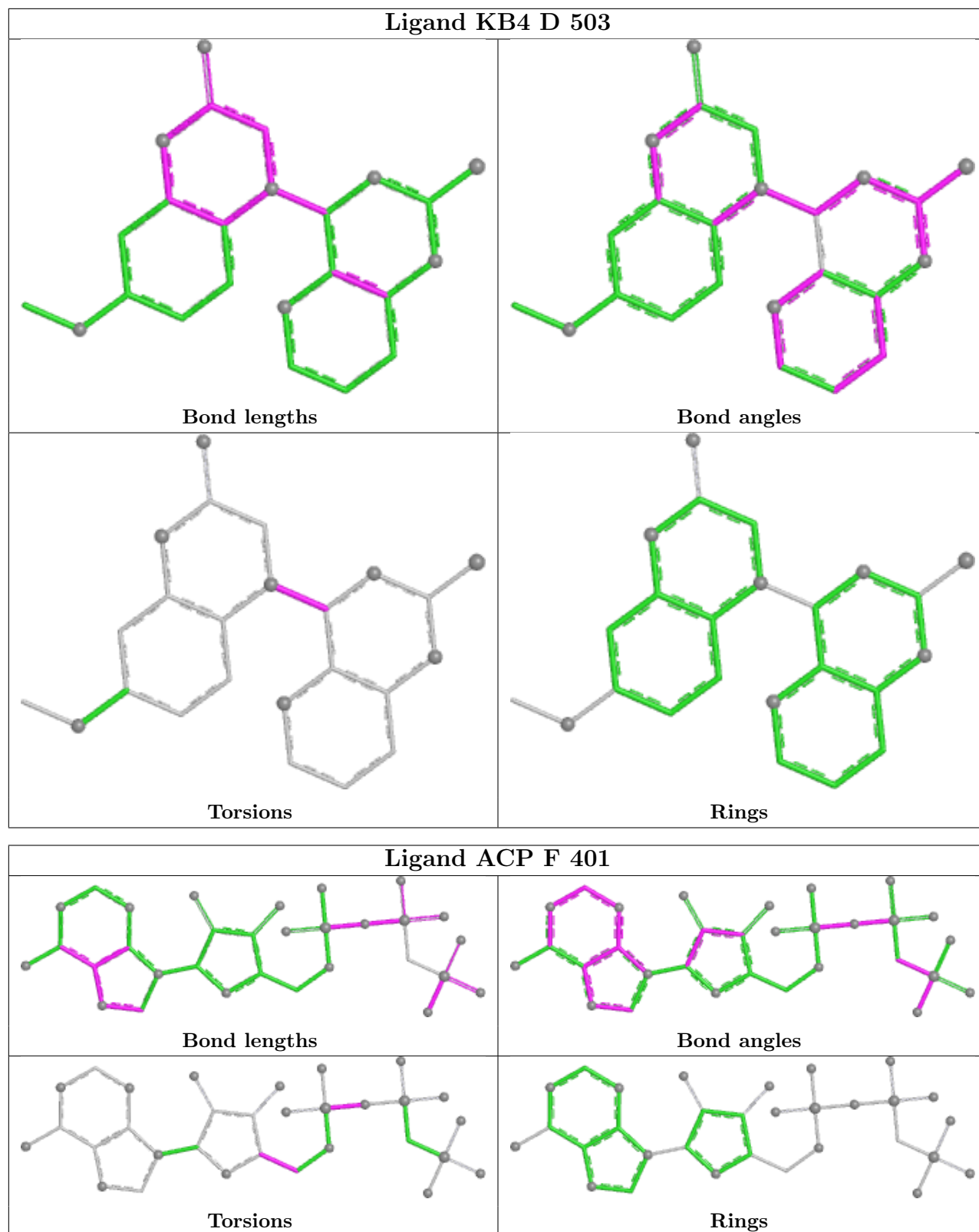


Torsions



Rings





5.7 Other polymers [\(i\)](#)

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	437/450 (97%)	0.01	7 (1%) 70 66	17, 38, 66, 92	0
1	C	441/450 (98%)	-0.32	8 (1%) 67 63	14, 28, 54, 99	1 (0%)
2	B	428/445 (96%)	0.05	13 (3%) 52 47	17, 35, 76, 106	3 (0%)
2	D	421/445 (94%)	0.63	28 (6%) 24 19	24, 55, 94, 125	3 (0%)
3	E	124/143 (86%)	0.69	7 (5%) 30 24	24, 53, 99, 120	1 (0%)
4	F	350/384 (91%)	1.00	76 (21%) 2 2	28, 66, 133, 170	0
All	All	2201/2317 (94%)	0.27	139 (6%) 26 20	14, 43, 97, 170	8 (0%)

