



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 26, 2026 – 05:19 AM UTC

PDB ID : 5LOV / pdb_00005lov
Title : DZ-2384 tubulin complex
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Deposited on : 2016-08-10
Resolution : 2.40 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

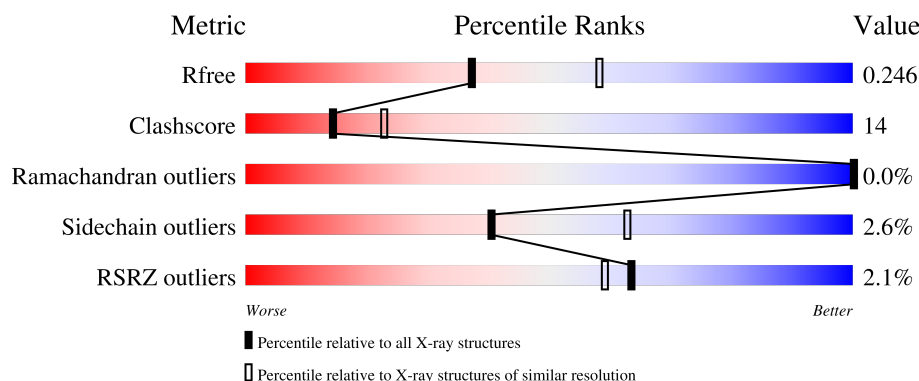
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	451	0% 71% 25% .
1	C	451	3% 78% 18% ..
2	B	445	0% 64% 29% 6%
2	D	445	2% 62% 32% 5%
3	E	143	4% 66% 15% 18%

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Mol	Chain	Length	Quality of chain
4	F	384	 A horizontal bar chart showing the quality of chain F. The bar is divided into four segments: a small red segment at the beginning labeled '3%', followed by a green segment labeled '50%', a yellow segment labeled '26%', and a grey segment at the end labeled '22%'. A small black dot is visible on the yellow segment.

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 17322 atoms, of which 49 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Tubulin alpha-1B chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	437	Total	C	N	O	S	0	6	0
			3442	2185	582	652	23			
1	C	437	Total	C	N	O	S	0	7	0
			3442	2182	581	655	24			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	417	Total	C	N	O	S	0	2	0
			3287	2068	558	634	27			
2	D	422	Total	C	N	O	S	0	2	0
			3323	2089	563	644	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
			970	599	177	190	4			

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

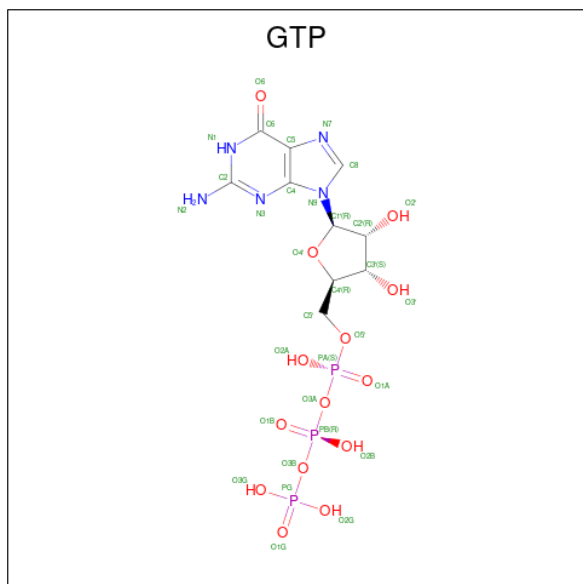
- Molecule 4 is a protein called Tubulin-tyrosine ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	298	Total	C	N	O	S	0	5	0
			2460	1596	409	443	12			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	379	HIS	-	expression tag	UNP E1BQ43
F	380	HIS	-	expression tag	UNP E1BQ43
F	381	HIS	-	expression tag	UNP E1BQ43
F	382	HIS	-	expression tag	UNP E1BQ43
F	383	HIS	-	expression tag	UNP E1BQ43
F	384	HIS	-	expression tag	UNP E1BQ43

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



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

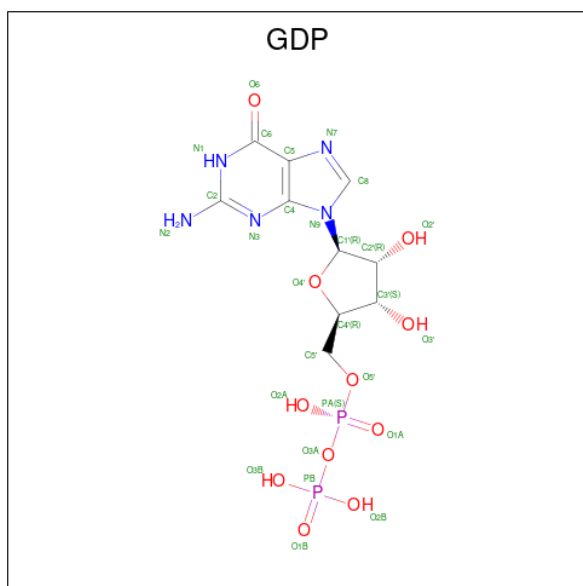
- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

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

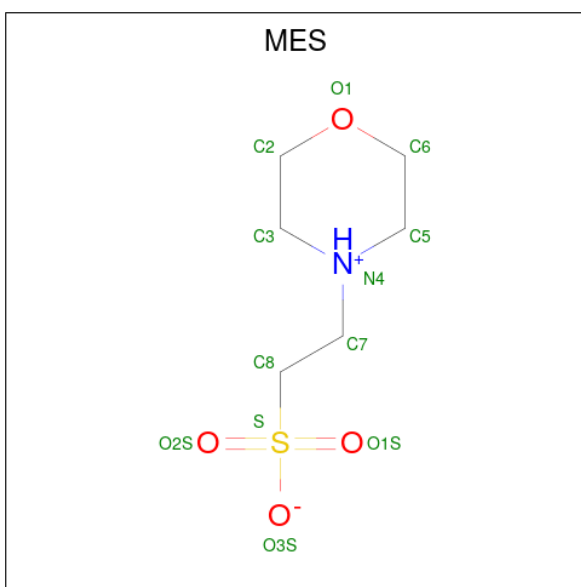
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Ca	0	0
			1	1		

