



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 08:00 PM UTC

PDB ID : 8WMU / pdb_00008wmu
Title : Structural basis of tubulin and heterocyclic podophyllotoxins complex for anticancer agents with dual-binding sites
Authors : Zhao, W.; Bi, J.
Deposited on : 2023-10-04
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

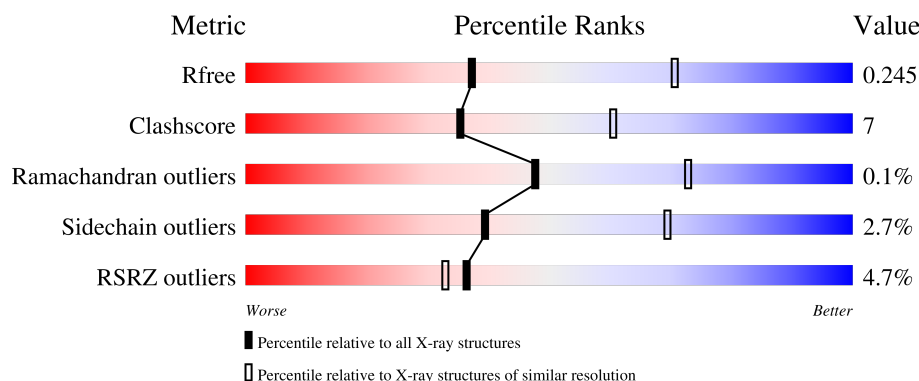
1 Overall quality at a glance

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	81% 17% .
1	C	440	85% 14%
2	B	431	3% 79% 18% ..
2	D	431	4% 81% 16% ..
3	E	138	2% 77% 8% . 14%

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Mol	Chain	Length	Quality of chain
4	F	380	14% 66% 16% • 18%

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 17170 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 Detyrosinated tubulin alpha-1B chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	434	Total	C	N	O	S	0	0	0
			3319	2105	565	627	22			
1	C	440	Total	C	N	O	S	0	0	0
			3423	2167	579	655	22			

- Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	423	Total	C	N	O	S	0	0	0
			3291	2072	555	637	27			
2	D	421	Total	C	N	O	S	0	0	0
			3244	2042	547	629	26			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	118	Total	C	N	O	S	0	0	0
			970	599	177	189	5			

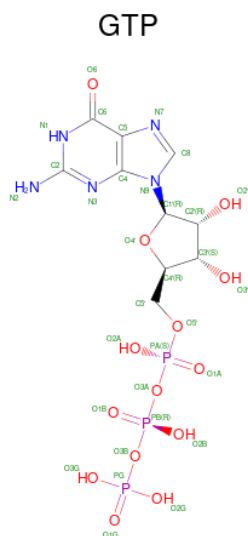
- Molecule 4 is a protein called Tubulin-tyrosine ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	313	Total	C	N	O	S	0	0	0
			2562	1651	436	461	14			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	379	HIS	-	expression tag	UNP A0A8C9FGJ1
F	380	HIS	-	expression tag	UNP A0A8C9FGJ1

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



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

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

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

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

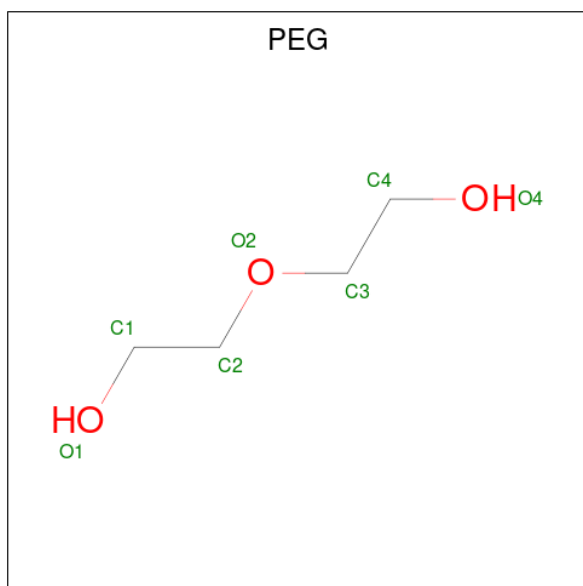
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total Ca 1 1	0	0
7	C	1	Total Ca 1 1	0	0

- Molecule 8 is GLYCEROL (CCD ID: GOL) (formula: $\text{C}_3\text{H}_8\text{O}_3$).



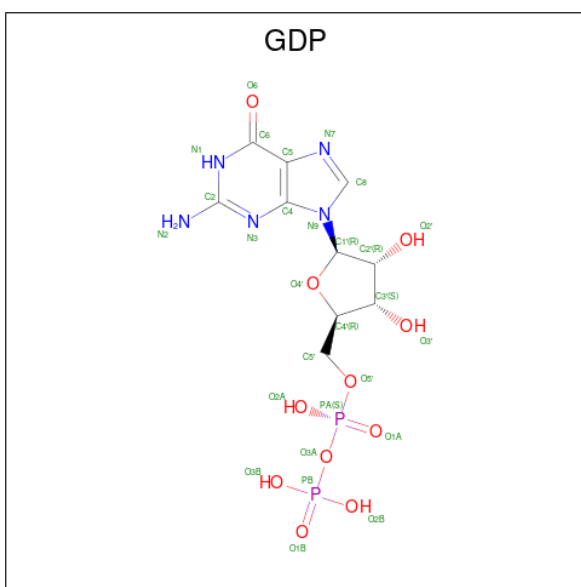
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 9 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



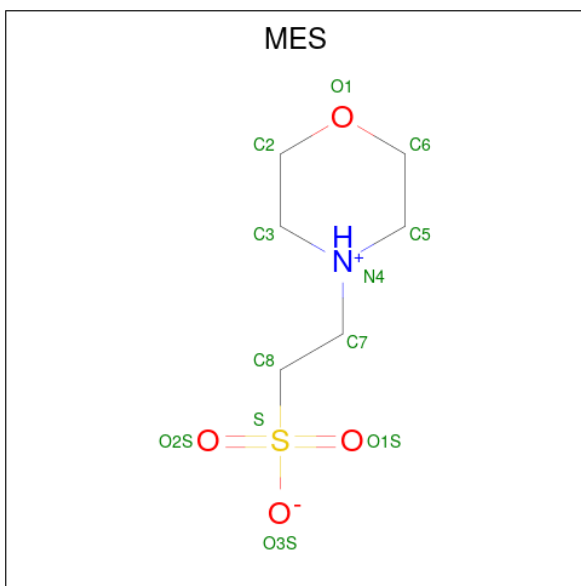
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			7	4	3		

- Molecule 10 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



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

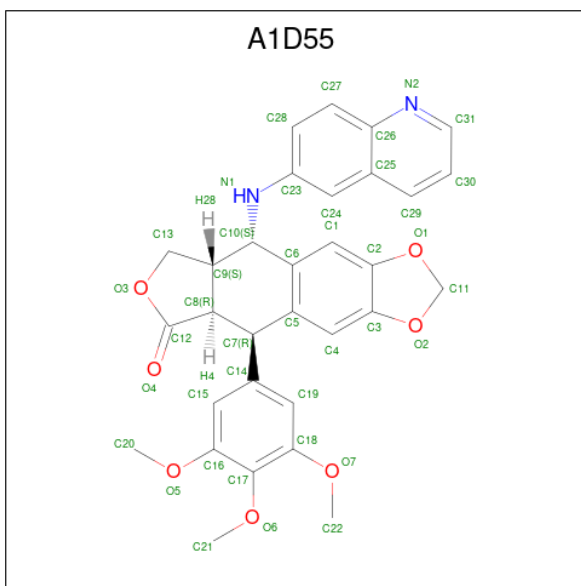
- Molecule 11 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: $C_6H_{13}NO_4S$).



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

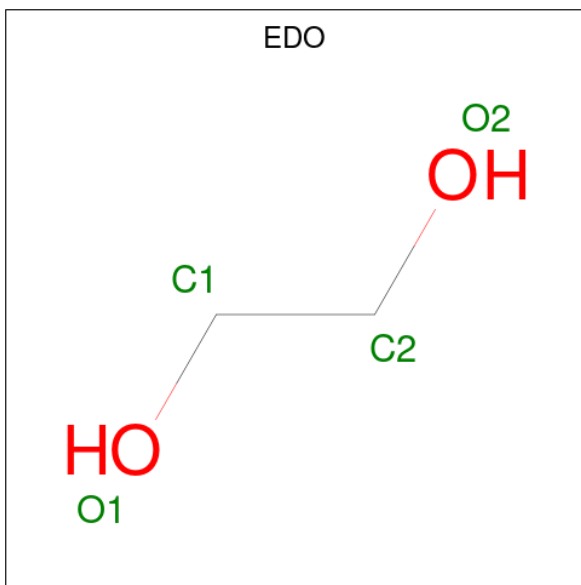
- Molecule 12 is (5 {S},5 {a} {S},8 {a} {R},9 {R})-5-(quinolin-6-ylamino)-9-(3,4,5-trimethoxyphenyl)-5 {a},6,8 {a},9-tetrahydro-5 {H}-[2]benzofuro[6,5-f][1,3]benzodioxol-8-one (CCD

ID: A1D55) (formula: $C_{31}H_{28}N_2O_7$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	B	1	Total	C	N	O	0	0
			40	31	2	7		

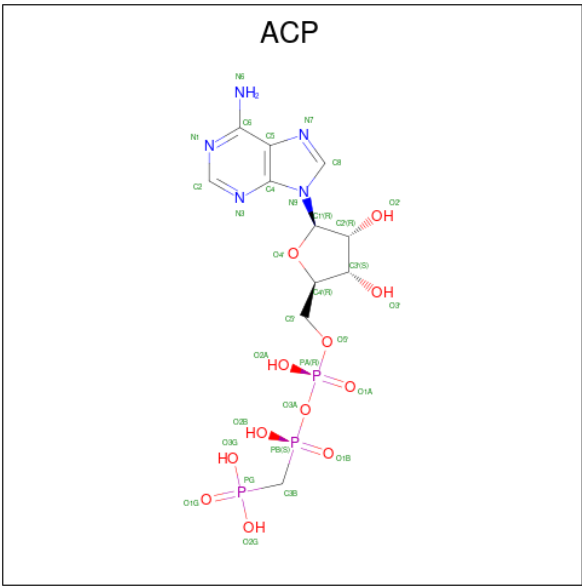
- Molecule 13 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	C	1	Total	C	O	0	0
			4	2	2		

- Molecule 14 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (CCD

ID: ACP) (formula: C₁₁H₁₈N₅O₁₂P₃).