All (139) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	170	LEU	4.9
2	D	1	MET	4.9
4	F	161	LEU	4.9
4	F	169	LEU	4.6
4	F	125	THR	4.6
2	D	73	MET	4.3
4	F	191	LEU	4.2
4	F	381	HIS	4.1
4	F	172	PHE	4.0
4	F	157	GLY	4.0
4	F	101	TYR	3.9
4	F	173	ILE	3.8
4	F	245	ILE	3.8
2	D	394	PHE	3.8
1	A	336	LYS	3.7
4	F	150	LYS	3.7
1	A	262	TYR	3.7
4	F	236	LYS	3.7
2	D	92	PHE	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	F	152	SER	3.6
2	D	245	GLN	3.6
4	F	382	HIS	3.5
3	E	29	PHE	3.5
4	F	132	LEU	3.5
2	B	323	MET	3.4
4	F	103	THR	3.4
2	B	428	ALA	3.4
4	F	372	THR	3.3
3	E	139	LEU	3.3
4	F	384	HIS	3.3
4	F	166	ALA	3.3
2	D	96	GLY	3.3
4	F	380	HIS	3.2
2	D	179	VAL	3.2
2	D	214	THR	3.2
4	F	159	GLY	3.2
4	F	130	VAL	3.2
2	D	291	GLN	3.2
4	F	254	GLY	3.2
4	F	249	TYR	3.1
1	C	441	GLU	3.1
4	F	383	HIS	3.1
1	C	285	GLN	3.1
4	F	233	PHE	3.1
4	F	253	TYR	3.1
2	B	279	GLN	3.1
4	F	374	ILE	3.1
4	F	244	CYS	3.0
3	E	131	GLU	3.0
2	B	55	THR	3.0
4	F	179	VAL	3.0
4	F	133	ALA	3.0
4	F	162	ILE	2.9
4	F	177	GLY	2.9
4	F	362	ALA	2.9
4	F	178	GLN	2.9
4	F	100	ILE	2.9
2	D	93	GLY	2.9
4	F	231	ALA	2.9
1	A	437	VAL	2.9
4	F	251	LYS	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	F	135	TYR	2.8
2	D	405	GLU	2.8
3	E	43	ARG	2.8
4	F	134	ALA	2.8
4	F	160	ILE	2.7
4	F	379	HIS	2.7
2	B	2	ARG	2.7
2	D	391	ARG	2.7
4	F	142	ARG	2.7
4	F	222	ARG	2.7
2	D	54	ALA	2.7
4	F	89	GLU	2.6
4	F	149	ALA	2.6
4	F	99	VAL	2.5
2	B	245	GLN	2.5
4	F	151	SER	2.5
1	C	1	MET	2.5
3	E	133	VAL	2.5
2	D	176	SER	2.5
4	F	73	ARG	2.5
2	D	55	THR	2.4
2	B	1	MET	2.4
2	D	83	GLN	2.4
4	F	181	VAL	2.4
4	F	237	THR	2.4
4	F	163	SER	2.4
4	F	176	GLN	2.4
2	B	72	THR	2.3
2	D	218	THR	2.3
2	D	395	LEU	2.3
2	B	48	ASN	2.3
3	E	52	LYS	2.3
4	F	167	SER	2.3
4	F	250	SER	2.3
2	D	396	HIS	2.3
2	B	281	TYR	2.3
4	F	164	SER	2.3
1	A	124	LYS	2.3
2	D	72	THR	2.3
4	F	257	GLU	2.2
2	B	390	ARG	2.2
1	C	357	TYR	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	2	ARG	2.2
4	F	136	ASN	2.2
2	D	15	GLN	2.2
4	F	263	PHE	2.2
1	A	282	TYR	2.2
4	F	234	GLN	2.2
3	E	24	LEU	2.2
1	A	88	HIS	2.2
1	C	283	HIS	2.2
2	D	397	TRP	2.2
4	F	180	HIS	2.2
2	D	393	ALA	2.2
4	F	248	GLU	2.2
4	F	238	CYS	2.2
2	B	246	LEU	2.2
4	F	1	MET	2.2
4	F	174	ASP	2.2
4	F	243	HIS	2.2
4	F	256	TYR	2.1
2	D	323	MET	2.1
2	D	217	LEU	2.1
4	F	320	MET	2.1
1	C	340	SER	2.1
4	F	230	SER	2.1
1	C	284	GLU	2.1
2	D	86	ARG	2.1
2	D	180	VAL	2.1
1	C	245	ASP	2.1
1	A	281	ALA	2.1
4	F	158	GLU	2.1
4	F	186	LEU	2.1
4	F	192	LEU	2.1
4	F	146	VAL	2.1
4	F	175	GLU	2.0
2	B	56	GLY	2.0
4	F	330	ILE	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 [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