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



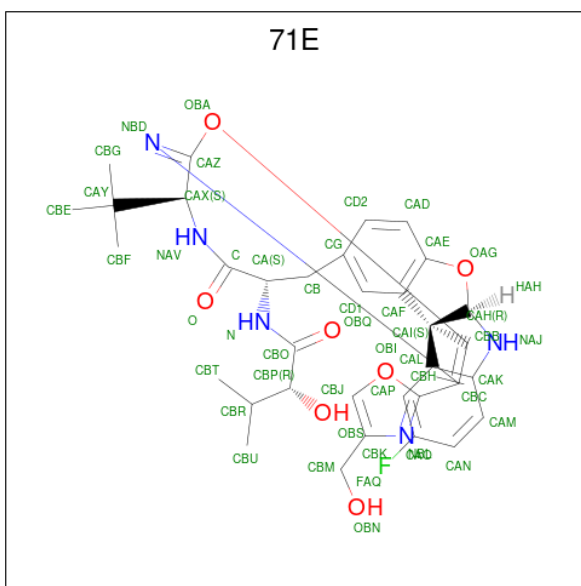
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	B	1	Total 28	C 10	N 5	O 11	P 2	0	0
8	D	1	Total 28	C 10	N 5	O 11	P 2	0	0

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



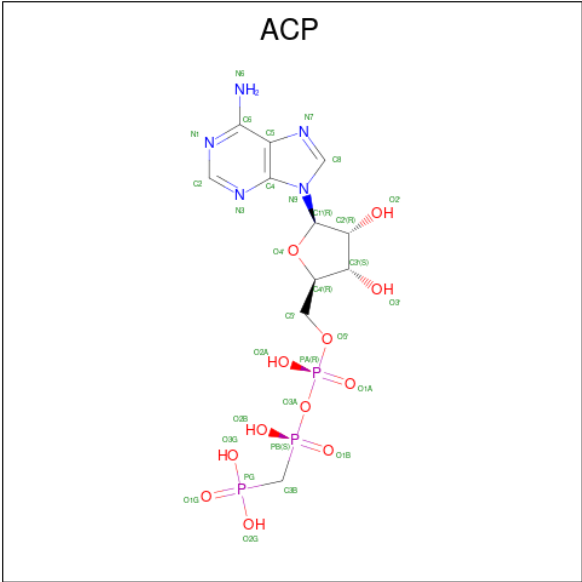
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
9	B	1	Total	C	H	N	O	S	0	0
			25	6	13	1	4	1		

- Molecule 10 is DZ 2384 (CCD ID: 71E) (formula: $\text{C}_{34}\text{H}_{36}\text{FN}_5\text{O}_7$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
10	C	1	Total	C	F	H	N	O	0	0
			83	34	1	36	5	7		

- 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	N	O	P	0	0
			31	11	5	12	3		

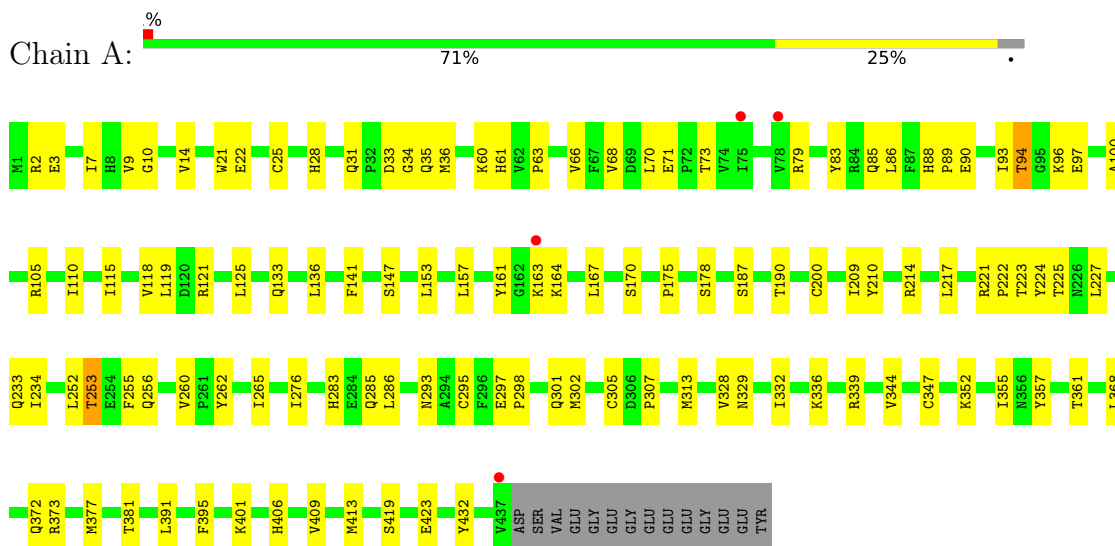
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	32	Total	O	0	0
			32	32		
12	B	30	Total	O	0	0
			30	30		
12	C	66	Total	O	0	0
			66	66		
12	D	7	Total	O	0	0
			7	7		

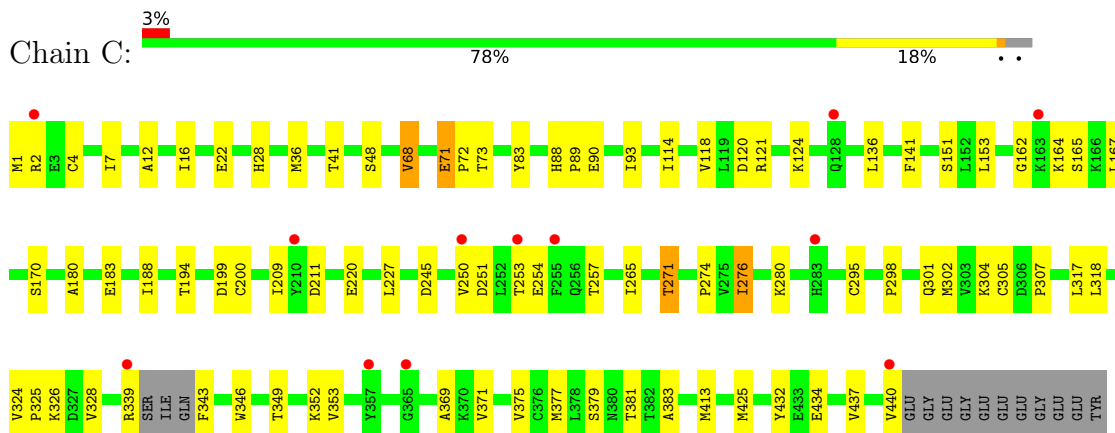
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

