



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:39 AM UTC

PDB ID : 5LYJ / pdb_00005lyj
Title : Tubulin-Combretastatin A4 complex
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Deposited on : 2016-09-28
Resolution : 2.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ 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

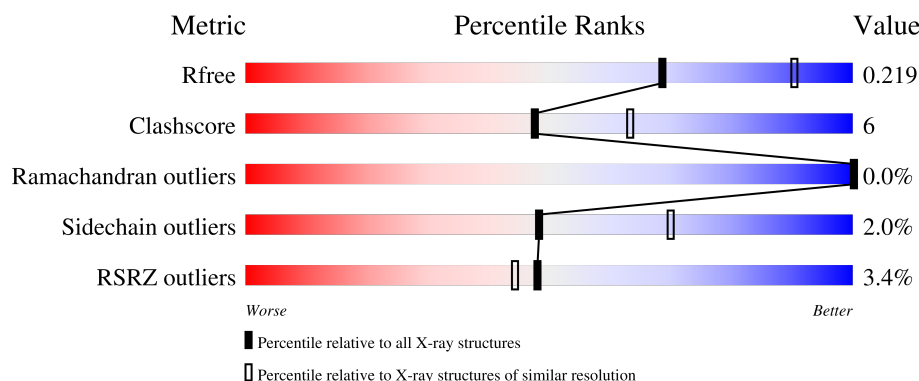
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	451	2% 85% 12%
1	C	451	0% 84% 13%
2	B	445	2% 79% 16%
2	D	445	4% 80% 16%
3	E	143	5% 78% 8% 14%

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Mol	Chain	Length	Quality of chain
4	F	384	 A horizontal bar chart showing the quality of chain F. The bar is divided into four segments: red (7%), green (69%), yellow (16%), and grey (14%). The segments are labeled with their respective percentages: 7%, 69%, 16%, and 14%.

2 Entry composition [i](#)

There are 13 unique types of molecules in this entry. The entry contains 17669 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	0	0
			3430	2170	583	655	22			
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	0	1	0
			3351	2106	573	646	26			
2	D	427	Total	C	N	O	S	0	0	0
			3349	2101	572	650	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			

There are 2 discrepancies between the modelled and reference sequences:

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

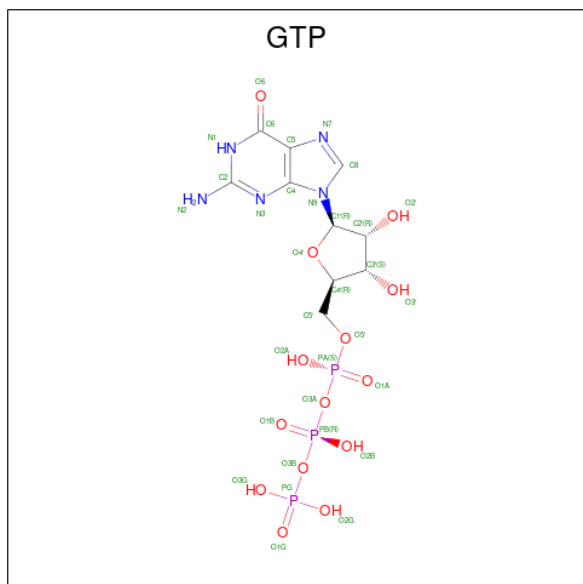
- Molecule 4 is a protein called Tubulin-tyrosine ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	332	Total	C	N	O	S	0	1	0
			2714	1740	464	495	15			

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		

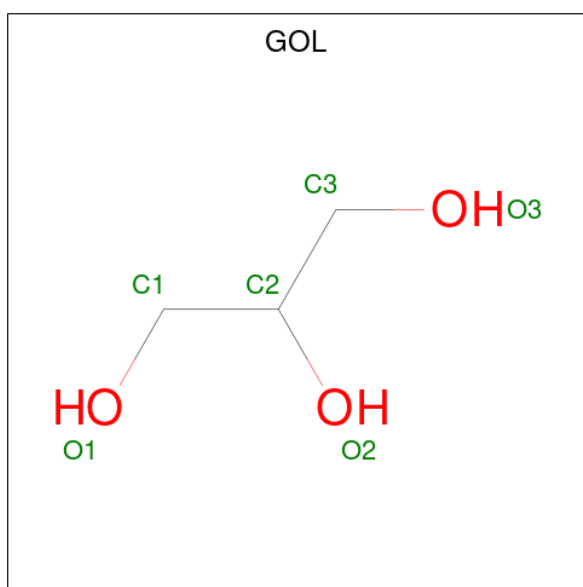
- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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		
6	D	1	Total	Mg	0	0
			1	1		

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

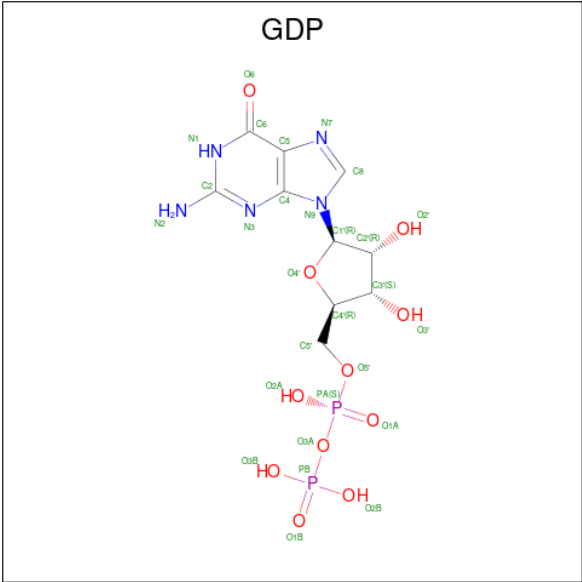
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Ca	0	0
			1	1		
7	B	2	Total	Ca	0	0
			2	2		
7	C	1	Total	Ca	0	0
			1	1		
7	E	1	Total	Ca	0	0
			1	1		

- Molecule 8 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



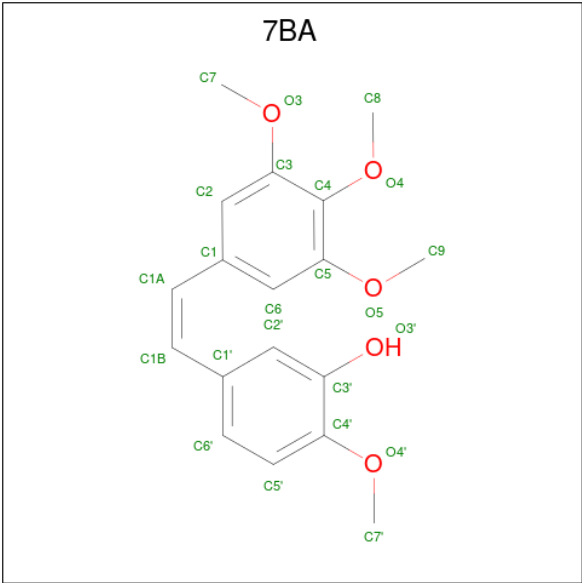
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			6	3	3		

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



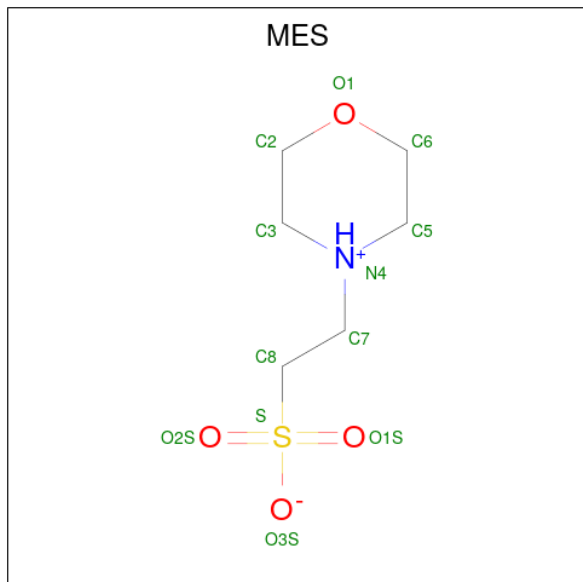
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	B	1	Total 28	C 10	N 5	O 11	P 2	0	0
9	D	1	Total 28	C 10	N 5	O 11	P 2	0	0

- Molecule 10 is Combretastatin A4 (CCD ID: 7BA) (formula: C₁₈H₂₀O₅).



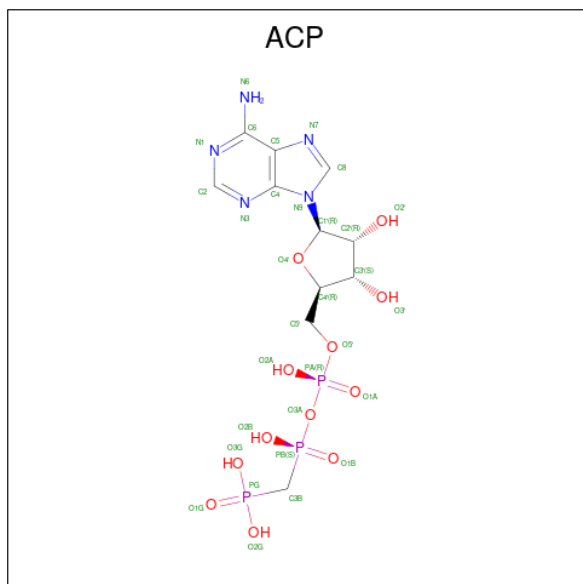
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	B	1	Total	C	O	0	0
			23	18	5		
10	D	1	Total	C	O	0	0
			23	18	5		

- Molecule 11 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: $C_6H_{13}NO_4S$).



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

- 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		

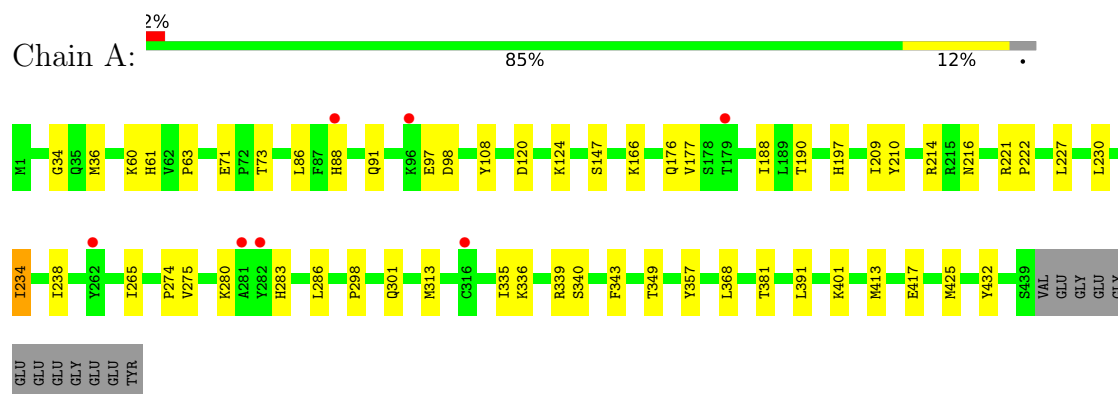
- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	30	Total 30	O 30	0	0
13	B	29	Total 29	O 29	0	0
13	C	75	Total 75	O 75	0	0
13	D	6	Total 6	O 6	0	0
13	E	3	Total 3	O 3	0	0
13	F	4	Total 4	O 4	0	0

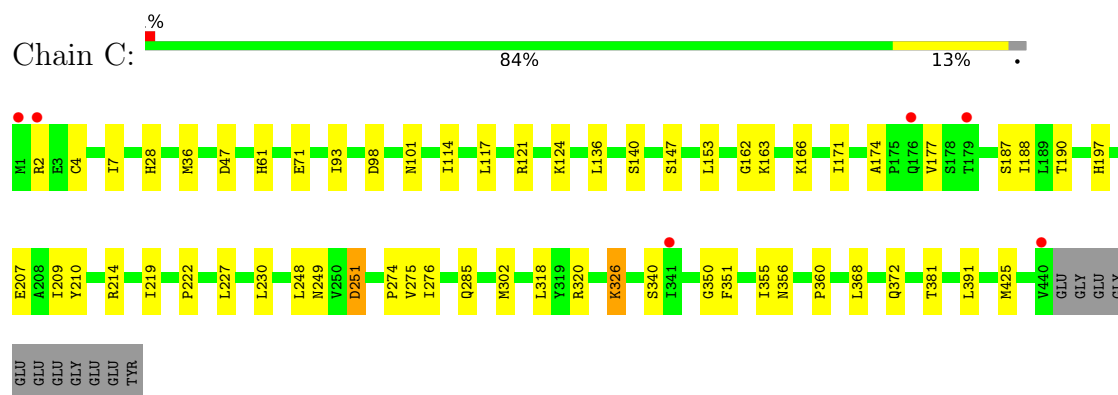
3 Residue-property plots

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.