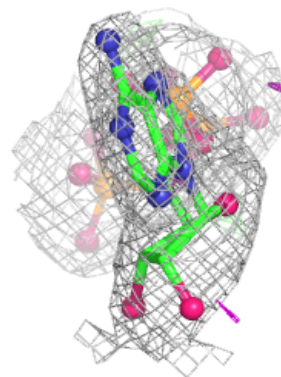
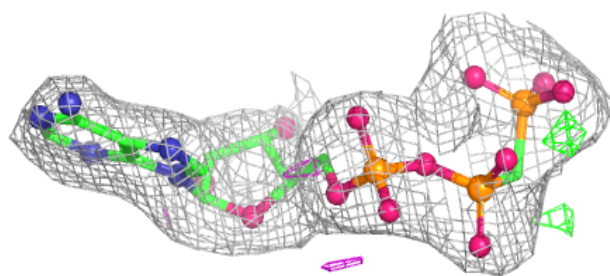
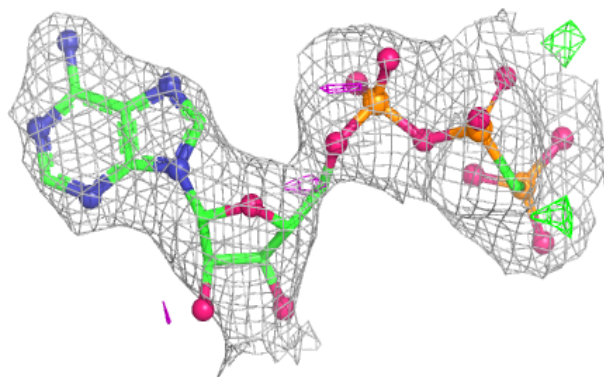
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	MG	D	502	1/1	0.80	0.15	68,68,68,68	0
7	CL	A	503	1/1	0.83	0.14	74,74,74,74	0
12	ACP	F	401	31/31	0.85	0.12	67,80,90,97	0
6	CA	E	201	1/1	0.86	0.11	73,73,73,73	0
10	MES	B	505	12/12	0.88	0.15	60,67,71,74	0
5	GTP	D	501	32/32	0.90	0.11	44,50,79,86	0
6	CA	B	503	1/1	0.91	0.10	73,73,73,73	0
10	MES	B	504	12/12	0.94	0.11	43,51,56,59	0
11	KB4	D	503	24/24	0.95	0.07	30,36,50,50	0
6	CA	A	502	1/1	0.98	0.04	55,55,55,55	0
5	GTP	A	501	32/32	0.98	0.05	20,24,26,28	0
11	KB4	B	506	24/24	0.98	0.05	24,28,33,35	0
8	MG	B	502	1/1	0.98	0.06	24,24,24,24	0
6	CA	C	503	1/1	0.98	0.04	43,43,43,43	0
9	GDP	B	501	28/28	0.99	0.05	18,21,23,26	0
5	GTP	C	501	32/32	0.99	0.04	18,20,23,24	0
8	MG	A	504	1/1	0.99	0.03	29,29,29,29	0
8	MG	C	502	1/1	1.00	0.03	22,22,22,22	0