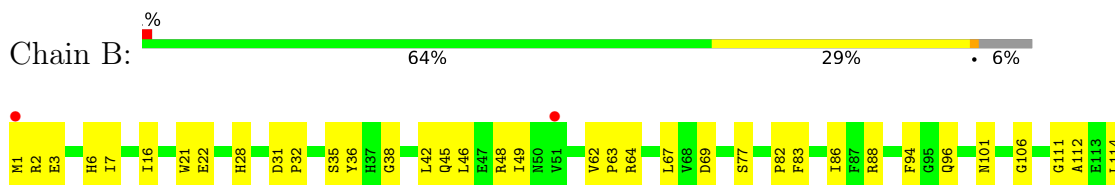
- Molecule 1: Tubulin alpha-1B chain

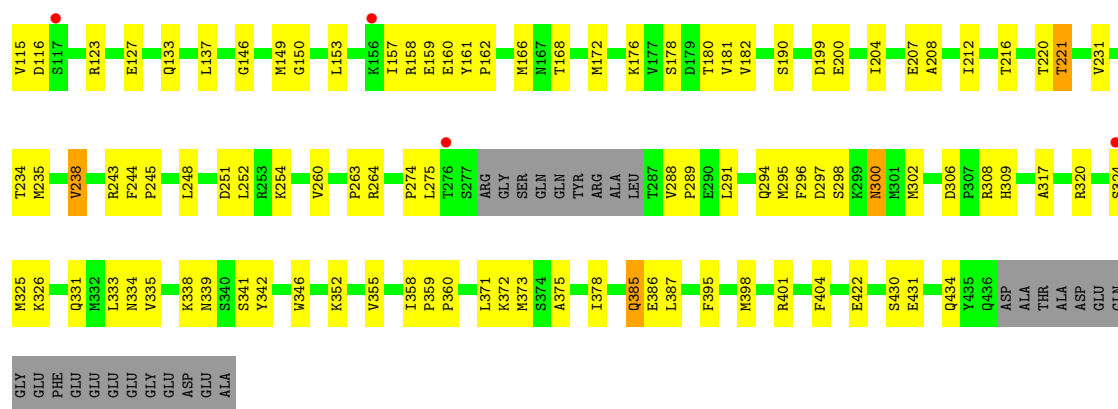


- Molecule 1: Tubulin alpha-1B chain

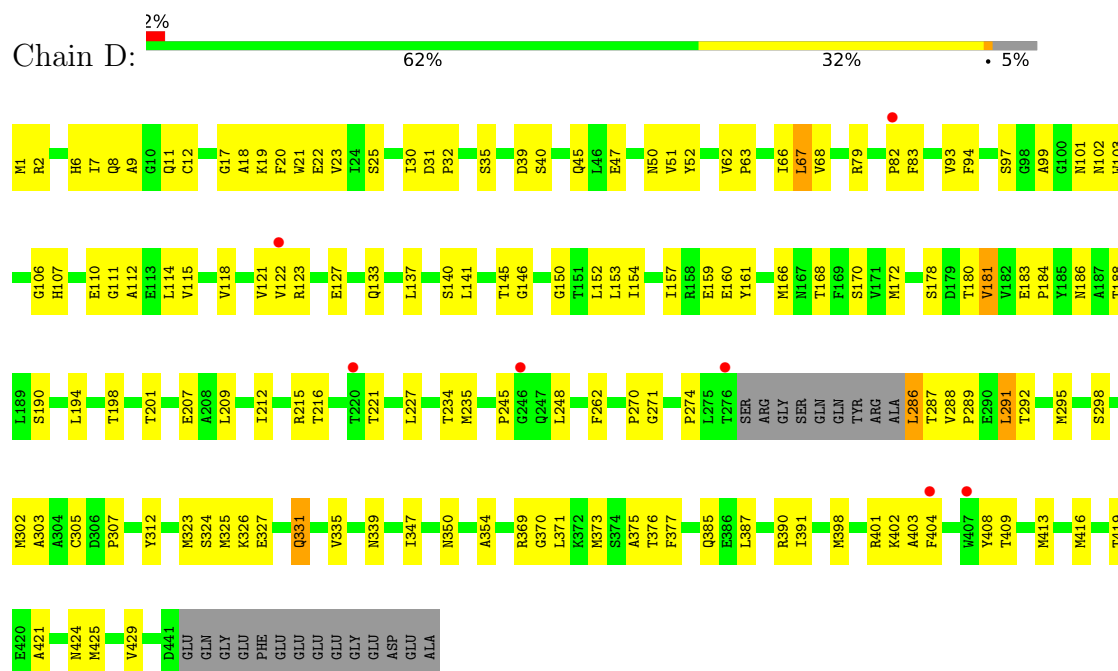


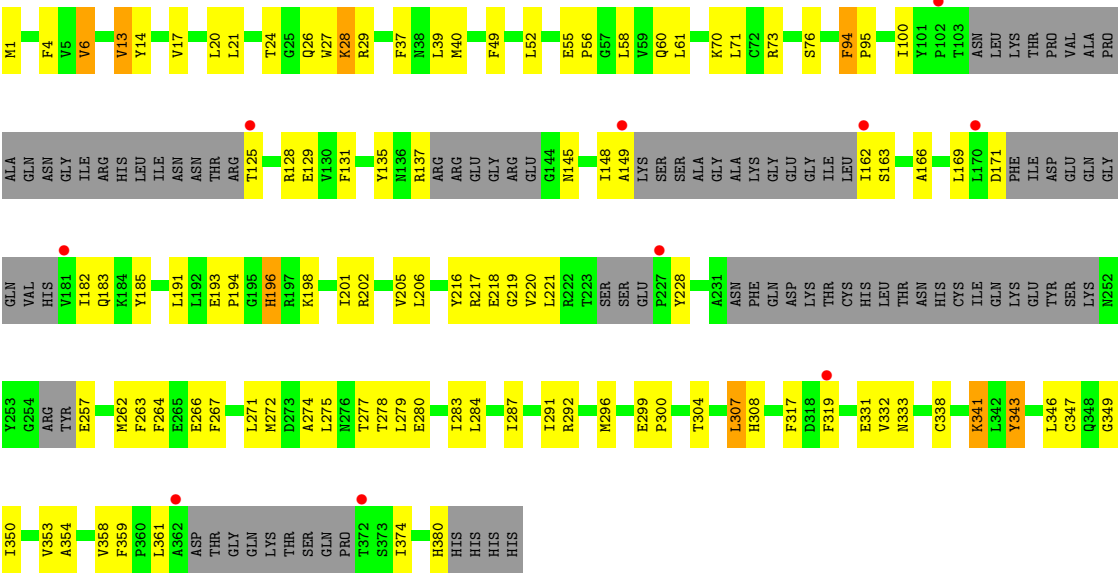
- Molecule 2: Tubulin beta-2B chain





• Molecule 2: Tubulin beta-2B chain





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	103.16Å 154.70Å 180.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	77.35 – 2.40 77.35 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.8 (77.35-2.40) 99.7 (77.35-2.40)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.08 (at 2.40Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.188 , 0.241 0.198 , 0.246	Depositor DCC
R_{free} test set	5650 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	64.7	Xtriage
Anisotropy	0.278	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 46.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	17322	wwPDB-VP
Average B, all atoms (Å ²)	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.35% 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: GTP, CA, 71E, GDP, MG, MES, ACP

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	0.33	0/3538	0.76	4/4804 (0.1%)
1	C	0.38	0/3540	0.75	2/4807 (0.0%)
2	B	0.35	0/3366	0.77	6/4559 (0.1%)
2	D	0.32	0/3402	0.75	3/4609 (0.1%)
