



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:49 AM UTC

PDB ID : 8YTX / pdb_00008ytx
Title : Tubulin-RB3-TTL in complex with compound SI9
Authors : Wu, C.Y.; Wang, Y.X.
Deposited on : 2024-03-26
Resolution : 2.53 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

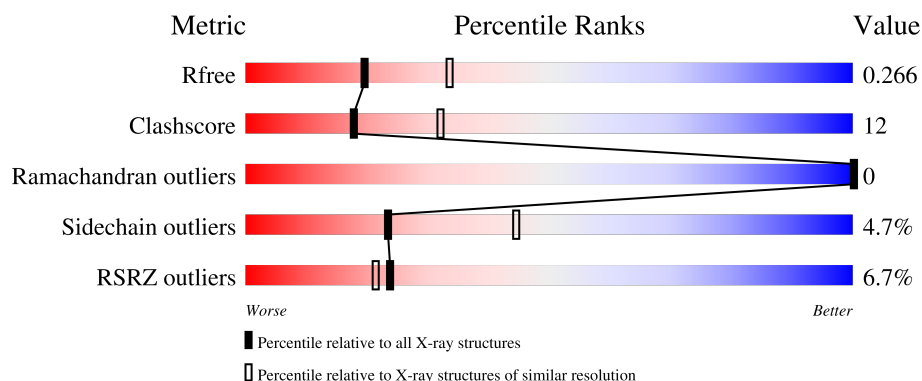
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.53 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	7383 (2.54-2.50)
Clashscore	190562	8079 (2.54-2.50)
Ramachandran outliers	187476	7944 (2.54-2.50)
Sidechain outliers	187428	7946 (2.54-2.50)
RSRZ outliers	180081	7387 (2.54-2.50)

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

Mol	Chain	Length	Quality of chain
1	A	440	2% 78% 21% ..
1	C	440	2% 82% 17% .
2	B	431	6% 77% 21% ..
2	D	431	10% 67% 28% ..
3	E	143	6% 59% 20% 18%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	F	380	 A horizontal bar chart showing the quality of chain F. The bar is divided into four segments: red (11%), green (47%), yellow (21%), and grey (29%). A small black dot is located on the yellow segment. The percentages are labeled below the bar: 11%, 47%, 21%, and 29%.

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 16858 atoms, of which 38 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	437	Total	C	N	O	S	0	0	0
			3405	2154	580	649	22			
1	C	440	Total	C	N	O	S	0	0	0
			3433	2172	583	656	22			

- Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	427	Total	C	N	O	S	0	0	0
			3351	2104	572	649	26			
2	D	418	Total	C	N	O	S	0	0	0
			3281	2065	555	634	27			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	117	Total	C	N	O	S	0	0	0
			962	594	176	187	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

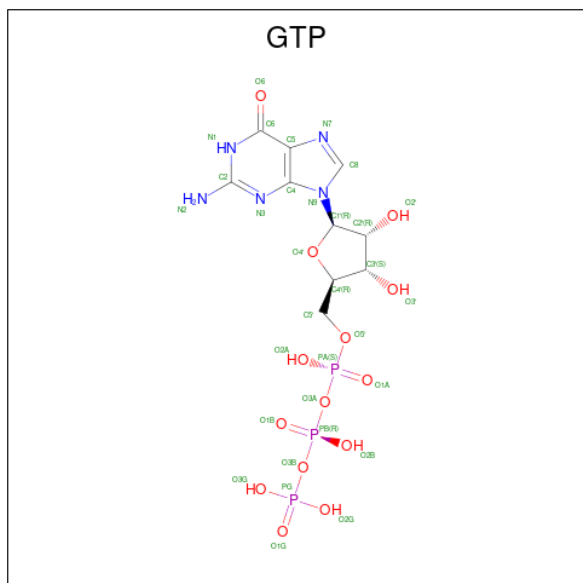
- Molecule 4 is a protein called Tubulin-tyrosine ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	268	Total	C	N	O	S	0	0	0
			2166	1397	366	389	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

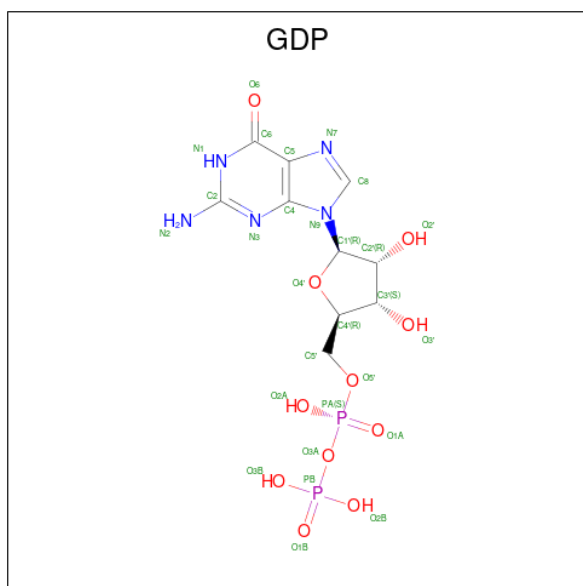
- Molecule 5 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



Continued from previous page...

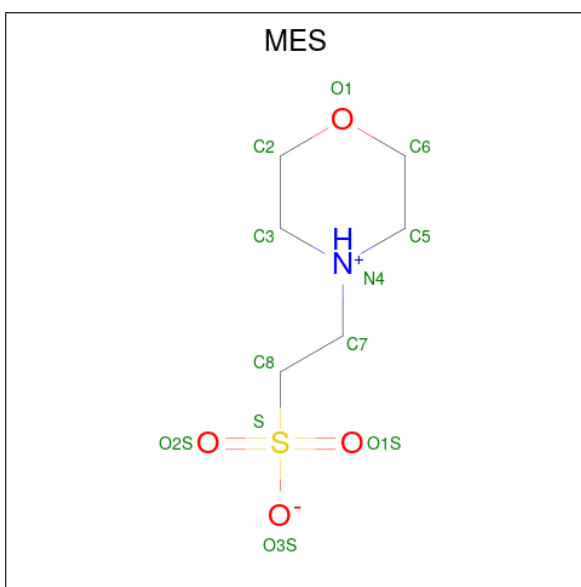
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	C	1	Total	Mg	1	0
			1	1		

- Molecule 8 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



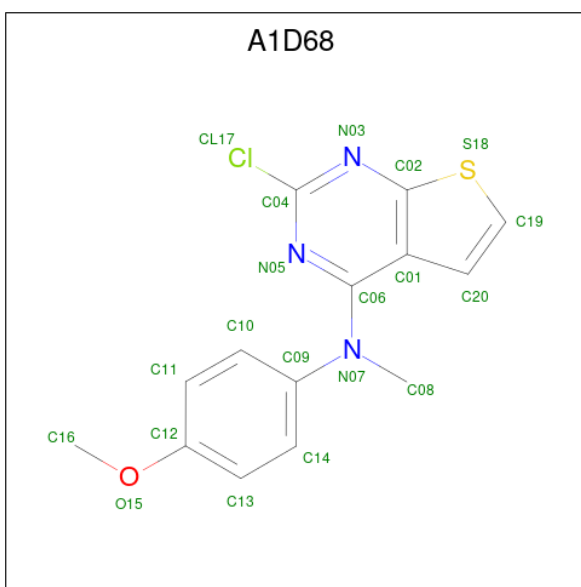
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	B	1	Total	C	N	O	P	28	0
			28	10	5	11	2		
8	D	1	Total	C	N	O	P	28	0
			28	10	5	11	2		

- Molecule 9 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: $C_6H_{13}NO_4S$).



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

- Molecule 10 is 2-chloranyl- {N}-(4-methoxyphenyl)- {N}-methyl-thieno[2,3-d]pyrimidin-4-amine (CCD ID: A1D68) (formula: $C_{14}H_{12}ClN_3OS$) (labeled as "Ligand of Interest" by depositor).



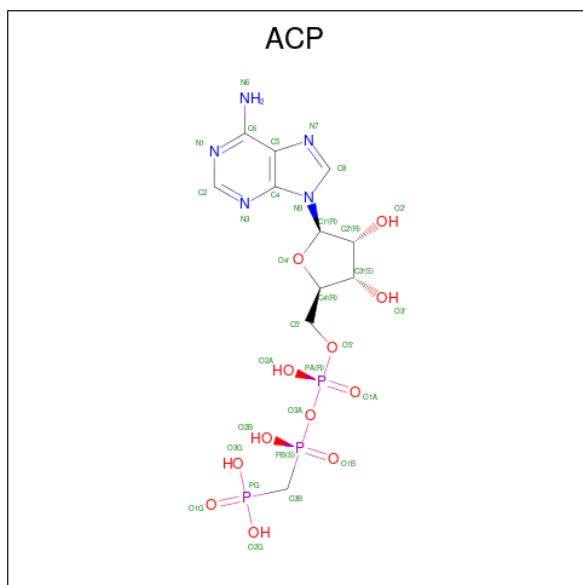
Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
10	B	1	Total	C	Cl	H	N	O	S	0	0
			32	14	1	12	3	1	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
10	D	1	Total	C	Cl	H	N	O	S	0	0
			32	14	1	12	3	1	1		

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



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
11	F	1	Total	C	H	N	O	P	45	0
			45	11	14	5	12	3		

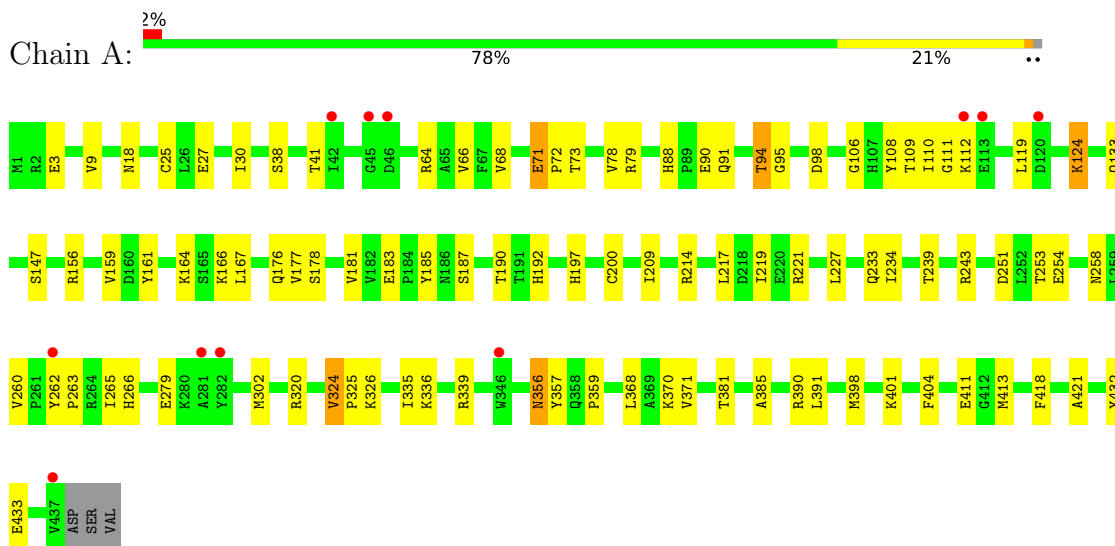
- Molecule 12 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	B	1	Total 1 O 1	0	0
12	D	1	Total 1 O 1	0	0

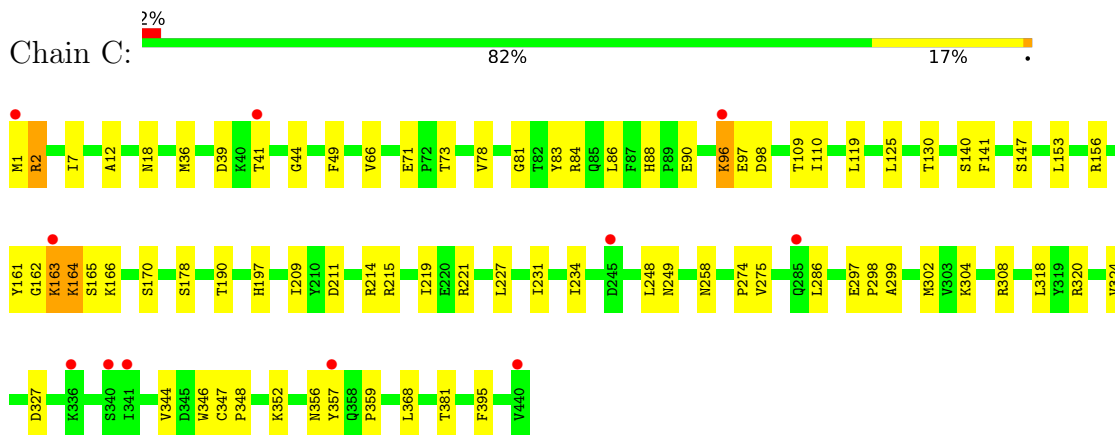
3 Residue-property plots

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.