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

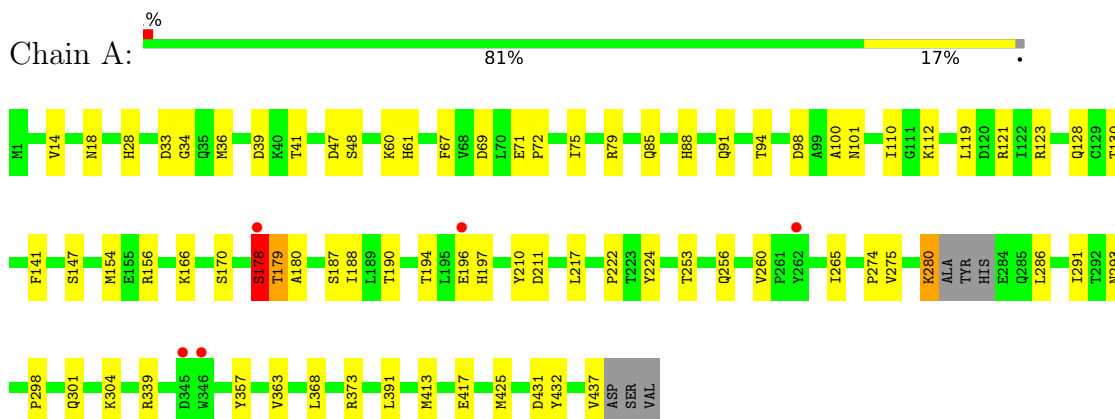
- Molecule 15 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	A	30	Total	O	0	0
			30	30		
15	B	29	Total	O	0	0
			29	29		
15	C	56	Total	O	0	0
			56	56		
15	D	6	Total	O	0	0
			6	6		
15	E	6	Total	O	0	0
			6	6		
15	F	5	Total	O	0	0
			5	5		

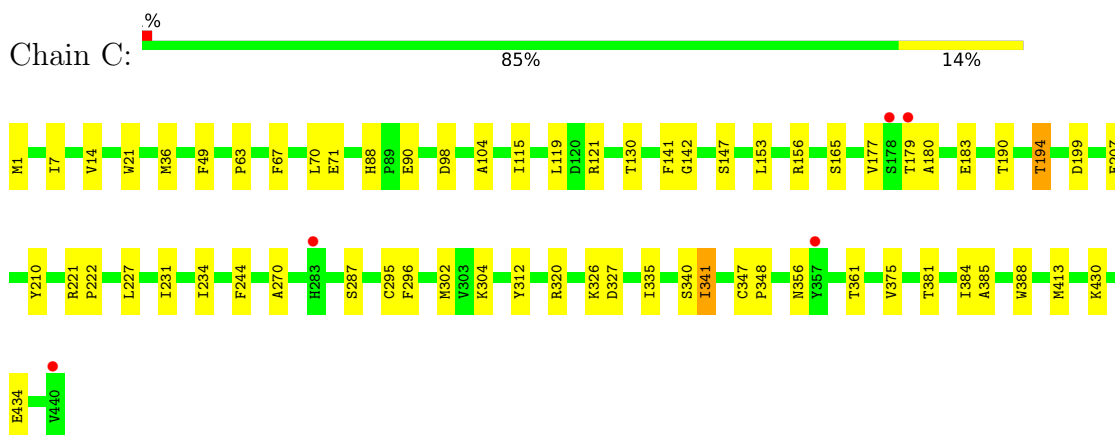
3 Residue-property plots [i](#)

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.

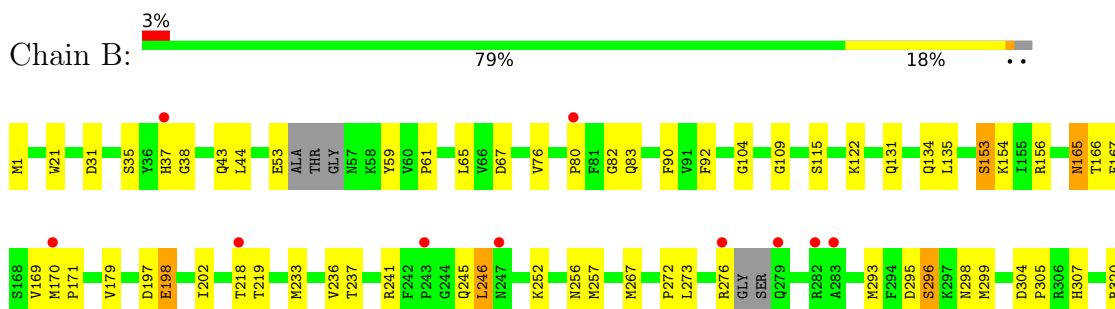
- Molecule 1: Detyrosinated tubulin alpha-1B chain

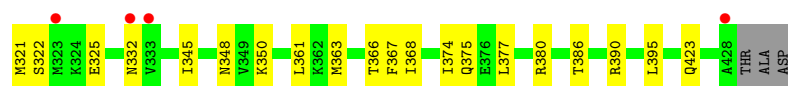


- Molecule 1: Detyrosinated tubulin alpha-1B chain

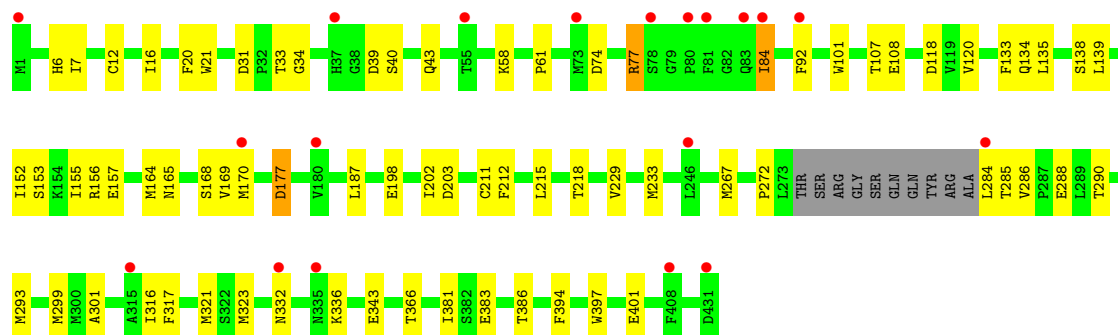
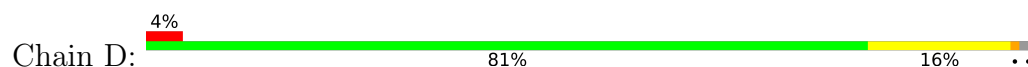


- Molecule 2: Tubulin beta chain

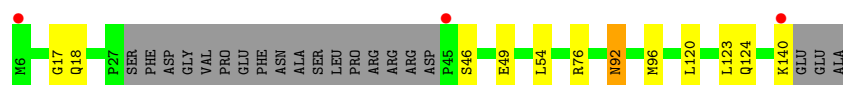
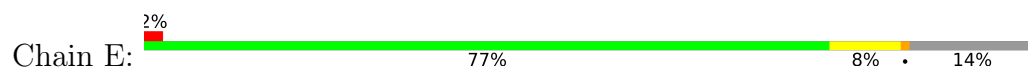




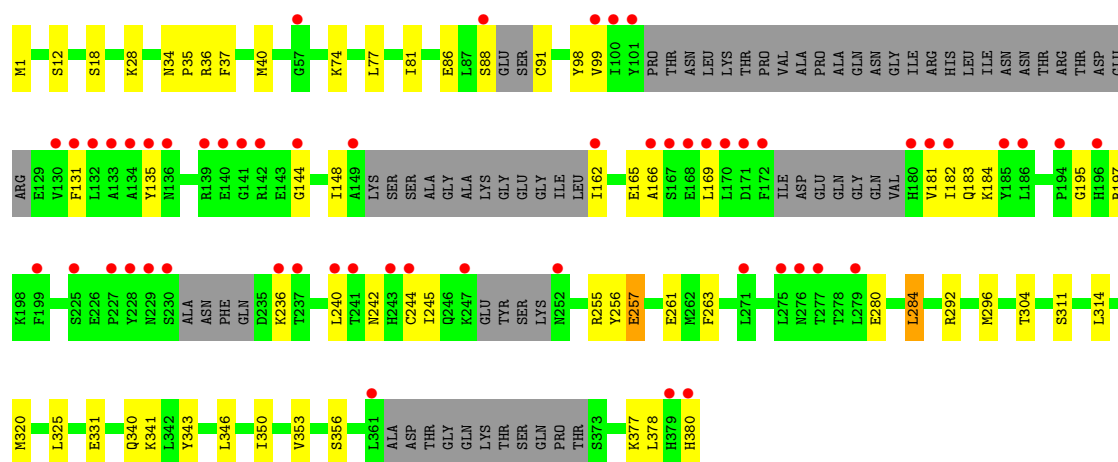
• Molecule 2: Tubulin beta chain



• 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	104.57Å 157.62Å 179.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.83 – 2.70 47.83 – 2.70	Depositor EDS
% Data completeness (in resolution range)	97.7 (47.83-2.70) 97.8 (47.83-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.13 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487, PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.197 , 0.245 0.197 , 0.245	Depositor DCC
R_{free} test set	4016 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	39.9	Xtriage
Anisotropy	0.063	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 43.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	17170	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.55% 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: GOL, EDO, CA, MG, PEG, ACP, MES, GDP, GTP, A1D55

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	0.38	0/3394	0.57	0/4616
1	C	0.51	0/3501	0.68	1/4756 (0.0%)
2	B	0.46	0/3364	0.61	0/4561
2	D	0.36	0/3316	0.56	0/4502
3	E	0.39	0/978	0.49	0/1297
4	F	0.30	0/2618	0.49	0/3533
All	All	0.41	0/17171	0.59	1/23265 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	115	ILE	N-CA-C	5.92	116.66	110.62

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	3319	0	3189	53	0
1	C	3423	0	3320	44	0
2	B	3291	0	3125	64	0
2	D	3244	0	3079	49	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	970	0	984	10	0
4	F	2562	0	2522	39	0
5	A	32	0	12	2	0
5	C	32	0	12	0	0
5	D	32	0	12	1	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
7	A	1	0	0	0	0
7	C	1	0	0	0	0
8	A	6	0	8	0	0
9	A	7	0	10	3	0
10	B	28	0	12	0	0
11	B	12	0	12	3	0
12	B	40	0	0	5	0
13	C	4	0	6	2	0
14	F	31	0	14	1	0
15	A	30	0	0	1	0
15	B	29	0	0	2	0
15	C	56	0	0	1	0
15	D	6	0	0	0	0
15	E	6	0	0	0	0
15	F	5	0	0	0	0
All	All	17170	0	16317	245	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 7.