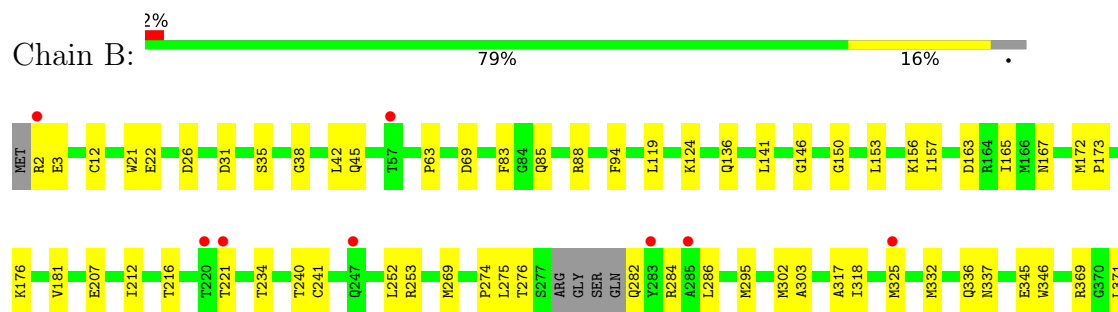
• Molecule 1: Tubulin alpha-1B chain

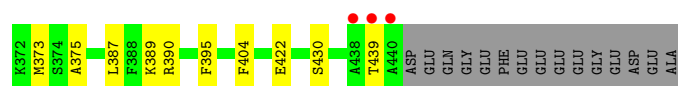


• Molecule 1: Tubulin alpha-1B chain

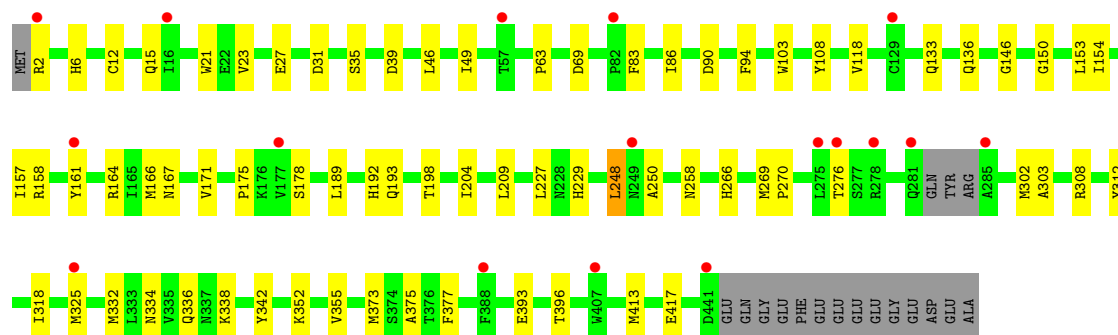
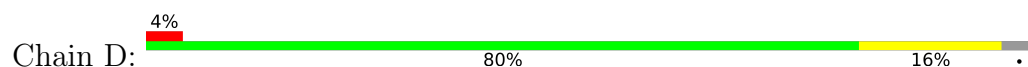


• Molecule 2: Tubulin beta-2B chain

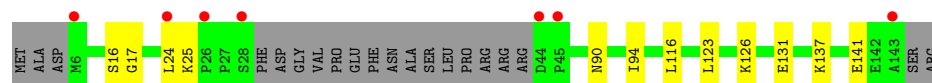
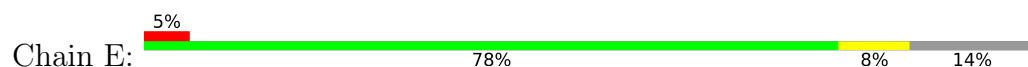




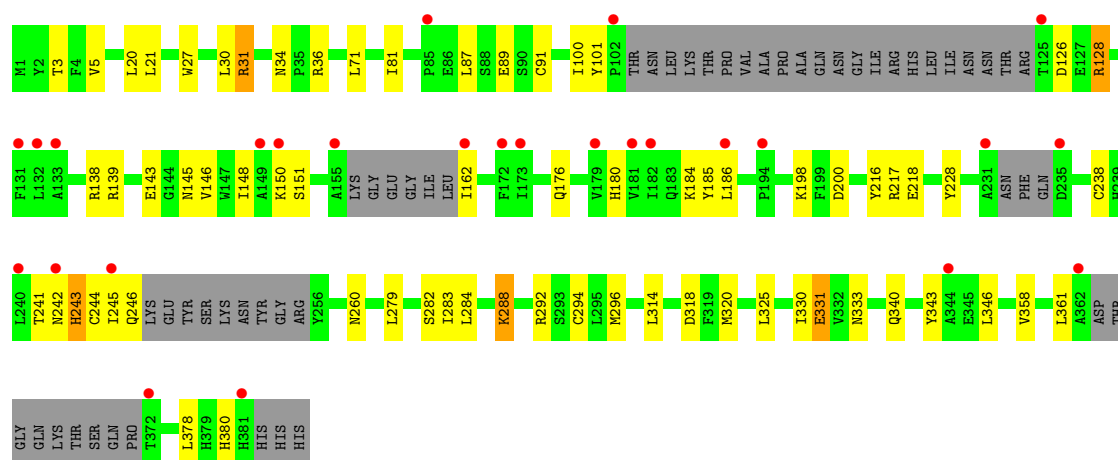
• Molecule 2: Tubulin beta-2B chain



• 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	104.59Å 157.17Å 180.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.43 – 2.40 49.43 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.6 (49.43-2.40) 99.6 (49.43-2.40)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.37 (at 2.39Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.191 , 0.217 0.194 , 0.219	Depositor DCC
R_{free} test set	5823 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	60.2	Xtriage
Anisotropy	0.160	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 52.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	17669	wwPDB-VP
Average B, all atoms (Å ²)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.63% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, MES, 7BA, CA, GTP, GDP, ACP, GOL

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	0.25	0/3508	0.48	0/4762
1	C	0.30	0/3521	0.51	0/4780
2	B	0.28	0/3428	0.50	0/4643
2	D	0.23	0/3422	0.45	0/4635
3	E	0.26	0/1022	0.36	0/1356
4	F	0.19	0/2777	0.40	0/3750
All	All	0.26	0/17678	0.47	0/23926

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 [i](#)

