WORLDWIDE wwPDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

Aug 16, 2023 – 06:55 AM EDT

PDB ID	:	1Z2B
Title	:	Tubulin-colchicine-vinblastine: stathmin-like domain complex
Authors	:	Gigant, B.; Wang, C.; Ravelli, R.B.G.; Roussi, F.; Steinmetz, M.O.; Curmi, P.A.; Sobel, A.; Knossow, M.
Deposited on	:	2005-03-08
Resolution	:	4.10 Å(reported)

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

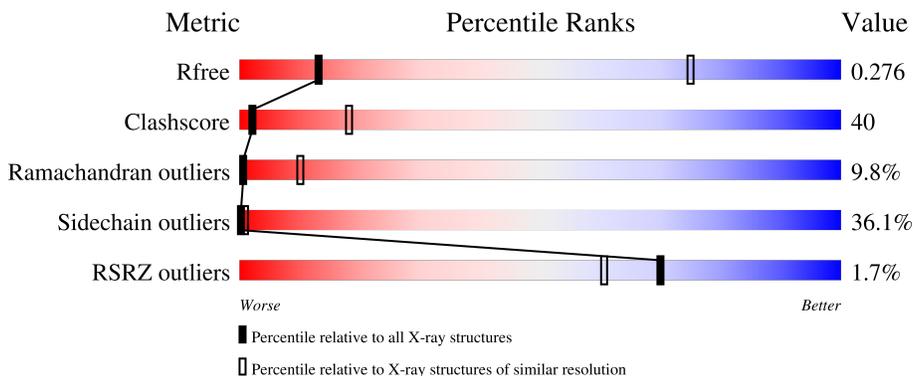|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 4.10 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	Percentile Ranks	Value
Rfree		0.276
Clashscore		40
Ramachandran outliers		9.8%
Sidechain outliers		36.1%
RSRZ outliers		1.7%

Worse   *Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1193 (4.50-3.70)
Clashscore	141614	1003 (4.44-3.76)
Ramachandran outliers	138981	1005 (4.48-3.72)
Sidechain outliers	138945	1199 (4.50-3.70)
RSRZ outliers	127900	1034 (4.50-3.70)

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 <=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	448	32% 43% 18% • 5%
1	C	448	2% 33% 42% 18% • 5%
2	B	445	2% 30% 38% 24% • 6%
2	D	445	2% 29% 40% 23% • 6%
3	E	142	% 33% 35% 16% • 13%

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The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
8	VLB	C	800	-	-	X	-

2 Entry composition ⓘ

There are 8 unique types of molecules in this entry. The entry contains 14173 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 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	427	Total 3290	C 2091	N 556	O 622	S 21	0	0	0
1	C	427	Total 3248	C 2058	N 552	O 618	S 20	38	0	0

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	7	ILE	VAL	SEE REMARK 999	GB 59858433
A	16	ILE	MET	SEE REMARK 999	GB 59858433
A	50	ASN	THR	SEE REMARK 999	GB 59858433
A	54	SER	CYS	SEE REMARK 999	GB 59858433
A	78	VAL	ILE	SEE REMARK 999	GB 59858433
A	80	THR	ASN	SEE REMARK 999	GB 59858433
A	82	THR	PRO	SEE REMARK 999	GB 59858433
A	117	LEU	PRO	SEE REMARK 999	GB 59858433
A	126	ALA	SER	SEE REMARK 999	GB 59858433
A	232	GLY	SER	SEE REMARK 999	GB 59858433
A	334	THR	ALA	SEE REMARK 999	GB 59858433
C	7	ILE	VAL	SEE REMARK 999	GB 59858433
C	16	ILE	MET	SEE REMARK 999	GB 59858433
C	50	ASN	THR	SEE REMARK 999	GB 59858433
C	54	SER	CYS	SEE REMARK 999	GB 59858433
C	78	VAL	ILE	SEE REMARK 999	GB 59858433
C	80	THR	ASN	SEE REMARK 999	GB 59858433
C	82	THR	PRO	SEE REMARK 999	GB 59858433
C	117	LEU	PRO	SEE REMARK 999	GB 59858433
C	126	ALA	SER	SEE REMARK 999	GB 59858433
C	232	GLY	SER	SEE REMARK 999	GB 59858433
C	334	THR	ALA	SEE REMARK 999	GB 59858433

- Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	419	Total 3240	C 2038	N 546	O 632	S 24	0	0	0
2	D	419	Total 3237	C 2037	N 544	O 632	S 24	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	172	VAL	MET	SEE REMARK 999	GB 50844501
B	318	VAL	ILE	SEE REMARK 999	GB 50844501
D	172	VAL	MET	SEE REMARK 999	GB 50844501
D	318	VAL	ILE	SEE REMARK 999	GB 50844501

- Molecule 3 is a protein called RB3 STATHMIN-LIKE DOMAIN 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	124	Total 917	C 555	N 174	O 183	S 5	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	4	ALA	-	SEE REMARK 999	UNP P63043

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 5 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).

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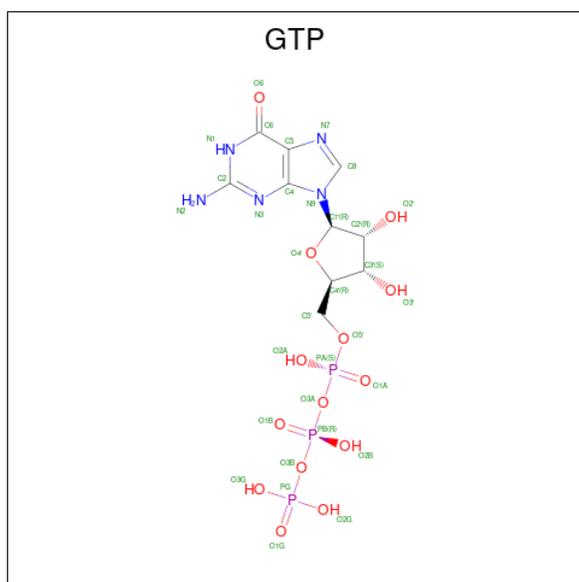
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
5	C	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

- Molecule 6 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).

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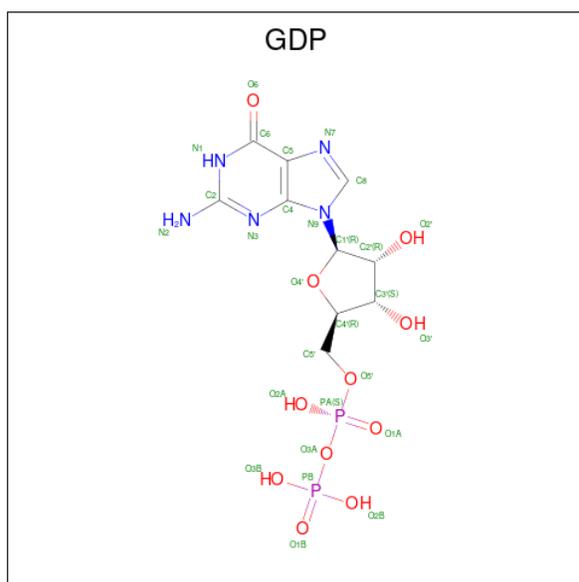
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	B	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

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

- Molecule 7 is 2-MERCAPTO-N-[1,2,3,10-TETRAMETHOXY-9-OXO-5,6,7,9-TETRA HYDRO-BENZO[A]HEPTALEN-7-YL]ACETAMIDE (three-letter code: CN2) (formula: $C_{22}H_{25}NO_6S$).
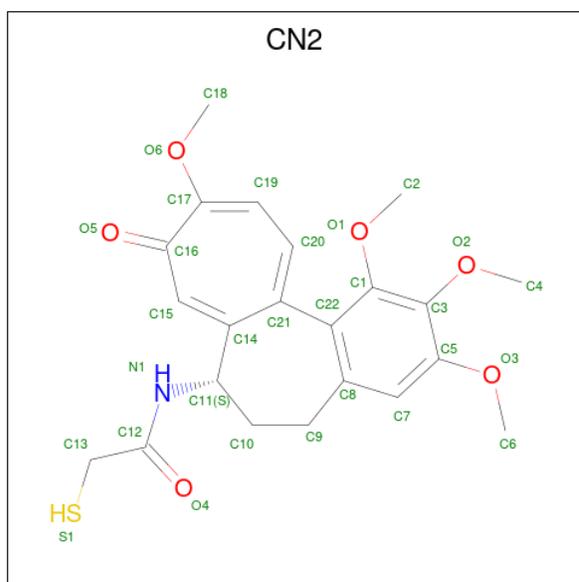
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	B	1	Total	C	N	O	S	0	0
			30	22	1	6	1		
7	D	1	Total	C	N	O	S	0	0
			30	22	1	6	1		

- Molecule 8 is (2ALPHA,2'BETA,3BETA,4ALPHA,5BETA)-VINCALEUKOBLASTINE (three-letter code: VLB) (formula: $C_{46}H_{58}N_4O_9$).