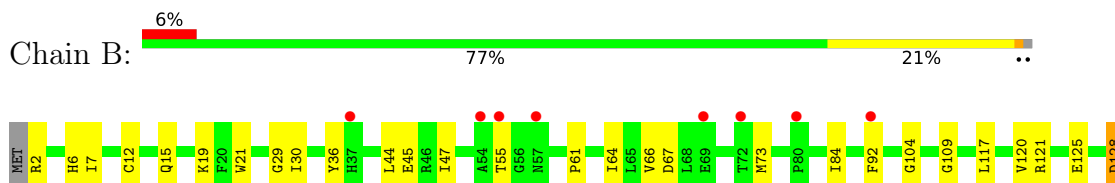
- Molecule 1: Detyrosinated tubulin alpha-1B chain

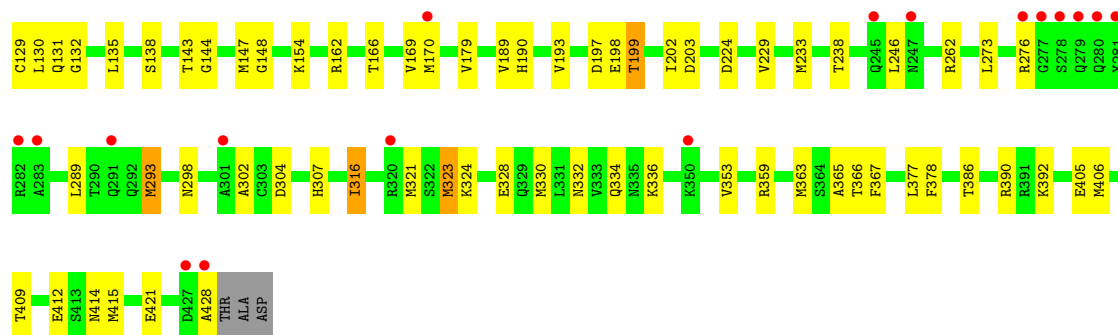


- Molecule 1: Detyrosinated tubulin alpha-1B chain

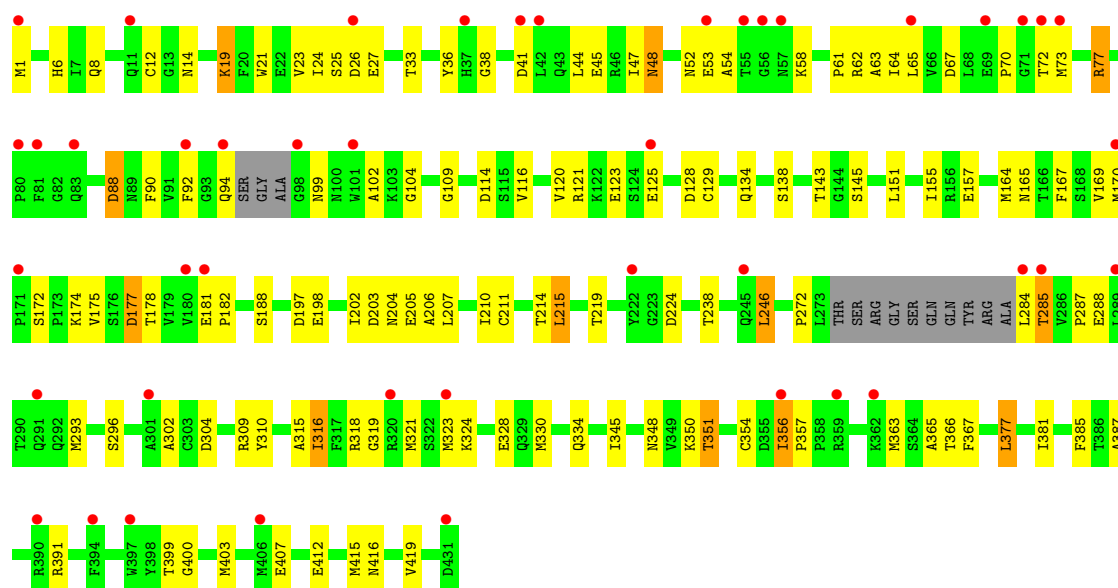


- Molecule 2: Tubulin beta chain

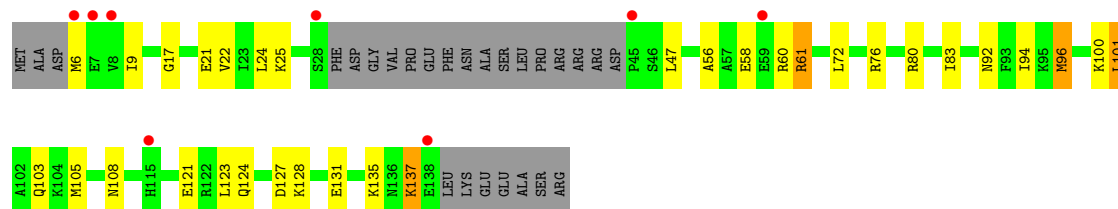




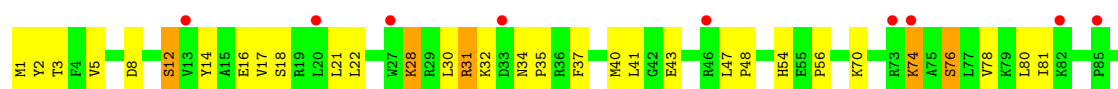
• Molecule 2: Tubulin beta chain

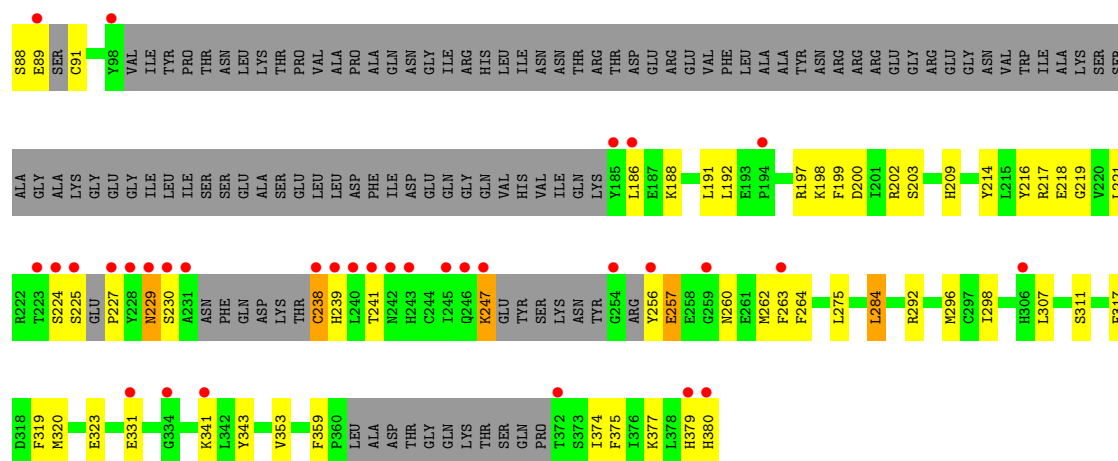


• Molecule 3: Stathmin-4



• 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	105.37Å 158.31Å 180.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.56 – 2.53 45.56 – 2.53	Depositor EDS
% Data completeness (in resolution range)	98.7 (45.56-2.53) 98.6 (45.56-2.53)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.22 (at 2.54Å)	Xtriage
Refinement program	PHENIX (1.21_5207: ???)	Depositor
R, R_{free}	0.222 , 0.266 0.222 , 0.266	Depositor DCC
R_{free} test set	2000 reflections (1.97%)	wwPDB-VP
Wilson B-factor (Å ²)	52.8	Xtriage
Anisotropy	0.195	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 36.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	16858	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.50% 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: GTP, MES, GDP, ACP, MG, A1D68, CA

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	0/3482	0.58	0/4728
1	C	0.44	0/3511	0.64	0/4768
2	B	0.39	0/3426	0.57	0/4643
2	D	0.32	0/3353	0.52	0/4543
3	E	0.37	0/970	0.52	0/1286
4	F	0.31	0/2215	0.49	0/2992
All	All	0.38	0/16957	0.57	0/22960

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	3405	0	3312	74	0
1	C	3433	0	3337	55	0
2	B	3351	0	3214	82	0
2	D	3281	0	3151	118	0
3	E	962	0	981	28	0
4	F	2166	0	2110	72	0
5	A	32	0	12	0	0

Continued on next page...

Continued from previous page...

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	C	1	0	0	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
8	B	28	0	12	0	0
8	D	28	0	11	0	0
9	B	24	0	26	0	0
10	B	20	12	0	0	0
10	D	20	12	0	0	0
11	F	31	14	14	0	0
12	B	1	0	0	0	0
12	D	1	0	0	0	0
All	All	16820	38	16192	403	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 12.