3	E	0.31	0/976	0.67	0/1292
4	F	0.27	0/2527	0.72	2/3413 (0.1%)
All	All	0.34	0/17349	0.75	17/23484 (0.1%)

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	324	VAL	CA-C-N	7.45	126.98	119.24
1	C	324	VAL	C-N-CA	7.45	126.98	119.24
2	B	161	TYR	CA-C-N	6.46	126.38	119.28
2	B	161	TYR	C-N-CA	6.46	126.38	119.28
2	D	262	PHE	CA-C-N	6.12	126.30	119.32
2	D	262	PHE	C-N-CA	6.12	126.30	119.32
1	A	262	TYR	CA-C-N	6.06	127.42	119.84
1	A	262	TYR	C-N-CA	6.06	127.42	119.84
2	D	288	VAL	CB-CA-C	-5.49	108.54	114.35
2	B	260	VAL	CA-C-N	5.40	124.73	118.85
2	B	260	VAL	C-N-CA	5.40	124.73	118.85
4	F	94	PHE	CA-C-N	5.39	125.39	119.89
4	F	94	PHE	C-N-CA	5.39	125.39	119.89
2	B	221	THR	CA-C-N	5.35	125.30	119.78
2	B	221	THR	C-N-CA	5.35	125.30	119.78
1	A	260	VAL	CA-C-N	5.15	124.32	118.97
1	A	260	VAL	C-N-CA	5.15	124.32	118.97

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	3442	0	3379	96	0
1	C	3442	0	3369	67	0
2	B	3287	0	3174	105	0
2	D	3323	0	3208	113	0
3	E	970	0	990	22	0
4	F	2460	0	2464	99	0
5	A	32	0	12	0	0
5	C	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
8	B	28	0	12	0	0
8	D	28	0	12	5	0
9	B	12	13	13	1	0
10	C	47	36	0	2	0
11	F	31	0	14	1	0
12	A	32	0	0	0	0
12	B	30	0	0	1	0
12	C	66	0	0	1	0
12	D	7	0	0	0	0
All	All	17273	49	16659	477	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 14.