VLB
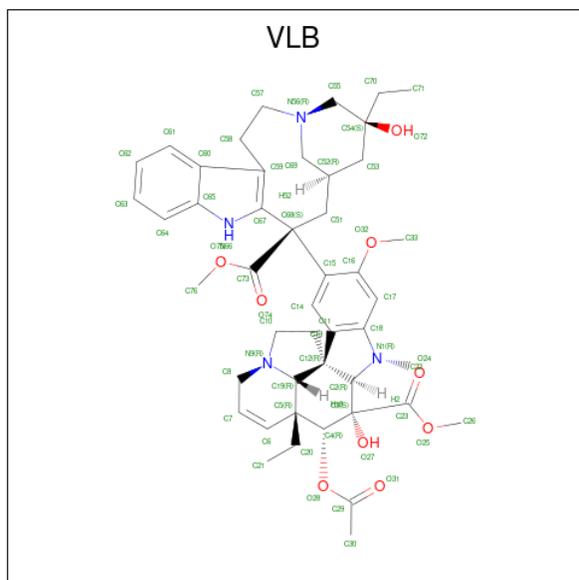
| Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	C	1	Total	C	N	O	0	0
			59	46	4	9		

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.
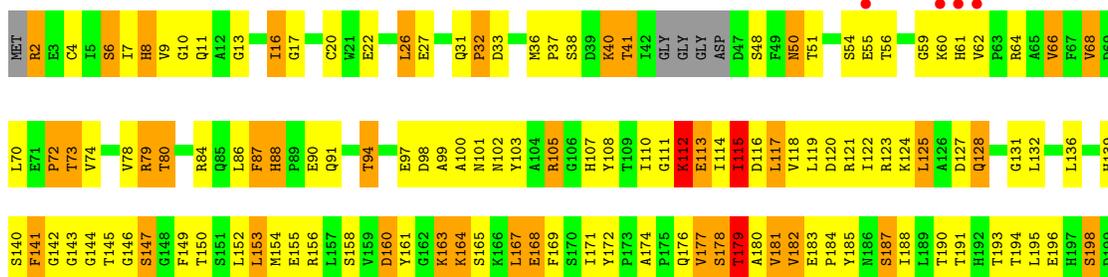
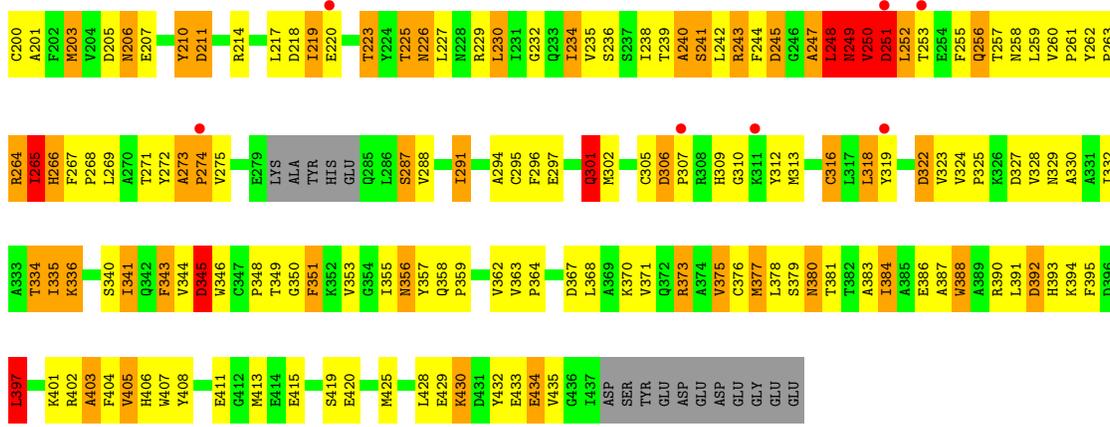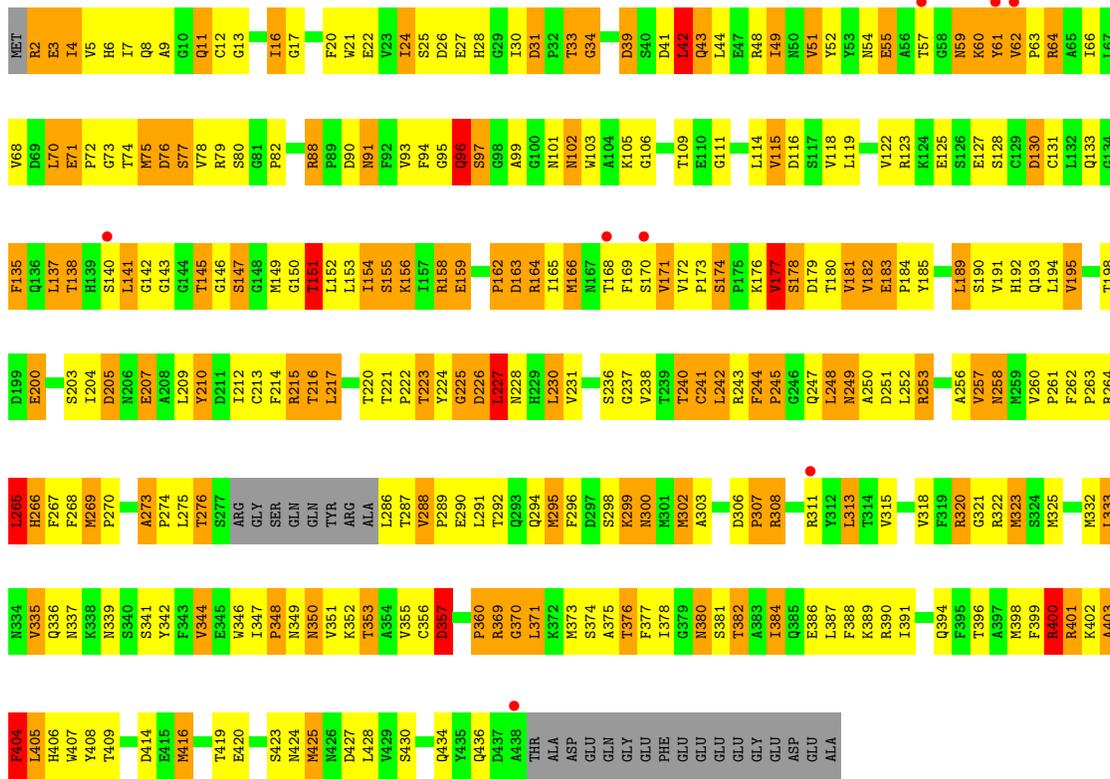- Molecule 1: Tubulin alpha chain
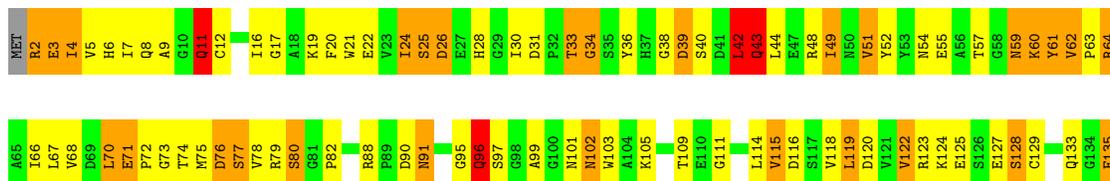
Chain A:
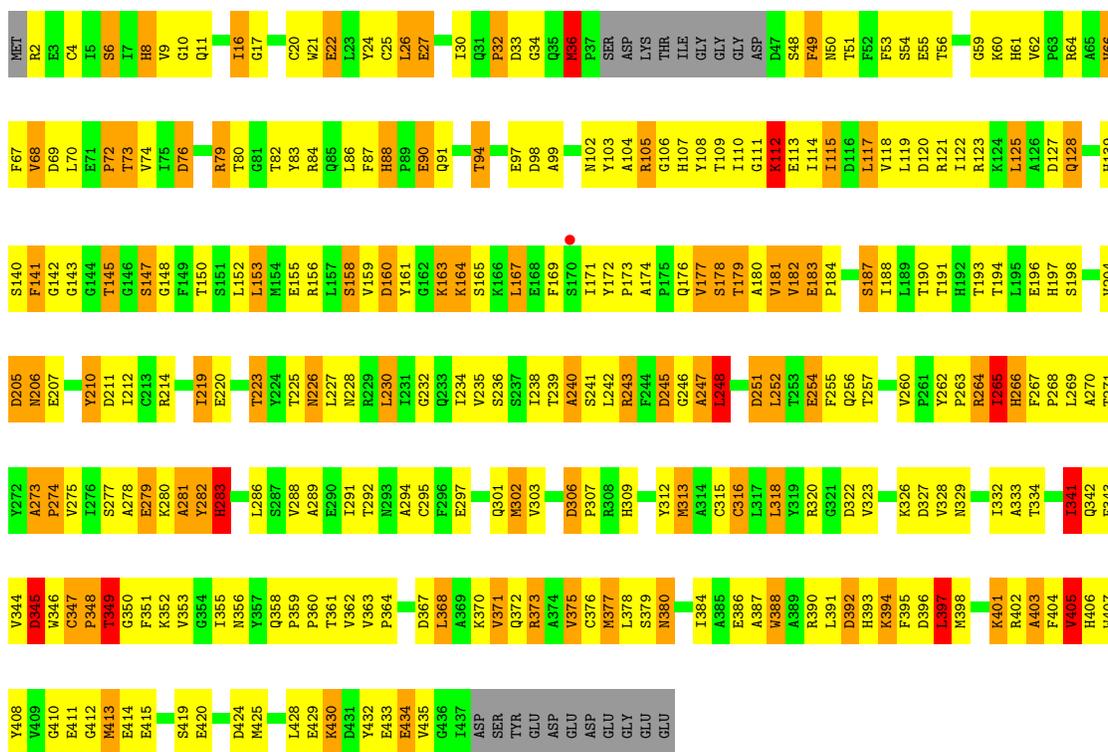
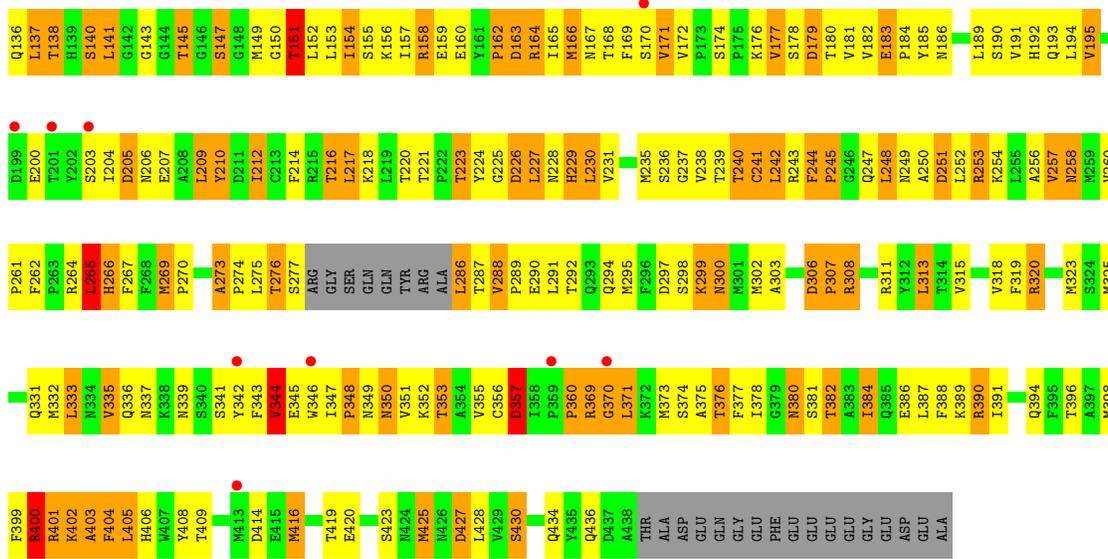- Molecule 1: Tubulin alpha chain