All (403) 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:73:MET:HE1	2:D:92:PHE:HB3	1.27	1.11
1:A:71:GLU:OE2	1:A:73:THR:HB	1.64	0.97
2:B:73:MET:HE2	2:B:92:PHE:HB3	1.48	0.96
2:D:73:MET:CE	2:D:92:PHE:HB3	1.96	0.95
2:B:238:THR:HB	2:B:316:ILE:HD13	1.46	0.93
4:F:186:LEU:HD12	4:F:320:MET:HG2	1.49	0.92
1:C:249:ASN:OD1	1:C:356:ASN:ND2	2.03	0.91
1:A:109:THR:HG21	1:A:411:GLU:OE1	1.71	0.90
1:A:90:GLU:OE1	1:A:124:LYS:NZ	2.03	0.90
2:D:170:MET:HE2	2:D:377:LEU:HD11	1.54	0.90
4:F:1:MET:HE1	4:F:28:LYS:HB3	1.55	0.89
2:B:143:THR:HG23	2:B:147:MET:HE2	1.55	0.86
2:D:272:PRO:HB3	2:D:284:LEU:HD22	1.58	0.85
2:D:272:PRO:HB3	2:D:284:LEU:CD2	2.09	0.82
4:F:188:LYS:HD3	4:F:323:GLU:OE1	1.82	0.80
2:B:324:LYS:HE2	2:B:328:GLU:OE2	1.80	0.80
2:D:330:MET:HG3	2:D:351:THR:HG21	1.62	0.80
2:B:406:MET:HE3	2:B:409:THR:HB	1.65	0.79
2:D:1:MET:HE3	2:D:128:ASP:HB2	1.66	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:239:THR:OG1	1:A:243:ARG:NH1	2.17	0.77
2:B:238:THR:HB	2:B:316:ILE:CD1	2.15	0.77
4:F:200:ASP:OD2	4:F:241:THR:OG1	2.02	0.77
1:A:370:LYS:HD3	1:A:371:VAL:N	2.00	0.76
2:B:238:THR:HG21	2:B:316:ILE:HD11	1.67	0.76
4:F:225:SER:O	4:F:227:PRO:HD3	1.88	0.74
2:D:285:THR:HG23	2:D:287:PRO:HD2	1.69	0.74
4:F:186:LEU:CD1	4:F:320:MET:HG2	2.16	0.74
1:C:248:LEU:HD12	1:C:357:TYR:OH	1.88	0.74
3:E:101:LEU:O	3:E:105:MET:HG2	1.88	0.74
1:A:166:LYS:NZ	1:A:197:HIS:O	2.19	0.73
2:D:330:MET:O	2:D:334:GLN:HG3	1.89	0.73
4:F:70:LYS:O	4:F:76:SER:HB2	1.89	0.73
4:F:263:PHE:CE2	4:F:341:LYS:HD3	2.24	0.72
2:B:179:VAL:HG12	1:C:348:PRO:HG2	1.71	0.72
2:B:262:ARG:NH2	2:B:414:ASN:OD1	2.21	0.72
2:B:189:VAL:HG11	2:B:415:MET:HE3	1.71	0.72
2:D:321:MET:O	2:D:323:MET:HE2	1.89	0.72
1:A:147:SER:HB2	1:A:190:THR:HB	1.72	0.71
1:A:18:ASN:HD21	1:A:78:VAL:CG2	2.03	0.71
2:B:378:PHE:HD1	2:B:415:MET:HE2	1.56	0.69
1:C:221:ARG:CZ	2:D:323:MET:HB3	2.22	0.69
2:D:21:TRP:CZ3	2:D:61:PRO:HB3	2.26	0.69
2:B:189:VAL:CB	2:B:415:MET:HE3	2.23	0.68
1:A:88:HIS:N	1:A:91:GLN:OE1	2.25	0.68
2:D:416:ASN:O	2:D:419:VAL:HG22	1.93	0.68
4:F:256:TYR:HB2	4:F:257:GLU:OE2	1.93	0.68
2:D:211:CYS:HA	2:D:215:LEU:HD23	1.76	0.67
2:D:63:ALA:C	2:D:64:ILE:HD13	2.19	0.67
4:F:192:LEU:HD21	4:F:262:MET:CE	2.24	0.67
2:B:224:ASP:OD1	2:B:276:ARG:NH2	2.28	0.67
2:B:238:THR:CG2	2:B:316:ILE:HD11	2.25	0.67
2:D:285:THR:HG22	2:D:288:GLU:HG3	1.75	0.67
1:A:112:LYS:HE3	3:E:61:ARG:HH22	1.60	0.66
4:F:224:SER:OG	4:F:238:CYS:HA	1.95	0.66
2:D:321:MET:HB3	2:D:363:MET:CE	2.26	0.66
4:F:247:LYS:NZ	4:F:247:LYS:HA	2.11	0.66
2:D:285:THR:HG22	2:D:288:GLU:CG	2.25	0.65
2:D:62:ARG:HG3	2:D:123:GLU:OE1	1.96	0.65
2:D:319:GLY:HA2	2:D:357:PRO:HG3	1.78	0.65
2:D:116:VAL:HG11	2:D:151:LEU:HD21	1.78	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:378:PHE:CD1	2:B:415:MET:HE2	2.32	0.65
2:D:321:MET:HB3	2:D:363:MET:HE1	1.78	0.65
1:C:162:GLY:HA2	3:E:94:ILE:HD11	1.79	0.64
2:B:170:MET:HG3	2:B:377:LEU:HD11	1.79	0.64
1:A:18:ASN:HD21	1:A:78:VAL:HG22	1.62	0.64
1:C:166:LYS:HE2	1:C:197:HIS:O	1.97	0.64
1:A:161:TYR:HB3	1:A:164:LYS:CG	2.28	0.63
2:B:189:VAL:CG1	2:B:415:MET:HE3	2.29	0.63
2:D:121:ARG:O	2:D:125:GLU:HG2	1.99	0.63
1:A:398:MET:HE3	1:A:404:PHE:HD2	1.64	0.63
2:D:318:ARG:HH21	2:D:356:ILE:HG12	1.62	0.63
1:A:233:GLN:HG3	1:A:368:LEU:CD1	2.29	0.63
2:B:166:THR:OG1	2:B:199:THR:HB	1.99	0.62
2:D:157:GLU:HA	3:E:123:LEU:HD13	1.80	0.62
4:F:80:LEU:HD21	4:F:298:ILE:CG2	2.30	0.62
4:F:296:MET:HE2	4:F:380:HIS:HB2	1.82	0.62
2:B:406:MET:HE3	2:B:406:MET:O	2.00	0.62
2:D:1:MET:HE3	2:D:128:ASP:CB	2.29	0.61
4:F:221:LEU:HD22	4:F:262:MET:CE	2.30	0.61
2:B:143:THR:CG2	2:B:147:MET:HE2	2.30	0.61
3:E:58:GLU:HG3	3:E:61:ARG:NH2	2.16	0.61
2:D:134:GLN:HA	2:D:165:ASN:O	2.01	0.61
2:D:321:MET:HE2	2:D:363:MET:HE2	1.83	0.61
2:D:324:LYS:HE2	2:D:328:GLU:OE2	2.00	0.61
1:A:161:TYR:HB3	1:A:164:LYS:HG2	1.83	0.60
4:F:216:TYR:CZ	4:F:218:GLU:HB2	2.36	0.60
2:D:73:MET:O	2:D:77:ARG:HG3	2.01	0.60
2:D:1:MET:HE3	2:D:128:ASP:CG	2.26	0.60
1:C:234:ILE:HD13	1:C:302:MET:SD	2.42	0.60
2:D:315:ALA:HB3	2:D:351:THR:CG2	2.31	0.60
2:B:406:MET:CE	2:B:409:THR:HB	2.31	0.60
3:E:121:GLU:O	3:E:124:GLN:HG3	2.02	0.59
1:A:119:LEU:HD11	1:A:156:ARG:HB3	1.84	0.59
4:F:192:LEU:HD21	4:F:262:MET:HE1	1.84	0.59
1:A:336:LYS:HD3	3:E:24:LEU:CD1	2.33	0.58
2:B:73:MET:HE2	2:B:92:PHE:CB	2.29	0.58
1:C:221:ARG:NH1	2:D:323:MET:HB3	2.16	0.58
2:B:386:THR:HG22	2:B:412:GLU:OE2	2.04	0.58
1:A:177:VAL:HG12	1:A:177:VAL:O	2.03	0.58
2:B:30:ILE:HD12	2:B:30:ILE:N	2.19	0.58
4:F:5:VAL:HG12	4:F:30:LEU:HB2	1.84	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:14:TYR:HA	4:F:17:VAL:HB	1.86	0.57
2:B:189:VAL:HG21	2:B:415:MET:CE	2.34	0.57
4:F:191:LEU:HA	4:F:197:ARG:O	2.04	0.57
4:F:247:LYS:HA	4:F:247:LYS:CE	2.34	0.57
2:D:315:ALA:HB3	2:D:351:THR:HG22	1.85	0.57
2:B:293:MET:HE2	2:B:367:PHE:HB2	1.87	0.57
4:F:377:LYS:HE2	4:F:379:HIS:CD2	2.40	0.57
1:C:320:ARG:HA	1:C:356:ASN:O	2.05	0.56
1:A:178:SER:HB2	1:A:183:GLU:OE2	2.06	0.56
2:D:157:GLU:CA	3:E:123:LEU:HD13	2.36	0.56
4:F:216:TYR:CE2	4:F:218:GLU:HB2	2.39	0.56
4:F:221:LEU:HD22	4:F:262:MET:HE3	1.87	0.56
1:C:324:VAL:HG22	1:C:327:ASP:OD2	2.05	0.56
2:D:23:VAL:O	2:D:27:GLU:HG3	2.06	0.56
2:D:210:ILE:O	2:D:215:LEU:HD22	2.06	0.56
4:F:1:MET:HE1	4:F:28:LYS:CB	2.32	0.56
2:B:169:VAL:HA	2:B:202:ILE:O	2.05	0.56
2:B:229:VAL:O	2:B:233:MET:HG3	2.04	0.55
1:C:71:GLU:HG2	1:C:98:ASP:HB3	1.88	0.55
2:D:6:HIS:CD2	2:D:21:TRP:HE1	2.25	0.55
1:C:275:VAL:HG13	1:C:368:LEU:HD21	1.88	0.55
2:D:102:ALA:HB2	2:D:403:MET:SD	2.47	0.55
1:C:215:ARG:CZ	1:C:299:ALA:HB1	2.37	0.55
2:D:272:PRO:HB3	2:D:284:LEU:HD21	1.89	0.55
2:D:316:ILE:HD12	2:D:366:THR:O	2.07	0.55
4:F:2:TYR:CZ	4:F:359:PHE:HB3	2.41	0.55
2:B:130:LEU:HB3	2:B:162:ARG:HE	1.72	0.55
2:D:88:ASP:OD1	2:D:88:ASP:N	2.39	0.55
1:A:119:LEU:HD11	1:A:156:ARG:CB	2.37	0.55
1:A:18:ASN:ND2	1:A:78:VAL:HG22	2.22	0.55
1:A:357:TYR:CE2	3:E:17:GLY:HA2	2.41	0.55
3:E:58:GLU:HG3	3:E:61:ARG:HH21	1.71	0.54
2:D:170:MET:HE2	2:D:377:LEU:CD1	2.33	0.54
1:A:279:GLU:HA	1:A:279:GLU:OE1	2.07	0.54
2:D:381:ILE:HG22	2:D:415:MET:HE1	1.88	0.54
4:F:219:GLY:HA3	4:F:264:PHE:CZ	2.42	0.54
1:C:344:VAL:HG21	1:C:346:TRP:CE2	2.43	0.54
2:B:238:THR:CB	2:B:316:ILE:CD1	2.85	0.54
2:D:293:MET:CG	2:D:367:PHE:HB2	2.38	0.54
1:A:94:THR:HG23	1:A:95:GLY:O	2.07	0.54
1:C:110:ILE:HD13	1:C:110:ILE:N	2.22	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:18:SER:O	4:F:22:LEU:HD12	2.08	0.53
1:C:81:GLY:O	1:C:84:ARG:NH1	2.40	0.53
2:D:48:ASN:H	2:D:48:ASN:ND2	2.06	0.53
2:D:70:PRO:HD3	2:D:94:GLN:HA	1.90	0.53
1:A:187:SER:HB3	1:A:391:LEU:HD21	1.89	0.53
1:A:254:GLU:HG2	1:A:258:ASN:ND2	2.23	0.53
1:C:141:PHE:CE1	1:C:170:SER:HB3	2.43	0.53
4:F:3:THR:HG22	4:F:28:LYS:HG3	1.91	0.53
1:A:221:ARG:NH1	2:B:323:MET:HE2	2.22	0.53
1:A:109:THR:HG22	3:E:61:ARG:HH11	1.73	0.53
2:B:262:ARG:NH1	2:B:421:GLU:OE1	2.37	0.53
1:C:178:SER:O	2:D:350:LYS:HE2	2.09	0.53
1:A:336:LYS:HD3	3:E:24:LEU:HD12	1.90	0.53
2:D:63:ALA:O	2:D:64:ILE:HD13	2.09	0.53
2:D:238:THR:OG1	2:D:318:ARG:HD2	2.09	0.53
2:D:285:THR:CG2	2:D:288:GLU:H	2.22	0.53
2:D:293:MET:HG2	2:D:367:PHE:HB2	1.90	0.53
2:D:145:SER:OG	2:D:188:SER:OG	2.26	0.53
3:E:127:ASP:O	3:E:131:GLU:HG2	2.08	0.53
2:D:155:ILE:HG21	2:D:164:MET:HE1	1.91	0.52
1:A:265:ILE:HG23	1:A:432:TYR:CE1	2.44	0.52
2:D:21:TRP:CE3	2:D:61:PRO:HB3	2.45	0.52
4:F:317:PHE:HB3	4:F:319:PHE:CE1	2.45	0.52
1:A:233:GLN:HG3	1:A:368:LEU:HD12	1.89	0.52
4:F:198:LYS:HE2	4:F:239:HIS:O	2.10	0.52
1:A:133:GLN:OE1	1:A:251:ASP:HA	2.09	0.52
2:D:318:ARG:NH2	2:D:356:ILE:HG12	2.24	0.52
3:E:92:ASN:OD1	3:E:96:MET:HE1	2.10	0.52
2:B:197:ASP:C	2:B:198:GLU:HG3	2.35	0.52
1:A:260:VAL:HG11	1:A:266:HIS:HB3	1.92	0.52
2:B:304:ASP:HB3	2:B:307:HIS:ND1	2.25	0.52
4:F:209:HIS:HA	4:F:311:SER:O	2.10	0.52
2:D:138:SER:HA	2:D:169:VAL:HB	1.93	0.51
1:A:209:ILE:HG22	1:A:227:LEU:HD22	1.92	0.51
2:D:104:GLY:O	2:D:109:GLY:HA3	2.09	0.51
2:D:400:GLY:O	3:E:137:LYS:HD2	2.10	0.51
3:E:6:MET:HG3	3:E:24:LEU:HD23	1.92	0.51
1:C:71:GLU:HB3	1:C:98:ASP:HB3	1.92	0.51
2:D:285:THR:HG23	2:D:287:PRO:CD	2.39	0.51
3:E:6:MET:HG3	3:E:24:LEU:CD2	2.41	0.51
4:F:353:VAL:HG21	4:F:375:PHE:CD2	2.46	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:67:ASP:HA	2:D:143:THR:HG21	1.92	0.51
1:A:401:LYS:HE3	2:B:428:ALA:HB1	1.92	0.50
1:A:398:MET:HE3	1:A:404:PHE:CD2	2.44	0.50
2:B:189:VAL:HG11	2:B:415:MET:CE	2.40	0.50
2:D:206:ALA:HB2	2:D:302:ALA:HB2	1.93	0.50
2:D:206:ALA:O	2:D:210:ILE:HG13	2.11	0.50
4:F:88:SER:HG	4:F:91:CYS:N	2.09	0.50
1:A:25:CYS:HB3	1:A:30:ILE:O	2.11	0.50
2:B:66:VAL:HG12	2:B:147:MET:HE1	1.94	0.50
2:B:189:VAL:HB	2:B:415:MET:HE3	1.91	0.50
4:F:192:LEU:HD21	4:F:262:MET:HE2	1.92	0.50
2:B:332:ASN:ND2	2:B:336:LYS:HE2	2.26	0.50
1:C:1:MET:HB3	1:C:130:THR:OG1	2.12	0.50
1:C:41:THR:OG1	1:C:44:GLY:O	2.30	0.50
1:C:109:THR:HG22	1:C:110:ILE:HD13	1.92	0.50
4:F:229:ASN:OD1	4:F:229:ASN:N	2.43	0.50
1:C:71:GLU:OE1	1:C:73:THR:HB	2.11	0.50
1:A:109:THR:HG22	3:E:61:ARG:NH1	2.27	0.49
3:E:9:ILE:HG12	3:E:21:GLU:HB3	1.93	0.49
4:F:3:THR:HG22	4:F:28:LYS:CG	2.42	0.49
4:F:192:LEU:CD2	4:F:262:MET:HE1	2.41	0.49
2:D:54:ALA:HB3	2:D:58:LYS:HB2	1.93	0.49
4:F:202:ARG:HG3	4:F:203:SER:N	2.27	0.49
1:A:185:TYR:CZ	1:A:398:MET:HE2	2.47	0.49
2:B:73:MET:CE	2:B:92:PHE:HB3	2.31	0.49
3:E:80:ARG:HA	3:E:83:ILE:HG22	1.95	0.49
2:D:12:CYS:HB3	2:D:138:SER:HB3	1.94	0.49
4:F:31:ARG:NH2	4:F:32:LYS:HG3	2.28	0.49
2:D:296:SER:OG	2:D:304:ASP:HA	2.12	0.49
4:F:197:ARG:HH12	4:F:257:GLU:CD	2.20	0.49
4:F:217:ARG:HG2	4:F:374:ILE:O	2.13	0.49
2:B:189:VAL:O	2:B:193:VAL:HG23	2.12	0.49
2:B:293:MET:CE	2:B:365:ALA:HB1	2.42	0.49
2:D:246:LEU:HD12	2:D:246:LEU:C	2.38	0.49
1:A:159:VAL:HG11	3:E:47:LEU:HB2	1.94	0.48
2:B:330:MET:O	2:B:334:GLN:HG3	2.12	0.48
2:D:310:TYR:CE1	2:D:367:PHE:HZ	2.31	0.48
1:A:187:SER:CB	1:A:391:LEU:HD21	2.44	0.48
1:A:324:VAL:HG13	1:A:325:PRO:HD2	1.94	0.48
1:A:413:MET:HE2	1:A:418:PHE:CE1	2.48	0.48
1:C:119:LEU:HD11	1:C:156:ARG:HB3	1.94	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:335:ILE:HG23	1:A:339:ARG:HG3	1.96	0.48
2:D:73:MET:HB3	2:D:90:PHE:CD2	2.49	0.48
2:B:29:GLY:O	2:B:36:TYR:HA	2.14	0.48
2:B:386:THR:O	2:B:390:ARG:HG2	2.13	0.48
1:C:83:TYR:CD1	1:C:86:LEU:HD22	2.48	0.48
2:D:1:MET:CE	2:D:128:ASP:HB2	2.39	0.48
1:C:357:TYR:O	1:C:359:PRO:HD3	2.14	0.48
2:D:134:GLN:HG3	2:D:167:PHE:HE1	1.78	0.48
4:F:225:SER:O	4:F:227:PRO:CD	2.59	0.48
2:B:104:GLY:O	2:B:109:GLY:HA3	2.14	0.47
2:B:273:LEU:HD11	2:B:298:ASN:HA	1.95	0.47
1:C:2:ARG:N	1:C:2:ARG:HD2	2.29	0.47
2:D:285:THR:HG22	2:D:288:GLU:CB	2.44	0.47
1:C:83:TYR:HD1	1:C:86:LEU:HD22	1.78	0.47
2:D:403:MET:HE3	2:D:407:GLU:CD	2.39	0.47
2:D:181:GLU:HB2	2:D:182:PRO:HD3	1.96	0.47
2:B:262:ARG:HH11	2:B:421:GLU:CD	2.23	0.47
1:A:221:ARG:HD2	2:B:323:MET:HB3	1.96	0.47
1:C:248:LEU:CD1	1:C:357:TYR:OH	2.60	0.47
1:C:18:ASN:HD21	1:C:78:VAL:HG22	1.80	0.47
4:F:320:MET:HE2	4:F:320:MET:HB2	1.83	0.47
1:C:274:PRO:CB	1:C:286:LEU:HD22	2.45	0.47
4:F:377:LYS:HE2	4:F:379:HIS:HD2	1.78	0.47
2:B:66:VAL:HG12	2:B:147:MET:CE	2.45	0.47
2:B:67:ASP:O	2:B:92:PHE:HA	2.15	0.47
2:D:64:ILE:HD11	2:D:123:GLU:HG3	1.97	0.47
2:D:285:THR:CG2	2:D:288:GLU:HG3	2.43	0.47
1:C:97:GLU:O	1:C:110:ILE:HG21	2.15	0.46
1:A:71:GLU:HG2	1:A:72:PRO:N	2.29	0.46
2:D:345:ILE:HG22	2:D:348:ASN:HB3	1.97	0.46
4:F:80:LEU:HD21	4:F:298:ILE:HG22	1.96	0.46
2:D:33:THR:O	2:D:58:LYS:HD2	2.15	0.46
1:A:234:ILE:HD13	1:A:302:MET:SD	2.55	0.46
1:A:370:LYS:HD3	1:A:370:LYS:C	2.40	0.46
1:C:12:ALA:HB3	1:C:140:SER:HB3	1.97	0.46
2:D:416:ASN:O	2:D:419:VAL:CG2	2.61	0.46
1:C:147:SER:HB2	1:C:190:THR:HB	1.97	0.46
2:D:172:SER:HB2	2:D:205:GLU:HB2	1.97	0.46
4:F:199:PHE:CD2	4:F:221:LEU:HD23	2.51	0.46
4:F:214:TYR:CD2	4:F:353:VAL:HG11	2.50	0.46
4:F:214:TYR:CE2	4:F:353:VAL:CG1	2.99	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:64:ILE:HD12	2:B:120:VAL:HG22	1.97	0.46
2:B:117:LEU:HD11	2:B:154:LYS:HD3	1.96	0.46
4:F:47:LEU:HD23	4:F:48:PRO:HD2	1.97	0.46
2:B:144:GLY:O	2:B:148:GLY:HA3	2.16	0.46
1:A:161:TYR:HB3	1:A:164:LYS:HG3	1.97	0.46
1:C:96:LYS:HB2	1:C:96:LYS:NZ	2.31	0.46
2:D:318:ARG:O	2:D:363:MET:HA	2.17	0.45
1:C:39:ASP:OD1	1:C:41:THR:OG1	2.35	0.45
2:D:385:PHE:CE1	2:D:412:GLU:HB2	2.51	0.45
2:D:387:ALA:O	2:D:391:ARG:HD3	2.17	0.45
1:C:163:LYS:HA	1:C:163:LYS:HD3	1.45	0.45
3:E:9:ILE:CG1	3:E:21:GLU:HB3	2.46	0.45
2:D:293:MET:SD	2:D:365:ALA:HB1	2.56	0.45
1:A:72:PRO:HB3	1:A:94:THR:HG21	1.99	0.45
1:C:227:LEU:O	1:C:231:ILE:HG13	2.16	0.45
2:D:203:ASP:O	2:D:207:LEU:HG	2.17	0.45
4:F:12:SER:HB2	4:F:343:TYR:CE1	2.51	0.45
1:A:390:ARG:HD2	4:F:54:HIS:CD2	2.51	0.45
2:B:2:ARG:HB3	2:B:131:GLN:HG2	1.98	0.45
2:D:155:ILE:CG2	2:D:164:MET:HE1	2.47	0.45
1:A:176:GLN:NE2	4:F:56:PRO:HB3	2.32	0.45
4:F:5:VAL:HG13	4:F:37:PHE:HB3	1.98	0.45
4:F:247:LYS:HA	4:F:247:LYS:HZ3	1.79	0.45
2:B:2:ARG:HB3	2:B:131:GLN:CG	2.47	0.45
2:B:321:MET:HE2	2:B:363:MET:HG2	1.99	0.45
4:F:14:TYR:HB3	4:F:41:LEU:HD13	1.97	0.45
1:C:161:TYR:O	1:C:162:GLY:C	2.61	0.44
1:A:27:GLU:CD	1:A:320:ARG:HH22	2.25	0.44
2:B:132:GLY:HA2	2:B:162:ARG:HB3	2.00	0.44
2:D:1:MET:HE3	2:D:128:ASP:OD2	2.17	0.44
2:D:44:LEU:HA	2:D:47:ILE:HB	2.00	0.44
1:A:9:VAL:HG22	1:A:68:VAL:CG1	2.47	0.44
2:D:65:LEU:N	2:D:65:LEU:HD12	2.33	0.44
1:C:7:ILE:HG21	1:C:153:LEU:HD21	1.99	0.44
1:C:66:VAL:HG23	1:C:125:LEU:CD1	2.47	0.44
2:D:151:LEU:HD12	2:D:151:LEU:HA	1.87	0.44
4:F:37:PHE:CZ	4:F:40:MET:HE3	2.52	0.44
1:C:41:THR:OG1	1:C:41:THR:O	2.34	0.44
3:E:72:LEU:O	3:E:76:ARG:HG2	2.17	0.44
4:F:377:LYS:HG2	4:F:379:HIS:CD2	2.52	0.44
2:B:316:ILE:HG23	2:B:366:THR:HB	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2:ARG:HA	2:B:129:CYS:O	2.18	0.44
1:C:221:ARG:NH1	2:D:323:MET:CB	2.81	0.44
1:A:385:ALA:HB2	1:A:432:TYR:CG	2.52	0.43
2:B:179:VAL:HG22	1:C:258:ASN:OD1	2.18	0.43
1:A:192:HIS:CG	1:A:421:ALA:HA	2.53	0.43
2:B:332:ASN:OD1	2:B:336:LYS:HD3	2.18	0.43
1:A:217:LEU:HD21	1:A:368:LEU:HD23	1.99	0.43
1:C:36:MET:HE1	1:C:49:PHE:CE2	2.54	0.43
1:C:274:PRO:HB3	1:C:286:LEU:HD22	2.00	0.43
2:D:197:ASP:C	2:D:198:GLU:HG3	2.44	0.43
1:A:18:ASN:HD21	1:A:78:VAL:HG21	1.81	0.43
2:B:61:PRO:HD3	2:B:84:ILE:HG12	2.01	0.43
2:D:73:MET:O	2:D:77:ARG:CG	2.65	0.43
1:A:326:LYS:HE2	1:A:326:LYS:HB3	1.57	0.43
2:D:24:ILE:HG13	2:D:25:SER:N	2.32	0.43
2:D:316:ILE:HD13	2:D:366:THR:HB	2.00	0.43
2:D:116:VAL:O	2:D:120:VAL:HG23	2.19	0.43
2:B:170:MET:HE3	2:B:170:MET:HB3	1.80	0.43
2:D:318:ARG:HA	2:D:354:CYS:O	2.19	0.43
1:A:262:TYR:HA	1:A:263:PRO:HD3	1.93	0.43
1:A:413:MET:CE	1:A:418:PHE:CE1	3.02	0.43
2:D:157:GLU:HA	3:E:123:LEU:CD1	2.48	0.43
1:A:3:GLU:HG2	1:A:64:ARG:CZ	2.49	0.42
2:B:12:CYS:HB3	2:B:138:SER:HB3	2.01	0.42
1:C:211:ASP:OD2	1:C:304:LYS:NZ	2.41	0.42
1:C:214:ARG:HG2	1:C:219:ILE:O	2.19	0.42
2:B:7:ILE:O	2:B:135:LEU:HA	2.19	0.42
2:D:285:THR:HG22	2:D:288:GLU:H	1.84	0.42
2:D:315:ALA:HB3	2:D:351:THR:HG23	1.99	0.42
2:B:128:ASP:OD1	2:B:128:ASP:N	2.52	0.42
2:B:170:MET:HE2	2:B:377:LEU:CD2	2.49	0.42
2:B:189:VAL:HG21	2:B:415:MET:HE3	2.01	0.42
4:F:191:LEU:HD23	4:F:197:ARG:O	2.20	0.42
2:D:73:MET:HB3	2:D:90:PHE:HD2	1.84	0.42
1:C:164:LYS:HE3	1:C:164:LYS:HB2	1.82	0.42
2:B:19:LYS:HD3	2:B:19:LYS:HA	1.80	0.42
2:D:36:TYR:CZ	2:D:38:GLY:HA3	2.54	0.42
4:F:284:LEU:HD12	4:F:284:LEU:HA	1.86	0.42
1:A:124:LYS:HB3	1:A:124:LYS:HE2	1.28	0.42
2:B:323:MET:HE3	2:B:353:VAL:HG11	2.00	0.42
1:A:357:TYR:O	1:A:359:PRO:HD3	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:234:ILE:CD1	1:C:302:MET:SD	3.08	0.42
4:F:353:VAL:HG21	4:F:375:PHE:CE2	2.53	0.42
2:B:190:HIS:ND1	2:B:414:ASN:ND2	2.61	0.41
2:B:332:ASN:HD21	2:B:336:LYS:HE2	1.85	0.41
2:D:321:MET:HB3	2:D:363:MET:HE2	2.01	0.41
2:B:121:ARG:HG2	2:B:125:GLU:OE2	2.20	0.41
2:B:324:LYS:O	2:B:328:GLU:HG3	2.20	0.41
1:C:209:ILE:HD11	1:C:302:MET:SD	2.61	0.41
2:D:21:TRP:CH2	2:D:61:PRO:HB3	2.55	0.41
4:F:17:VAL:O	4:F:21:LEU:HG	2.21	0.41
4:F:74:LYS:HA	4:F:74:LYS:HD3	1.88	0.41
4:F:198:LYS:HG2	4:F:199:PHE:N	2.34	0.41
1:A:79:ARG:HH22	1:A:94:THR:HB	1.86	0.41
1:A:320:ARG:HA	1:A:356:ASN:O	2.21	0.41
1:C:88:HIS:ND1	1:C:90:GLU:HB2	2.36	0.41
1:C:96:LYS:HG3	2:D:129:CYS:HB2	2.03	0.41
1:A:108:TYR:CE2	1:A:413:MET:HG3	2.56	0.41
1:C:395:PHE:CD1	1:C:395:PHE:C	2.98	0.41
3:E:56:ALA:HB1	3:E:60:ARG:HH12	1.84	0.41
2:D:52:ASN:ND2	2:D:123:GLU:OE1	2.53	0.41
2:D:210:ILE:HG22	2:D:215:LEU:CD2	2.51	0.41
4:F:292:ARG:O	4:F:296:MET:HG2	2.21	0.41
1:A:112:LYS:HE3	3:E:61:ARG:NH2	2.31	0.41
1:A:167:LEU:HG	1:A:200:CYS:HB3	2.03	0.41
2:B:67:ASP:HA	2:B:143:THR:HG21	2.02	0.41
2:B:392:LYS:HE3	2:B:405:GLU:OE2	2.20	0.41
2:D:214:THR:HG22	2:D:215:LEU:HD13	2.03	0.41
2:D:323:MET:HE3	2:D:323:MET:H	1.85	0.41
2:D:354:CYS:SG	2:D:356:ILE:HG23	2.60	0.41
4:F:12:SER:HB2	4:F:343:TYR:OH	2.19	0.41
4:F:89:GLU:O	4:F:91:CYS:N	2.53	0.41
4:F:217:ARG:NH1	4:F:374:ILE:HA	2.36	0.41
2:D:64:ILE:HD13	2:D:64:ILE:N	2.36	0.41
1:A:106:GLY:O	1:A:111:GLY:HA3	2.21	0.40
1:C:298:PRO:HG2	1:C:308:ARG:NH2	2.36	0.40
2:D:19:LYS:HD3	2:D:19:LYS:HA	1.85	0.40
2:D:169:VAL:HA	2:D:202:ILE:O	2.20	0.40
2:D:175:VAL:HG21	2:D:204:ASN:ND2	2.36	0.40
2:D:177:ASP:O	2:D:178:THR:C	2.64	0.40
4:F:34:ASN:OD1	4:F:35:PRO:HD2	2.21	0.40
1:A:68:VAL:O	1:A:68:VAL:HG13	2.22	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:GLU:CB	1:A:98:ASP:HB3	2.51	0.40
1:A:357:TYR:CZ	3:E:17:GLY:HA2	2.57	0.40
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.39	0.40
2:B:189:VAL:CG2	2:B:415:MET:HE3	2.51	0.40
2:B:203:ASP:OD2	2:B:302:ALA:HB3	2.21	0.40
2:D:134:GLN:HG3	2:D:167:PHE:CE1	2.55	0.40
4:F:8:ASP:HB2	4:F:43:GLU:HA	2.03	0.40
2:B:44:LEU:HA	2:B:47:ILE:HB	2.04	0.40
2:B:289:LEU:HD23	2:B:289:LEU:HA	1.89	0.40
3:E:135:LYS:HE2	3:E:135:LYS:HB3	1.61	0.40
4:F:2:TYR:CE1	4:F:359:PHE:HB3	2.55	0.40
1:A:214:ARG:HG2	1:A:219:ILE:O	2.21	0.40
2:D:1:MET:HG3	2:D:128:ASP:HB3	2.04	0.40
2:D:8:GLN:NE2	2:D:14:ASN:HA	2.37	0.40
4:F:214:TYR:CE2	4:F:353:VAL:HG11	2.57	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	435/440 (99%)	427 (98%)	8 (2%)	0	100	100
1	C	438/440 (100%)	425 (97%)	13 (3%)	0	100	100
2	B	425/431 (99%)	418 (98%)	7 (2%)	0	100	100
2	D	412/431 (96%)	405 (98%)	7 (2%)	0	100	100
3	E	113/143 (79%)	111 (98%)	2 (2%)	0	100	100
4	F	253/380 (67%)	247 (98%)	6 (2%)	0	100	100
All	All	2076/2265 (92%)	2033 (98%)	43 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	366/371 (99%)	353 (96%)	13 (4%)	31	55
1	C	370/371 (100%)	360 (97%)	10 (3%)	39	65
2	B	367/372 (99%)	357 (97%)	10 (3%)	39	65
2	D	360/372 (97%)	336 (93%)	24 (7%)	15	29
3	E	104/127 (82%)	94 (90%)	10 (10%)	8	16
4	F	235/338 (70%)	217 (92%)	18 (8%)	12	23
All	All	1802/1951 (92%)	1717 (95%)	85 (5%)	23	44