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	3430	0	3339	40	0
1	C	3440	0	3353	36	0
2	B	3351	0	3233	45	0
2	D	3349	0	3223	40	0
3	E	1014	0	1029	8	0
4	F	2714	0	2682	38	0
5	A	32	0	12	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
6	D	1	0	0	0	0
7	A	1	0	0	0	0
7	B	2	0	0	0	0
7	C	1	0	0	0	0
7	E	1	0	0	0	0
8	A	6	0	8	1	0
9	B	28	0	12	1	0
9	D	28	0	12	1	0
10	B	23	0	0	0	0
10	D	23	0	0	1	0
11	B	12	0	12	1	0
12	F	31	0	14	3	0
13	A	30	0	0	1	0
13	B	29	0	0	0	0
13	C	75	0	0	1	0
13	D	6	0	0	0	0
13	E	3	0	0	0	0
13	F	4	0	0	0	0
All	All	17669	0	16941	193	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 (193) 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:270:PRO:HG2	2:D:302:MET:HB2	1.68	0.73
4:F:186:LEU:HD12	4:F:320:MET:HG2	1.72	0.70
1:A:71:GLU:HG2	1:A:98:ASP:HB3	1.73	0.70
2:B:253[A]:ARG:NH1	11:B:504:MES:O2S	2.20	0.69
1:C:101:ASN:HD22	2:D:258:ASN:HD21	1.43	0.67
2:B:173:PRO:O	2:B:390:ARG:NH2	2.28	0.66
4:F:246:GLN:OE1	4:F:260:ASN:ND2	2.29	0.65
2:B:2:ARG:NH1	2:B:3:GLU:OE1	2.29	0.65
4:F:184:LYS:NZ	4:F:185:TYR:O	2.27	0.65
1:C:47:ASP:OD2	13:C:601:HOH:O	2.13	0.65
1:A:221:ARG:HD2	2:B:325:MET:HB3	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:MET:HB3	1:A:61:HIS:CE1	2.35	0.61
2:B:345:GLU:OE1	2:B:345:GLU:N	2.30	0.61
2:B:295:MET:HE3	2:B:375:ALA:HB1	1.83	0.60
2:B:439:THR:HG21	4:F:31:ARG:HH21	1.65	0.60
1:C:71:GLU:HG2	1:C:98:ASP:HB3	1.82	0.60
2:D:175:PRO:HA	2:D:178:SER:HB2	1.82	0.60
1:A:343:PHE:CD1	1:A:349:THR:HG23	2.37	0.60
1:C:285:GLN:OE1	1:C:372:GLN:NE2	2.34	0.60
1:C:163:LYS:HE2	3:E:90:ASN:HA	1.83	0.59
1:A:97:GLU:OE2	2:B:253[B]:ARG:NH1	2.31	0.59
2:B:119:LEU:HD11	2:B:156:LYS:HB3	1.84	0.59
2:B:274:PRO:HB3	2:B:286:LEU:HD22	1.85	0.59
1:A:166:LYS:HE2	1:A:197:HIS:O	2.03	0.58
4:F:318:ASP:OD2	12:F:401:ACP:O3G	2.22	0.58
1:A:210:TYR:CE2	1:A:214:ARG:HD2	2.39	0.57
2:D:269:MET:HG3	2:D:303:ALA:HB3	1.85	0.57
4:F:139:ARG:HG2	4:F:145:ASN:HD22	1.71	0.56
1:C:209:ILE:HG22	1:C:227:LEU:HD22	1.88	0.56
2:B:172:MET:HG3	2:B:387:LEU:HD11	1.87	0.56
2:B:241:CYS:SG	2:B:318:ILE:HD12	2.47	0.55
4:F:282:SER:HB2	4:F:325:LEU:HD13	1.89	0.55
2:B:240:THR:HB	2:B:318:ILE:HD13	1.90	0.54
4:F:5:VAL:HG12	4:F:30:LEU:HB2	1.89	0.54
2:B:136:GLN:HA	2:B:167:ASN:O	2.09	0.54
2:B:146:GLY:O	2:B:150:GLY:HA3	2.08	0.53
1:C:249:ASN:OD1	1:C:356:ASN:ND2	2.41	0.53
1:C:7:ILE:HG21	1:C:153:LEU:HD21	1.90	0.53
2:D:193:GLN:OE1	3:E:126:LYS:NZ	2.29	0.53
1:C:4[B]:CYS:SG	1:C:136:LEU:HG	2.50	0.52
1:A:88:HIS:N	1:A:91:GLN:OE1	2.39	0.52
2:D:118:VAL:HG11	2:D:153:LEU:HD11	1.92	0.52
2:D:393:GLU:O	2:D:396:THR:HG22	2.10	0.52
4:F:284:LEU:O	4:F:288:LYS:HG3	2.10	0.52
1:A:209:ILE:HG23	1:A:230:LEU:HD23	1.92	0.51
1:C:209:ILE:HG23	1:C:230:LEU:HD23	1.91	0.51
2:D:6:HIS:CD2	2:D:21:TRP:HE1	2.28	0.51
2:D:248:LEU:HD23	2:D:250:ALA:HB2	1.91	0.51
3:E:137:LYS:O	3:E:141:GLU:HG2	2.10	0.51
1:A:34:GLY:HA3	1:A:60:LYS:HG3	1.93	0.51
2:B:69:ASP:O	2:B:94:PHE:HA	2.11	0.51
1:A:280:LYS:O	1:A:283:HIS:NE2	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:12:CYS:HB2	9:D:501:GDP:C8	2.45	0.50
1:A:209:ILE:HG22	1:A:227:LEU:HD22	1.94	0.50
1:C:210:TYR:CZ	1:C:222:PRO:HD2	2.46	0.50
2:D:171:VAL:HA	2:D:204:ILE:O	2.12	0.49
1:C:320:ARG:HA	1:C:356:ASN:O	2.11	0.49
4:F:331:GLU:OE2	12:F:401:ACP:O3G	2.29	0.49
2:B:337:ASN:OD1	4:F:36:ARG:NH1	2.46	0.49
4:F:71:LEU:HD11	4:F:294:CYS:HB3	1.93	0.49
2:B:395:PHE:CE1	2:B:422:GLU:HB2	2.48	0.49
4:F:138:ARG:HG3	4:F:143:GLU:HB3	1.93	0.49
1:A:336:LYS:HG2	3:E:24:LEU:HD23	1.94	0.49
1:A:108:TYR:CE2	1:A:413:MET:HG3	2.48	0.48
2:D:108:TYR:OH	2:D:417:GLU:OE2	2.28	0.48
2:B:31:ASP:OD2	2:B:35:SER:HB2	2.13	0.48
1:A:188:ILE:HG13	1:A:425:MET:HG3	1.96	0.48
2:B:141:LEU:HD12	2:B:172:MET:SD	2.54	0.48
1:C:147:SER:HB2	1:C:190:THR:HB	1.95	0.48
1:A:176:GLN:HG2	1:A:210:TYR:CE2	2.48	0.48
2:D:198:THR:HG1	2:D:266:HIS:HE2	1.62	0.48
4:F:151:SER:HB3	4:F:180:HIS:CD2	2.49	0.48
4:F:296[A]:MET:HE2	4:F:380:HIS:HB2	1.95	0.48
1:C:93:ILE:HD11	1:C:121:ARG:HG3	1.94	0.48
1:A:147:SER:HB2	1:A:190:THR:HB	1.95	0.47
4:F:148:ILE:HD12	4:F:162:ILE:HG12	1.95	0.47
2:D:325:MET:SD	2:D:355:VAL:HG11	2.54	0.47
1:C:209:ILE:HD11	1:C:302:MET:SD	2.55	0.47
1:C:117:LEU:HD11	1:C:121:ARG:NH2	2.29	0.47
1:A:274:PRO:HB3	1:A:286:LEU:HD12	1.96	0.47
2:D:153:LEU:O	2:D:157:ILE:HG13	2.14	0.47
4:F:139:ARG:HG2	4:F:145:ASN:ND2	2.29	0.47
1:A:401:LYS:HG3	2:B:346:TRP:CE3	2.49	0.47
2:B:234:THR:OG1	2:B:302:MET:SD	2.71	0.47
2:B:276:THR:HG21	2:B:371:LEU:HD21	1.97	0.46
1:C:36:MET:HB3	1:C:61:HIS:CE1	2.50	0.46
1:C:174:ALA:HB1	1:C:207:GLU:HB2	1.97	0.46
1:A:176:GLN:HG2	1:A:210:TYR:CD2	2.50	0.46
1:C:2:ARG:NH2	1:C:251:ASP:OD2	2.47	0.46
2:B:181:VAL:HG21	2:B:404:PHE:CZ	2.51	0.46
1:C:350:GLY:C	1:C:351:PHE:HD1	2.23	0.46
2:D:209:LEU:HB3	2:D:227:LEU:HD22	1.97	0.46
1:A:216:ASN:ND2	8:A:504:GOL:H2	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:176:LYS:HD2	2:B:207:GLU:HG3	1.98	0.46
4:F:242:ASN:O	4:F:243:HIS:HB3	2.15	0.46
1:A:413:MET:HE3	1:A:417:GLU:HB3	1.98	0.46
2:B:212:ILE:HG23	2:B:275:LEU:HD13	1.97	0.46
2:B:373:MET:HE2	2:B:373:MET:HB3	1.75	0.46
4:F:292:ARG:HG3	4:F:378:LEU:HD23	1.97	0.46
1:A:63:PRO:HD3	1:A:86:LEU:HG	1.97	0.45
2:B:26:ASP:OD2	2:B:369:ARG:HD2	2.16	0.45
1:A:275:VAL:HG13	1:A:368:LEU:HD21	1.97	0.45
2:D:189:LEU:O	2:D:192:HIS:HB3	2.16	0.45
1:A:298:PRO:HA	1:A:301:GLN:CD	2.42	0.45
4:F:228:TYR:HA	4:F:238:CYS:SG	2.57	0.45
4:F:217:ARG:HG3	4:F:218:GLU:HG2	1.99	0.45
2:B:163:ASP:O	2:B:253[A]:ARG:NH2	2.45	0.45
1:A:176:GLN:HB2	13:A:621:HOH:O	2.17	0.45
2:B:21:TRP:CZ3	2:B:63:PRO:HB3	2.52	0.44
2:B:165:ILE:HG21	2:B:252:LEU:HB3	1.98	0.44
1:A:391:LEU:HD12	1:A:391:LEU:HA	1.89	0.44
2:D:146:GLY:O	2:D:150:GLY:HA3	2.17	0.44
4:F:340:GLN:HA	4:F:343:TYR:CD2	2.52	0.44
1:C:274:PRO:HB2	1:C:276:ILE:HG12	2.00	0.44
4:F:284:LEU:HD12	4:F:284:LEU:HA	1.75	0.44
2:B:153:LEU:O	2:B:157:ILE:HG13	2.18	0.44
2:D:318:ILE:HG12	10:D:503:7BA:C8	2.48	0.44
2:D:334:ASN:OD1	2:D:338:LYS:HE3	2.16	0.44
1:C:188:ILE:HG13	1:C:425:MET:HG3	2.00	0.44
1:C:248:LEU:HD13	1:C:355:ILE:HD12	1.99	0.44
1:C:320:ARG:HG3	1:C:360:PRO:HG3	1.99	0.44
1:C:368:LEU:HD23	1:C:368:LEU:HA	1.68	0.44
2:D:136:GLN:HA	2:D:167:ASN:O	2.17	0.44
2:D:103:TRP:CE3	2:D:189:LEU:HD13	2.53	0.44
2:D:158:ARG:HG2	3:E:123:LEU:HD11	1.99	0.44
1:A:265:ILE:HG23	1:A:432:TYR:CZ	2.53	0.43
2:D:312:TYR:CE1	2:D:377:PHE:HZ	2.36	0.43
2:D:2:ARG:HB3	2:D:133:GLN:HE21	1.83	0.43
1:C:210:TYR:CE1	1:C:222:PRO:HD2	2.53	0.43
1:C:214:ARG:HG2	1:C:219:ILE:O	2.19	0.43
2:B:38:GLY:HA3	2:B:45:GLN:OE1	2.17	0.43
2:B:269:MET:HG2	2:B:303:ALA:HB3	2.01	0.43
1:C:166:LYS:HE2	1:C:197:HIS:O	2.19	0.43
4:F:279:LEU:HD12	4:F:283:ILE:HB	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:ASP:OD2	1:A:124:LYS:HE2	2.18	0.43
2:B:163:ASP:OD1	2:B:163:ASP:N	2.49	0.43
2:D:23:VAL:O	2:D:27:GLU:HG3	2.17	0.43
1:A:234:ILE:O	1:A:238:ILE:HG13	2.18	0.43
1:A:336:LYS:HD2	1:A:336:LYS:HA	1.82	0.43
4:F:185:TYR:OH	4:F:198:LYS:NZ	2.44	0.43
2:D:318:ILE:O	2:D:375:ALA:HA	2.19	0.42
2:B:221:THR:HG21	1:C:326:LYS:HA	2.01	0.42
1:A:280:LYS:HB2	1:A:280:LYS:HE3	1.79	0.42
1:C:28:HIS:O	1:C:36:MET:HE3	2.20	0.42
2:D:161:TYR:HB3	2:D:164:ARG:HG2	2.01	0.42
2:B:389:LYS:HE3	2:B:389:LYS:HB2	1.87	0.42
1:A:335:ILE:HG23	1:A:339:ARG:HG3	2.00	0.42
2:D:31:ASP:OD2	2:D:35:SER:HB2	2.19	0.42
2:D:46:LEU:HA	2:D:49:ILE:HB	2.00	0.42
1:A:221:ARG:CD	2:B:325:MET:HB3	2.47	0.42
4:F:340:GLN:HA	4:F:343:TYR:HD2	1.84	0.42
2:D:332:MET:O	2:D:336:GLN:HG3	2.20	0.42
1:A:210:TYR:CE1	1:A:222:PRO:HD2	2.55	0.42
1:C:124:LYS:HB3	1:C:124:LYS:HE3	1.84	0.42
2:B:332:MET:O	2:B:336:GLN:HG3	2.20	0.42
1:C:140:SER:HA	1:C:171:ILE:HB	2.02	0.42
2:D:39:ASP:OD1	2:D:39:ASP:N	2.46	0.42
1:A:357:TYR:CE2	3:E:17:GLY:HA2	2.55	0.41
2:B:282:GLN:HG3	2:B:284:ARG:H	1.85	0.41
4:F:101:TYR:HD1	4:F:126:ASP:HB2	1.84	0.41
1:C:93:ILE:HG22	1:C:114:ILE:HD11	2.02	0.41
2:D:154:ILE:HG23	2:D:166:MET:HG2	2.01	0.41
4:F:89:GLU:OE1	4:F:89:GLU:N	2.34	0.41
2:B:22:GLU:HG2	2:B:83:PHE:CD1	2.55	0.41
1:C:187:SER:HB3	1:C:391:LEU:HD21	2.02	0.41
2:B:88:ARG:HH21	2:B:124:LYS:NZ	2.19	0.41
1:A:280:LYS:HB3	1:A:283:HIS:NE2	2.35	0.41
2:B:216:THR:HG21	2:B:275:LEU:HD12	2.02	0.41
1:C:162:GLY:HA2	3:E:94:ILE:HD11	2.02	0.41
2:D:21:TRP:CZ3	2:D:63:PRO:HB3	2.55	0.41
2:D:69:ASP:O	2:D:94:PHE:HA	2.20	0.41
2:D:373:MET:HE2	2:D:373:MET:HB3	1.92	0.41
2:D:413:MET:HE2	2:D:413:MET:HB3	1.92	0.41
4:F:81:ILE:HG12	4:F:87:LEU:HD13	2.03	0.41
1:A:313:MET:HE3	1:A:313:MET:HB2	1.92	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:12:CYS:HB2	9:B:501:GDP:C8	2.56	0.41
2:D:83:PHE:O	2:D:86:ILE:HG22	2.21	0.41
2:D:308:ARG:HG2	2:D:342:TYR:CZ	2.56	0.41
4:F:101:TYR:N	4:F:126:ASP:OD1	2.47	0.41
1:A:71:GLU:OE2	1:A:73:THR:OG1	2.31	0.41
1:A:98:ASP:HB2	5:A:501:GTP:O1G	2.20	0.41
1:C:275:VAL:HG13	1:C:368:LEU:HD21	2.01	0.41
4:F:27:TRP:HE1	4:F:361:LEU:HD21	1.86	0.41
4:F:30:LEU:HD13	4:F:34:ASN:ND2	2.35	0.41
4:F:100:ILE:HD12	4:F:128:ARG:HA	2.03	0.41
4:F:216:TYR:CD2	4:F:346:LEU:HD13	2.56	0.41
4:F:21:LEU:O	4:F:27:TRP:HB2	2.20	0.41
3:E:116:LEU:HD23	3:E:116:LEU:HA	1.86	0.40
2:B:295:MET:HE1	2:B:317:ALA:HB1	2.02	0.40
4:F:150:LYS:NZ	12:F:401:ACP:O2A	2.54	0.40
4:F:330:ILE:HD13	4:F:330:ILE:HA	1.92	0.40
4:F:146:VAL:O	4:F:184:LYS:NZ	2.39	0.40
2:D:21:TRP:CE3	2:D:63:PRO:HB3	2.56	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	437/451 (97%)	423 (97%)	14 (3%)	0	100	100
1	C	439/451 (97%)	427 (97%)	12 (3%)	0	100	100
2	B	422/445 (95%)	414 (98%)	8 (2%)	0	100	100
2	D	423/445 (95%)	415 (98%)	8 (2%)	0	100	100
3	E	119/143 (83%)	117 (98%)	2 (2%)	0	100	100
4	F	321/384 (84%)	306 (95%)	14 (4%)	1 (0%)	36	50