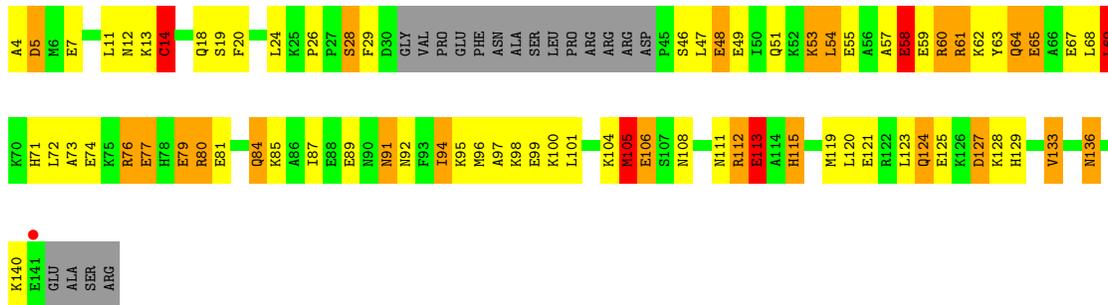Chain C:
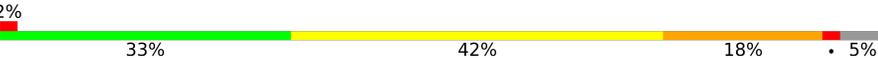
• Molecule 2: Tubulin beta chain

Chain B:

• Molecule 2: Tubulin beta chain

Chain D:

• Molecule 3: RB3 STATHMIN-LIKE DOMAIN 4

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α, β, γ	324.85Å 324.85Å 54.21Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 4.10 38.31 – 4.09	Depositor EDS
% Data completeness (in resolution range)	95.4 (20.00-4.10) 94.7 (38.31-4.09)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.12 (at 4.13Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.209 , 0.269 0.211 , 0.276	Depositor DCC
R_{free} test set	1283 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	197.5	Xtriage
Anisotropy	0.058	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 195.7	EDS
L-test for twinning[2]	$< |L| > = 0.48, < L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.035 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	14173	wwPDB-VP
Average B, all atoms (Å^2)	117.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.78% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GTP, CN2, GDP, VLB, MG

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	0.80	1/3367 (0.0%)	0.97	12/4579 (0.3%)
1	C	0.79	3/3320 (0.1%)	1.02	16/4520 (0.4%)
2	B	0.75	0/3312	0.97	9/4498 (0.2%)
2	D	0.73	0/3309	1.00	13/4494 (0.3%)
3	E	0.73	1/925 (0.1%)	0.92	3/1241 (0.2%)
All	All	0.76	5/14233 (0.0%)	0.98	53/19332 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	4
2	B	0	1
2	D	0	1
3	E	0	1
All	All	0	8

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	306	ASP	C-N	-6.13	1.22	1.34
3	E	105	MET	SD-CE	5.45	2.08	1.77
1	A	36	MET	SD-CE	5.41	2.08	1.77
1	C	203	MET	SD-CE	5.34	2.07	1.77
1	C	168	GLU	CD-OE1	5.03	1.31	1.25

The worst 5 of 53 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	301	GLN	O-C-N	-14.33	99.77	122.70
1	C	120	ASP	CB-CG-OD2	7.82	125.33	118.30
1	C	301	GLN	CA-C-N	7.40	133.48	117.20
1	C	160	ASP	CB-CG-OD2	7.29	124.86	118.30
1	A	205	ASP	CB-CG-OD2	7.25	124.83	118.30

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	177	VAL	Peptide
2	B	162	PRO	Peptide
1	C	177	VAL	Peptide
1	C	248	LEU	Peptide
1	C	249	ASN	Peptide

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	3290	0	3154	240	0
1	C	3248	0	3087	258	0
2	B	3240	0	3056	300	0
2	D	3237	0	3054	272	0
3	E	917	0	803	66	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
5	A	32	0	12	4	0
5	C	32	0	12	5	0
6	B	28	0	12	5	0
6	D	28	0	12	7	0
7	B	30	0	23	7	0
7	D	30	0	23	8	0
8	C	59	0	58	21	0
All	All	14173	0	13306	1096	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 40.