All (245) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:221:ARG:HG3	2:D:323:MET:HG2	1.33	1.09
4:F:1:MET:HE3	4:F:28:LYS:HB2	1.52	0.89
1:A:178:SER:OG	1:A:179:THR:N	2.01	0.84
1:A:88:HIS:HB2	1:A:91:GLN:HG3	1.68	0.76
1:A:196:GLU:HG3	15:A:603:HOH:O	1.87	0.75
2:B:350:LYS:HG3	12:B:504:A1D55:C1	2.16	0.74
2:B:165:ASN:HB2	2:B:198:GLU:HG2	1.70	0.73
1:C:71:GLU:HB2	1:C:98:ASP:HB3	1.70	0.73
2:B:293:MET:HE2	2:B:367:PHE:HB2	1.75	0.69
1:A:154:MET:HG3	1:A:194:THR:HG23	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:170:MET:HE1	2:D:381:ILE:HD11	1.73	0.68
2:B:197:ASP:OD2	11:B:503:MES:H52	1.94	0.68
4:F:135:TYR:CE2	4:F:166:ALA:HB2	2.29	0.68
2:B:179:VAL:HG12	1:C:348:PRO:HG2	1.77	0.67
1:C:327:ASP:HB3	13:C:504:EDO:H22	1.78	0.66
2:D:286:VAL:HG22	2:D:321:MET:HE3	1.78	0.66
2:D:170:MET:HB2	2:D:203:ASP:HA	1.79	0.65
1:A:413:MET:HE3	1:A:417:GLU:HB3	1.78	0.64
2:D:211:CYS:HA	2:D:215:LEU:HB2	1.81	0.63
1:C:190:THR:O	1:C:194:THR:HG23	1.98	0.63
2:D:332:ASN:OD1	2:D:336:LYS:HD2	1.98	0.62
2:B:256:ASN:HD22	12:B:504:A1D55:C1	2.12	0.62
1:A:211:ASP:OD2	1:A:304:LYS:NZ	2.31	0.61
1:C:7:ILE:HG21	1:C:153:LEU:HD21	1.81	0.61
4:F:195:GLY:HA3	4:F:197:ARG:HD2	1.83	0.61
1:C:234:ILE:HG21	1:C:302:MET:SD	2.42	0.60
1:A:71:GLU:HB2	1:A:98:ASP:HB3	1.83	0.60
9:A:505:PEG:H41	2:B:245:GLN:CB	2.31	0.60
1:C:90:GLU:HG2	1:C:121:ARG:NH2	2.16	0.60
4:F:166:ALA:O	4:F:169:LEU:N	2.32	0.59
2:B:156:ARG:CZ	11:B:503:MES:H21	2.33	0.59
2:D:177:ASP:N	2:D:177:ASP:OD1	2.35	0.58
2:B:170:MET:HG3	2:B:377:LEU:HD11	1.86	0.58
4:F:280:GLU:HA	4:F:284:LEU:HB2	1.84	0.58
1:A:179:THR:HG22	2:B:350:LYS:HE2	1.84	0.58
1:A:224:TYR:H	9:A:505:PEG:H31	1.67	0.58
2:B:218:THR:HG21	1:C:326:LYS:HZ3	1.68	0.58
1:A:112:LYS:HD2	3:E:54:LEU:HB3	1.85	0.57
3:E:46:SER:N	3:E:49:GLU:OE2	2.37	0.57
1:C:1:MET:HB3	1:C:130:THR:OG1	2.05	0.57
1:A:71:GLU:HG2	1:A:72:PRO:HD2	1.85	0.57
2:B:375:GLN:HE22	2:B:423:GLN:HG2	1.70	0.57
2:B:1:MET:HG3	2:B:131:GLN:HG2	1.86	0.56
4:F:34:ASN:ND2	4:F:36:ARG:H	2.04	0.56
4:F:162:ILE:HD11	4:F:240:LEU:HD21	1.88	0.56
4:F:197:ARG:NH2	4:F:257:GLU:OE2	2.39	0.56
3:E:120:LEU:O	3:E:124:GLN:HG2	2.05	0.56
1:A:119:LEU:HD11	1:A:156:ARG:HB3	1.88	0.55
1:A:265:ILE:HG23	1:A:432:TYR:CZ	2.41	0.55
1:A:180:ALA:HA	2:B:256:ASN:HD21	1.69	0.55
1:A:293:ASN:CG	1:A:339:ARG:HH21	2.14	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:148:ILE:HG13	4:F:162:ILE:HG13	1.89	0.55
2:D:12:CYS:HB2	5:D:501:GTP:C8	2.42	0.55
2:D:77:ARG:HH12	2:D:92:PHE:HE2	1.55	0.55
2:D:120:VAL:HG11	2:D:155:ILE:CD1	2.37	0.55
1:A:274:PRO:HB3	1:A:286:LEU:HD12	1.88	0.55
2:B:257:MET:HE1	2:B:368:ILE:HB	1.88	0.55
2:B:170:MET:HE3	2:B:377:LEU:HD21	1.90	0.54
2:B:134:GLN:HA	2:B:165:ASN:O	2.06	0.54
2:D:290:THR:HA	2:D:293:MET:HE2	1.90	0.54
2:B:218:THR:HG21	1:C:326:LYS:NZ	2.24	0.53
4:F:131:PHE:CZ	4:F:182:ILE:HG12	2.44	0.53
2:B:350:LYS:HG3	12:B:504:A1D55:C2	2.38	0.53
2:D:152:ILE:HG23	2:D:164:MET:HG2	1.91	0.53
2:D:212:PHE:HE1	2:D:218:THR:O	1.92	0.53
2:D:343:GLU:OE1	2:D:343:GLU:N	2.30	0.53
1:A:69:ASP:O	1:A:94:THR:HA	2.09	0.53
2:D:229:VAL:O	2:D:233:MET:HG3	2.09	0.53
2:D:101:TRP:CE3	2:D:187:LEU:HD13	2.44	0.53
2:B:31:ASP:HB3	2:B:37:HIS:CE1	2.44	0.52
4:F:341:LYS:HD3	4:F:341:LYS:N	2.24	0.52
1:A:147:SER:HB2	1:A:190:THR:HB	1.91	0.52
1:A:298:PRO:O	1:A:301:GLN:HG3	2.10	0.52
4:F:88:SER:HG	4:F:91:CYS:N	2.08	0.52
4:F:346:LEU:O	4:F:350:ILE:HG13	2.09	0.52
2:D:6:HIS:CD2	2:D:134:GLN:HE21	2.28	0.52
2:B:273:LEU:HD11	2:B:298:ASN:HA	1.92	0.52
1:C:14:VAL:HG13	1:C:67:PHE:HD2	1.75	0.52
1:A:217:LEU:HD21	1:A:368:LEU:HD23	1.92	0.52
2:B:165:ASN:HB2	2:B:198:GLU:CG	2.40	0.51
2:B:135:LEU:HB3	2:B:166:THR:HG22	1.91	0.51
1:C:90:GLU:O	1:C:121:ARG:HG2	2.10	0.51
1:C:295:CYS:SG	1:C:375:VAL:HG13	2.51	0.51
2:B:219:THR:HG21	1:C:326:LYS:HA	1.93	0.51
2:D:157:GLU:HG3	3:E:123:LEU:HD13	1.93	0.51
4:F:148:ILE:HG22	4:F:183:GLN:O	2.10	0.51
4:F:304:THR:HG21	4:F:311:SER:HB2	1.93	0.51
1:C:36:MET:HE1	1:C:49:PHE:CE2	2.45	0.51
1:C:296:PHE:CE2	1:C:341:ILE:HD11	2.46	0.51
1:A:101:ASN:OD1	2:B:252:LYS:HG2	2.11	0.50
5:A:501:GTP:H5''	12:B:504:A1D55:C30	2.42	0.50
1:C:385:ALA:HA	1:C:388:TRP:CD1	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:267:MET:HG2	2:D:301:ALA:HB3	1.93	0.50
2:D:6:HIS:HD2	2:D:134:GLN:HE21	1.60	0.50
1:C:227:LEU:O	1:C:231:ILE:HG13	2.11	0.50
2:B:167:PHE:CE2	2:B:233:MET:HG2	2.47	0.50
2:D:134:GLN:HA	2:D:165:ASN:O	2.12	0.50
2:B:237:THR:O	2:B:241:ARG:HG3	2.11	0.49
1:A:166:LYS:HE2	1:A:197:HIS:O	2.12	0.49
4:F:244:CYS:SG	4:F:245:ILE:N	2.85	0.49
1:A:100:ALA:HA	2:B:252:LYS:HG3	1.93	0.49
1:A:256:GLN:NE2	1:A:260:VAL:O	2.45	0.49
2:B:21:TRP:CZ3	2:B:61:PRO:HB3	2.47	0.49
2:B:67:ASP:O	2:B:92:PHE:HA	2.13	0.49
2:D:20:PHE:CD1	2:D:233:MET:HE2	2.47	0.49
4:F:98:TYR:HB2	4:F:182:ILE:CG2	2.43	0.49
1:C:287:SER:HB2	13:C:504:EDO:H11	1.95	0.49
1:C:142:GLY:HA3	1:C:183:GLU:OE1	2.13	0.48
1:A:275:VAL:HG13	1:A:368:LEU:HD21	1.94	0.48
4:F:236:LYS:HB2	4:F:240:LEU:HG	1.96	0.48
1:A:79:ARG:HH12	1:A:94:THR:HG21	1.79	0.48
2:B:104:GLY:O	2:B:109:GLY:HA3	2.14	0.48
11:B:503:MES:H82	11:B:503:MES:H51	1.65	0.48
1:C:320:ARG:HA	1:C:356:ASN:O	2.14	0.48
2:B:377:LEU:C	2:B:377:LEU:HD23	2.38	0.47
1:A:265:ILE:HD11	1:A:431:ASP:HB3	1.95	0.47
1:C:244:PHE:HB2	1:C:356:ASN:HD21	1.80	0.47
1:A:34:GLY:O	1:A:61:HIS:HD2	1.97	0.47
1:C:179:THR:O	1:C:179:THR:OG1	2.28	0.47
4:F:135:TYR:OH	4:F:165:GLU:HA	2.14	0.47
2:D:156:ARG:HG2	3:E:123:LEU:HD11	1.95	0.47
4:F:77:LEU:O	4:F:81:ILE:HG13	2.14	0.47
4:F:261:GLU:OE1	4:F:341:LYS:NZ	2.45	0.47
1:A:39:ASP:OD2	1:A:61:HIS:HE1	1.97	0.47
2:D:267:MET:CE	2:D:299:MET:HG3	2.45	0.47
2:B:171:PRO:O	2:B:380:ARG:NH2	2.48	0.46
4:F:255:ARG:HB3	4:F:256:TYR:CD1	2.49	0.46
1:A:210:TYR:CE1	1:A:222:PRO:HD2	2.51	0.46
1:C:119:LEU:HD11	1:C:156:ARG:HB3	1.96	0.46
2:D:272:PRO:HB3	2:D:284:LEU:HD21	1.98	0.46
4:F:86:GLU:OE1	4:F:86:GLU:N	2.44	0.46
1:C:210:TYR:CE1	1:C:222:PRO:HD2	2.50	0.46
1:C:234:ILE:HD13	1:C:302:MET:SD	2.56	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:21:TRP:CZ3	2:D:61:PRO:HB3	2.51	0.46
1:A:14:VAL:HG13	1:A:67:PHE:HD2	1.81	0.46
2:B:65:LEU:HD22	2:B:90:PHE:CE2	2.51	0.46
2:D:133:PHE:HB2	2:D:164:MET:HE1	1.98	0.46
1:A:79:ARG:HH22	1:A:94:THR:HG23	1.81	0.46
2:B:293:MET:HE1	2:B:366:THR:C	2.41	0.46
2:D:6:HIS:CE1	2:D:21:TRP:HE1	2.34	0.46
4:F:37:PHE:CZ	4:F:40:MET:HE3	2.51	0.46
1:A:88:HIS:HB2	1:A:91:GLN:CG	2.44	0.45
2:B:345:ILE:HG22	2:B:348:ASN:HB3	1.99	0.45
1:A:224:TYR:CD2	9:A:505:PEG:H42	2.51	0.45
2:B:304:ASP:HB3	2:B:307:HIS:ND1	2.31	0.45
1:C:88:HIS:CE1	1:C:90:GLU:HB2	2.51	0.45
3:E:92:ASN:ND2	3:E:96:MET:HE3	2.31	0.45
1:C:244:PHE:HB2	1:C:356:ASN:ND2	2.31	0.45
2:B:395:LEU:HD23	2:B:395:LEU:HA	1.79	0.45
1:A:187:SER:HB3	1:A:391:LEU:HD21	1.97	0.45
2:B:296:SER:HA	2:B:299:MET:HG2	1.98	0.45
2:D:133:PHE:HB2	2:D:164:MET:CE	2.47	0.45
1:A:265:ILE:HD12	1:A:265:ILE:N	2.32	0.45
2:B:246:LEU:HD11	12:B:504:A1D55:C9	2.46	0.45
2:D:316:ILE:HG23	2:D:366:THR:HB	1.99	0.45
2:B:380:ARG:HD3	15:B:620:HOH:O	2.16	0.45
2:D:139:LEU:HD21	2:D:168:SER:HB3	1.99	0.45
4:F:242:ASN:HB2	4:F:245:ILE:HB	1.99	0.45
2:B:276:ARG:H	2:B:276:ARG:HG3	1.55	0.44
1:A:357:TYR:CE2	3:E:17:GLY:HA2	2.52	0.44
1:C:430:LYS:HD3	1:C:434:GLU:OE2	2.17	0.44
2:D:74:ASP:HA	2:D:77:ARG:HG3	1.99	0.44
1:A:128:GLN:HA	1:A:128:GLN:OE1	2.17	0.44
2:D:383:GLU:O	2:D:386:THR:HG22	2.18	0.44
4:F:263:PHE:CZ	4:F:341:LYS:HG2	2.53	0.44
2:B:154:LYS:HE2	3:E:76:ARG:NE	2.33	0.44
1:C:165:SER:HA	1:C:199:ASP:OD2	2.17	0.44
2:D:316:ILE:CG2	2:D:366:THR:HB	2.48	0.44
4:F:284:LEU:HA	4:F:284:LEU:HD22	1.85	0.44
2:D:34:GLY:O	2:D:58:LYS:HA	2.19	0.43
1:C:302:MET:HB3	1:C:302:MET:HE3	1.63	0.43
3:E:140:LYS:HB2	3:E:140:LYS:HE2	1.73	0.43
2:B:31:ASP:OD1	2:B:35:SER:N	2.33	0.43
2:D:170:MET:HB3	2:D:170:MET:HE3	1.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:74:LYS:HD2	4:F:74:LYS:HA	1.65	0.43
1:A:291:ILE:HD13	1:A:373:ARG:HG3	2.01	0.43
1:A:425:MET:HE3	1:A:425:MET:HB3	1.75	0.43
2:B:321:MET:HB3	2:B:363:MET:SD	2.58	0.43
1:C:340:SER:HA	15:C:605:HOH:O	2.18	0.43
1:A:280:LYS:C	1:A:280:LYS:HD2	2.44	0.43
4:F:98:TYR:HB2	4:F:182:ILE:HG22	2.00	0.43
2:B:169:VAL:HA	2:B:202:ILE:O	2.19	0.43
1:C:312:TYR:CE2	1:C:341:ILE:HD13	2.54	0.43
1:A:28:HIS:O	1:A:36:MET:HE3	2.18	0.43
1:C:296:PHE:HE2	1:C:341:ILE:HD11	1.84	0.43
1:A:180:ALA:HA	2:B:256:ASN:ND2	2.34	0.42
2:B:295:ASP:OD1	2:B:296:SER:N	2.51	0.42
4:F:377:LYS:HD3	4:F:380:HIS:CE1	2.54	0.42
2:B:153:SER:HB3	3:E:76:ARG:HH22	1.84	0.42
2:B:320:ARG:HA	2:B:320:ARG:NH1	2.34	0.42
1:C:104:ALA:HB2	1:C:413:MET:SD	2.59	0.42
4:F:340:GLN:HA	4:F:343:TYR:HD2	1.85	0.42
2:B:267:MET:HE1	2:B:305:PRO:HG3	2.02	0.42
1:C:207:GLU:HG2	1:C:304:LYS:HE2	2.01	0.42
4:F:292:ARG:HD2	4:F:378:LEU:O	2.19	0.42
2:D:120:VAL:HG21	2:D:155:ILE:HD11	2.01	0.42
1:A:98:ASP:HB2	5:A:501:GTP:O2G	2.20	0.42
1:A:141:PHE:CE1	1:A:170:SER:HB3	2.55	0.42
1:A:275:VAL:HG13	1:A:368:LEU:CD2	2.50	0.42
1:A:47:ASP:OD1	1:A:47:ASP:N	2.50	0.41
2:B:53:GLU:HG3	2:B:59:TYR:CE1	2.55	0.41
2:B:76:VAL:O	2:B:82:GLY:HA3	2.20	0.41
2:B:246:LEU:HD23	2:B:246:LEU:HA	1.78	0.41
2:B:267:MET:HG2	2:B:374:ILE:HD13	2.02	0.41
2:D:7:ILE:O	2:D:135:LEU:HA	2.20	0.41
2:D:12:CYS:HB3	2:D:138:SER:HB3	2.02	0.41
2:D:31:ASP:HB3	2:D:33:THR:H	1.85	0.41
1:C:270:ALA:HB3	1:C:302:MET:HE2	2.02	0.41
4:F:256:TYR:CD1	4:F:256:TYR:N	2.88	0.41
2:B:38:GLY:HA3	2:B:43:GLN:OE1	2.20	0.41
2:B:83:GLN:NE2	15:B:608:HOH:O	2.48	0.41
1:A:154:MET:HG3	1:A:194:THR:CG2	2.48	0.41
2:B:122:LYS:HD2	2:B:122:LYS:HA	1.79	0.41
2:B:299:MET:HE3	2:B:305:PRO:HG2	2.03	0.41
1:C:88:HIS:CE1	1:C:90:GLU:H	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:107:THR:HG21	2:D:401:GLU:OE1	2.20	0.41
2:D:169:VAL:HA	2:D:202:ILE:O	2.21	0.41
1:C:21:TRP:CZ3	1:C:63:PRO:HB3	2.55	0.41
1:C:141:PHE:O	1:C:147:SER:HB3	2.21	0.41
1:C:180:ALA:O	1:C:183:GLU:HG3	2.20	0.41
2:D:61:PRO:HD2	2:D:84:ILE:O	2.20	0.41
4:F:99:VAL:HG22	4:F:181:VAL:HG12	2.03	0.41
2:B:21:TRP:CE3	2:B:61:PRO:HB3	2.55	0.41
2:B:293:MET:HE2	2:B:367:PHE:CB	2.48	0.41
2:D:61:PRO:HG2	2:D:84:ILE:HG23	2.01	0.41
1:A:121:ARG:HH11	1:A:121:ARG:HG3	1.85	0.41
2:D:285:THR:OG1	2:D:288:GLU:HG3	2.21	0.41
1:A:123:ARG:HA	1:A:123:ARG:HD3	1.89	0.41
1:A:196:GLU:HB2	1:A:197:HIS:CD2	2.55	0.41
2:B:272:PRO:HD2	2:B:361:LEU:HD13	2.02	0.41
2:B:322:SER:HB3	2:B:325:GLU:HB2	2.03	0.41
1:C:70:LEU:HD23	1:C:70:LEU:HA	1.82	0.41
1:C:147:SER:HB2	1:C:190:THR:HB	2.03	0.41
2:D:293:MET:HE1	2:D:317:PHE:CZ	2.56	0.41
2:D:394:PHE:O	2:D:397:TRP:HD1	2.04	0.41
2:D:40:SER:HB3	2:D:43:GLN:HG3	2.02	0.41
2:D:107:THR:OG1	2:D:108:GLU:N	2.50	0.41
4:F:34:ASN:HD22	4:F:35:PRO:N	2.19	0.41
4:F:292:ARG:HB3	4:F:296:MET:HE2	2.02	0.41
4:F:320:MET:HE1	14:F:401:ACP:C4	2.52	0.40
4:F:325:LEU:HD23	4:F:325:LEU:HA	1.96	0.40
1:A:60:LYS:NZ	1:A:85:GLN:O	2.40	0.40
4:F:314:LEU:HD22	4:F:350:ILE:HD11	2.04	0.40
1:A:156:ARG:HA	1:A:156:ARG:HD2	1.92	0.40
2:B:386:THR:O	2:B:390:ARG:HG2	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	430/440 (98%)	420 (98%)	9 (2%)	1 (0%)	43	68
1	C	438/440 (100%)	428 (98%)	10 (2%)	0	100	100
2	B	417/431 (97%)	402 (96%)	14 (3%)	1 (0%)	43	68
2	D	417/431 (97%)	404 (97%)	13 (3%)	0	100	100
3	E	114/138 (83%)	111 (97%)	3 (3%)	0	100	100
4	F	297/380 (78%)	279 (94%)	17 (6%)	1 (0%)	36	60
All	All	2113/2260 (94%)	2044 (97%)	66 (3%)	3 (0%)	48	73