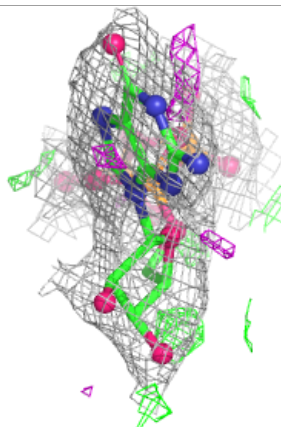
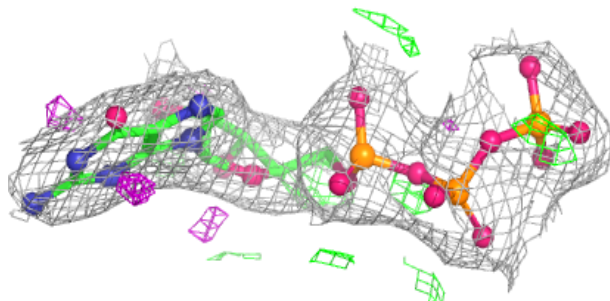
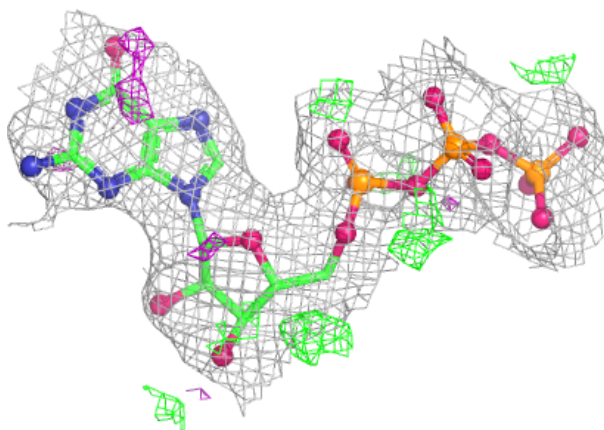
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ACP F 401:

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

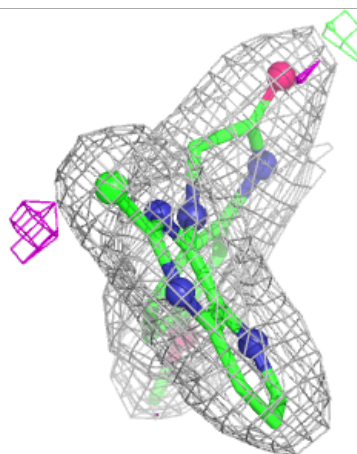
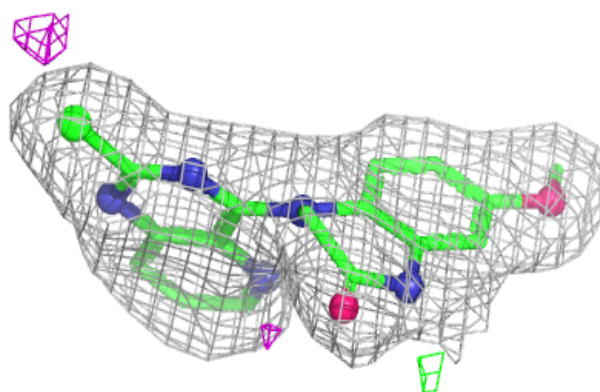
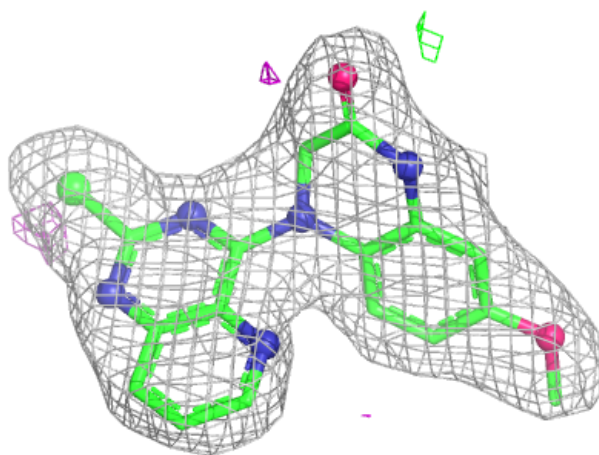
**Electron density around GTP D 501:**

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



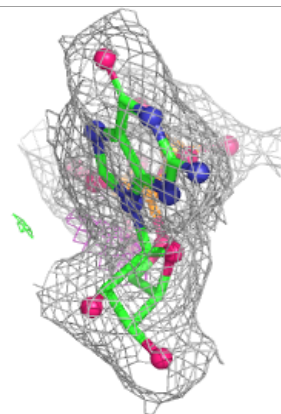
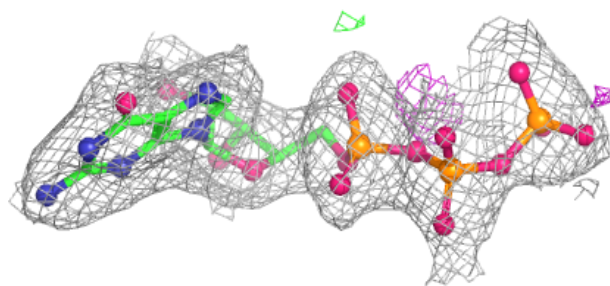
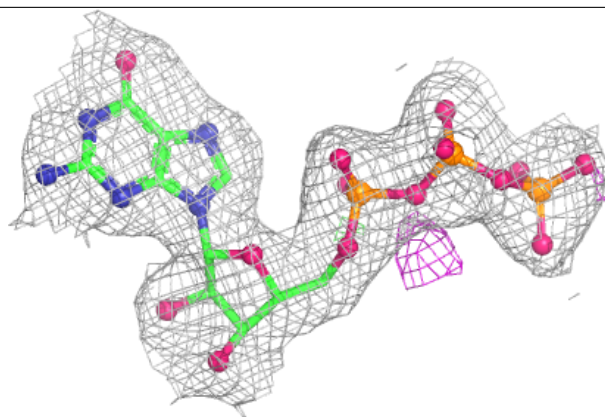
Electron density around KB4 D 503:

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



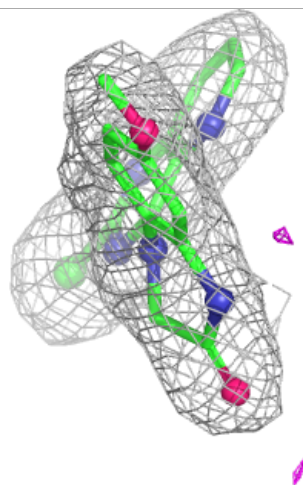
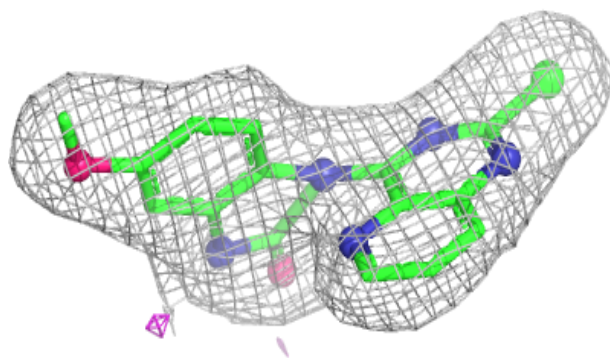
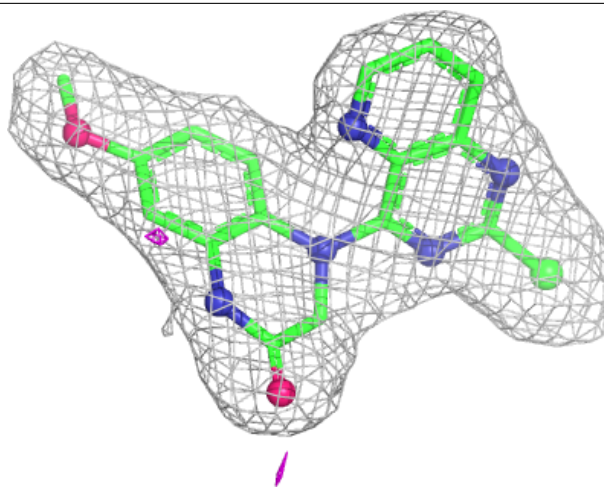
Electron density around GTP A 501:

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



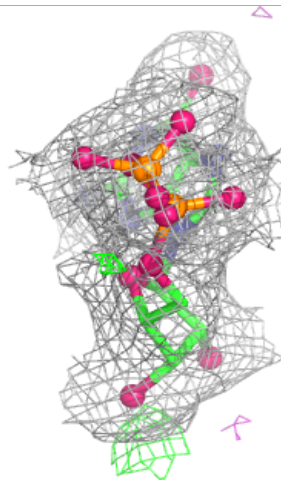
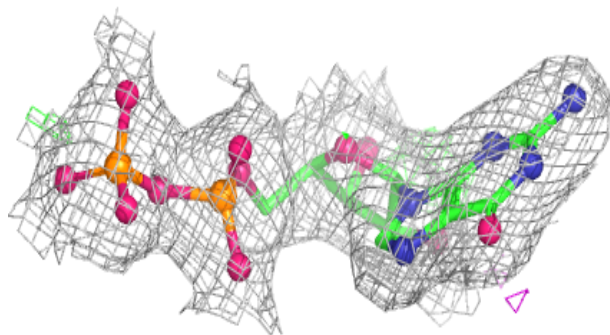
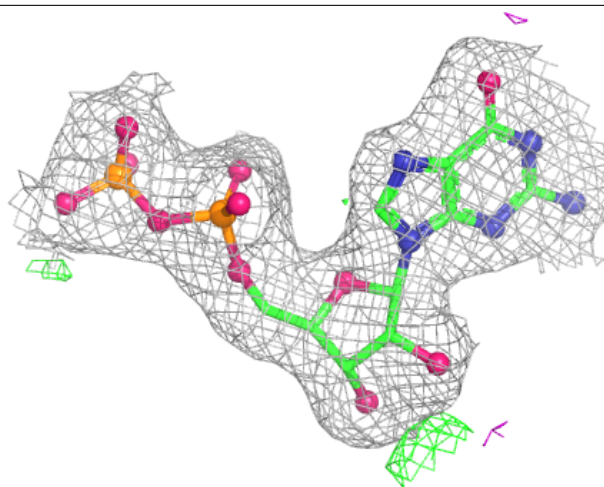
Electron density around KB4 B 506:

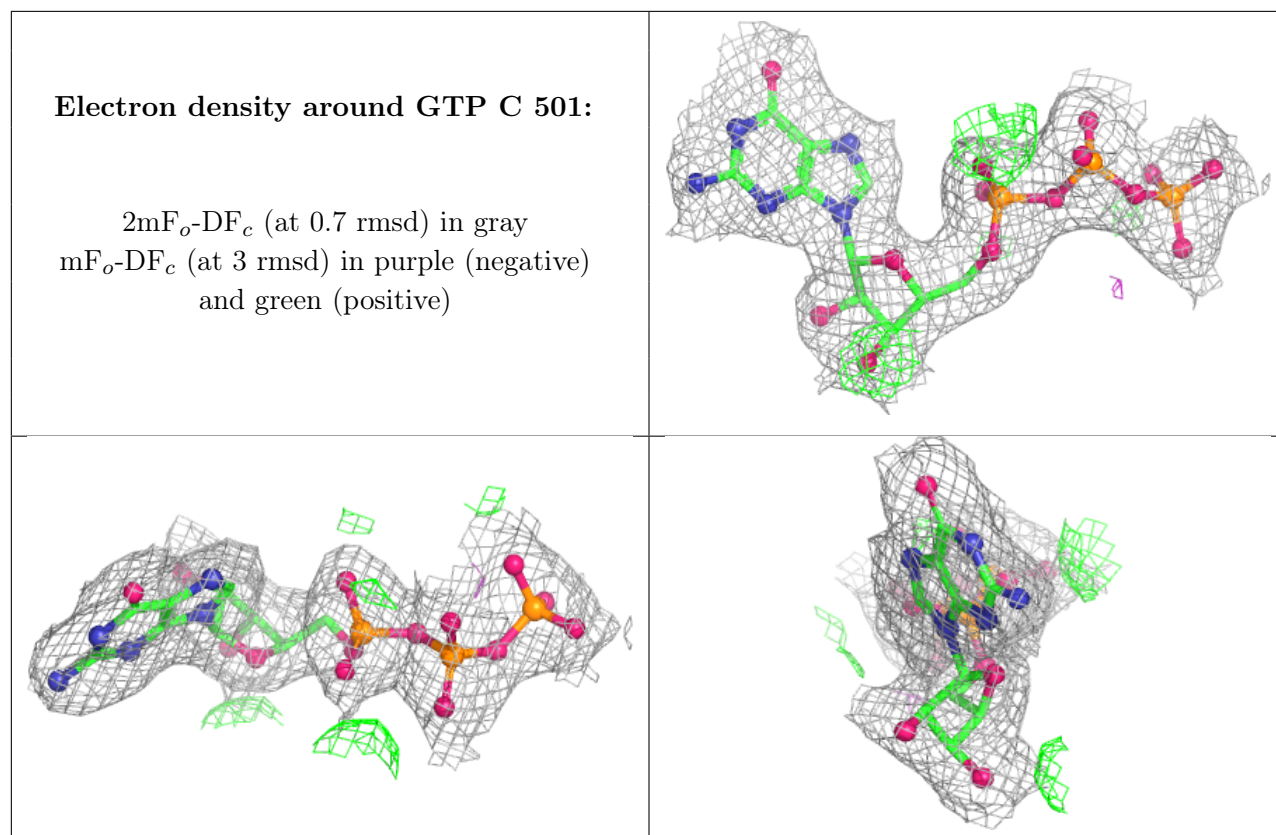
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around GDP B 501:

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





6.5 Other polymers [i](#)

There are no such residues in this entry.