The worst 5 of 1096 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:203:MET:SD	1:C:203:MET:CE	2.07	1.42
1:A:36:MET:SD	1:A:36:MET:CE	2.08	1.40
3:E:105:MET:SD	3:E:105:MET:CE	2.08	1.39
2:B:241:CYS:HB3	2:B:247:GLN:NE2	1.55	1.20
1:A:346:TRP:HE3	1:A:346:TRP:O	1.27	1.17

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	423/448 (94%)	317 (75%)	75 (18%)	31 (7%)	1	16
1	C	421/448 (94%)	315 (75%)	68 (16%)	38 (9%)	1	12
2	B	415/445 (93%)	298 (72%)	71 (17%)	46 (11%)	0	7
2	D	415/445 (93%)	297 (72%)	73 (18%)	45 (11%)	0	7
3	E	120/142 (84%)	68 (57%)	36 (30%)	16 (13%)	0	4
All	All	1794/1928 (93%)	1295 (72%)	323 (18%)	176 (10%)	0	10

5 of 176 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	55	GLU
1	A	62	VAL
1	A	72	PRO
1	A	112	LYS
1	A	240	ALA

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	345/377 (92%)	228 (66%)	117 (34%)	0	1
1	C	336/377 (89%)	224 (67%)	112 (33%)	0	2
2	B	348/383 (91%)	217 (62%)	131 (38%)	0	0
2	D	348/383 (91%)	218 (63%)	130 (37%)	0	0
3	E	80/126 (64%)	44 (55%)	36 (45%)	0	0
All	All	1457/1646 (88%)	931 (64%)	526 (36%)	0	1

5 of 526 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	350	ASN
2	D	390	ARG
2	D	349	ASN
3	E	119	MET
2	B	248	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 59 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	350	ASN
3	E	12	ASN
1	C	107	HIS
2	D	436	GLN
2	D	309	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 ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 9 ligands modelled in this entry, 2 are monoatomic - leaving 7 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$|Z| > 2$	Counts	RMSZ	#$|Z| > 2$
8	VLB	C	800	-	63,67,67	1.56	10 (15%)	79,108,108	2.52	26 (32%)
7	CN2	B	700	-	27,32,32	3.70	7 (25%)	26,45,45	4.95	12 (46%)
7	CN2	D	701	-	27,32,32	3.46	8 (29%)	26,45,45	5.07	12 (46%)
5	GTP	A	600	4	26,34,34	1.33	3 (11%)	32,54,54	1.75	8 (25%)
5	GTP	C	601	4	26,34,34	1.30	3 (11%)	32,54,54	1.94	9 (28%)
6	GDP	B	602	-	24,30,30	1.05	1 (4%)	30,47,47	1.86	10 (33%)
6	GDP	D	603	-	24,30,30	1.19	1 (4%)	30,47,47	1.82	8 (26%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	VLB	C	800	-	-	16/38/131/131	0/7/9/9
7	CN2	B	700	-	-	2/10/27/27	0/3/3/3
7	CN2	D	701	-	-	3/10/27/27	0/3/3/3
5	GTP	A	600	4	-	5/18/38/38	0/3/3/3
5	GTP	C	601	4	-	6/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	GDP	B	602	-	-	4/12/32/32	0/3/3/3
6	GDP	D	603	-	-	3/12/32/32	0/3/3/3

The worst 5 of 33 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	700	CN2	C20-C19	-11.34	1.19	1.38
7	D	701	CN2	C20-C19	-10.44	1.21	1.38
7	B	700	CN2	C19-C17	-8.37	1.24	1.39
7	D	701	CN2	C19-C17	-8.34	1.24	1.39
7	B	700	CN2	C20-C21	-7.60	1.23	1.39

The worst 5 of 85 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	D	701	CN2	C19-C20-C21	21.96	147.72	129.68
7	B	700	CN2	C19-C20-C21	21.87	147.65	129.68
8	C	800	VLB	C4-O28-C29	-9.58	102.87	117.65
8	C	800	VLB	C57-C58-C59	6.86	127.27	114.30
7	D	701	CN2	C20-C19-C17	6.72	145.96	129.69

There are no chirality outliers.

5 of 39 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	600	GTP	C5'-O5'-PA-O1A
5	C	601	GTP	C5'-O5'-PA-O1A
6	B	602	GDP	PA-O3A-PB-O2B
6	B	602	GDP	O4'-C4'-C5'-O5'
6	D	603	GDP	O4'-C4'-C5'-O5'

There are no ring outliers.

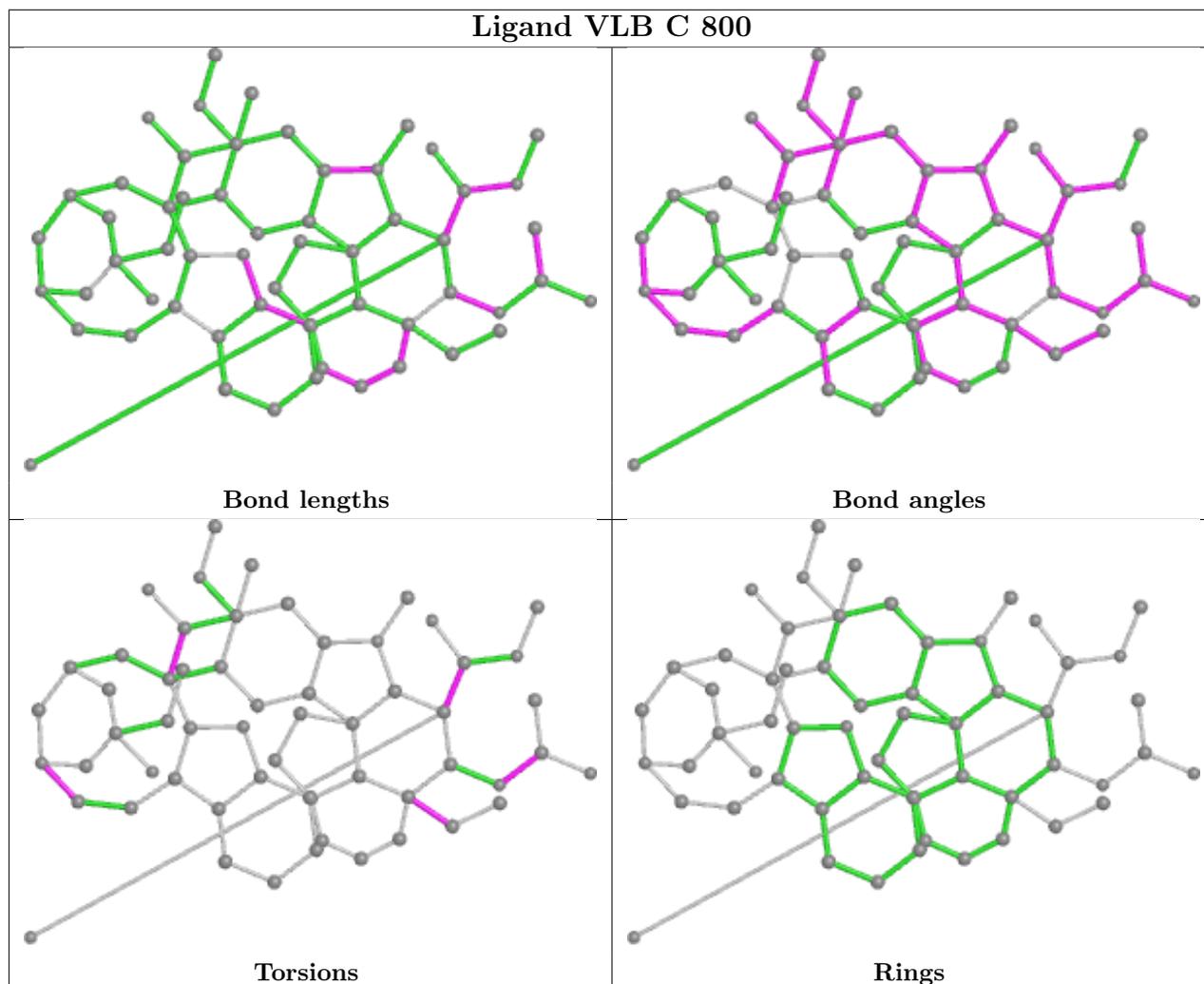7 monomers are involved in 57 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	C	800	VLB	21	0
7	B	700	CN2	7	0
7	D	701	CN2	8	0
5	A	600	GTP	4	0
5	C	601	GTP	5	0