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	2161/2319 (93%)	2102 (97%)	58 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	F	243	HIS

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	370/379 (98%)	366 (99%)	4 (1%)	65	82
1	C	372/379 (98%)	366 (98%)	6 (2%)	55	76
2	B	368/383 (96%)	365 (99%)	3 (1%)	73	86
2	D	368/383 (96%)	362 (98%)	6 (2%)	55	76
3	E	110/127 (87%)	107 (97%)	3 (3%)	39	62
4	F	298/342 (87%)	283 (95%)	15 (5%)	22	38
All	All	1886/1993 (95%)	1849 (98%)	37 (2%)	48	70

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	177	VAL
1	A	234	ILE
1	A	340	SER
1	A	381	THR
2	B	42	LEU
2	B	85	GLN
2	B	430	SER
1	C	177	VAL
1	C	251	ASP
1	C	318	LEU
1	C	326	LYS

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Mol	Chain	Res	Type
1	C	340	SER
1	C	381	THR
2	D	15	GLN
2	D	90	ASP
2	D	229	HIS
2	D	248	LEU
2	D	276	THR
2	D	352	LYS
3	E	16	SER
3	E	25	LYS
3	E	131	GLU
4	F	3	THR
4	F	20	LEU
4	F	31	ARG
4	F	91	CYS
4	F	128	ARG
4	F	176	GLN
4	F	200	ASP
4	F	241	THR
4	F	244	CYS
4	F	245	ILE
4	F	288	LYS
4	F	314	LEU
4	F	331	GLU
4	F	333	ASN
4	F	358	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	A	285	GLN
1	A	300	ASN
1	A	301	GLN
2	B	8	GLN
2	B	14	ASN
2	B	37	HIS
2	B	85	GLN
2	B	136	GLN
2	B	385	GLN
2	B	433	GLN
1	C	393	HIS

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Mol	Chain	Res	Type
2	D	331	GLN
2	D	436	GLN
3	E	12	ASN
3	E	108	ASN
4	F	269	GLN
4	F	333	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	$\# Z > 2$
10	7BA	B	503	-	24,24,24	0.95	2 (8%)	32,32,32	2.23	10 (31%)
10	7BA	D	503	-	24,24,24	0.99	2 (8%)	32,32,32	2.95	10 (31%)
12	ACP	F	401	-	31,33,33	1.91	10 (32%)	47,52,52	1.75	10 (21%)
9	GDP	D	501	6	29,30,30	1.20	4 (13%)	45,47,47	1.71	6 (13%)
9	GDP	B	501	6	29,30,30	1.15	3 (10%)	45,47,47	1.77	9 (20%)
5	GTP	A	501	6	33,34,34	0.91	0	50,54,54	1.58	12 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	GOL	A	504	-	5,5,5	0.34	0	5,5,5	0.37	0
11	MES	B	504	-	12,12,12	2.21	1 (8%)	15,16,16	1.84	2 (13%)
5	GTP	C	501	6	33,34,34	1.00	2 (6%)	50,54,54	1.61	11 (22%)

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
10	7BA	B	503	-	-	9/13/13/13	0/2/2/2
10	7BA	D	503	-	-	13/13/13/13	0/2/2/2
12	ACP	F	401	-	-	9/19/38/38	0/3/3/3
9	GDP	D	501	6	-	5/16/32/32	0/3/3/3
9	GDP	B	501	6	-	5/16/32/32	0/3/3/3
5	GTP	A	501	6	-	7/22/38/38	0/3/3/3
8	GOL	A	504	-	-	3/4/4/4	-
11	MES	B	504	-	-	1/6/14/14	0/1/1/1
5	GTP	C	501	6	-	8/22/38/38	0/3/3/3

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	B	504	MES	C8-S	-7.40	1.67	1.77
12	F	401	ACP	C5-C4	4.68	1.47	1.39
12	F	401	ACP	PB-O1B	4.23	1.61	1.51
12	F	401	ACP	PB-O2B	-3.33	1.48	1.56
12	F	401	ACP	PB-O3A	3.22	1.62	1.58
9	D	501	GDP	C5-C4	3.08	1.47	1.38
12	F	401	ACP	PG-O2G	2.88	1.61	1.55
12	F	401	ACP	PG-O3G	2.84	1.61	1.55
9	B	501	GDP	C5-C4	2.82	1.46	1.38
12	F	401	ACP	C5-C6	2.65	1.48	1.41
9	B	501	GDP	C6-N1	-2.59	1.34	1.38
10	B	503	7BA	C1'-C1B	-2.54	1.40	1.47
10	D	503	7BA	C1'-C1B	-2.33	1.40	1.47
12	F	401	ACP	C5-N7	-2.32	1.34	1.39
12	F	401	ACP	C8-N7	2.25	1.36	1.31
9	D	501	GDP	C6-N1	-2.25	1.34	1.38
5	C	501	GTP	PB-O3A	2.25	1.61	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	D	503	7BA	C1-C1A	-2.24	1.41	1.47
12	F	401	ACP	PA-O3A	2.24	1.61	1.59
9	B	501	GDP	PA-O3A	2.23	1.61	1.59
9	D	501	GDP	PA-O3A	2.23	1.61	1.59
10	B	503	7BA	C1-C1A	-2.22	1.41	1.47
9	D	501	GDP	C5-N7	-2.14	1.34	1.39
5	C	501	GTP	PA-O3A	2.11	1.61	1.59

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	D	503	7BA	O4'-C4'-C3'	8.81	127.77	114.55
10	D	503	7BA	C7'-O4'-C4'	7.23	128.12	117.51
10	D	503	7BA	C7-O3-C3	6.43	126.95	117.51
9	D	501	GDP	C5-C4-N3	-5.85	119.09	128.39
9	B	501	GDP	C5-C4-N3	-5.78	119.19	128.39
12	F	401	ACP	C5-C4-N3	-5.58	119.04	126.72
10	D	503	7BA	O4'-C4'-C5'	-5.52	114.99	124.30
11	B	504	MES	C5-N4-C3	5.26	120.18	108.84
10	B	503	7BA	C7'-O4'-C4'	5.19	125.12	117.51
10	B	503	7BA	O4'-C4'-C3'	5.07	122.15	114.55
9	B	501	GDP	C2-N3-C4	4.77	120.51	112.30
9	D	501	GDP	C2-N3-C4	4.75	120.49	112.30
10	D	503	7BA	O5-C5-C4	4.74	123.26	115.14
9	B	501	GDP	N9-C4-N3	4.65	135.26	125.95
12	F	401	ACP	N3-C4-N9	4.59	134.97	127.17
5	C	501	GTP	C2-N3-C4	4.44	119.95	112.30
5	A	501	GTP	C2-N3-C4	4.40	119.88	112.30
5	C	501	GTP	C5-C4-N3	-4.34	121.48	128.39
10	B	503	7BA	C8-O4-C4	4.30	126.42	114.74
10	B	503	7BA	C7-O3-C3	4.24	123.73	117.51
9	D	501	GDP	N9-C4-N3	4.24	134.43	125.95
5	A	501	GTP	C5-C4-N3	-4.18	121.74	128.39
10	B	503	7BA	O5-C5-C4	3.91	121.84	115.14
12	F	401	ACP	C2-N3-C4	3.60	120.62	111.83
10	D	503	7BA	O5-C5-C6	-3.37	118.27	124.08
5	C	501	GTP	N9-C8-N7	-3.33	107.23	113.40
9	B	501	GDP	C6-C5-N7	3.28	136.27	130.29
9	D	501	GDP	C6-C5-N7	3.25	136.21	130.29
12	F	401	ACP	N3-C2-N1	-3.25	123.67	128.58
12	F	401	ACP	C4-C5-N7	-3.21	106.91	110.58
10	B	503	7BA	O4'-C4'-C5'	-3.11	119.06	124.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	B	504	MES	O1S-S-C8	2.99	111.25	106.73
10	D	503	7BA	O3-C3-C2	-2.88	119.12	124.08
10	D	503	7BA	O3-C3-C4	2.88	120.07	115.14
5	C	501	GTP	N9-C4-N3	2.87	131.69	125.95
5	A	501	GTP	N9-C8-N7	-2.87	108.08	113.40
12	F	401	ACP	C4-N9-C8	2.84	108.72	105.74
5	C	501	GTP	C8-N7-C5	2.83	109.30	104.26
5	A	501	GTP	O3'-C3'-C4'	-2.82	102.97	111.08
10	B	503	7BA	O3-C3-C2	-2.82	119.22	124.08
5	C	501	GTP	O2B-PB-O3A	2.80	114.85	107.27
10	B	503	7BA	O5-C5-C6	-2.76	119.31	124.08
10	B	503	7BA	O4-C4-C5	2.74	124.06	120.12
5	C	501	GTP	C2-N1-C6	-2.68	120.25	125.11
10	B	503	7BA	O3-C3-C4	2.63	119.64	115.14
5	C	501	GTP	O3'-C3'-C4'	-2.62	103.56	111.08
9	D	501	GDP	C4-C5-N7	-2.58	106.58	110.67
5	A	501	GTP	C2-N1-C6	-2.56	120.47	125.11
9	B	501	GDP	C4-C5-N7	-2.50	106.70	110.67
5	A	501	GTP	C8-N7-C5	2.50	108.71	104.26
5	A	501	GTP	O2G-PG-O3B	2.45	112.84	104.64
5	C	501	GTP	O6-C6-C5	-2.41	120.17	126.53
5	A	501	GTP	N9-C4-N3	2.39	130.74	125.95
5	C	501	GTP	C5-C6-N1	2.39	119.33	113.25
10	D	503	7BA	C9-O5-C5	2.34	120.95	117.51
12	F	401	ACP	C5-N7-C8	2.32	107.10	103.45
12	F	401	ACP	PB-O3A-PA	-2.29	124.88	132.37
9	B	501	GDP	O2A-PA-O3A	2.29	113.46	107.27
9	B	501	GDP	O6-C6-C5	-2.28	120.51	126.53
5	A	501	GTP	O2A-PA-O3A	2.28	113.43	107.27
12	F	401	ACP	C3'-C2'-C1'	2.27	105.75	101.46
5	A	501	GTP	O6-C6-C5	-2.26	120.56	126.53
5	A	501	GTP	C5-C6-N1	2.25	118.98	113.25
10	D	503	7BA	C5'-C4'-C3'	-2.24	117.22	119.87
9	D	501	GDP	O6-C6-C5	-2.21	120.70	126.53
5	A	501	GTP	N2-C2-N1	2.17	121.34	116.76
9	B	501	GDP	O3'-C3'-C4'	-2.11	105.01	111.08
12	F	401	ACP	C2'-C1'-N9	-2.06	108.20	113.30
9	B	501	GDP	C5-C6-N1	2.05	118.47	113.25
5	C	501	GTP	N2-C2-N1	2.02	121.03	116.76