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	178	SER
4	F	144	GLY
2	B	80	PRO

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	348/371 (94%)	334 (96%)	14 (4%)	28	56
1	C	368/371 (99%)	360 (98%)	8 (2%)	45	74
2	B	356/372 (96%)	347 (98%)	9 (2%)	42	71
2	D	349/372 (94%)	341 (98%)	8 (2%)	44	73
3	E	104/123 (85%)	102 (98%)	2 (2%)	50	77
4	F	279/338 (82%)	271 (97%)	8 (3%)	37	67
All	All	1804/1947 (93%)	1755 (97%)	49 (3%)	39	69

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

Mol	Chain	Res	Type
1	A	18	ASN
1	A	33	ASP
1	A	41	THR
1	A	48	SER
1	A	75	ILE
1	A	110	ILE
1	A	130	THR
1	A	178	SER
1	A	179	THR
1	A	188	ILE
1	A	253	THR
1	A	280	LYS
1	A	363	VAL
1	A	437	VAL
2	B	44	LEU
2	B	115	SER
2	B	153	SER
2	B	165	ASN
2	B	198	GLU
2	B	236	VAL
2	B	246	LEU
2	B	296	SER
2	B	332	ASN
1	C	177	VAL
1	C	194	THR
1	C	335	ILE
1	C	341	ILE
1	C	347	CYS
1	C	361	THR
1	C	381	THR
1	C	384	ILE
2	D	16	ILE
2	D	39	ASP
2	D	77	ARG
2	D	84	ILE
2	D	118	ASP
2	D	153	SER
2	D	177	ASP
2	D	198	GLU
3	E	18	GLN
3	E	92	ASN
4	F	12	SER
4	F	18	SER