All (85) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	SER
1	A	41	THR
1	A	66	VAL
1	A	71	GLU
1	A	94	THR
1	A	110	ILE
1	A	124	LYS
1	A	181	VAL
1	A	253	THR
1	A	324	VAL
1	A	356	ASN
1	A	381	THR
1	A	433	GLU
2	B	15	GLN
2	B	45	GLU
2	B	55	THR
2	B	128	ASP
2	B	199	THR
2	B	246	LEU
2	B	293	MET
2	B	316	ILE
2	B	323	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	359	ARG
1	C	2	ARG
1	C	96	LYS
1	C	163	LYS
1	C	164	LYS
1	C	165	SER
1	C	297	GLU
1	C	318	LEU
1	C	347	CYS
1	C	352	LYS
1	C	381	THR
2	D	19	LYS
2	D	26	ASP
2	D	41	ASP
2	D	45	GLU
2	D	48	ASN
2	D	53	GLU
2	D	72	THR
2	D	77	ARG
2	D	88	ASP
2	D	99	ASN
2	D	114	ASP
2	D	174	LYS
2	D	177	ASP
2	D	215	LEU
2	D	219	THR
2	D	224	ASP
2	D	246	LEU
2	D	285	THR
2	D	309	ARG
2	D	316	ILE
2	D	351	THR
2	D	356	ILE
2	D	377	LEU
2	D	399	THR
3	E	22	VAL
3	E	25	LYS
3	E	61	ARG
3	E	96	MET
3	E	100	LYS
3	E	101	LEU
3	E	103	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	E	108	ASN
3	E	128	LYS
3	E	137	LYS
4	F	12	SER
4	F	16	GLU
4	F	28	LYS
4	F	31	ARG
4	F	74	LYS
4	F	76	SER
4	F	78	VAL
4	F	81	ILE
4	F	229	ASN
4	F	230	SER
4	F	238	CYS
4	F	247	LYS
4	F	257	GLU
4	F	260	ASN
4	F	275	LEU
4	F	284	LEU
4	F	307	LEU
4	F	331	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	A	18	ASN
1	A	301	GLN
1	A	393	HIS
2	B	11	GLN
2	B	15	GLN
2	B	165	ASN
2	B	245	GLN
2	B	347	ASN
1	C	128	GLN
1	C	372	GLN
2	D	134	GLN
2	D	165	ASN
2	D	329	GLN
3	E	12	ASN
3	E	108	ASN
4	F	260	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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 14 ligands modelled in this entry, 5 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
11	ACP	F	401	-	31,33,33	2.04	2 (6%)	47,52,52	0.94	3 (6%)
5	GTP	A	501	7	33,34,34	0.94	1 (3%)	50,54,54	1.58	9 (18%)
10	A1D68	D	502	-	22,22,22	1.17	1 (4%)	28,31,31	4.72	12 (42%)
9	MES	B	502	-	12,12,12	1.25	1 (8%)	15,16,16	0.66	0
9	MES	B	503	-	12,12,12	1.26	1 (8%)	15,16,16	0.70	0
5	GTP	C	501	7	33,34,34	0.97	1 (3%)	50,54,54	1.58	9 (18%)
8	GDP	D	501	-	29,30,30	1.16	2 (6%)	45,47,47	1.87	8 (17%)
8	GDP	B	501	7	29,30,30	1.17	3 (10%)	45,47,47	1.79	7 (15%)
10	A1D68	B	505	-	22,22,22	1.21	2 (9%)	28,31,31	5.10	10 (35%)