There are no chirality outliers.

All (60) 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-O3A
5	A	501	GTP	C5'-O5'-PA-O1A
5	A	501	GTP	C5'-O5'-PA-O2A
5	C	501	GTP	C5'-O5'-PA-O3A
5	C	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O2A
8	A	504	GOL	O1-C1-C2-C3
9	B	501	GDP	C5'-O5'-PA-O3A
9	B	501	GDP	C5'-O5'-PA-O1A
9	B	501	GDP	C5'-O5'-PA-O2A
9	D	501	GDP	C5'-O5'-PA-O3A
9	D	501	GDP	C5'-O5'-PA-O1A
12	F	401	ACP	PG-C3B-PB-O1B
12	F	401	ACP	PG-C3B-PB-O2B
12	F	401	ACP	PG-C3B-PB-O3A
12	F	401	ACP	C5'-O5'-PA-O2A
10	D	503	7BA	C5'-C4'-O4'-C7'
10	D	503	7BA	C3'-C4'-O4'-C7'
12	F	401	ACP	O4'-C4'-C5'-O5'
10	D	503	7BA	C6-C5-O5-C9
10	D	503	7BA	C2-C3-O3-C7
10	B	503	7BA	C5'-C4'-O4'-C7'
10	D	503	7BA	C4-C3-O3-C7
10	B	503	7BA	C3'-C4'-O4'-C7'
10	D	503	7BA	C4-C5-O5-C9
8	A	504	GOL	O1-C1-C2-O2
10	B	503	7BA	C2-C1-C1A-C1B
10	B	503	7BA	C3-C4-O4-C8
12	F	401	ACP	C3'-C4'-C5'-O5'
10	B	503	7BA	C6-C1-C1A-C1B
10	D	503	7BA	C6'-C1'-C1B-C1A
10	D	503	7BA	C3-C4-O4-C8
10	D	503	7BA	C2-C1-C1A-C1B
10	D	503	7BA	C2'-C1'-C1B-C1A
11	B	504	MES	C8-C7-N4-C3
10	B	503	7BA	C6'-C1'-C1B-C1A
10	D	503	7BA	C6-C1-C1A-C1B
10	B	503	7BA	C2'-C1'-C1B-C1A
10	D	503	7BA	C5-C4-O4-C8
10	B	503	7BA	C5-C4-O4-C8
9	D	501	GDP	C5'-O5'-PA-O2A
12	F	401	ACP	C5'-O5'-PA-O1A

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Mol	Chain	Res	Type	Atoms
12	F	401	ACP	C5'-O5'-PA-O3A
12	F	401	ACP	PB-O3A-PA-O1A
9	D	501	GDP	PB-O3A-PA-O2A
5	C	501	GTP	C4'-C5'-O5'-PA
5	A	501	GTP	PB-O3B-PG-O1G
5	C	501	GTP	PB-O3B-PG-O1G
8	A	504	GOL	C1-C2-C3-O3
5	A	501	GTP	PB-O3B-PG-O3G
5	C	501	GTP	PB-O3B-PG-O3G
5	A	501	GTP	PB-O3A-PA-O2A
5	C	501	GTP	PB-O3A-PA-O2A
9	B	501	GDP	PB-O3A-PA-O1A
9	B	501	GDP	PB-O3A-PA-O2A
10	B	503	7BA	C1-C1A-C1B-C1'
10	D	503	7BA	C1-C1A-C1B-C1'
5	C	501	GTP	PB-O3A-PA-O1A
9	D	501	GDP	PB-O3A-PA-O1A

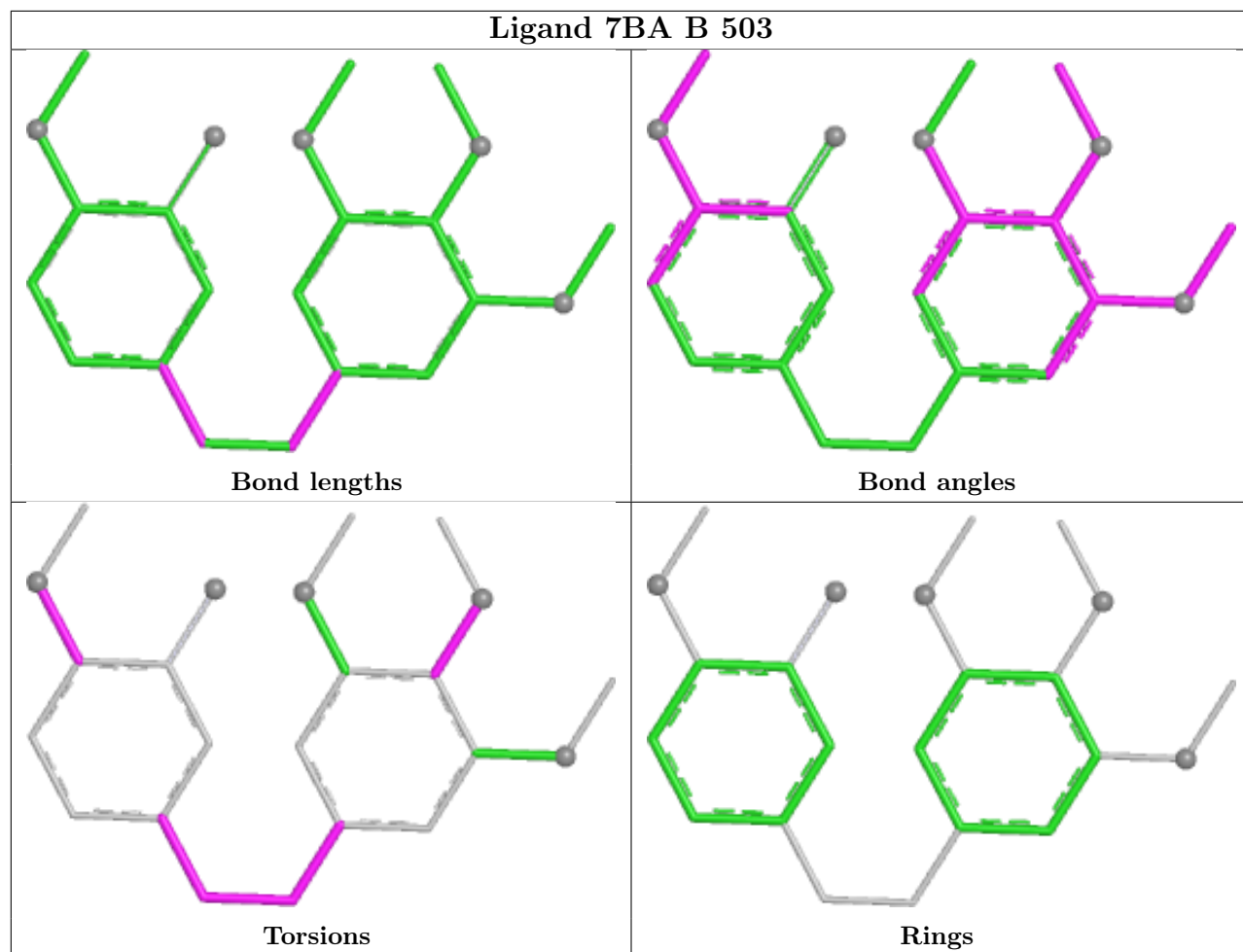
There are no ring outliers.

7 monomers are involved in 9 short contacts:

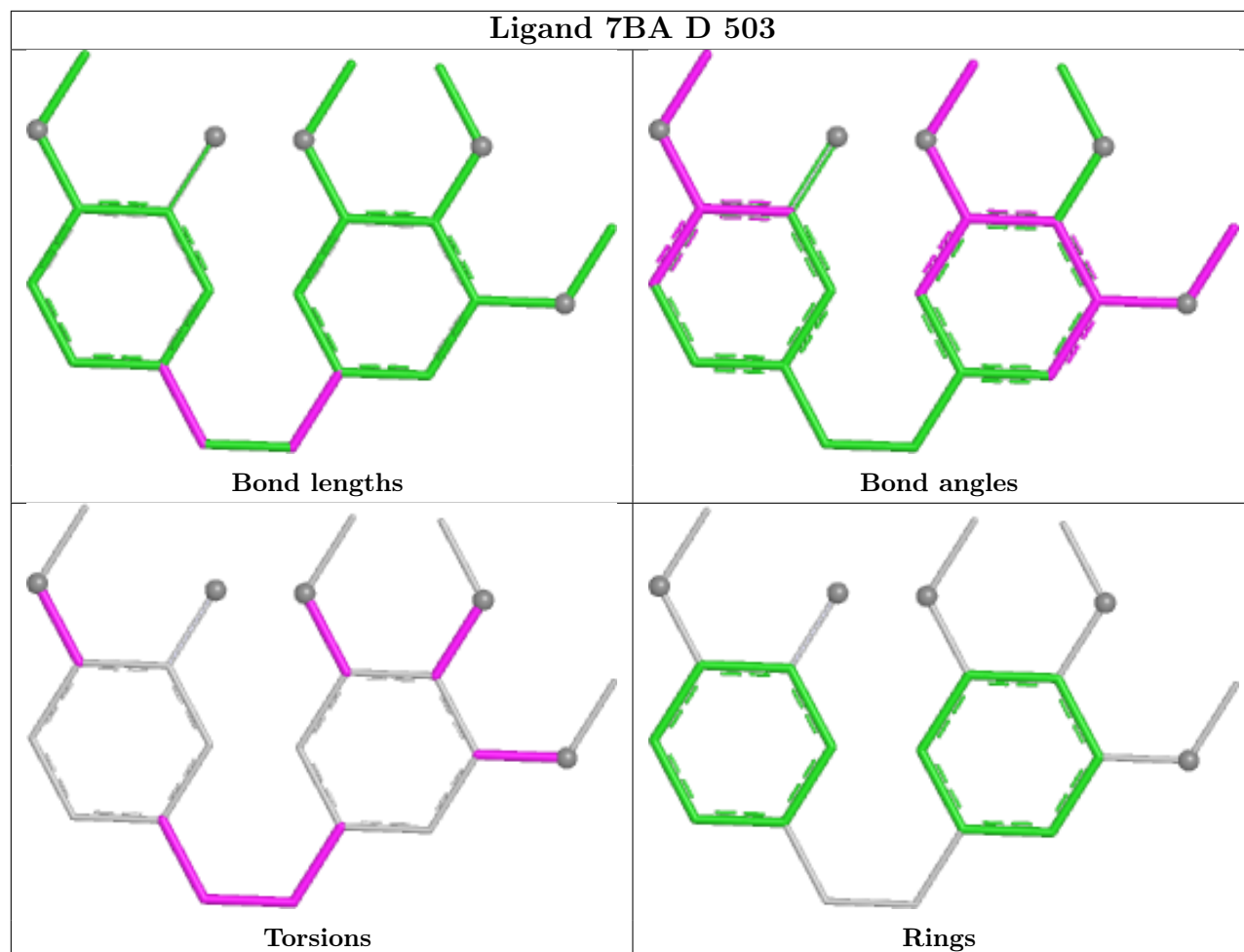
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	D	503	7BA	1	0
12	F	401	ACP	3	0
9	D	501	GDP	1	0
9	B	501	GDP	1	0
5	A	501	GTP	1	0
8	A	504	GOL	1	0
11	B	504	MES	1	0