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Mol	Chain	Res	Type
4	F	184	LYS
4	F	257	GLU
4	F	284	LEU
4	F	331	GLU
4	F	353	VAL
4	F	356	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	50	ASN
1	A	61	HIS
1	A	85	GLN
1	A	393	HIS
2	B	37	HIS
2	B	256	ASN
2	B	414	ASN
2	B	424	GLN
1	C	85	GLN
1	C	101	ASN
1	C	256	GLN
1	C	356	ASN
1	C	406	HIS
2	D	6	HIS
2	D	100	ASN
2	D	292	GLN
3	E	84	GLN
3	E	92	ASN
4	F	34	ASN
4	F	333	ASN
4	F	380	HIS

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 5 are monoatomic - leaving 10 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$
13	EDO	C	504	-	3,3,3	0.70	0	2,2,2	0.17	0
14	ACP	F	401	-	31,33,33	1.11	2 (6%)	47,52,52	0.82	1 (2%)
5	GTP	A	501	6	33,34,34	1.12	3 (9%)	50,54,54	1.41	8 (16%)
5	GTP	D	501	-	33,34,34	0.91	1 (3%)	50,54,54	1.73	11 (22%)
11	MES	B	503	-	12,12,12	2.14	1 (8%)	15,16,16	2.39	7 (46%)
12	A1D55	B	504	-	46,46,46	1.16	6 (13%)	66,68,68	1.64	11 (16%)
5	GTP	C	501	6	33,34,34	1.07	2 (6%)	50,54,54	1.54	11 (22%)
8	GOL	A	504	-	5,5,5	0.80	0	5,5,5	1.35	1 (20%)
10	GDP	B	501	6	29,30,30	1.25	3 (10%)	45,47,47	1.83	8 (17%)
9	PEG	A	505	-	6,6,6	0.22	0	5,5,5	0.16	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
13	EDO	C	504	-	-	1/1/1/1	-
14	ACP	F	401	-	-	10/19/38/38	0/3/3/3
5	GTP	A	501	6	-	5/22/38/38	0/3/3/3
5	GTP	D	501	-	-	5/22/38/38	0/3/3/3
11	MES	B	503	-	-	1/6/14/14	0/1/1/1
12	A1D55	B	504	-	-	3/14/49/49	0/7/7/7
5	GTP	C	501	6	-	7/22/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	GOL	A	504	-	-	4/4/4/4	-
10	GDP	B	501	6	-	3/16/32/32	0/3/3/3
9	PEG	A	505	-	-	1/4/4/4	-

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	B	503	MES	C8-S	-7.07	1.67	1.77
14	F	401	ACP	PB-O3A	5.20	1.64	1.58
10	B	501	GDP	PA-O3A	3.30	1.63	1.59
14	F	401	ACP	PA-O3A	3.18	1.62	1.59
5	A	501	GTP	PB-O3A	2.99	1.62	1.59
5	C	501	GTP	PB-O3A	2.88	1.62	1.59
12	B	504	A1D55	C9-C10	2.79	1.56	1.53
10	B	501	GDP	C5-C4	2.65	1.46	1.38
10	B	501	GDP	C6-N1	-2.56	1.34	1.38
12	B	504	A1D55	O3-C13	-2.41	1.41	1.45
12	B	504	A1D55	O6-C17	-2.36	1.34	1.38
12	B	504	A1D55	C8-C7	-2.33	1.51	1.56
5	C	501	GTP	PA-O3A	2.33	1.62	1.59
12	B	504	A1D55	C6-C10	2.29	1.55	1.51
5	A	501	GTP	PB-O3B	2.22	1.61	1.59
5	D	501	GTP	C2-N3	2.21	1.38	1.33
12	B	504	A1D55	C8-C9	-2.09	1.50	1.54
5	A	501	GTP	PA-O3A	2.02	1.61	1.59

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	B	503	MES	C5-N4-C3	6.10	121.97	108.84
10	B	501	GDP	C5-C4-N3	-5.59	119.49	128.39
5	D	501	GTP	C5-C4-N3	-5.26	120.02	128.39
10	B	501	GDP	C2-N3-C4	5.15	121.17	112.30
14	F	401	ACP	PB-O3A-PA	-4.87	116.49	132.37
5	D	501	GTP	C2-N3-C4	4.67	120.34	112.30
5	C	501	GTP	C2-N3-C4	4.48	120.01	112.30
12	B	504	A1D55	O7-C18-C17	4.31	122.52	115.14
5	C	501	GTP	C5-C4-N3	-4.28	121.58	128.39
12	B	504	A1D55	O7-C18-C19	-4.08	117.05	124.08
10	B	501	GDP	N9-C4-N3	3.91	133.77	125.95
12	B	504	A1D55	C6-C10-N1	3.84	120.63	111.70
10	B	501	GDP	C6-C5-N7	3.80	137.20	130.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	501	GTP	C5-C4-N3	-3.60	122.67	128.39
5	A	501	GTP	C2-N3-C4	3.49	118.32	112.30
5	D	501	GTP	C2-N1-C6	-3.26	119.19	125.11
12	B	504	A1D55	C14-C7-C5	3.22	117.91	112.95
5	D	501	GTP	N9-C4-N3	3.17	132.30	125.95
5	C	501	GTP	N9-C8-N7	-3.14	107.58	113.40
12	B	504	A1D55	O2-C3-C4	3.10	131.98	127.86
11	B	503	MES	O1-C6-C5	-3.06	105.18	111.77
12	B	504	A1D55	C15-C14-C7	2.99	126.12	120.41
5	C	501	GTP	C8-N7-C5	2.98	109.57	104.26
11	B	503	MES	O3S-S-C8	2.94	111.76	106.00
5	D	501	GTP	C8-N7-C5	2.83	109.30	104.26
5	C	501	GTP	N9-C4-N3	2.82	131.60	125.95
12	B	504	A1D55	C6-C5-C7	2.76	121.56	114.39
5	D	501	GTP	N9-C8-N7	-2.76	108.28	113.40
10	B	501	GDP	O6-C6-C5	-2.75	119.26	126.53
11	B	503	MES	C7-N4-C5	2.73	118.51	111.24
5	A	501	GTP	N9-C8-N7	-2.72	108.36	113.40
5	D	501	GTP	O4'-C1'-N9	-2.63	102.40	108.36
5	A	501	GTP	O2B-PB-O3A	2.62	114.37	107.27
5	D	501	GTP	C5-C6-N1	2.55	119.73	113.25
5	A	501	GTP	O6-C6-C5	-2.50	119.93	126.53
10	B	501	GDP	O2B-PB-O3A	2.43	112.79	104.64
10	B	501	GDP	C4-C5-N7	-2.43	106.83	110.67
5	C	501	GTP	O2B-PB-O3A	2.34	113.59	107.27
12	B	504	A1D55	C14-C7-C8	2.33	117.20	113.22
12	B	504	A1D55	O1-C2-C1	2.32	130.95	127.86
11	B	503	MES	O3S-S-O2S	-2.32	105.60	111.40
5	C	501	GTP	N1-C2-N3	-2.28	119.15	123.32
10	B	501	GDP	C5-C6-N1	2.27	119.04	113.25
5	C	501	GTP	C5-C6-N1	2.25	118.97	113.25
5	A	501	GTP	C2-N1-C6	-2.23	121.07	125.11
12	B	504	A1D55	O6-C17-C16	2.21	123.29	120.12
8	A	504	GOL	C3-C2-C1	-2.20	103.74	111.80
11	B	503	MES	C6-C5-N4	-2.16	106.84	110.12
5	D	501	GTP	C4-C5-N7	-2.16	107.25	110.67
12	B	504	A1D55	C23-N1-C10	2.15	126.37	122.16
5	A	501	GTP	C8-N7-C5	2.15	108.09	104.26
11	B	503	MES	C7-N4-C3	2.12	116.89	111.24
5	D	501	GTP	O6-C6-C5	-2.08	121.05	126.53
5	C	501	GTP	C4-C5-N7	-2.07	107.39	110.67
5	D	501	GTP	O2A-PA-O3A	2.07	112.86	107.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	501	GTP	N2-C2-N1	2.04	121.06	116.76
5	C	501	GTP	O2A-PA-O3A	2.03	112.77	107.27
5	C	501	GTP	C2-N1-C6	-2.02	121.45	125.11

There are no chirality outliers.

All (40) 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	C5'-O5'-PA-O3A
5	C	501	GTP	C5'-O5'-PA-O1A
5	D	501	GTP	C5'-O5'-PA-O3A
5	D	501	GTP	C5'-O5'-PA-O1A
8	A	504	GOL	O1-C1-C2-C3
10	B	501	GDP	C5'-O5'-PA-O3A
10	B	501	GDP	C5'-O5'-PA-O1A
10	B	501	GDP	C5'-O5'-PA-O2A
11	B	503	MES	C8-C7-N4-C5
12	B	504	A1D55	C9-C10-N1-C23
14	F	401	ACP	PG-C3B-PB-O1B
14	F	401	ACP	PG-C3B-PB-O3A
14	F	401	ACP	PB-O3A-PA-O5'
14	F	401	ACP	C5'-O5'-PA-O1A
14	F	401	ACP	C5'-O5'-PA-O2A
14	F	401	ACP	C5'-O5'-PA-O3A
14	F	401	ACP	O4'-C4'-C5'-O5'
14	F	401	ACP	C3'-C4'-C5'-O5'
12	B	504	A1D55	C24-C23-N1-C10
8	A	504	GOL	C1-C2-C3-O3
8	A	504	GOL	O1-C1-C2-O2
9	A	505	PEG	O2-C3-C4-O4
12	B	504	A1D55	C28-C23-N1-C10
13	C	504	EDO	O1-C1-C2-O2
5	A	501	GTP	PB-O3B-PG-O3G
14	F	401	ACP	C4'-C5'-O5'-PA
5	A	501	GTP	C5'-O5'-PA-O2A
5	C	501	GTP	C5'-O5'-PA-O2A
5	D	501	GTP	C5'-O5'-PA-O2A
14	F	401	ACP	PG-C3B-PB-O2B
5	D	501	GTP	PB-O3A-PA-O2A
5	C	501	GTP	PB-O3B-PG-O1G

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Mol	Chain	Res	Type	Atoms
8	A	504	GOL	O2-C2-C3-O3
5	C	501	GTP	PB-O3B-PG-O3G
5	C	501	GTP	PB-O3A-PA-O1A
5	C	501	GTP	PB-O3A-PA-O2A
5	D	501	GTP	PB-O3A-PA-O1A
5	A	501	GTP	PG-O3B-PB-O2B

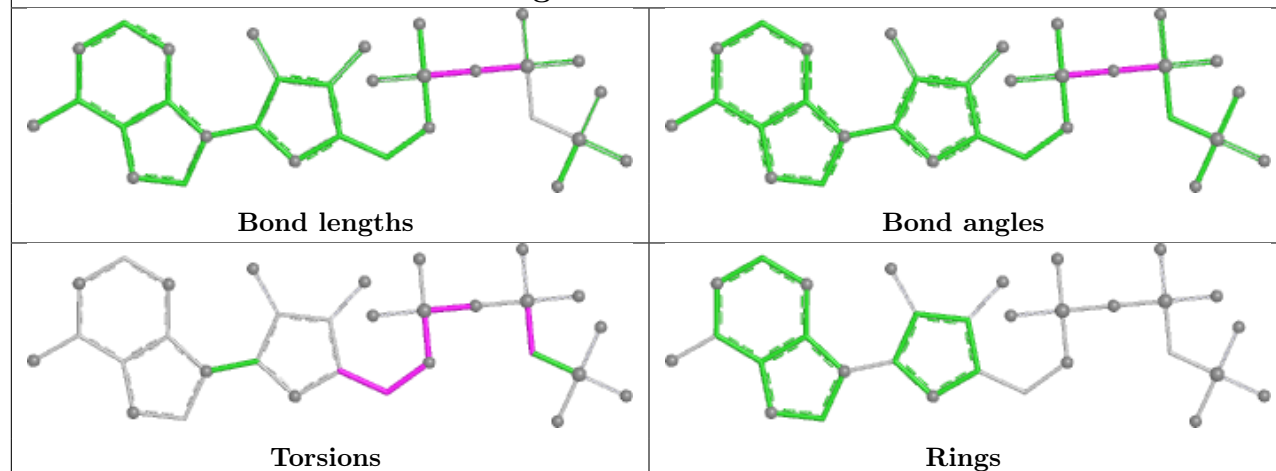
There are no ring outliers.