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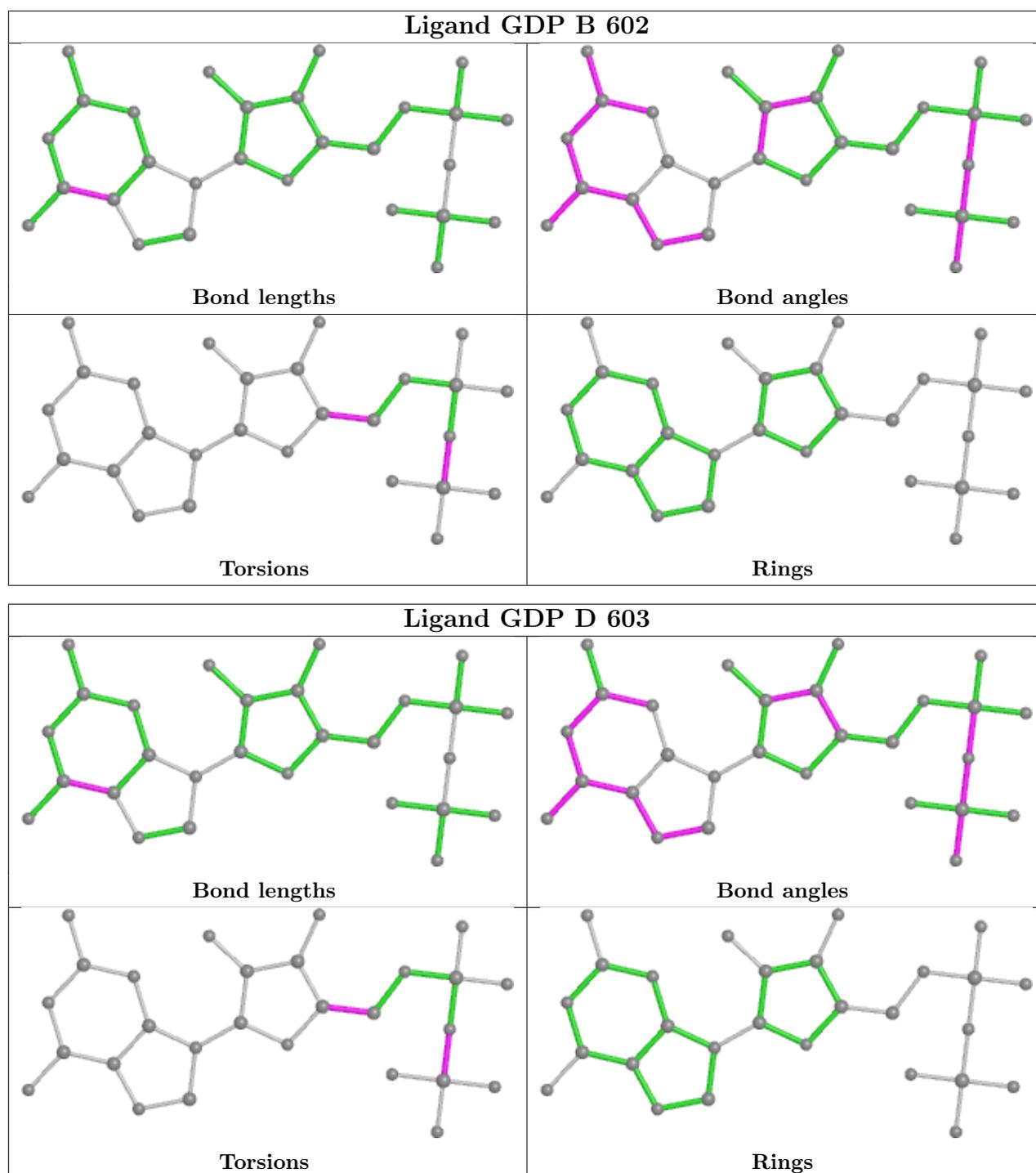| Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	602	GDP	5	0
6	D	603	GDP	7	0