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

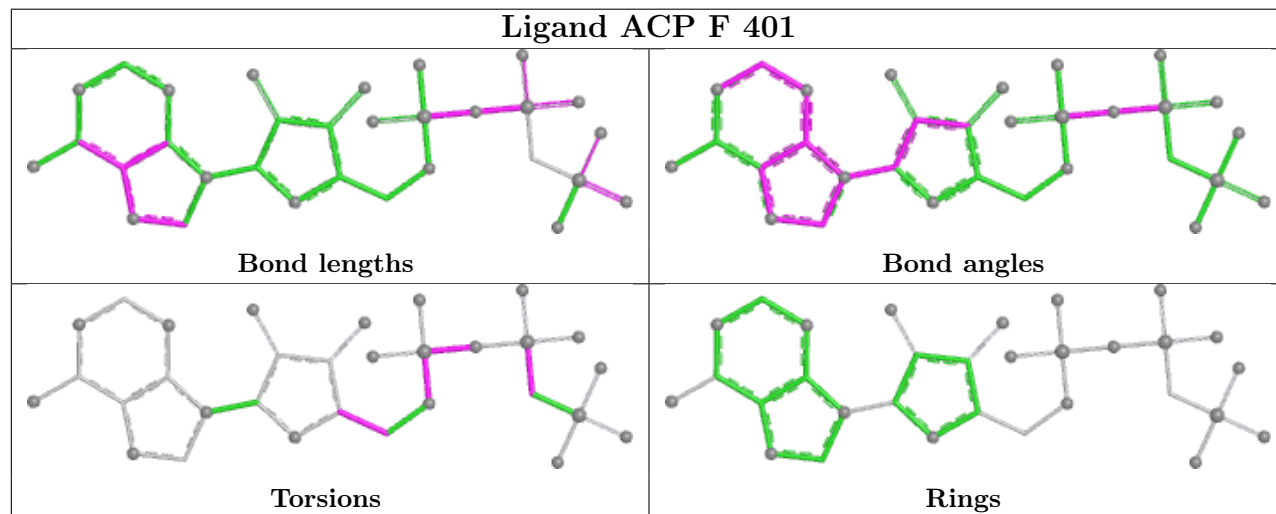
Ligand 7BA B 503

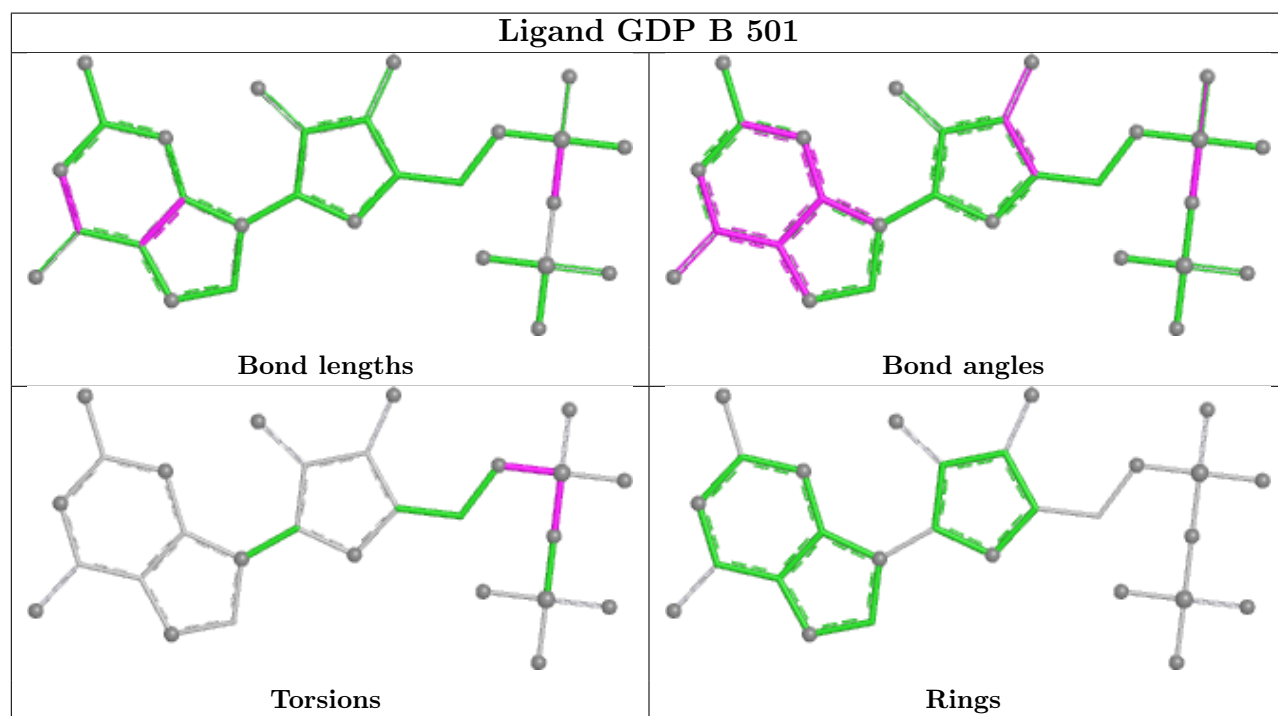
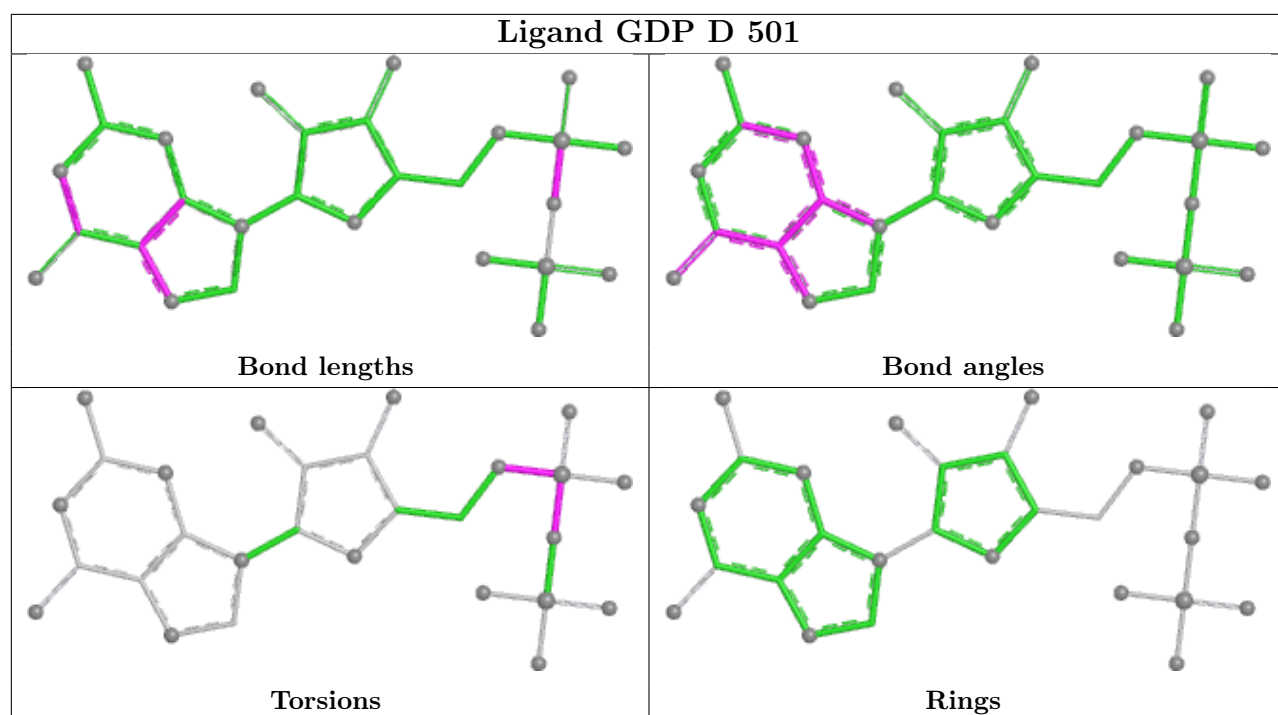