7 monomers are involved in 16 short contacts:

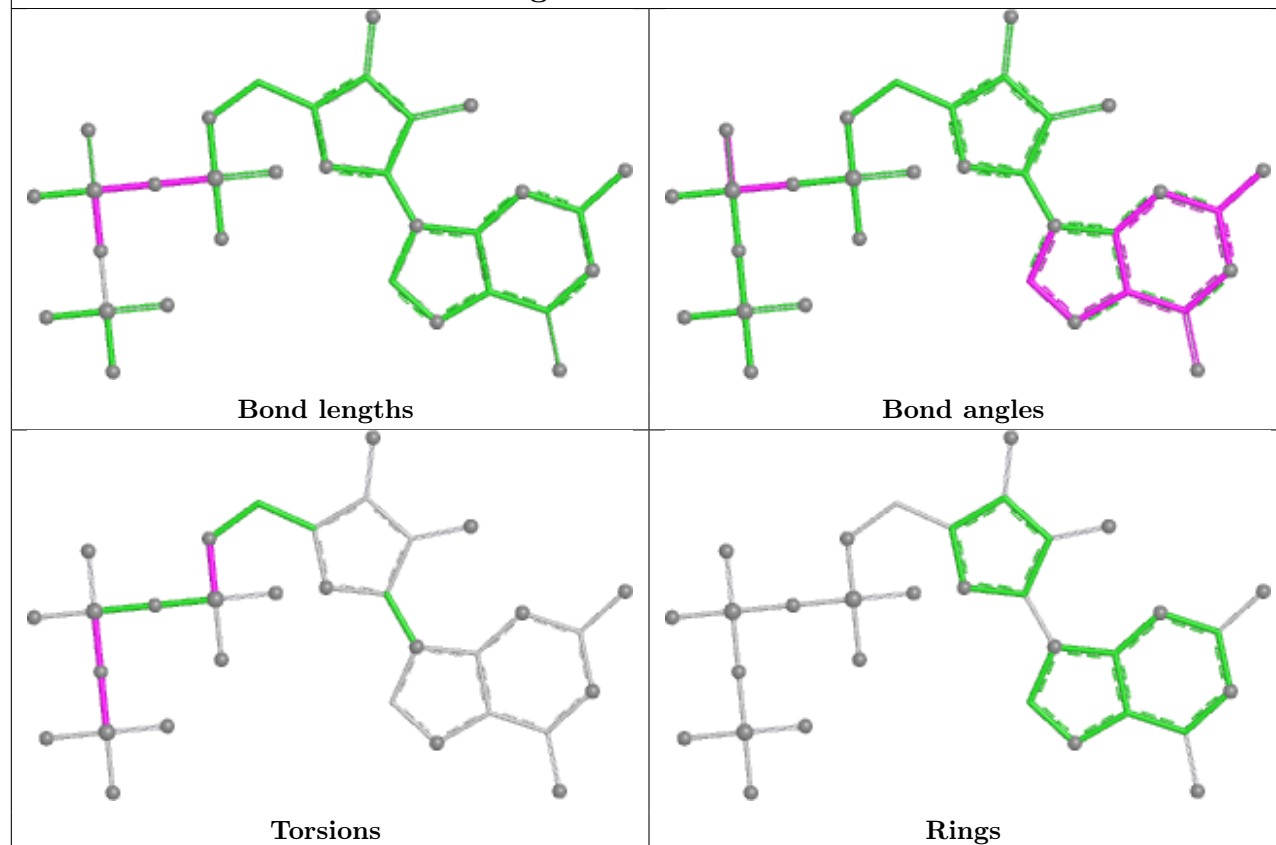
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	C	504	EDO	2	0
14	F	401	ACP	1	0
5	A	501	GTP	2	0
5	D	501	GTP	1	0
11	B	503	MES	3	0
12	B	504	A1D55	5	0
9	A	505	PEG	3	0

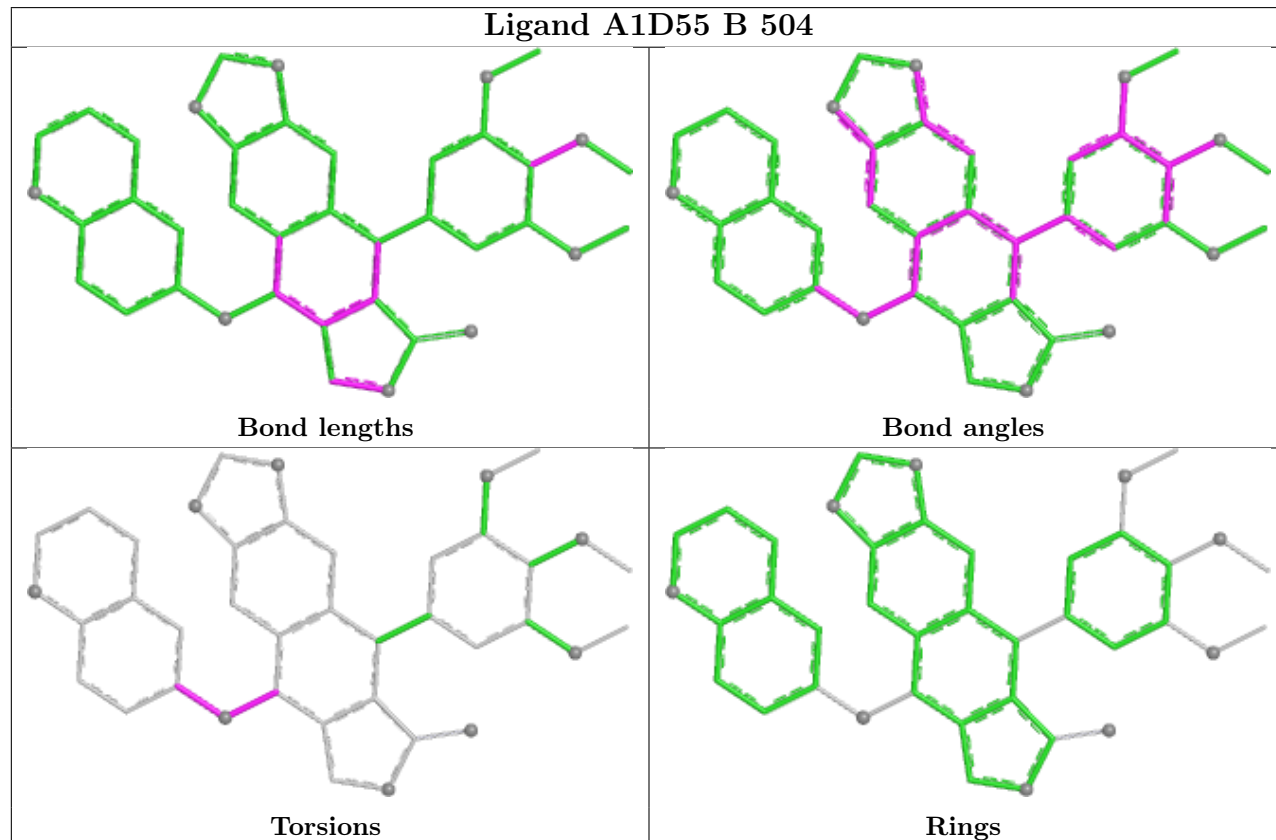
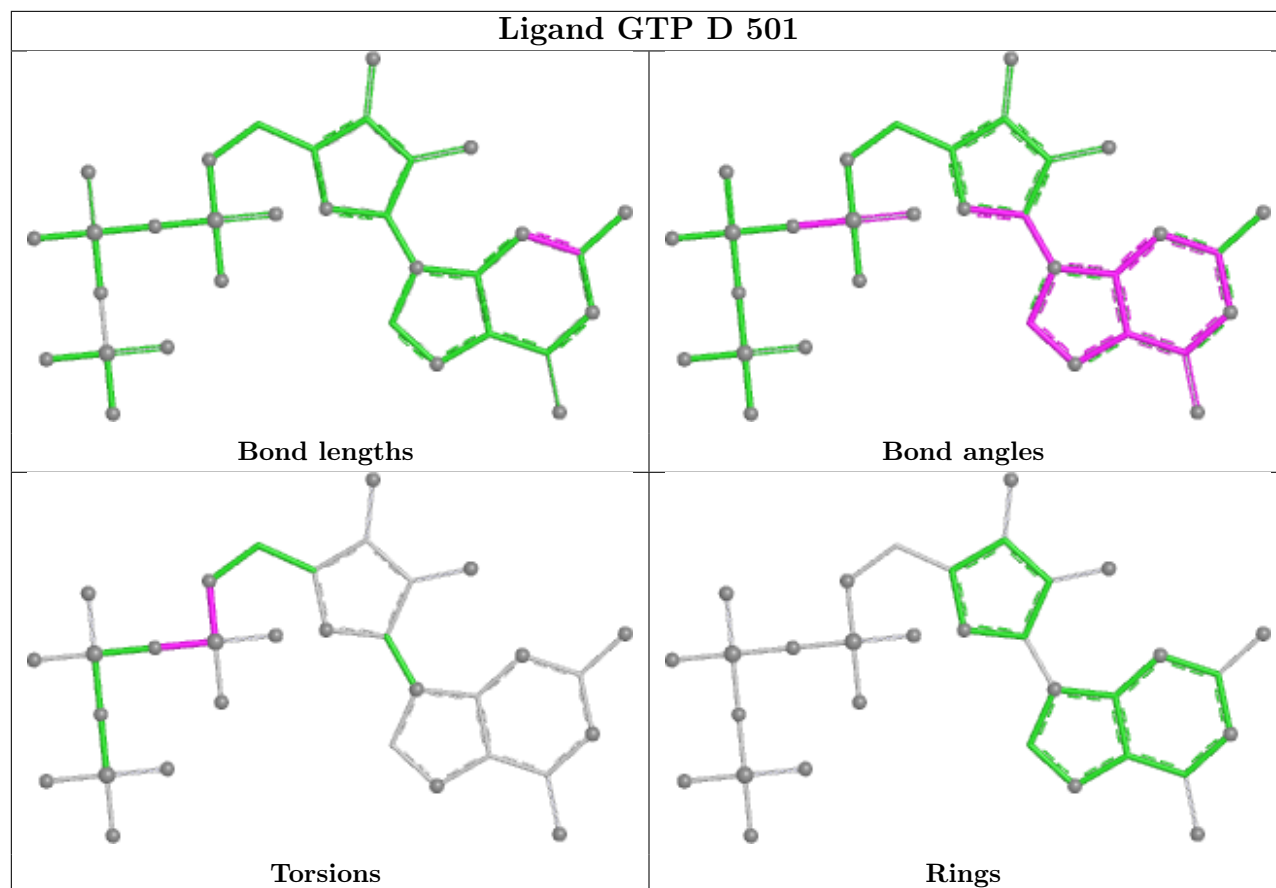
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