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
11	ACP	F	401	-	-	1/19/38/38	0/3/3/3
5	GTP	A	501	7	-	9/22/38/38	0/3/3/3
10	A1D68	D	502	-	-	2/10/10/10	0/3/3/3
9	MES	B	502	-	-	5/6/14/14	0/1/1/1
9	MES	B	503	-	-	3/6/14/14	0/1/1/1
5	GTP	C	501	7	-	6/22/38/38	0/3/3/3
8	GDP	D	501	-	-	3/16/32/32	0/3/3/3
8	GDP	B	501	7	-	3/16/32/32	0/3/3/3
10	A1D68	B	505	-	-	2/10/10/10	0/3/3/3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	F	401	ACP	PB-O3A	10.30	1.69	1.58
10	D	502	A1D68	C06-N07	3.48	1.46	1.39
9	B	503	MES	C8-S	3.40	1.82	1.77
9	B	502	MES	C8-S	3.34	1.82	1.77
8	B	501	GDP	C5-C4	3.19	1.47	1.38
8	D	501	GDP	C5-C4	3.06	1.47	1.38
10	B	505	A1D68	C01-C02	-2.83	1.38	1.41
8	B	501	GDP	C6-N1	-2.41	1.34	1.38
5	C	501	GTP	C2-N3	2.20	1.38	1.33
8	D	501	GDP	C6-N1	-2.17	1.34	1.38
10	B	505	A1D68	C06-N07	2.16	1.43	1.39
5	A	501	GTP	C2-N3	2.13	1.38	1.33
11	F	401	ACP	PB-O2B	-2.11	1.51	1.56
8	B	501	GDP	C5-N7	-2.04	1.35	1.39

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	505	A1D68	C02-S18-C19	21.06	96.87	90.62
10	D	502	A1D68	C02-S18-C19	18.56	96.13	90.62
10	D	502	A1D68	C01-C02-N03	-9.09	120.43	126.55
10	D	502	A1D68	S18-C02-N03	8.76	132.71	122.51
10	B	505	A1D68	S18-C02-N03	8.74	132.69	122.51
10	B	505	A1D68	C01-C02-N03	-7.86	121.25	126.55

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	505	A1D68	C01-C02-S18	-6.59	106.06	111.38
8	D	501	GDP	C5-C4-N3	-6.31	118.35	128.39
8	B	501	GDP	C5-C4-N3	-6.20	118.53	128.39
8	D	501	GDP	C2-N3-C4	5.60	121.94	112.30
10	D	502	A1D68	C01-C02-S18	-5.59	106.86	111.38
5	C	501	GTP	C5-C4-N3	-5.06	120.34	128.39
8	B	501	GDP	C2-N3-C4	5.06	121.01	112.30
5	A	501	GTP	C5-C4-N3	-5.01	120.42	128.39
10	B	505	A1D68	C02-C01-C20	4.99	116.20	111.76
5	C	501	GTP	C2-N3-C4	4.67	120.35	112.30
8	B	501	GDP	N9-C4-N3	4.61	135.16	125.95
5	A	501	GTP	C2-N3-C4	4.59	120.21	112.30
8	D	501	GDP	N9-C4-N3	4.50	134.94	125.95
10	D	502	A1D68	C04-N03-C02	3.84	119.34	115.16
10	B	505	A1D68	N05-C04-N03	-3.80	122.58	129.52
10	B	505	A1D68	C20-C19-S18	-3.69	106.32	113.90
10	D	502	A1D68	C04-N05-C06	3.59	121.15	110.98
10	D	502	A1D68	N05-C04-N03	-3.55	123.03	129.52
10	B	505	A1D68	C04-N03-C02	3.51	118.98	115.16
8	D	501	GDP	C6-C5-N7	3.48	136.63	130.29
10	D	502	A1D68	C20-C19-S18	-3.41	106.89	113.90
10	D	502	A1D68	C02-C01-C20	3.37	114.75	111.76
10	B	505	A1D68	CL17-C04-N05	3.27	119.77	115.17
10	B	505	A1D68	C04-N05-C06	3.25	120.19	110.98
8	B	501	GDP	C6-C5-N7	3.19	136.09	130.29
5	C	501	GTP	N9-C4-N3	3.18	132.32	125.95
5	A	501	GTP	N9-C4-N3	3.15	132.26	125.95
11	F	401	ACP	O2B-PB-O1B	3.12	120.12	109.95
5	A	501	GTP	C2-N1-C6	-2.94	119.77	125.11
5	C	501	GTP	C2-N1-C6	-2.89	119.87	125.11
8	D	501	GDP	C4-C5-N7	-2.69	106.41	110.67
11	F	401	ACP	O1G-PG-C3B	-2.64	105.61	111.37
5	A	501	GTP	N9-C8-N7	-2.60	108.58	113.40
10	D	502	A1D68	CL17-C04-N05	2.58	118.81	115.17
5	C	501	GTP	N9-C8-N7	-2.57	108.63	113.40
8	B	501	GDP	C4-C5-N7	-2.55	106.63	110.67
5	A	501	GTP	C8-N7-C5	2.50	108.72	104.26
5	C	501	GTP	C5-C6-N1	2.49	119.60	113.25
5	C	501	GTP	C8-N7-C5	2.49	108.70	104.26
5	A	501	GTP	C5-C6-N1	2.48	119.57	113.25
11	F	401	ACP	PB-O3A-PA	-2.45	124.37	132.37
10	D	502	A1D68	C16-O15-C12	-2.43	112.29	117.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	501	GTP	O6-C6-C5	-2.40	120.20	126.53
5	A	501	GTP	O6-C6-C5	-2.38	120.24	126.53
8	B	501	GDP	C3'-C2'-C1'	2.31	105.83	101.46
5	C	501	GTP	C3'-C2'-C1'	2.19	105.61	101.46
5	A	501	GTP	C3'-C2'-C1'	2.17	105.57	101.46
8	D	501	GDP	O6-C6-C5	-2.15	120.87	126.53
10	D	502	A1D68	CL17-C04-N03	2.12	118.16	115.17
8	B	501	GDP	O6-C6-C5	-2.10	120.98	126.53
8	D	501	GDP	N2-C2-N1	2.06	121.10	116.76
8	D	501	GDP	C5-C6-N1	2.05	118.46	113.25

There are no chirality outliers.

All (34) 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-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	B	501	GDP	C5'-O5'-PA-O3A
8	B	501	GDP	C5'-O5'-PA-O1A
8	B	501	GDP	C5'-O5'-PA-O2A
8	D	501	GDP	C5'-O5'-PA-O3A
8	D	501	GDP	C5'-O5'-PA-O2A
9	B	503	MES	C7-C8-S-O1S
9	B	503	MES	C7-C8-S-O2S
9	B	503	MES	C7-C8-S-O3S
10	D	502	A1D68	C11-C12-O15-C16
10	D	502	A1D68	C13-C12-O15-C16
9	B	502	MES	C7-C8-S-O3S
10	B	505	A1D68	C13-C12-O15-C16
10	B	505	A1D68	C11-C12-O15-C16
5	A	501	GTP	C3'-C4'-C5'-O5'
5	C	501	GTP	C3'-C4'-C5'-O5'
9	B	502	MES	C7-C8-S-O1S
9	B	502	MES	C7-C8-S-O2S
5	C	501	GTP	O4'-C4'-C5'-O5'
5	A	501	GTP	O4'-C4'-C5'-O5'
5	A	501	GTP	C5'-O5'-PA-O1A
9	B	502	MES	C8-C7-N4-C3

Continued on next page...