All (477) 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)
4:F:1:MET:HE3	4:F:28:LYS:HB2	1.38	1.02
2:D:295:MET:HE3	2:D:375:ALA:HB1	1.41	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:333:LEU:HD21	4:F:58:LEU:HD13	1.43	1.00
2:B:42:LEU:HD23	2:B:358:ILE:HD11	1.44	0.98
4:F:148:ILE:HA	4:F:162:ILE:HG22	1.47	0.97
1:C:71:GLU:HG2	1:C:72:PRO:HD2	1.48	0.96
4:F:262:MET:HE3	4:F:266:GLU:HG2	1.46	0.95
1:A:70:LEU:HD13	1:A:110:ILE:HG21	1.50	0.93
4:F:262:MET:HE2	4:F:267:PHE:HA	1.51	0.92
1:C:271:THR:HG21	1:C:295[A]:CYS:HA	1.59	0.83
1:C:271:THR:HG21	1:C:295[B]:CYS:HA	1.59	0.82
2:B:176:LYS:HD2	2:B:207:GLU:HG3	1.61	0.81
2:D:323:MET:HE2	2:D:373:MET:HE2	1.64	0.80
1:A:223:THR:HG22	1:A:225:THR:H	1.46	0.80
4:F:272:MET:HE3	4:F:278:THR:HG22	1.61	0.80
1:A:2:ARG:HB3	1:A:133:GLN:HG2	1.65	0.79
2:D:1:MET:HG2	2:D:50:ASN:CB	2.12	0.78
2:B:216:THR:HG21	2:B:275:LEU:HD12	1.65	0.78
2:D:1:MET:HG2	2:D:50:ASN:HB2	1.65	0.78
2:D:391:ILE:HG22	2:D:425:MET:HE1	1.66	0.78
1:A:297:GLU:HG3	1:A:339:ARG:HH12	1.48	0.77
1:C:71:GLU:HG2	1:C:72:PRO:CD	2.14	0.77
2:B:320:ARG:HG2	2:B:359:PRO:HA	1.65	0.77
1:A:175:PRO:HA	1:A:178:SER:HB3	1.66	0.76
1:A:221:ARG:HD2	2:B:325:MET:HB3	1.65	0.76
4:F:28:LYS:HE3	4:F:28:LYS:HA	1.68	0.76
1:C:381:THR:HG22	1:C:383:ALA:H	1.47	0.76
4:F:149:ALA:HB2	4:F:182:ILE:HD13	1.67	0.76
4:F:201:ILE:HD13	4:F:221:LEU:HG	1.66	0.75
2:B:325:MET:HE2	2:B:355:VAL:HB	1.66	0.74
2:D:11:GLN:HB3	8:D:501:GDP:O2A	1.87	0.74
2:D:93:VAL:HG12	2:D:114:LEU:HD11	1.70	0.73
2:D:8:GLN:HE21	2:D:67:LEU:HG	1.54	0.73
1:A:234:ILE:HD13	1:A:302:MET:SD	2.28	0.72
2:B:360:PRO:HG2	2:B:371:LEU:HD12	1.72	0.71
1:A:217:LEU:HD21	1:A:368:LEU:HD23	1.71	0.71
4:F:262:MET:HE2	4:F:267:PHE:CA	2.20	0.70
1:A:167:LEU:HD22	1:A:200:CYS:HB3	1.72	0.70
4:F:349:GLY:O	4:F:353[B]:VAL:HG12	1.90	0.70
1:A:70:LEU:CD1	1:A:110:ILE:HG21	2.22	0.70
2:D:123:ARG:O	2:D:127:GLU:HG2	1.91	0.70
2:D:270:PRO:HG2	2:D:302:MET:HB2	1.73	0.69
4:F:131:PHE:CE1	4:F:182:ILE:HG21	2.27	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:12:ALA:O	1:C:16:ILE:HG12	1.92	0.68
1:C:271:THR:HG21	1:C:295[A]:CYS:CA	2.23	0.68
1:C:271:THR:CG2	1:C:295[A]:CYS:HA	2.23	0.68
1:C:271:THR:CG2	1:C:295[B]:CYS:HA	2.23	0.68
1:C:209:ILE:HG22	1:C:227:LEU:HD22	1.76	0.68
2:D:347:ILE:HG22	2:D:350:ASN:HB3	1.76	0.68
1:C:276:ILE:HD13	1:C:369:ALA:HB3	1.77	0.67
4:F:338:CYS:HB3	4:F:343:TYR:CE1	2.30	0.67
5:C:501:GTP:O1G	12:C:601:HOH:O	2.13	0.67
1:C:88:HIS:CD2	1:C:90:GLU:HG2	2.30	0.66
4:F:163:SER:HB2	4:F:169:LEU:HD13	1.78	0.66
1:C:93:ILE:HD11	1:C:121:ARG:HG3	1.77	0.66
1:A:276:ILE:HD12	1:A:283:HIS:HD2	1.61	0.66
4:F:304:THR:HG22	4:F:307:LEU:HD12	1.78	0.65
2:D:295:MET:CE	2:D:375:ALA:HB1	2.21	0.65
4:F:279:LEU:HG	4:F:284[B]:LEU:HD23	1.77	0.65
2:D:97:SER:HB3	2:D:110:GLU:HG2	1.79	0.65
1:A:175:PRO:HA	1:A:178:SER:CB	2.27	0.65
2:B:333:LEU:CD2	4:F:58:LEU:HD13	2.22	0.64
1:C:88:HIS:CD2	1:C:89:PRO:HD2	2.32	0.64
2:B:137:LEU:HB3	2:B:168[B]:THR:HG22	1.78	0.64
1:A:329:ASN:HD21	3:E:8:VAL:CG2	2.11	0.64
2:D:31:ASP:HB2	2:D:32:PRO:HD2	1.80	0.64
2:D:1:MET:HE3	2:D:50:ASN:HB2	1.80	0.64
4:F:216:TYR:CE2	4:F:218:GLU:HB2	2.33	0.64
4:F:287:ILE:O	4:F:291:ILE:HG12	1.97	0.64
2:D:289:PRO:HA	2:D:331:GLN:HG2	1.80	0.63
2:B:320:ARG:NE	2:B:360:PRO:HD3	2.14	0.63
2:D:248:LEU:HD23	2:D:354:ALA:HB2	1.81	0.62
4:F:61:LEU:HD22	4:F:358:VAL:HG11	1.82	0.62
4:F:279:LEU:HG	4:F:284[B]:LEU:CD2	2.30	0.62
2:B:306:ASP:HB3	2:B:309:HIS:ND1	2.14	0.62
4:F:185:TYR:OH	4:F:198:LYS:NZ	2.33	0.62
2:B:360:PRO:CG	2:B:371:LEU:HD12	2.29	0.62
2:D:188:THR:HG22	2:D:421:ALA:HB1	1.82	0.62
1:A:336:LYS:HE3	3:E:25:LYS:HZ3	1.65	0.62
2:D:1:MET:HG2	2:D:50:ASN:HB3	1.82	0.62
2:D:409:THR:O	3:E:140:LYS:NZ	2.33	0.61