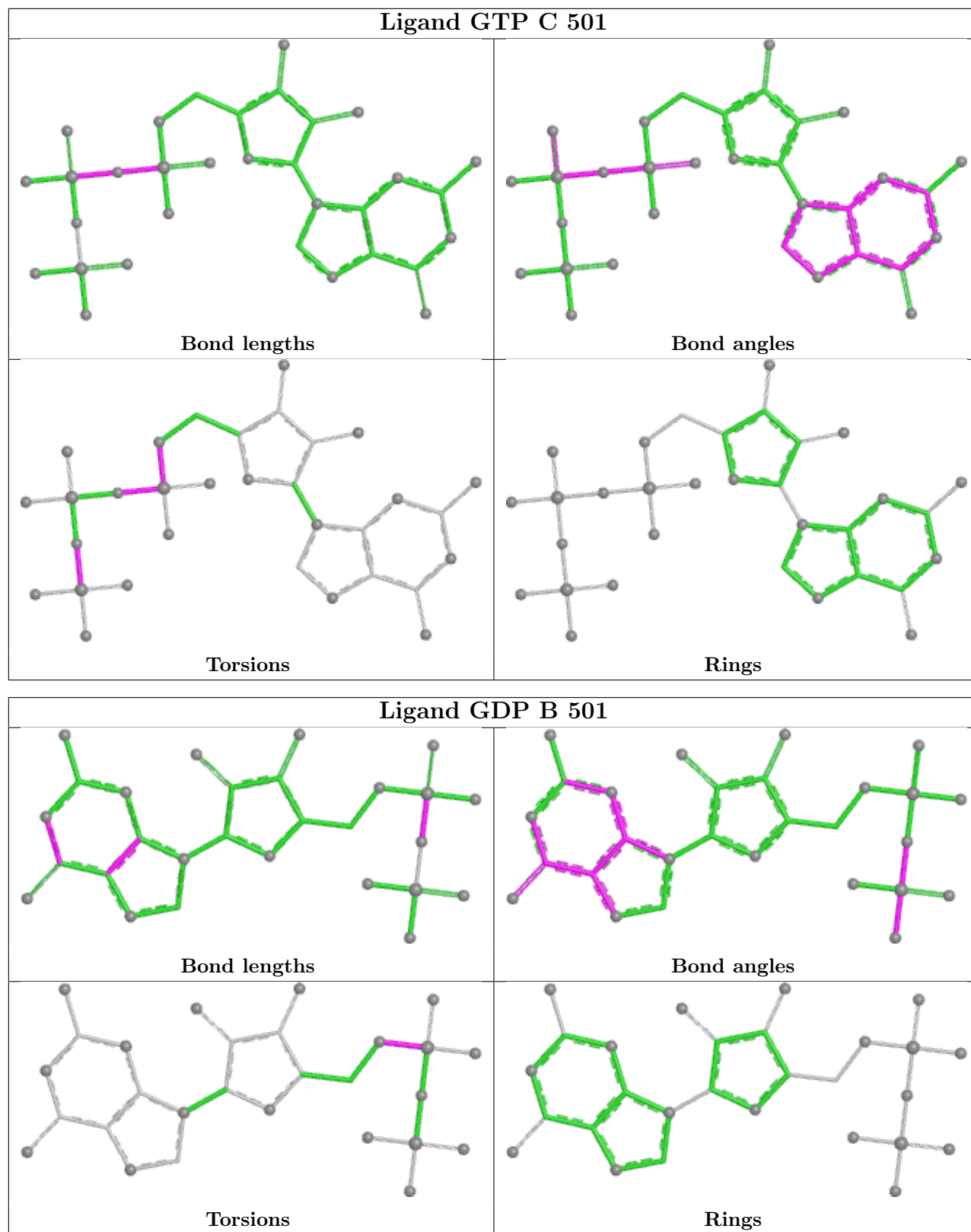
Ligand ACP F 401



Ligand GTP A 501







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	434/440 (98%)	0.05	5 (1%) 76 75	25, 41, 61, 69	0
1	C	440/440 (100%)	-0.18	5 (1%) 78 76	18, 30, 48, 62	0
2	B	423/431 (98%)	0.06	14 (3%) 49 45	18, 36, 60, 68	0
2	D	421/431 (97%)	0.26	19 (4%) 38 34	27, 48, 66, 80	0
3	E	118/138 (85%)	0.24	3 (2%) 58 55	31, 48, 69, 78	0
4	F	313/380 (82%)	1.07	55 (17%) 4 3	40, 65, 94, 105	0
All	All	2149/2260 (95%)	0.20	101 (4%) 36 33	18, 43, 76, 105	0

All (101) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	149	ALA	4.7
4	F	131	PHE	4.6
4	F	101	TYR	4.5
4	F	130	VAL	4.4
3	E	6	MET	4.4
4	F	228	TYR	4.1
4	F	237	THR	4.0
1	A	178	SER	3.9
4	F	194	PRO	3.8
2	B	247	ASN	3.8
4	F	169	LEU	3.8
4	F	182	ILE	3.7
2	D	332	ASN	3.6
4	F	252	ASN	3.6
2	D	170	MET	3.6
4	F	166	ALA	3.5
3	E	45	PRO	3.5
4	F	172	PHE	3.5
1	A	345	ASP	3.5

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Mol	Chain	Res	Type	RSRZ
4	F	170	LEU	3.5
2	D	37	HIS	3.4
4	F	100	ILE	3.4
2	D	80	PRO	3.3
2	D	1	MET	3.3
4	F	186	LEU	3.3
4	F	380	HIS	3.2
4	F	135	TYR	3.2
4	F	171	ASP	3.0
1	C	283	HIS	3.0
4	F	276	ASN	2.9
2	D	78	SER	2.9
2	B	279	GLN	2.9
4	F	99	VAL	2.9
2	B	170	MET	2.9
1	C	357	TYR	2.9
2	B	282	ARG	2.8
4	F	279	LEU	2.8
2	B	37	HIS	2.8
4	F	134	ALA	2.8
3	E	140	LYS	2.8
2	D	246	LEU	2.8
2	D	284	LEU	2.8
4	F	57	GLY	2.8
2	B	218	THR	2.7
4	F	141	GLY	2.7
2	D	83	GLN	2.7
2	D	73	MET	2.7
2	D	55	THR	2.7
1	A	262	TYR	2.7
4	F	243	HIS	2.7
4	F	132	LEU	2.6
4	F	240	LEU	2.6
4	F	230	SER	2.6
4	F	180	HIS	2.6
2	B	80	PRO	2.6
4	F	88	SER	2.5
4	F	162	ILE	2.5
4	F	140	GLU	2.5
2	D	180	VAL	2.5
1	A	346	TRP	2.5
4	F	361	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
4	F	379	HIS	2.5
4	F	277	THR	2.5
4	F	236	LYS	2.4
2	B	243	PRO	2.4
4	F	144	GLY	2.4
4	F	196	HIS	2.4
4	F	244	CYS	2.4
2	D	315	ALA	2.4
2	B	276	ARG	2.3
4	F	168	GLU	2.3
1	C	440	VAL	2.3
4	F	181	VAL	2.3
2	D	81	PHE	2.3
2	D	92	PHE	2.3
4	F	225	SER	2.3
2	D	335	ASN	2.2
2	B	333	VAL	2.2
4	F	247	LYS	2.2
2	D	84	ILE	2.2
1	A	196	GLU	2.2
4	F	199	PHE	2.2
2	B	428	ALA	2.2
4	F	142	ARG	2.2
4	F	229	ASN	2.1
4	F	271	LEU	2.1
4	F	167	SER	2.1
2	D	408	PHE	2.1
2	B	283	ALA	2.1
4	F	139	ARG	2.1
4	F	227	PRO	2.1
2	B	323	MET	2.1
4	F	185	TYR	2.1
2	D	431	ASP	2.1
1	C	179	THR	2.0
4	F	241	THR	2.0
4	F	275	LEU	2.0
2	B	332	ASN	2.0
4	F	133	ALA	2.0
1	C	178	SER	2.0
4	F	136	ASN	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 ⓘ

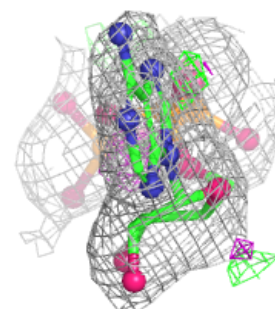
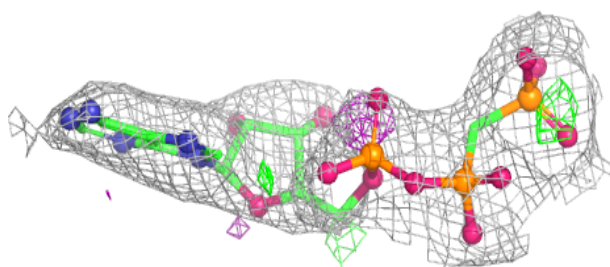
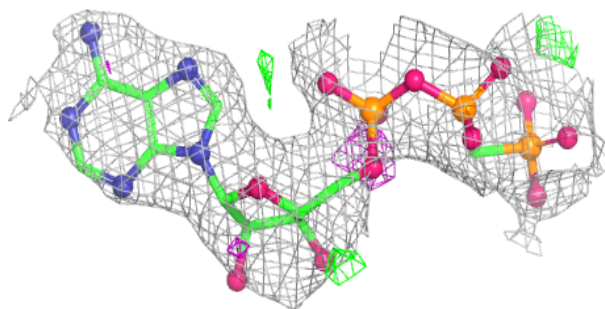
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	PEG	A	505	7/7	0.80	0.23	54,58,61,64	0
14	ACP	F	401	31/31	0.84	0.16	70,76,88,99	0
12	A1D55	B	504	40/40	0.85	0.18	31,35,44,48	40
8	GOL	A	504	6/6	0.89	0.14	37,43,50,52	6
6	MG	C	502	1/1	0.89	0.23	32,32,32,32	0
6	MG	A	502	1/1	0.90	0.27	36,36,36,36	0
13	EDO	C	504	4/4	0.91	0.13	42,44,49,51	0
6	MG	B	502	1/1	0.91	0.18	22,22,22,22	0
11	MES	B	503	12/12	0.94	0.11	27,35,49,50	0
5	GTP	D	501	32/32	0.94	0.09	43,49,65,84	0
7	CA	A	503	1/1	0.96	0.05	67,67,67,67	0
5	GTP	A	501	32/32	0.97	0.07	26,28,31,35	0
7	CA	C	503	1/1	0.98	0.03	41,41,41,41	0
10	GDP	B	501	28/28	0.98	0.07	17,26,28,33	0
5	GTP	C	501	32/32	0.98	0.05	22,22,25,29	0