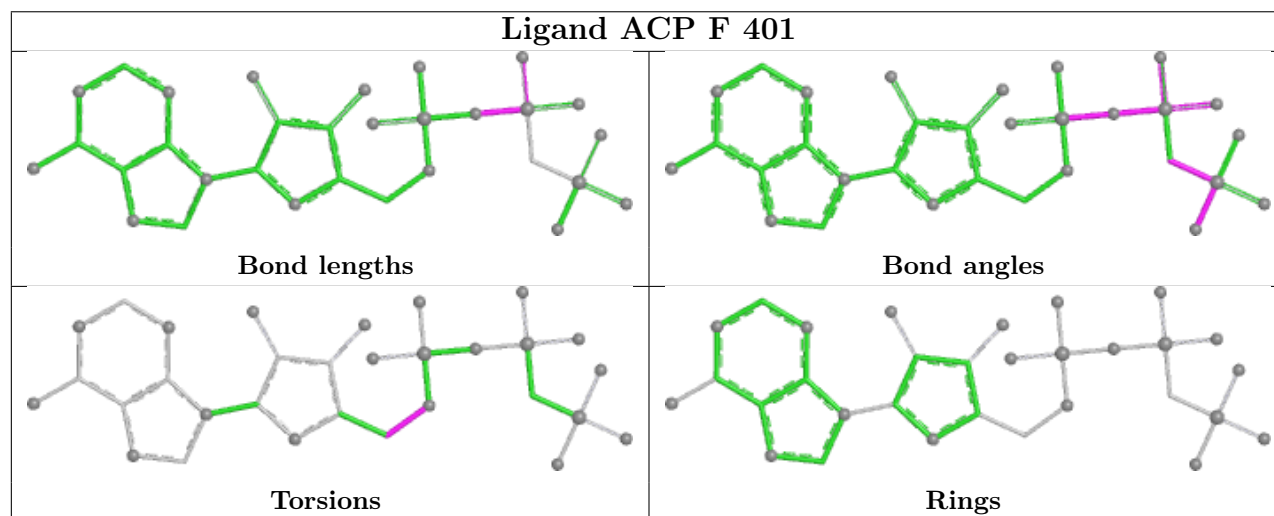
Continued from previous page...

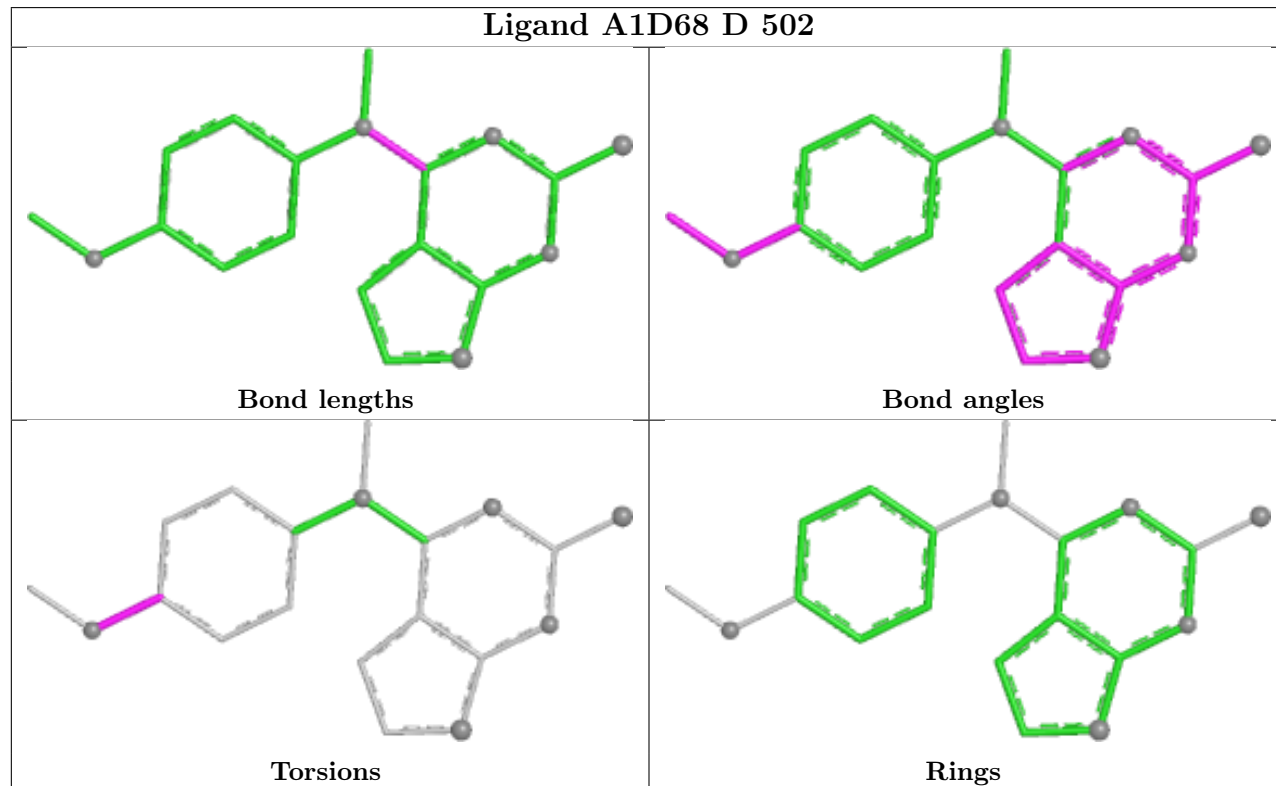
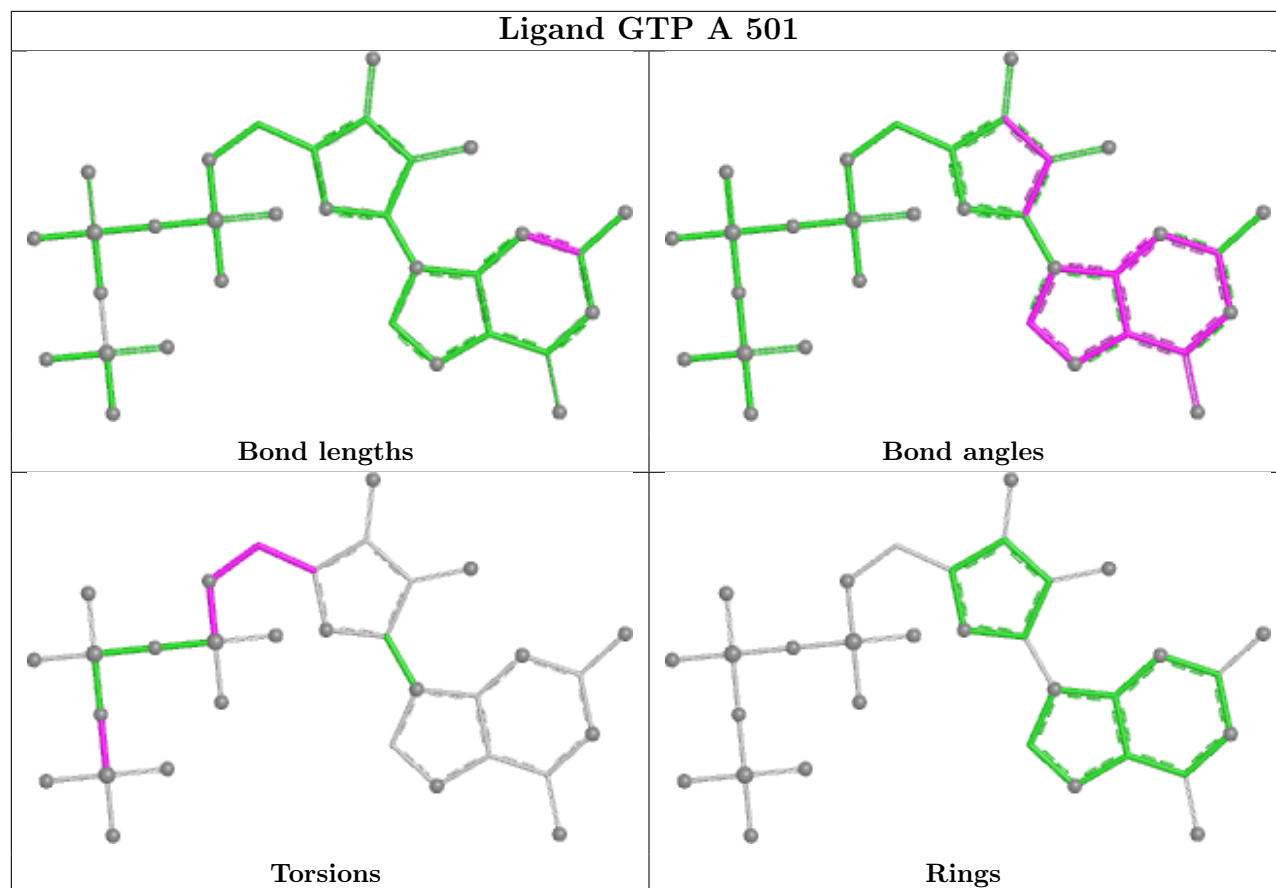
Mol	Chain	Res	Type	Atoms
9	B	502	MES	C8-C7-N4-C5
5	A	501	GTP	C4'-C5'-O5'-PA
5	C	501	GTP	C4'-C5'-O5'-PA
11	F	401	ACP	C4'-C5'-O5'-PA
5	A	501	GTP	PB-O3B-PG-O3G
8	D	501	GDP	C3'-C4'-C5'-O5'
5	A	501	GTP	PB-O3B-PG-O1G

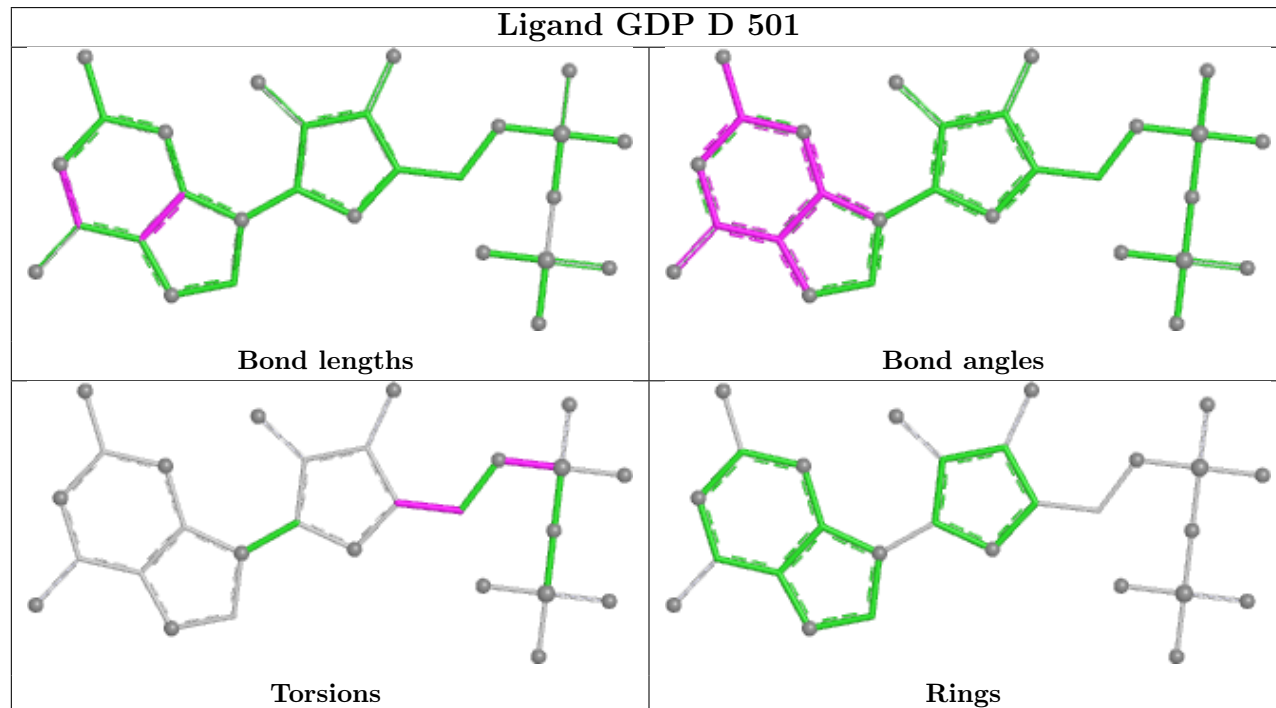
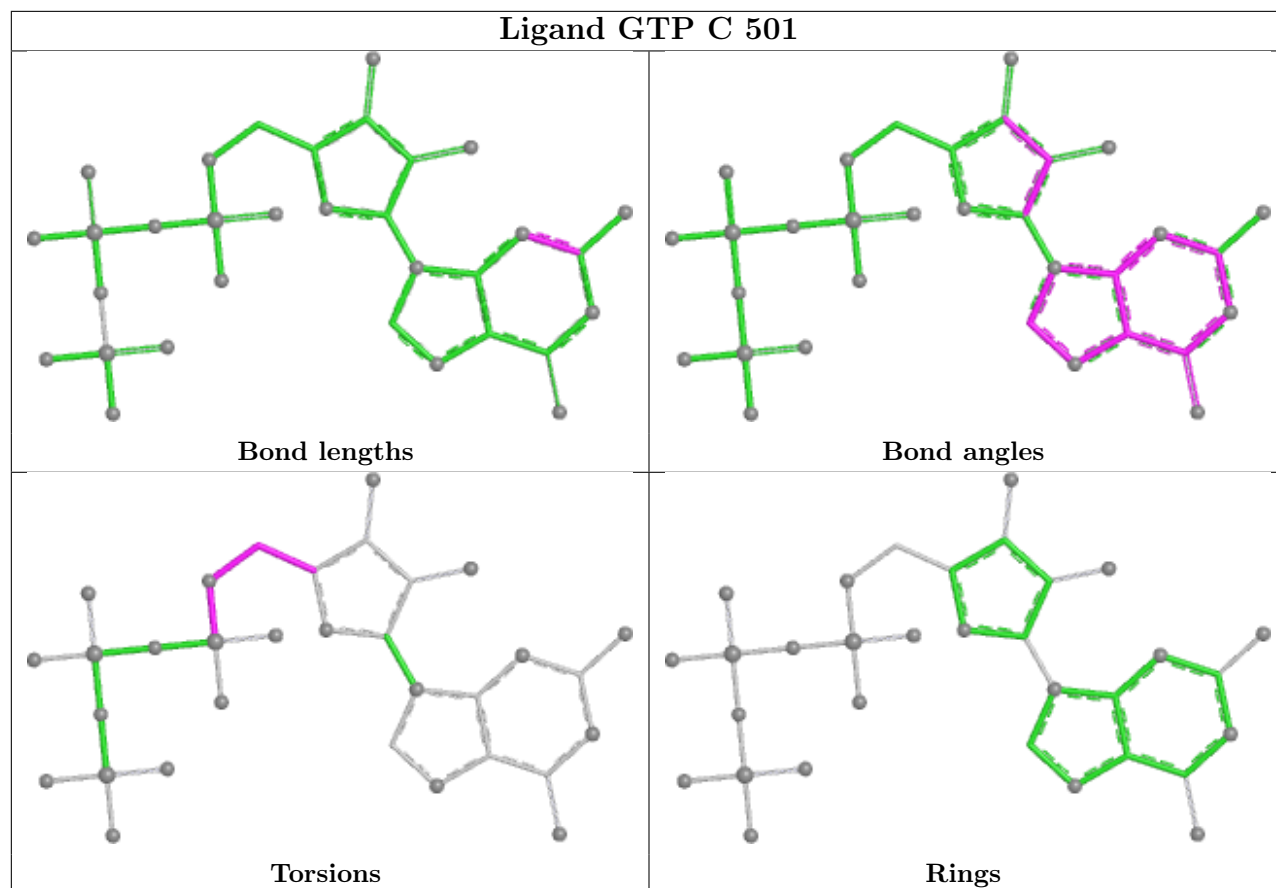
There are no ring outliers.