Ligand 7BA D 503

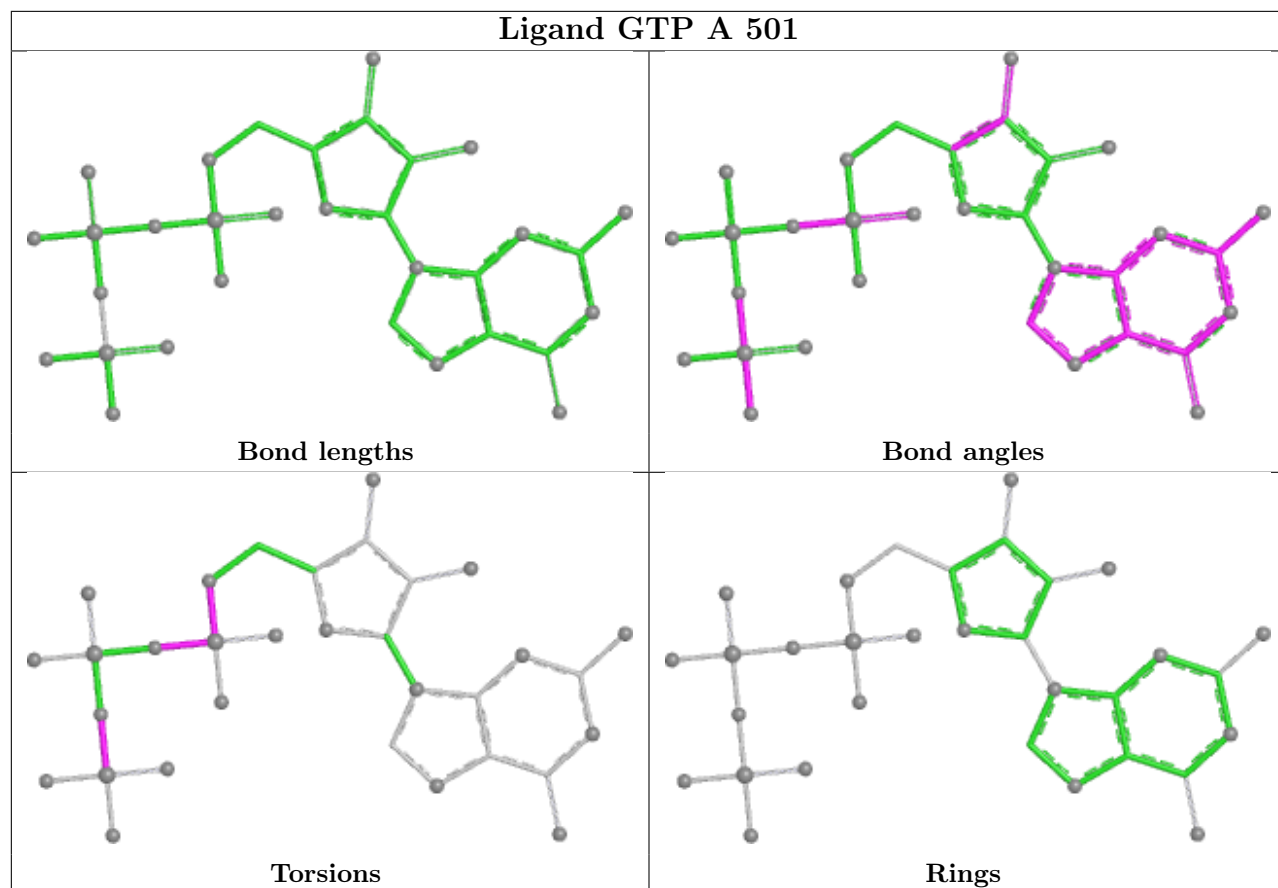


Ligand ACP F 401

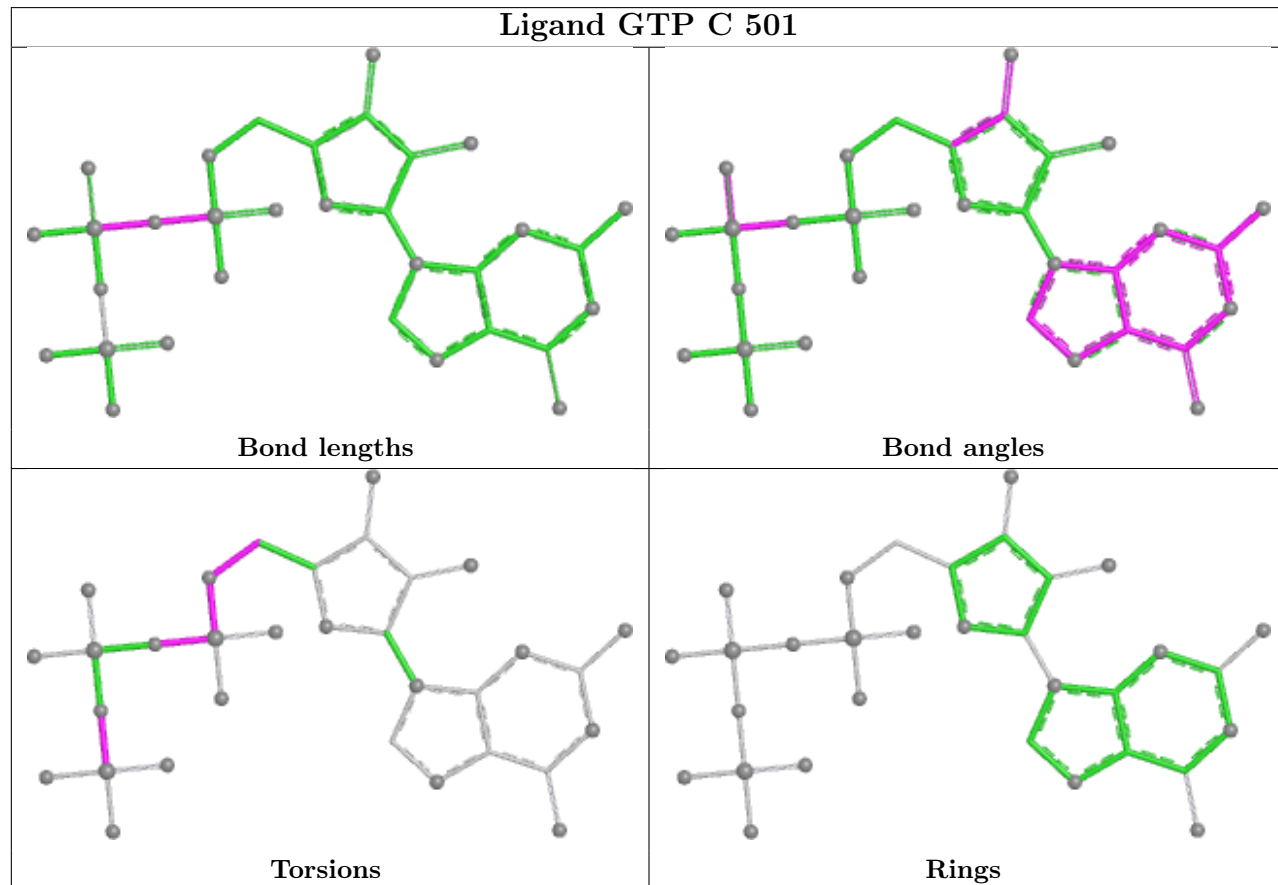




Ligand GTP A 501



Ligand GTP C 501



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	439/451 (97%)	0.20	7 (1%) 70 66	48, 73, 105, 152	0
1	C	440/451 (97%)	-0.14	6 (1%) 73 69	33, 56, 85, 100	1 (0%)
2	B	425/445 (95%)	0.07	11 (2%) 57 53	34, 64, 103, 143	3 (0%)
2	D	427/445 (95%)	0.45	17 (3%) 42 38	49, 87, 122, 145	4 (0%)
3	E	123/143 (86%)	0.43	7 (5%) 29 25	54, 84, 135, 161	0
4	F	332/384 (86%)	0.73	26 (7%) 19 15	41, 108, 161, 181	1 (0%)
All	All	2186/2319 (94%)	0.25	74 (3%) 48 44	33, 75, 131, 181	9 (0%)

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	155	ALA	5.2
2	D	285	ALA	5.2
1	C	176	GLN	4.6
4	F	231	ALA	4.6
4	F	186	LEU	4.0
1	C	440	VAL	3.9
2	B	438	ALA	3.8
4	F	372	THR	3.6
2	D	281	GLN	3.5
2	D	2	ARG	3.3
2	B	57	THR	3.2
4	F	125	THR	3.2
3	E	143	ALA	3.2
2	D	276	THR	3.2
2	B	440	ALA	3.2
4	F	240	LEU	3.2
1	C	179	THR	3.1
2	D	407	TRP	3.0
2	D	325	MET	3.0

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Mol	Chain	Res	Type	RSRZ
2	D	82	PRO	3.0
1	A	282	TYR	3.0
4	F	381	HIS	2.9
1	A	179	THR	2.9
2	B	325	MET	2.9
3	E	45	PRO	2.9
2	B	220	THR	2.9
4	F	344	ALA	2.8
4	F	179	VAL	2.8
4	F	362	ALA	2.8
4	F	245	ILE	2.7
1	A	96	LYS	2.6
2	B	221	THR	2.6
4	F	102	PRO	2.6
2	D	388	PHE	2.6
4	F	132	LEU	2.5
3	E	44	ASP	2.5
4	F	131	PHE	2.5
1	A	262	TYR	2.5
4	F	242	ASN	2.5
4	F	149	ALA	2.4
3	E	24	LEU	2.4
4	F	235	ASP	2.4
1	C	1	MET	2.3
1	A	316	CYS	2.3
2	D	161	TYR	2.3
4	F	85	PRO	2.3
1	C	341	ILE	2.3
4	F	173	ILE	2.3
4	F	181	VAL	2.3
2	D	278	ARG	2.3
1	C	2	ARG	2.3
2	D	57	THR	2.3
2	D	249	ASN	2.2
2	B	247	GLN	2.2
2	D	177	VAL	2.2
2	B	2	ARG	2.2
1	A	281	ALA	2.2
4	F	172	PHE	2.2
3	E	6	MET	2.2
2	B	283	TYR	2.2
4	F	182	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
2	D	441	ASP	2.2
3	E	26	PRO	2.2
4	F	133	ALA	2.2
2	B	439	THR	2.1
2	D	275	LEU	2.1
4	F	194	PRO	2.1
2	D	129	CYS	2.1
3	E	28	SER	2.1
4	F	150	LYS	2.1
2	B	285	ALA	2.0
2	D	16	ILE	2.0
4	F	162	ILE	2.0
1	A	88	HIS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	MG	D	502	1/1	0.73	0.14	99,99,99,99	0
12	ACP	F	401	31/31	0.87	0.10	119,125,136,138	0
8	GOL	A	504	6/6	0.90	0.14	87,90,98,101	0
9	GDP	D	501	28/28	0.92	0.10	70,77,85,87	0
7	CA	B	505	1/1	0.92	0.10	120,120,120,120	0
10	7BA	D	503	23/23	0.94	0.13	56,75,94,98	0
10	7BA	B	503	23/23	0.95	0.13	50,67,86,91	0
7	CA	B	506	1/1	0.95	0.12	94,94,94,94	0
7	CA	E	201	1/1	0.95	0.10	108,108,108,108	0
11	MES	B	504	12/12	0.96	0.08	63,67,71,71	0

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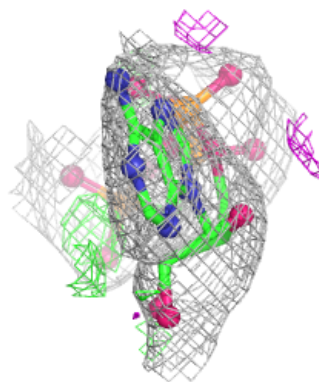
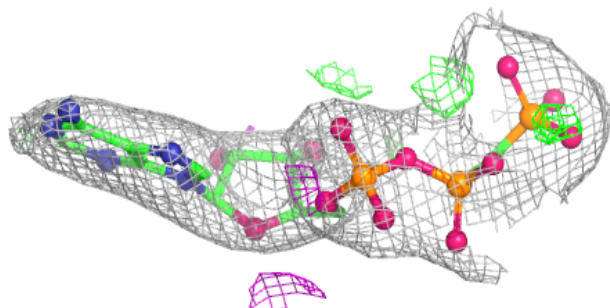
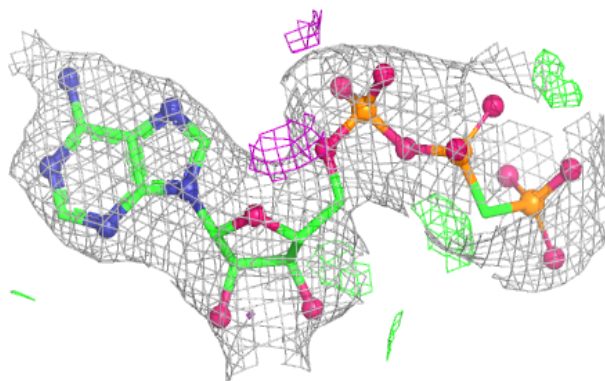
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	MG	C	502	1/1	0.96	0.10	53,53,53,53	0
9	GDP	B	501	28/28	0.98	0.06	38,47,53,58	0
5	GTP	A	501	32/32	0.98	0.05	46,57,62,66	0
5	GTP	C	501	32/32	0.98	0.05	41,46,51,52	0
7	CA	C	503	1/1	0.99	0.03	82,82,82,82	0
6	MG	B	502	1/1	0.99	0.08	47,47,47,47	0
7	CA	A	503	1/1	0.99	0.04	91,91,91,91	0
6	MG	A	502	1/1	1.00	0.06	69,69,69,69	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.