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

Ligand VLB C 800

Bond lengths

Bond angles

Torsions

Rings

Ligand CN2 B 700

Bond lengths

Bond angles

Torsions

Rings

Ligand CN2 D 701

Bond lengths

Bond angles

Torsions

Rings

Ligand GTP A 600

Bond lengths

Bond angles

Torsions

Rings

Ligand GTP C 601

Bond lengths

Bond angles

Torsions

Rings

Ligand GDP B 602

Bond lengths

Bond angles

Torsions

Rings

Ligand GDP D 603

Bond lengths

Bond angles

Torsions

Rings
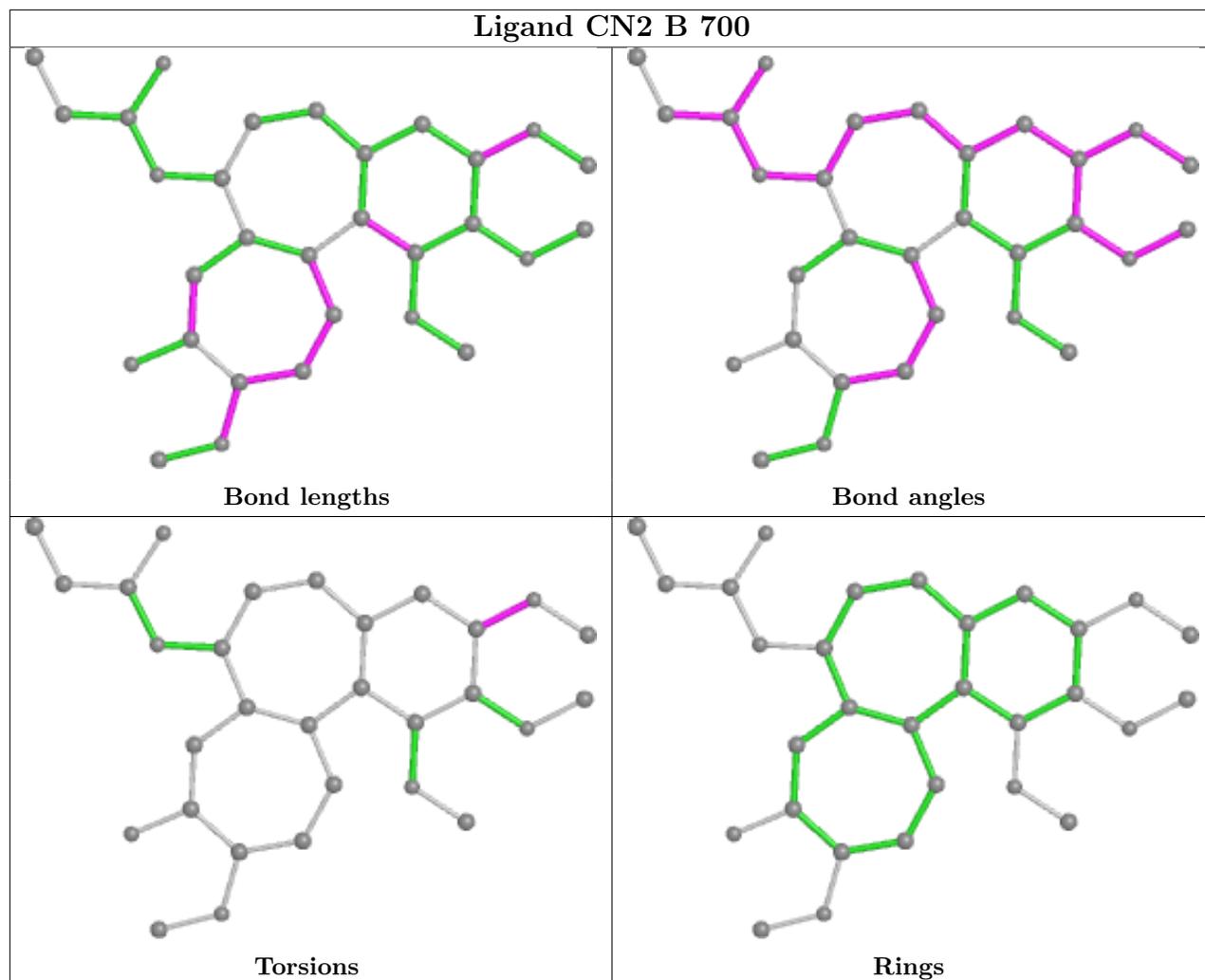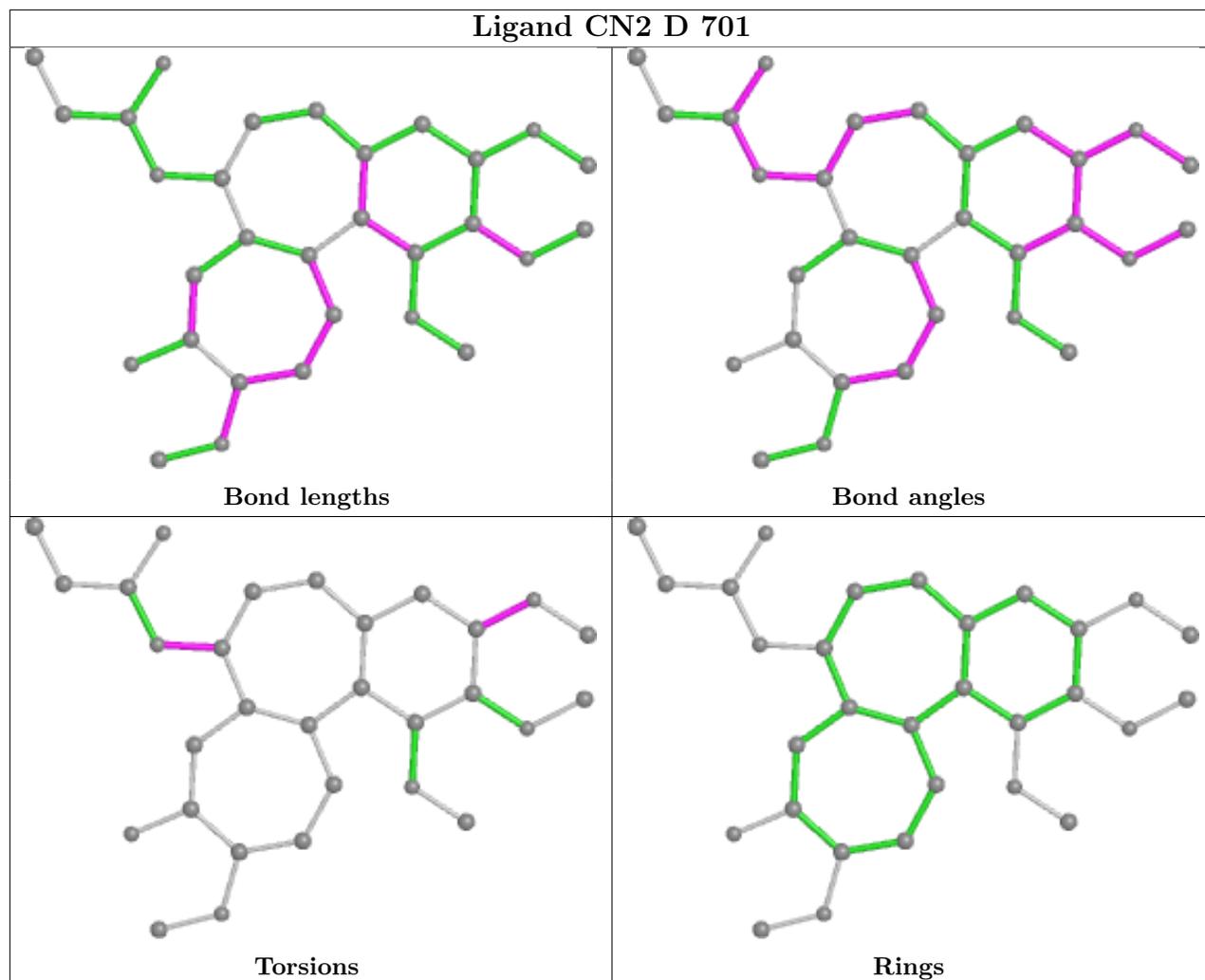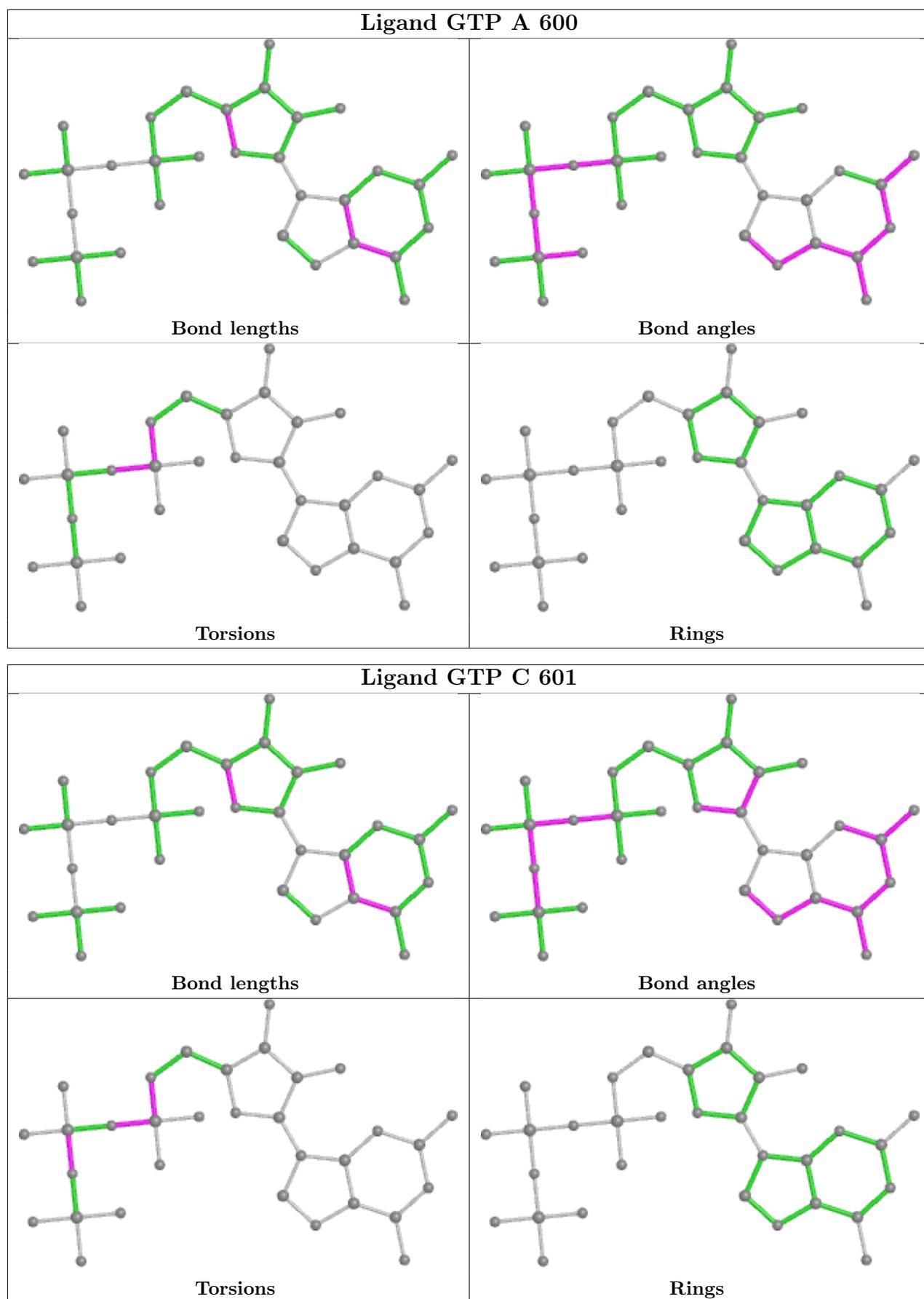
5.7 Other polymers ⓘ

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	427/448 (95%)	-0.31	1 (0%)	95	93	118, 118, 118, 118	1 (0%)
1	C	422/448 (94%)	-0.05	11 (2%)	56	45	118, 118, 118, 118	0
2	B	419/445 (94%)	-0.08	8 (1%)	66	58	118, 118, 118, 118	0
2	D	419/445 (94%)	-0.07	9 (2%)	63	54	118, 118, 118, 118	0
3	E	124/142 (87%)	-0.23	1 (0%)	86	79	118, 118, 118, 118	0
All	All	1811/1928 (93%)	-0.13	30 (1%)	70	60	118, 118, 118, 118	1 (0%)

The worst 5 of 30 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	61	TYR	3.8
1	C	311	LYS	3.2
2	B	62	VAL	3.1
1	C	61	HIS	3.1
2	D	203	SER	2.9