1:A:2:ARG:CB	1:A:133:GLN:HG2	2.30	0.61
2:D:8:GLN:OE1	2:D:17:GLY:HA3	1.99	0.61
1:A:210:TYR:CE1	1:A:214:ARG:HD2	2.36	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:288:VAL:HG12	2:B:331:GLN:HG3	1.82	0.61
4:F:135:TYR:O	4:F:145:ASN:ND2	2.34	0.61
2:B:28:HIS:HB3	2:B:49:ILE:CD1	2.30	0.61
1:C:343:PHE:CD2	1:C:349:THR:HG23	2.36	0.60
1:A:36:MET:HB3	1:A:61:HIS:CE1	2.35	0.60
4:F:20:LEU:O	4:F:24:THR:HG23	2.01	0.60
4:F:274:ALA:C	4:F:275:LEU:HD23	2.26	0.60
2:B:238:VAL:HB	2:B:378:ILE:HD11	1.83	0.60
1:A:344:VAL:HG23	1:A:347:CYS:HB2	1.84	0.59
2:D:295:MET:HE3	2:D:375:ALA:CB	2.25	0.59
1:C:434:GLU:O	1:C:437:VAL:HG12	2.03	0.59
1:A:147:SER:HB2	1:A:190:THR:HB	1.84	0.59
2:B:325:MET:CE	2:B:355:VAL:HB	2.32	0.59
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.21	0.58
1:A:66[B]:VAL:HG23	1:A:125:LEU:CD1	2.33	0.58
1:A:221:ARG:CD	2:B:325:MET:HB3	2.31	0.58
1:C:93:ILE:HG22	1:C:114:ILE:HD11	1.85	0.58
2:B:159:GLU:OE1	3:E:76:ARG:NH1	2.34	0.58
1:C:167:LEU:HD22	1:C:200:CYS:HB3	1.85	0.58
2:B:220:THR:HG23	2:B:221:THR:H	1.67	0.58
1:C:276:ILE:HD11	1:C:371:VAL:CG1	2.34	0.57
1:C:41:THR:O	1:C:41:THR:OG1	2.22	0.57
2:D:207:GLU:HB3	2:D:390:ARG:HH12	1.69	0.57
2:D:209:LEU:HB3	2:D:227:LEU:HD22	1.85	0.57
2:D:391:ILE:CG2	2:D:425:MET:HE1	2.34	0.57
2:B:178:SER:HB2	1:C:349:THR:O	2.02	0.57
1:A:357:TYR:CE2	3:E:17:GLY:HA2	2.40	0.57
1:C:1:MET:O	1:C:2:ARG:HB2	2.04	0.57
1:C:180:ALA:O	1:C:183:GLU:HG3	2.05	0.57
2:B:83:PHE:O	2:B:86:ILE:HG12	2.05	0.56
2:B:434:GLN:NE2	12:B:602:HOH:O	2.38	0.56
4:F:148:ILE:HG12	4:F:149:ALA:N	2.20	0.56
4:F:202:ARG:HB3	4:F:220:VAL:CG1	2.34	0.56
1:A:409:VAL:HA	1:A:413:MET:O	2.05	0.56
1:C:220:GLU:HG2	2:D:326:LYS:HD3	1.87	0.56
4:F:338:CYS:HB3	4:F:343:TYR:CD1	2.40	0.56
1:C:271:THR:HG21	1:C:295[B]:CYS:CA	2.23	0.56
2:D:298:SER:OG	2:D:307:PRO:HD2	2.04	0.56
2:D:79:ARG:HH12	2:D:94:PHE:HZ	1.52	0.56
1:A:187:SER:HB3	1:A:391:LEU:HD21	1.88	0.56
1:C:4[A]:CYS:SG	1:C:136:LEU:HG	2.46	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:36:TYR:CD1	2:B:46:LEU:HD21	2.41	0.56
3:E:44:ASP:HB2	3:E:45:PRO:HD2	1.88	0.56
1:C:298:PRO:HA	1:C:301:GLN:OE1	2.06	0.55
3:E:139:LEU:H	3:E:139:LEU:HD22	1.70	0.55
4:F:191:LEU:HD21	4:F:228:TYR:HB3	1.88	0.55
4:F:262:MET:CE	4:F:266:GLU:HG2	2.29	0.55
2:D:12:CYS:HB3	2:D:140:SER:HB3	1.89	0.55
2:B:83:PHE:HB3	2:B:86:ILE:HD13	1.87	0.55
1:C:276:ILE:CD1	1:C:369:ALA:HB3	2.37	0.55
4:F:13:VAL:HG23	4:F:347:CYS:SG	2.47	0.55
1:A:34:GLY:HA3	1:A:60:LYS:HG3	1.88	0.55
2:B:306:ASP:OD2	2:B:308:ARG:NH2	2.33	0.55
2:D:118:VAL:O	2:D:121:VAL:HG22	2.07	0.55
2:D:181:VAL:O	2:D:398:MET:HE1	2.07	0.55
1:A:31:GLN:NE2	1:A:35:GLN:HB2	2.21	0.54
1:C:71:GLU:OE2	1:C:73:THR:OG1	2.24	0.54
4:F:13:VAL:HG13	4:F:14:TYR:CD1	2.42	0.54
1:A:141:PHE:CE1	1:A:170:SER:HB3	2.42	0.54
2:B:42:LEU:HD23	2:B:358:ILE:CD1	2.30	0.54
2:B:248:LEU:HD21	2:B:352:LYS:HB2	1.90	0.54
2:B:234:THR:O	2:B:238:VAL:HG13	2.08	0.54
1:A:336:LYS:HE3	3:E:25:LYS:NZ	2.23	0.54
2:D:160:GLU:HG2	2:D:161:TYR:CE1	2.42	0.54
4:F:283:ILE:O	4:F:287:ILE:HG12	2.08	0.54
2:D:31:ASP:HB2	2:D:32:PRO:CD	2.37	0.54
4:F:95:PRO:HB2	4:F:183:GLN:HG3	1.90	0.54
2:B:288:VAL:N	2:B:289:PRO:HD2	2.24	0.53
2:D:106:GLY:O	2:D:111:GLY:HA3	2.09	0.53
4:F:202:ARG:HB3	4:F:220:VAL:HG12	1.90	0.53
2:D:295:MET:HE2	2:D:376:THR:O	2.09	0.53
2:B:216:THR:HG21	2:B:275:LEU:CD1	2.37	0.53
1:C:162:GLY:HA2	3:E:94:ILE:HD11	1.90	0.53
1:A:210:TYR:CE2	1:A:222:PRO:HD2	2.44	0.53
2:D:67:LEU:HD12	2:D:67:LEU:H	1.73	0.53
4:F:299:GLU:N	4:F:300:PRO:HD2	2.24	0.53
2:B:69:ASP:O	2:B:94:PHE:HA	2.08	0.53
1:C:343:PHE:CE2	1:C:349:THR:HG23	2.44	0.53
4:F:280:GLU:HA	4:F:284[B]:LEU:HB2	1.91	0.53
2:D:172:MET:HG3	2:D:387:LEU:HD11	1.91	0.52