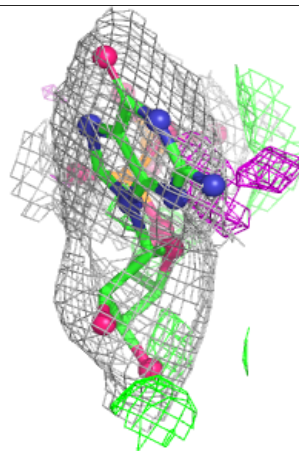
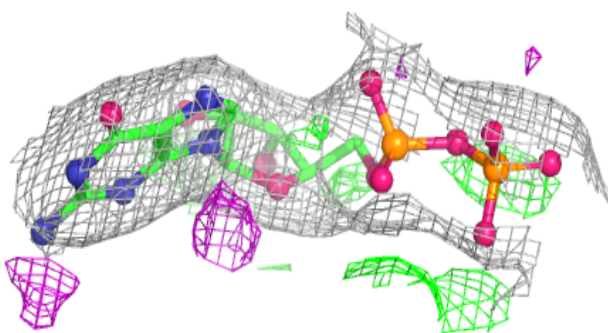
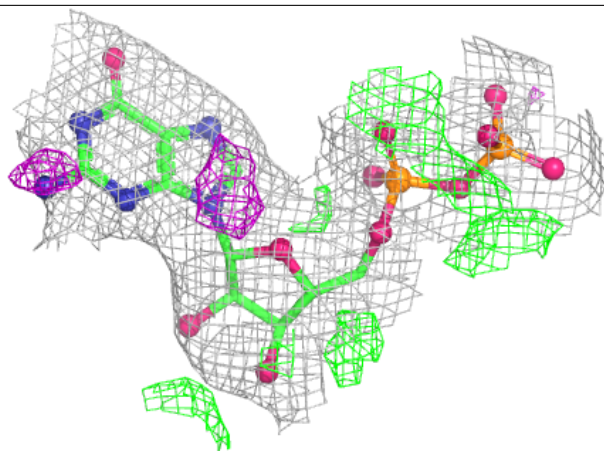
Electron density around ACP F 401:

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

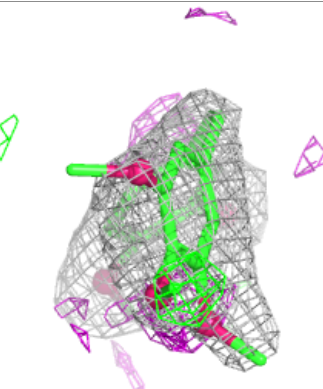
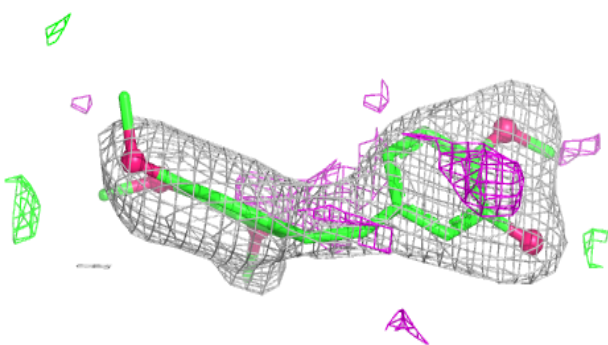
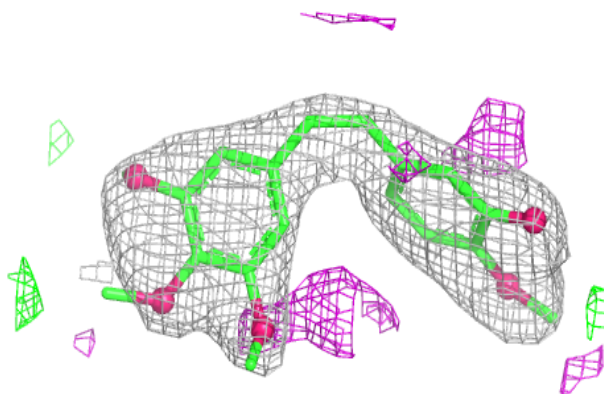


Electron density around GDP D 501:

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

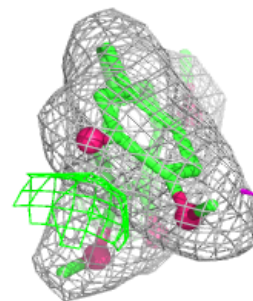
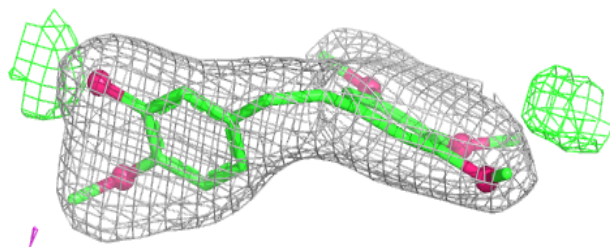
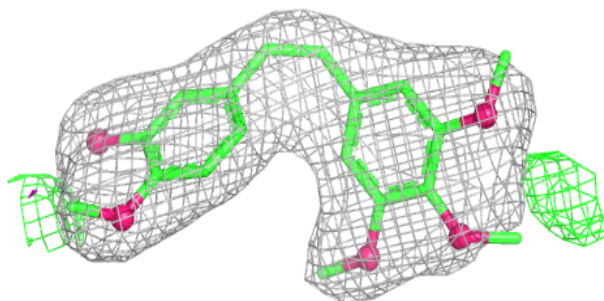
**Electron density around 7BA D 503:**

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



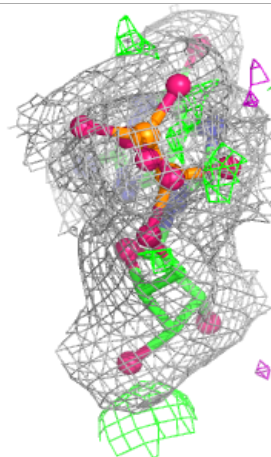
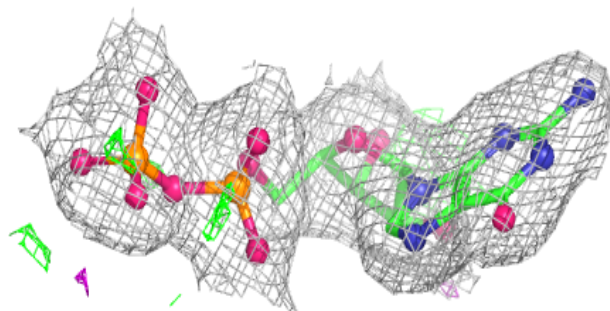
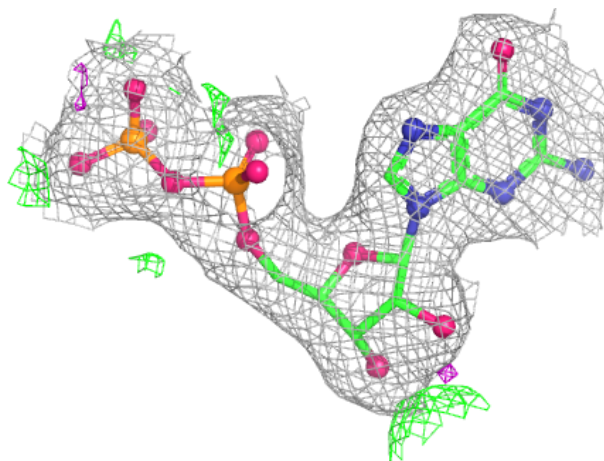
Electron density around 7BA B 503:

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



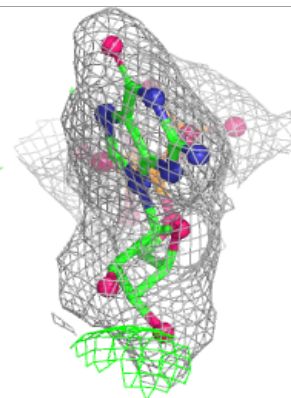
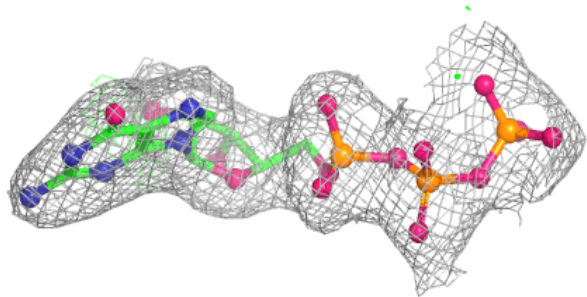
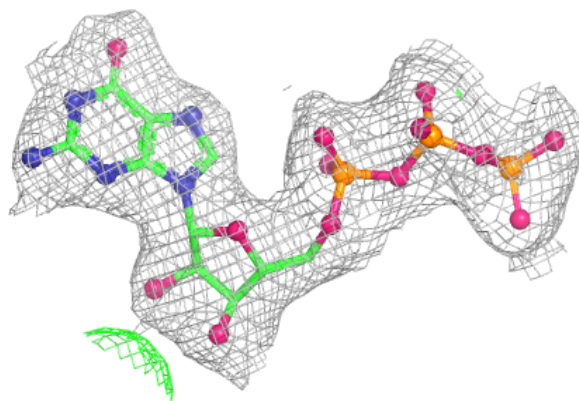
Electron density around GDP B 501:

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

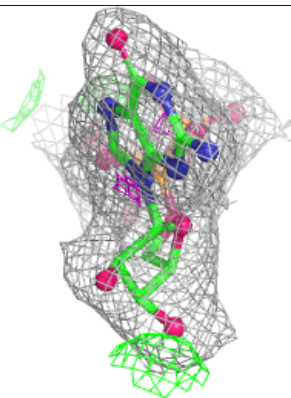
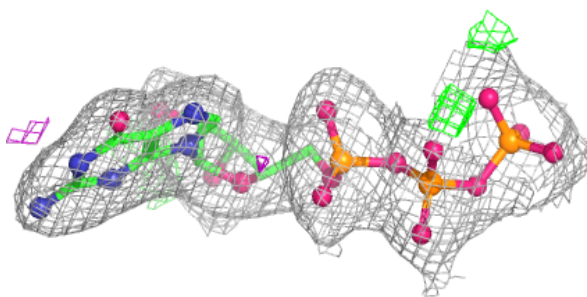
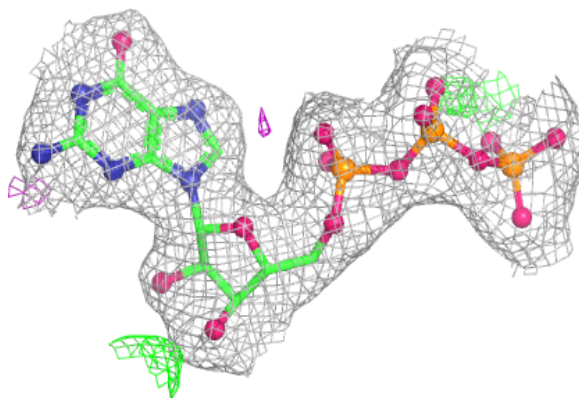


Electron density around GTP A 501:

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

**Electron density around 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.