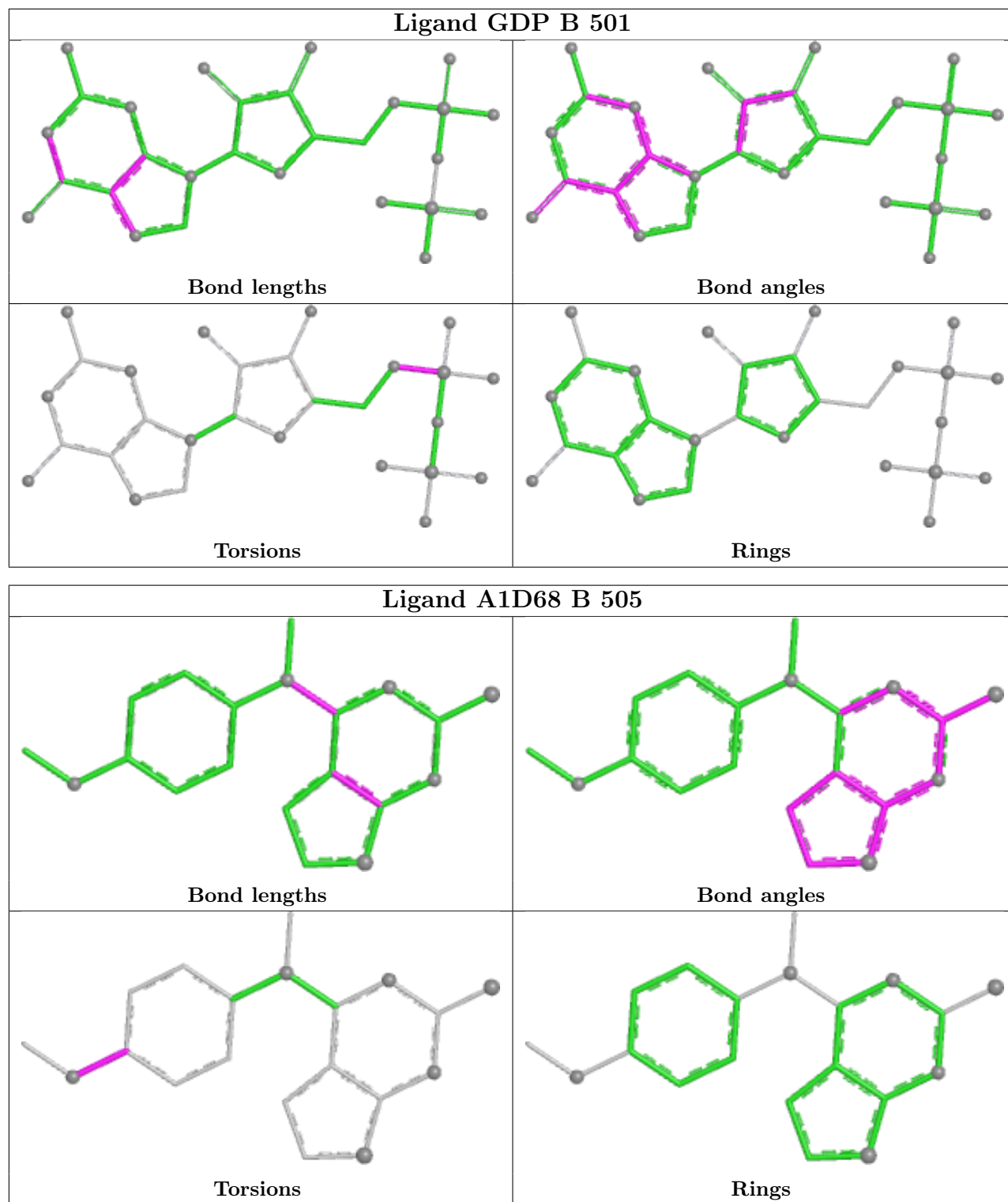
No monomer is involved in short contacts.

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.









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	437/440 (99%)	0.20	11 (2%) 58 55	37, 53, 79, 96	0
1	C	440/440 (100%)	-0.00	11 (2%) 58 55	30, 43, 66, 110	0
2	B	427/431 (99%)	0.34	25 (5%) 28 25	32, 51, 87, 140	0
2	D	418/431 (96%)	0.78	44 (10%) 11 10	39, 69, 101, 132	0
3	E	117/143 (81%)	0.72	8 (6%) 23 21	44, 64, 100, 113	0
4	F	268/380 (70%)	0.96	42 (15%) 5 4	45, 69, 104, 130	0
All	All	2107/2265 (93%)	0.43	141 (6%) 24 21	30, 57, 93, 140	0

All (141) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	231	ALA	5.1
4	F	225	SER	5.1
4	F	238	CYS	5.1
2	B	428	ALA	4.6
4	F	254	GLY	4.4
3	E	45	PRO	4.3
2	D	397	TRP	4.2
4	F	246	GLN	4.1
4	F	239	HIS	4.1
2	D	92	PHE	4.1
2	D	1	MET	4.0
1	C	340	SER	4.0
1	A	437	VAL	3.9
3	E	28	SER	3.8
4	F	186	LEU	3.8
1	C	1	MET	3.7
2	B	278	SER	3.7
4	F	89	GLU	3.7
4	F	256	TYR	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	F	194	PRO	3.7
3	E	6	MET	3.6
1	C	357	TYR	3.6
4	F	230	SER	3.6
4	F	380	HIS	3.5
2	D	170	MET	3.5
3	E	138	GLU	3.5
2	D	284	LEU	3.5
2	B	55	THR	3.5
4	F	229	ASN	3.4
4	F	46	ARG	3.4
1	A	282	TYR	3.3
4	F	33	ASP	3.3
4	F	240	LEU	3.3
2	D	42	LEU	3.3
2	D	72	THR	3.3
2	D	181	GLU	3.2
2	B	280	GLN	3.2
2	D	431	ASP	3.2
2	B	57	ASN	3.2
4	F	247	LYS	3.1
4	F	372	THR	3.1
4	F	306	HIS	3.1
4	F	20	LEU	3.0
4	F	185	TYR	3.0
4	F	227	PRO	3.0
2	D	94	GLN	3.0
4	F	245	ILE	3.0
2	D	56	GLY	3.0
2	B	320	ARG	2.9
2	B	69	GLU	2.9
2	D	394	PHE	2.9
2	B	245	GLN	2.8
1	C	440	VAL	2.8
1	C	41	THR	2.8
2	B	54	ALA	2.8
2	D	53	GLU	2.8
4	F	224	SER	2.7
2	B	427	ASP	2.7
2	D	57	ASN	2.7
2	D	301	ALA	2.7
4	F	334	GLY	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	346	TRP	2.7
2	B	301	ALA	2.7
1	C	96	LYS	2.6
4	F	259	GLY	2.6
4	F	74	LYS	2.6
2	D	356	ILE	2.6
2	B	281	TYR	2.6
4	F	228	TYR	2.6
2	D	98	GLY	2.6
3	E	7	GLU	2.5
1	A	113	GLU	2.5
2	D	362	LYS	2.5
2	B	350	LYS	2.5
2	D	80	PRO	2.5
2	D	101	TRP	2.5
2	D	37	HIS	2.5
4	F	13	VAL	2.5
2	D	55	THR	2.5
3	E	59	GLU	2.4
1	A	112	LYS	2.4
2	D	323	MET	2.4
2	B	72	THR	2.4
1	C	245	ASP	2.4
2	B	170	MET	2.4
4	F	242	ASN	2.4
2	D	41	ASP	2.4
4	F	73	ARG	2.4
1	A	262	TYR	2.4
2	D	73	MET	2.4
2	D	285	THR	2.4
2	D	81	PHE	2.4
2	D	406	MET	2.4
2	B	80	PRO	2.3
2	B	282	ARG	2.3
2	B	37	HIS	2.3
2	D	171	PRO	2.3
4	F	243	HIS	2.3
2	D	26	ASP	2.3
4	F	263	PHE	2.3
2	B	277	GLY	2.3
3	E	115	HIS	2.3
4	F	27	TRP	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	120	ASP	2.3
2	D	180	VAL	2.3
2	D	320	ARG	2.3
4	F	223	THR	2.2
1	A	46	ASP	2.2
2	D	125	GLU	2.2
4	F	331	GLU	2.2
1	A	281	ALA	2.2
2	D	11	GLN	2.2
2	D	245	GLN	2.2
4	F	341	LYS	2.2
2	B	276	ARG	2.2
2	D	359	ARG	2.2
4	F	379	HIS	2.2
2	D	65	LEU	2.2
2	B	247	ASN	2.2
2	B	283	ALA	2.2
1	C	285	GLN	2.1
2	B	279	GLN	2.1
2	D	83	GLN	2.1
2	D	222	TYR	2.1
4	F	98	TYR	2.1
2	B	291	GLN	2.1
1	A	45	GLY	2.1
2	D	289	LEU	2.1
1	C	341	ILE	2.1
1	C	163	LYS	2.1
4	F	85	PRO	2.1
2	B	92	PHE	2.1
3	E	8	VAL	2.1
2	D	71	GLY	2.1
4	F	241	THR	2.1
4	F	82	LYS	2.1
2	D	291	GLN	2.0
2	D	69	GLU	2.0
1	A	42	ILE	2.0
2	D	390	ARG	2.0
1	C	336	LYS	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 ⓘ

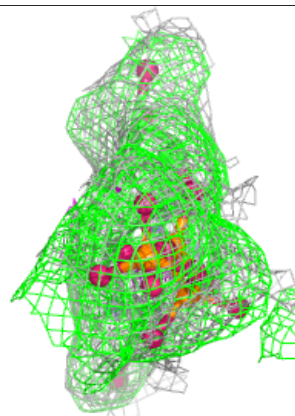
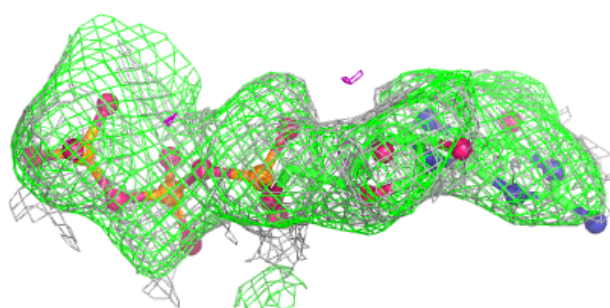
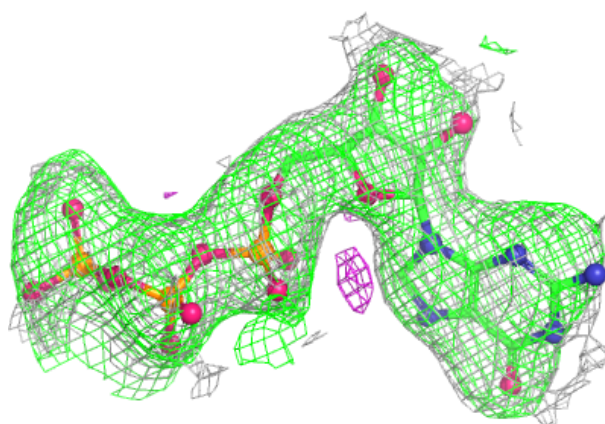
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	GTP	A	501	32/32	-	-	39,41,43,44	32
5	GTP	C	501	32/32	-	-	34,36,38,40	32
6	CA	A	502	1/1	-	-	78,78,78,78	1
6	CA	C	502	1/1	-	-	56,56,56,56	1
7	MG	A	503	1/1	-	-	45,45,45,45	1
7	MG	B	504	1/1	-	-	47,47,47,47	1
7	MG	C	503	1/1	-	-	40,40,40,40	1
8	GDP	B	501	28/28	-	-	37,42,43,45	28
8	GDP	D	501	28/28	-	-	68,74,78,81	28
9	MES	B	502	12/12	-	-	44,46,50,50	12
9	MES	B	503	12/12	-	-	59,60,60,61	12
10	A1D68	B	505	20/20	0.92	0.11	39,45,52,76	0
10	A1D68	D	502	20/20	0.92	0.11	43,54,61,87	0
11	ACP	F	401	31/31	-	-	76,86,104,106	45