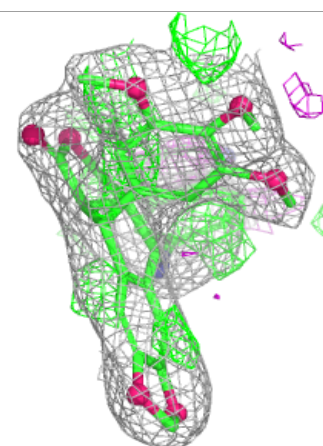
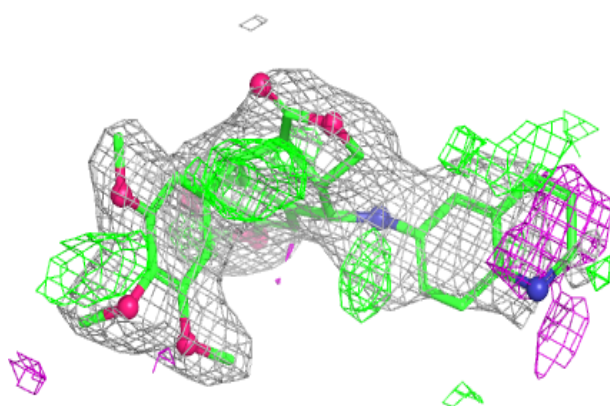
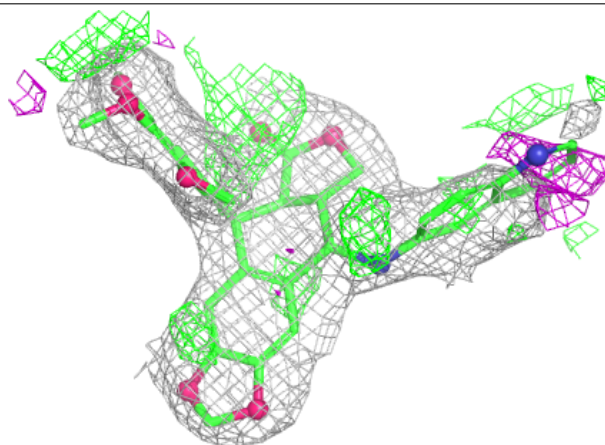
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

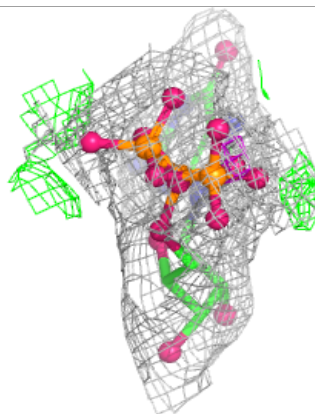
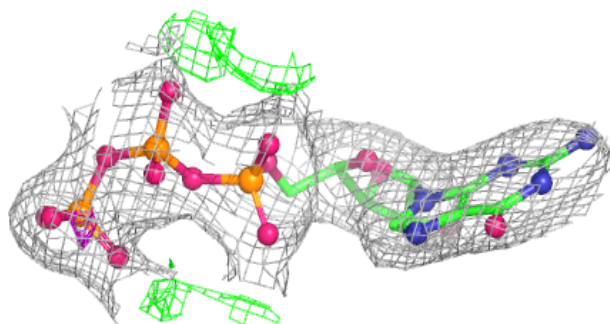
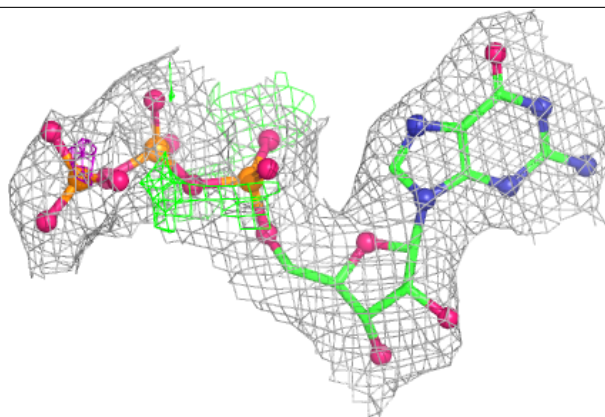
**Electron density around A1D55 B 504:**

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

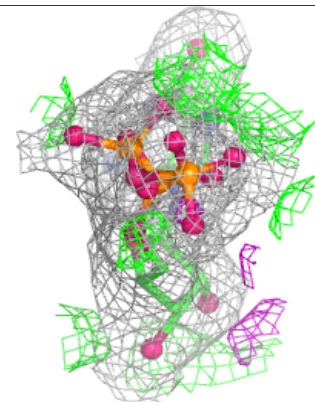
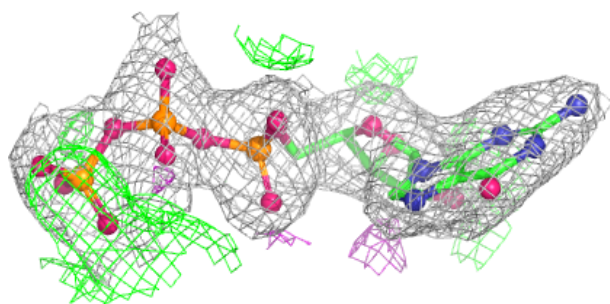
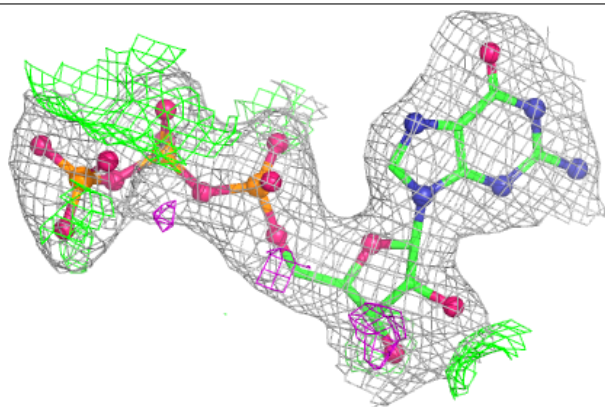


Electron density around GTP D 501:

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

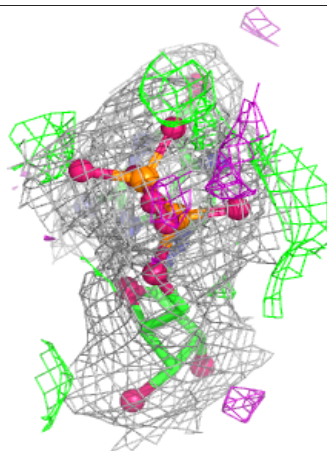
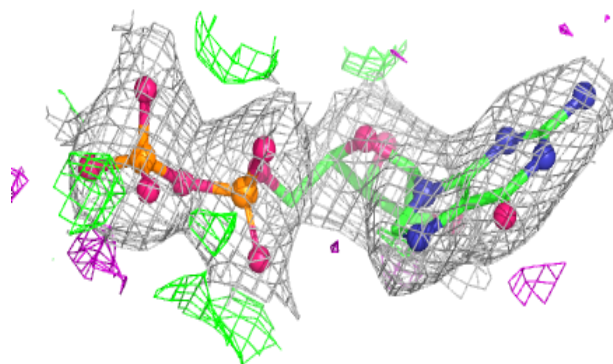
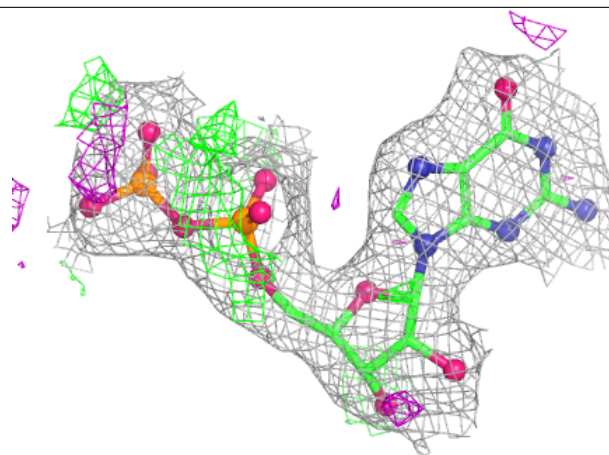
**Electron density around GTP A 501:**

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

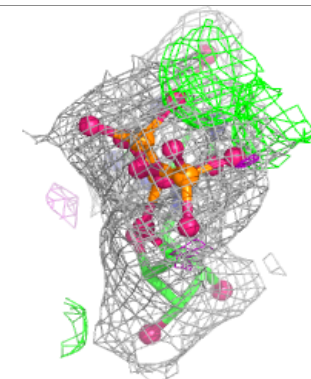
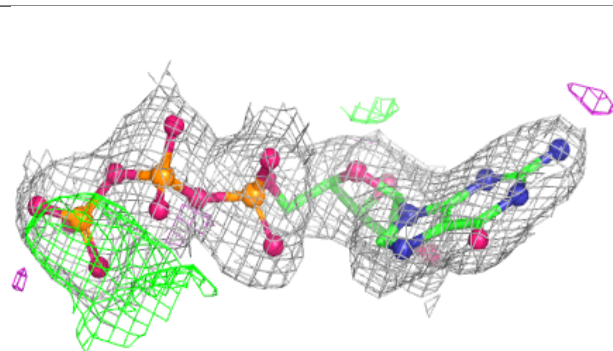
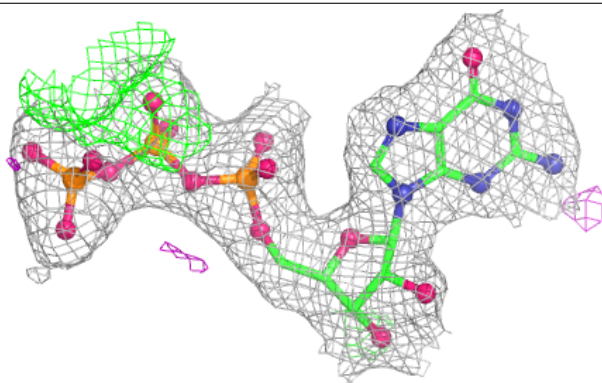


Electron density around GDP B 501:

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

**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.