1:A:141:PHE:HB3	1:A:187:SER:OG	2.09	0.52
2:B:244:PHE:HB3	2:B:245:PRO:HD2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:51:VAL:HG12	2:D:52:TYR:CD2	2.44	0.52
4:F:28:LYS:HA	4:F:28:LYS:CE	2.37	0.52
4:F:292:ARG:O	4:F:296:MET:HB2	2.09	0.52
1:A:66[B]:VAL:HG23	1:A:125:LEU:HD11	1.92	0.52
1:C:251:ASP:OD2	1:C:253:THR:HG22	2.10	0.52
1:A:406:HIS:CG	2:B:263:PRO:HD3	2.44	0.52
2:B:248:LEU:HD21	2:B:352:LYS:CB	2.39	0.52
1:A:209:ILE:HG22	1:A:227:LEU:HD22	1.91	0.52
2:B:67:LEU:N	2:B:67:LEU:HD12	2.24	0.52
2:B:264:ARG:NE	2:B:431:GLU:OE2	2.30	0.52
2:B:358:ILE:N	2:B:358:ILE:HD12	2.25	0.52
1:A:406:HIS:ND1	2:B:263:PRO:HD3	2.24	0.52
2:B:28:HIS:HA	2:B:45:GLN:HB3	1.92	0.52
1:A:223:THR:HG22	1:A:224:TYR:N	2.25	0.52
1:A:276:ILE:HD12	1:A:283:HIS:CD2	2.43	0.52
2:B:48:ARG:HB2	2:B:243:ARG:O	2.09	0.51
1:C:22:GLU:HG3	1:C:83:TYR:OH	2.10	0.51
1:C:254:GLU:HG2	1:C:352:LYS:HE2	1.93	0.51
2:D:118:VAL:O	2:D:122:VAL:HG23	2.10	0.51
2:D:324:SER:HB3	2:D:327:GLU:HB2	1.93	0.51
4:F:202:ARG:NH2	4:F:333:ASN:HD22	2.08	0.51
2:B:96:GLN:HG3	1:C:1:MET:HG2	1.93	0.51
2:D:154:ILE:HG23	2:D:166:MET:HG2	1.92	0.51
2:D:7:ILE:O	2:D:137:LEU:HD12	2.10	0.51
4:F:26:GLN:HE22	4:F:361:LEU:HA	1.76	0.51
2:B:62:VAL:HG11	2:B:88:ARG:HG3	1.93	0.51
4:F:37:PHE:O	4:F:60:GLN:HG2	2.11	0.51
1:A:9:VAL:HG22	1:A:68[B]:VAL:CG1	2.41	0.51
2:D:20:PHE:CD1	2:D:235:MET:HE2	2.46	0.51
4:F:169:LEU:CD2	4:F:182:ILE:HD12	2.41	0.51
2:B:291:LEU:HD13	2:B:373:MET:HG2	1.93	0.50
2:D:291:LEU:HD22	2:D:375:ALA:CB	2.41	0.50
1:A:285:GLN:HG2	1:A:372[B]:GLN:NE2	2.25	0.50
1:C:2:ARG:NH1	1:C:251:ASP:OD1	2.45	0.50
2:D:145:THR:N	8:D:501:GDP:O2B	2.44	0.50
10:C:503:71E:OBA	10:C:503:71E:CD1	2.56	0.50
1:A:357:TYR:CZ	3:E:17:GLY:HA2	2.47	0.50
4:F:135:TYR:CE2	4:F:166:ALA:HB2	2.46	0.50
2:B:153:LEU:O	2:B:157:ILE:HG12	2.10	0.50
4:F:350:ILE:O	4:F:354:ALA:HB3	2.12	0.50
2:D:234:THR:OG1	2:D:302:MET:HE3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:287:ILE:HG23	4:F:319:PHE:CE2	2.48	0.49
1:A:265:ILE:HG23	1:A:432:TYR:CZ	2.48	0.49
1:A:7:ILE:HG21	1:A:153:LEU:HD21	1.94	0.49
4:F:263:PHE:CZ	4:F:341:LYS:HG3	2.47	0.49
4:F:148:ILE:HG22	4:F:183:GLN:O	2.12	0.49
2:D:274:PRO:HD2	2:D:371:LEU:HD13	1.95	0.49
2:B:291:LEU:HD21	2:B:375:ALA:HB2	1.94	0.49
2:D:12:CYS:CB	2:D:140:SER:HB3	2.42	0.49
2:B:31:ASP:HB2	2:B:32:PRO:HD2	1.95	0.49
2:D:82:PRO:O	2:D:83:PHE:HB2	2.12	0.49
2:D:66:ILE:HD13	2:D:122:VAL:HG22	1.95	0.49
11:F:401:ACP:O2A	11:F:401:ACP:O1B	2.31	0.49
1:A:93:ILE:CD1	1:A:118:VAL:HA	2.43	0.48
1:A:253:THR:O	1:A:256:GLN:HG2	2.12	0.48
2:B:160:GLU:C	2:B:162:PRO:HD3	2.37	0.48
1:C:68[A]:VAL:HG11	1:C:118:VAL:HG21	1.94	0.48
1:C:141:PHE:CE1	1:C:170:SER:HB3	2.48	0.48
2:D:159:GLU:HG3	3:E:123:LEU:HD13	1.94	0.48
4:F:14:TYR:HA	4:F:17:VAL:HB	1.95	0.48
1:A:21:TRP:CZ3	1:A:63:PRO:HB3	2.48	0.48
1:A:265:ILE:HG23	1:A:432:TYR:CE1	2.48	0.48
1:A:401:LYS:HG3	2:B:346:TRP:CD2	2.48	0.48
2:D:323:MET:HB3	2:D:373:MET:CE	2.44	0.48
1:A:33:ASP:HA	1:A:85:GLN:HB2	1.95	0.48
1:A:298:PRO:HA	1:A:301:GLN:CD	2.38	0.48
2:D:19:LYS:O	2:D:23:VAL:HG23	2.12	0.48
2:B:181:VAL:HG11	2:B:404:PHE:CZ	2.49	0.48
2:B:294:GLN:HG2	2:B:300:ASN:OD1	2.14	0.48
2:B:133:GLN:OE1	2:B:252:LEU:HG	2.13	0.48
4:F:267:PHE:CD2	4:F:279:LEU:HD13	2.48	0.48
2:B:114:LEU:HD23	2:B:149:MET:HE1	1.96	0.48
3:E:70:LYS:O	3:E:74:GLU:HG3	2.12	0.48
2:D:66:ILE:CD1	2:D:122:VAL:HG22	2.44	0.48
2:D:295:MET:HE2	2:D:376:THR:C	2.39	0.48
2:B:339:ASN:HB3	2:B:342:TYR:HD2	1.79	0.48
1:C:48:SER:HB3	1:C:245:ASP:CG	2.38	0.48
1:C:28:HIS:O	1:C:36:MET:HE3	2.14	0.47
1:C:377:MET:HE3	1:C:379:SER:OG	2.13	0.47
2:D:12:CYS:HB2	8:D:501:GDP:C8	2.49	0.47
1:A:141:PHE:O	1:A:147:SER:HB3	2.14	0.47