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 monosaccharides in this entry.
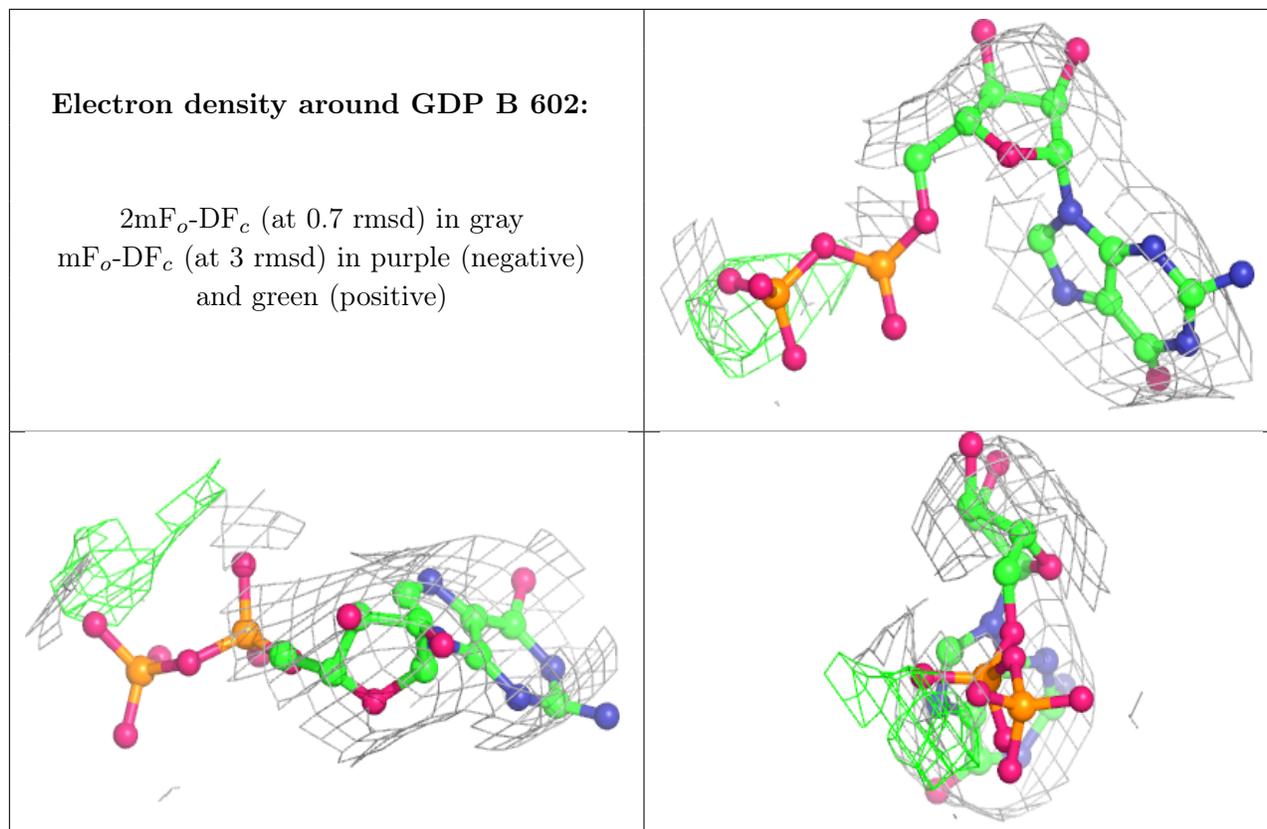
6.4 Ligands ⓘ

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
6	GDP	B	602	28/28	0.85	0.44	117,117,117,117	0
8	VLB	C	800	59/59	0.88	0.28	117,117,117,117	0
7	CN2	B	700	30/30	0.89	0.28	117,117,117,117	0
7	CN2	D	701	30/30	0.94	0.22	117,117,117,117	0
5	GTP	A	600	32/32	0.94	0.29	117,117,117,117	0
5	GTP	C	601	32/32	0.95	0.25	117,117,117,117	0
6	GDP	D	603	28/28	0.97	0.23	117,117,117,117	0
4	MG	C	501	1/1	0.97	0.26	117,117,117,117	0
4	MG	A	500	1/1	0.98	0.34	117,117,117,117	0

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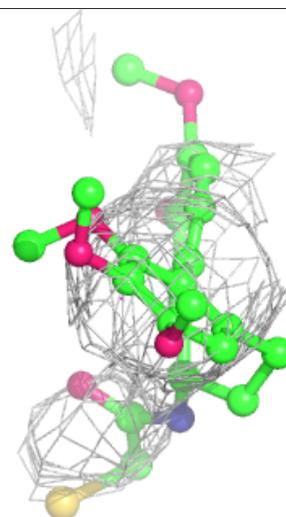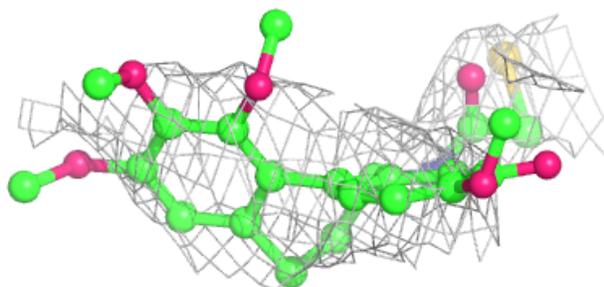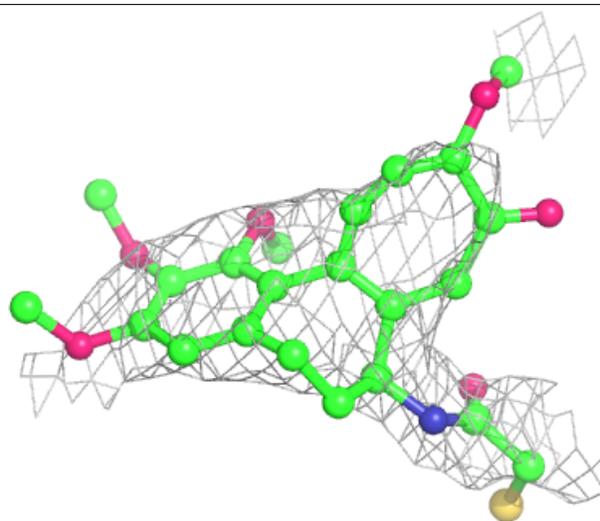

Electron density around GDP B 602:

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 VLB C 800:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
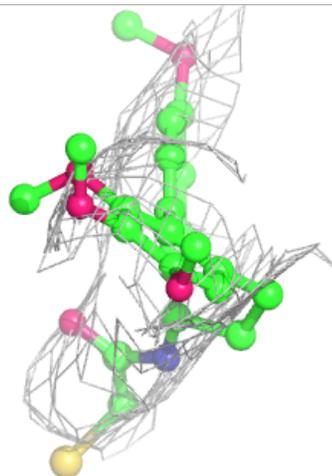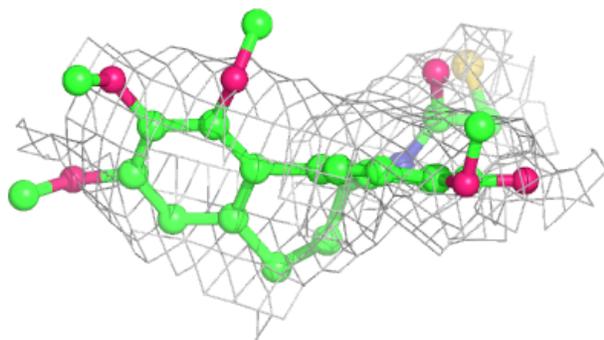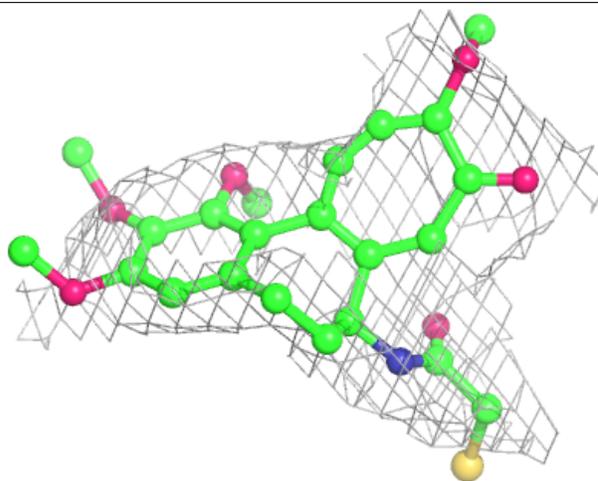and green (positive)
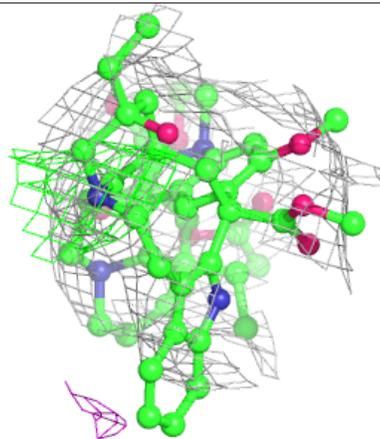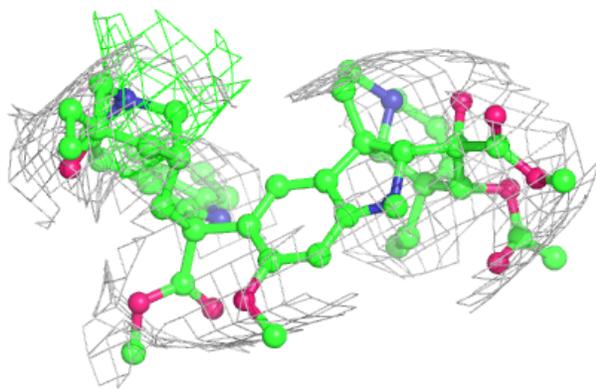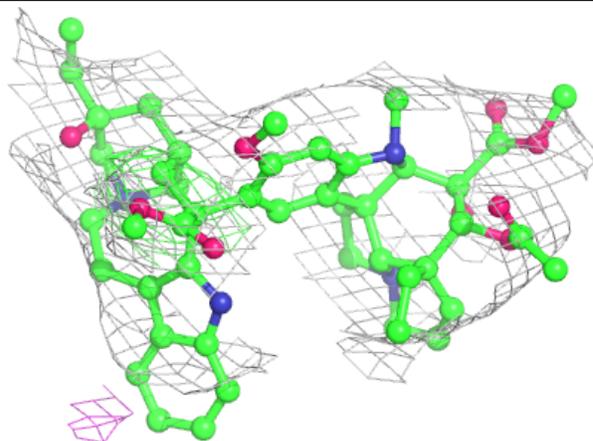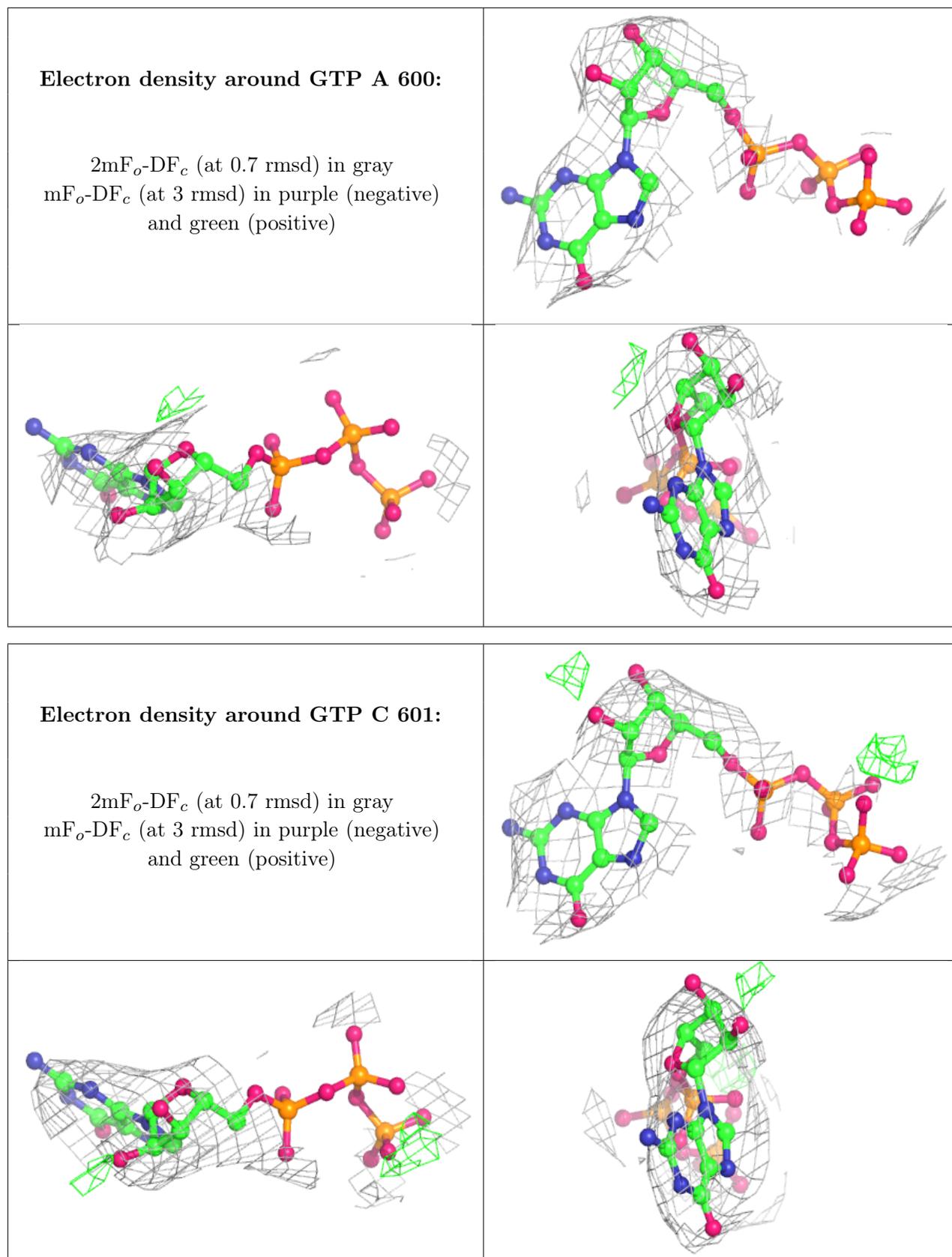
Electron density around CN2 B 700:

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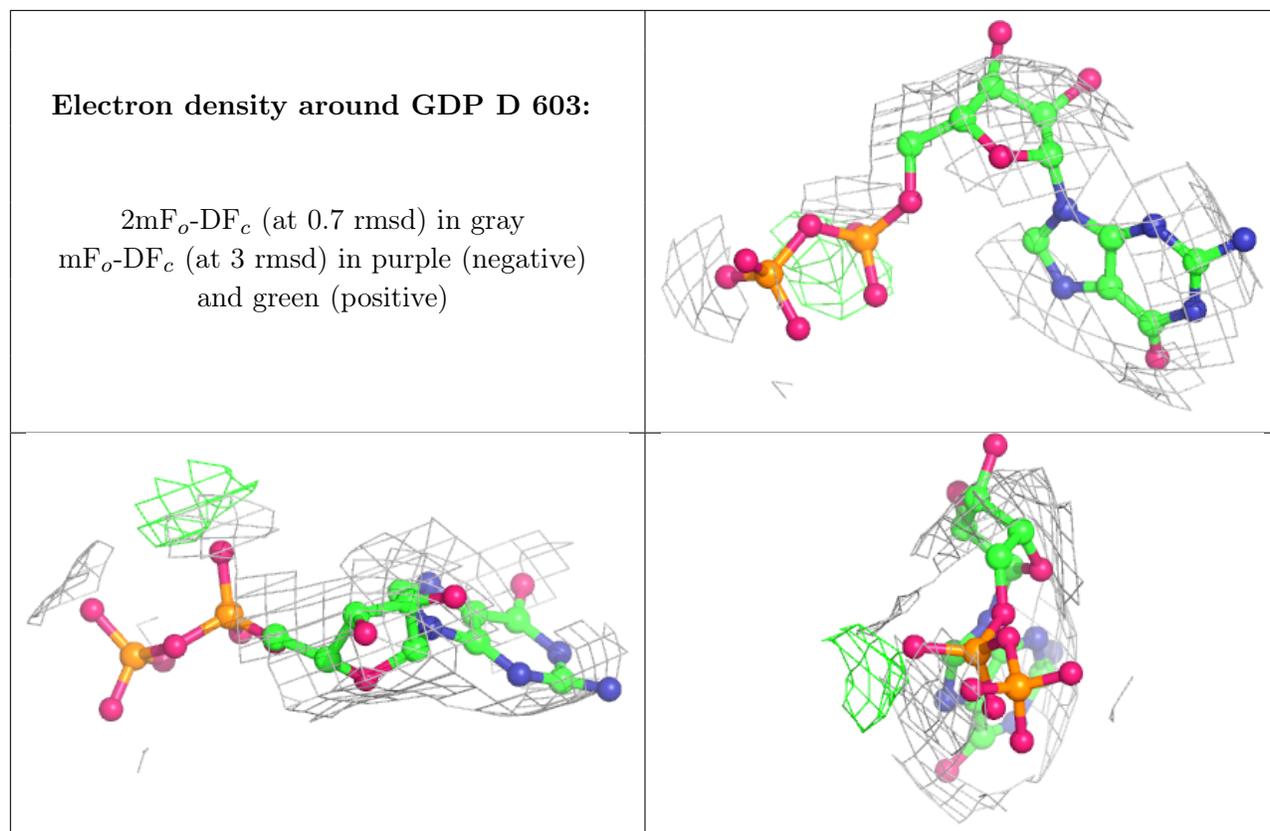mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around CN2 D 701:

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

Electron density around GTP A 600:

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

Electron density around GTP C 601:

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

Electron density around GDP D 603:

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

6.5 Other polymers ⓘ

There are no such residues in this entry.