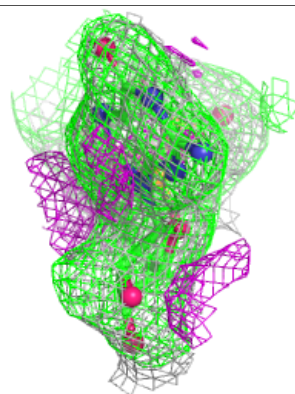
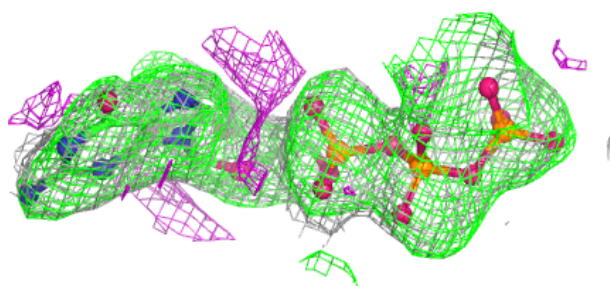
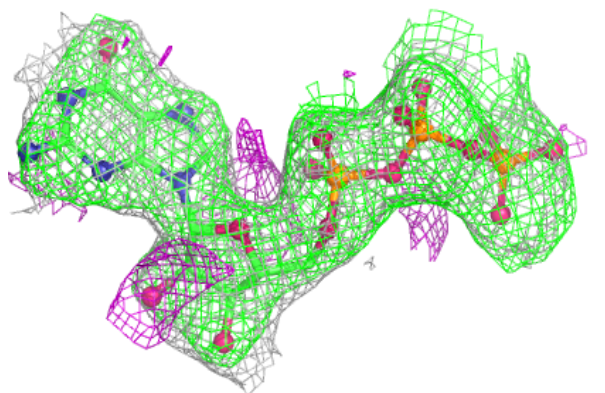
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 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)

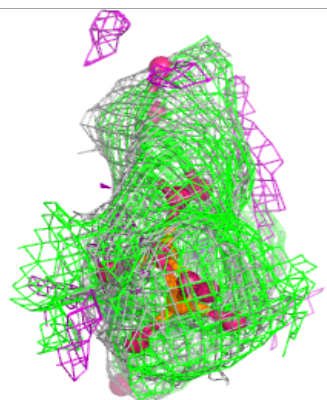
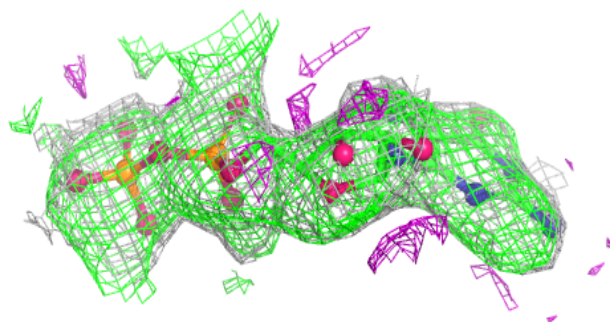
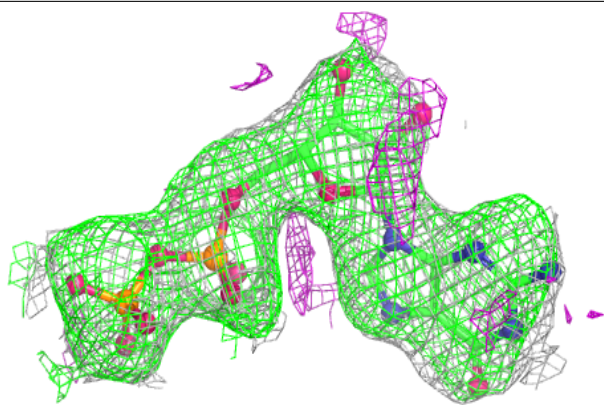
**Electron density around GTP C 501:**

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



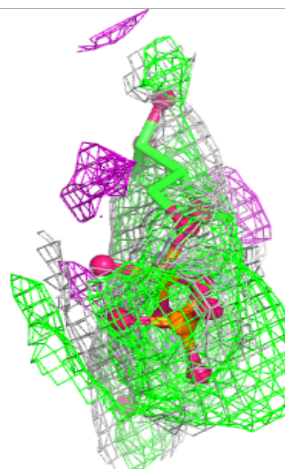
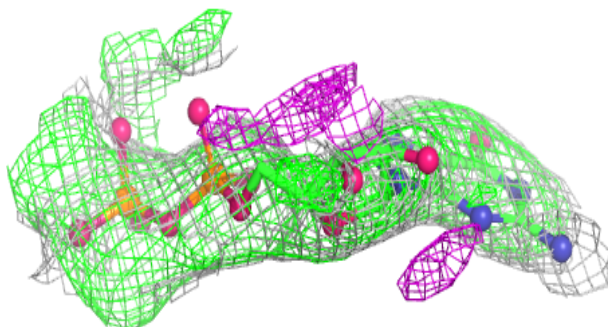
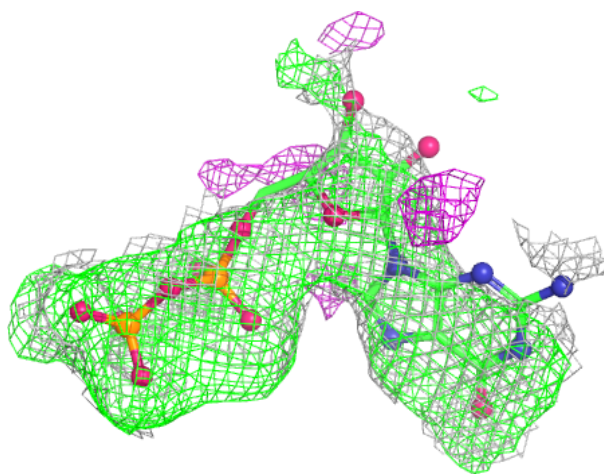
Electron density around GDP B 501:

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



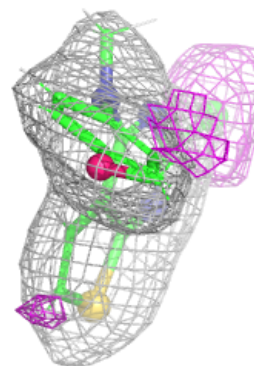
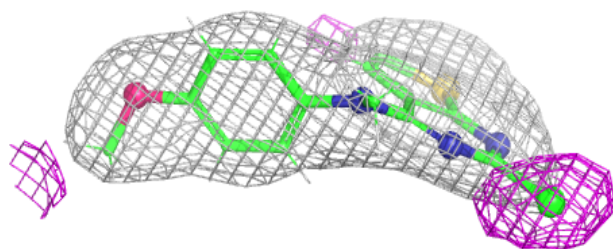
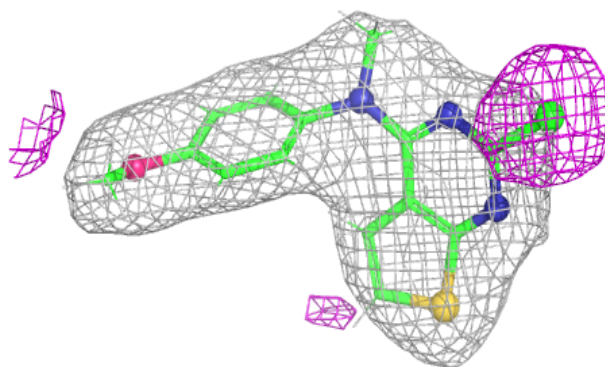
Electron density around GDP D 501:

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

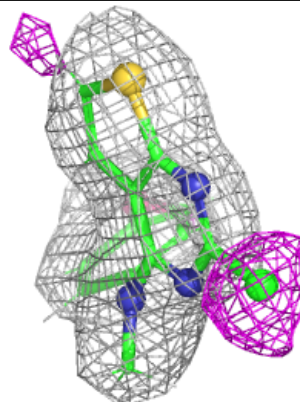
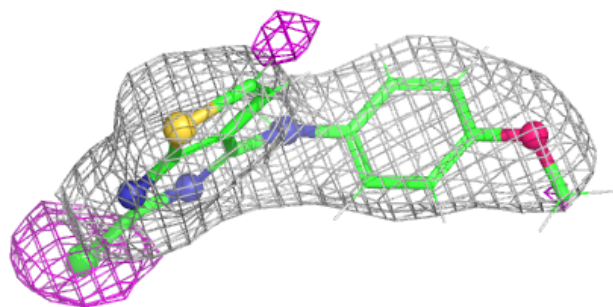
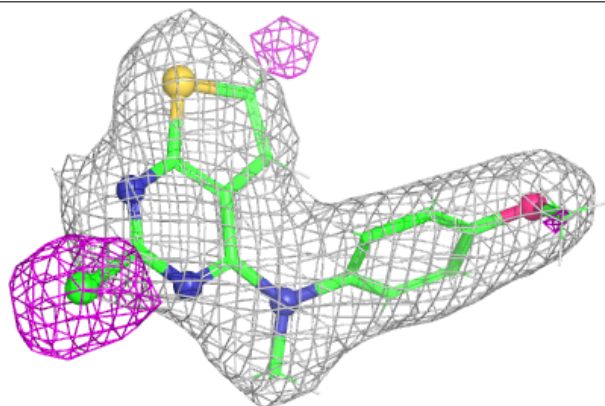


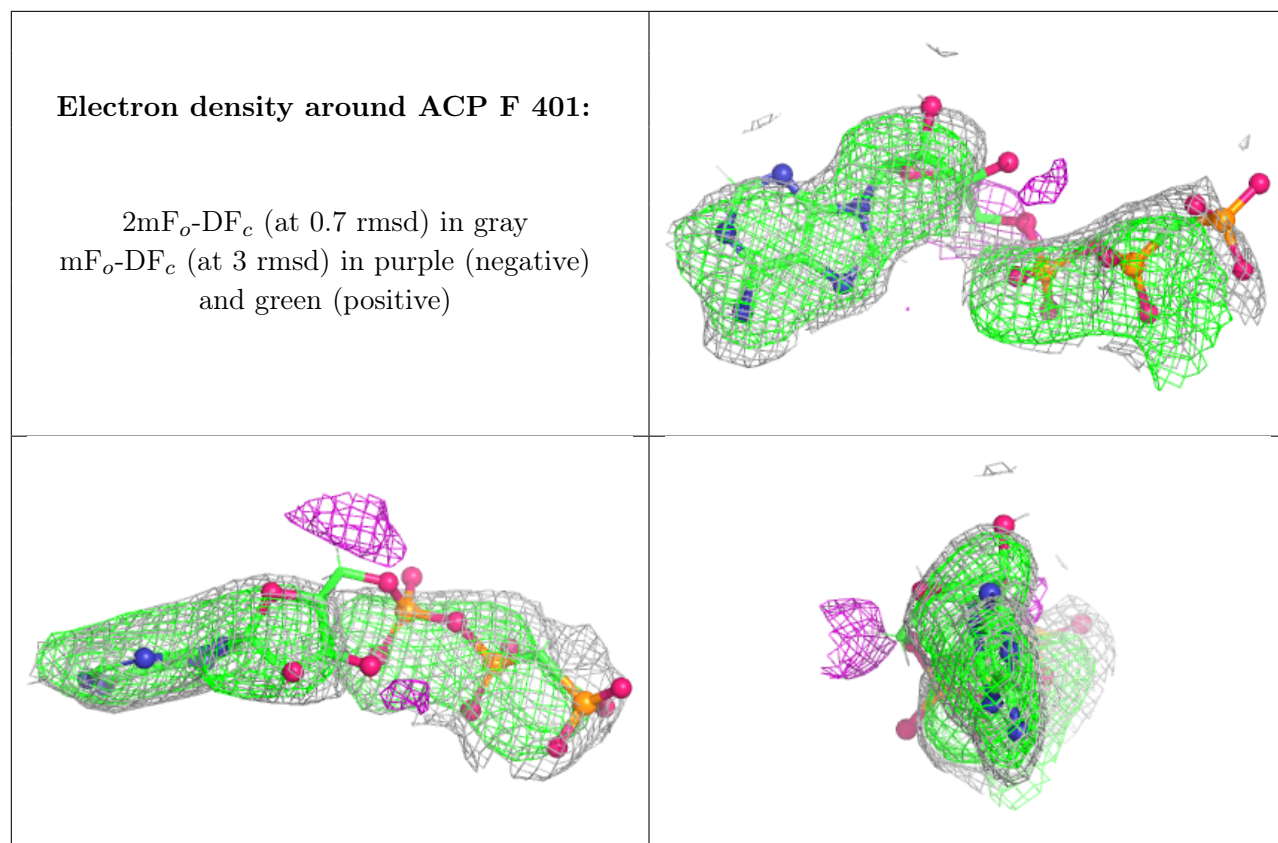
Electron density around A1D68 B 505:

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

**Electron density around A1D68 D 502:**

$2mF_o-DF_c$ (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.