2:D:172:MET:HE2	2:D:387:LEU:HD21	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:73:ARG:HB2	4:F:76:SER:HB2	1.94	0.47
2:D:103:TRP:HB2	2:D:186:ASN:OD1	2.14	0.47
2:D:387:LEU:HD23	2:D:387:LEU:C	2.39	0.47
1:A:25:CYS:SG	1:A:86:LEU:HD21	2.55	0.47
1:A:79:ARG:HH22	1:A:94:THR:CG2	2.27	0.47
1:A:217:LEU:HD21	1:A:368:LEU:CD2	2.40	0.47
4:F:267:PHE:CZ	4:F:271[B]:LEU:HD11	2.49	0.47
1:A:372[B]:GLN:HE21	1:A:373:ARG:HH12	1.61	0.47
4:F:277[B]:THR:HG22	4:F:278:THR:N	2.30	0.47
1:A:100:ALA:HA	2:B:254:LYS:HG3	1.96	0.47
1:A:163:LYS:O	1:A:164:LYS:HD3	2.15	0.47
1:C:165:SER:HA	1:C:199:ASP:OD2	2.14	0.47
4:F:193:GLU:OE1	4:F:194:PRO:HA	2.15	0.47
2:B:371:LEU:C	2:B:373:MET:H	2.23	0.47
1:A:293:ASN:O	1:A:339:ARG:NH2	2.48	0.47
2:B:220:THR:HG23	2:B:221:THR:N	2.29	0.47
1:C:305:CYS:O	1:C:307:PRO:HD3	2.15	0.47
2:D:31:ASP:OD2	2:D:35:SER:HB2	2.15	0.47
3:E:44:ASP:HB2	3:E:45:PRO:CD	2.45	0.47
4:F:129:GLU:CD	4:F:129:GLU:H	2.22	0.47
1:A:153:LEU:O	1:A:157:LEU:HG	2.14	0.46
2:B:199:ASP:C	2:B:200:GLU:HG3	2.40	0.46
4:F:206:LEU:HD21	4:F:353[B]:VAL:HG13	1.96	0.46
1:A:66[B]:VAL:HG23	1:A:125:LEU:HD12	1.98	0.46
2:B:298:SER:C	2:B:300:ASN:H	2.23	0.46
2:B:324:SER:C	2:B:326:LYS:H	2.23	0.46
1:C:7:ILE:HG21	1:C:153:LEU:HD21	1.97	0.46
1:C:120[A]:ASP:OD2	1:C:124:LYS:HE3	2.15	0.46
1:C:151:SER:HA	1:C:194[B]:THR:HG22	1.97	0.46
3:E:139:LEU:HD22	3:E:139:LEU:N	2.29	0.46
4:F:279:LEU:O	4:F:284[B]:LEU:HD23	2.15	0.46
2:D:25:SER:CB	2:D:30:ILE:HD11	2.44	0.46
1:A:97:GLU:HG3	2:B:2:ARG:CZ	2.45	0.46
2:B:28:HIS:ND1	2:B:49:ILE:HD12	2.30	0.46
2:B:133:GLN:OE1	2:B:251:ASP:HB2	2.15	0.46
2:D:323:MET:HB3	2:D:373:MET:HE1	1.97	0.46
2:D:416:MET:HA	2:D:419:THR:HG22	1.97	0.46
3:E:46:SER:O	3:E:50:ILE:HG13	2.15	0.46
1:A:328:VAL:O	1:A:332:ILE:HG13	2.14	0.46
1:A:161:TYR:HB3	1:A:164:LYS:CG	2.46	0.46
2:D:8:GLN:HE21	2:D:67:LEU:CG	2.24	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:21:TRP:O	2:D:25:SER:OG	2.20	0.46
2:B:157:ILE:HG21	2:B:166:MET:HE1	1.98	0.46
2:D:323:MET:HE2	2:D:373:MET:CE	2.42	0.46
2:D:18:ALA:O	2:D:22:GLU:HG3	2.16	0.46
4:F:13:VAL:HG13	4:F:14:TYR:HD1	1.81	0.46
4:F:17:VAL:O	4:F:21:LEU:HG	2.16	0.46
4:F:267:PHE:CE2	4:F:271[B]:LEU:HD11	2.50	0.46
4:F:277[A]:THR:HG22	4:F:278:THR:H	1.81	0.46
2:B:106:GLY:O	2:B:111:GLY:HA3	2.16	0.46
2:D:331:GLN:O	2:D:335:VAL:HG13	2.16	0.45
1:A:71:GLU:OE1	1:A:73:THR:HB	2.15	0.45
1:A:295:CYS:HB3	1:A:377:MET:HE2	1.98	0.45
1:A:355:ILE:O	3:E:17:GLY:HA3	2.16	0.45
2:D:1:MET:CG	2:D:50:ASN:HB2	2.40	0.45
2:D:292:THR:HG22	2:D:335:VAL:HG11	1.99	0.45
4:F:219:GLY:HA3	4:F:264:PHE:CZ	2.51	0.45
1:A:136[A]:LEU:HD11	1:A:252:LEU:HD21	1.97	0.45
2:B:82:PRO:O	2:B:83:PHE:HB2	2.17	0.45
2:B:339:ASN:O	2:B:341:SER:N	2.49	0.45
2:D:47:GLU:HG2	2:D:245:PRO:HG3	1.97	0.45
4:F:100:ILE:HG21	4:F:128:ARG:HG3	1.99	0.45
3:E:134:ARG:C	3:E:136:ASN:H	2.24	0.45
4:F:4:PHE:CZ	4:F:29:ARG:HB2	2.51	0.45
4:F:277[B]:THR:HG22	4:F:278:THR:H	1.81	0.45
2:B:21:TRP:CZ3	2:B:63:PRO:HB3	2.52	0.45
2:D:25:SER:HB3	2:D:30:ILE:CD1	2.47	0.45
1:A:105:ARG:HG2	1:A:110:ILE:HD13	1.99	0.45
2:B:123:ARG:O	2:B:127:GLU:HG3	2.15	0.45
2:B:204:ILE:HG22	2:B:302:MET:HB2	1.99	0.45
2:D:67:LEU:HD12	2:D:67:LEU:N	2.32	0.45
2:B:306:ASP:HB3	2:B:309:HIS:CE1	2.51	0.45
2:D:141:LEU:HD12	2:D:172:MET:SD	2.57	0.45
2:B:101:ASN:OD1	1:C:254:GLU:HG3	2.16	0.45
2:B:112:ALA:O	2:B:115:VAL:HG12	2.17	0.45
2:B:208:ALA:O	2:B:212:ILE:HD13	2.17	0.45
2:B:274:PRO:HA	2:B:294:GLN:OE1	2.17	0.45
4:F:277[A]:THR:HG22	4:F:278:THR:N	2.31	0.45
1:A:285:GLN:HG2	1:A:372[B]:GLN:CD	2.42	0.44
2:B:137:LEU:HB3	2:B:168[A]:THR:HG22	1.97	0.44
2:B:28:HIS:HD1	2:B:49:ILE:HD12	1.82	0.44
2:D:221:THR:O	2:D:221:THR:OG1	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:6:HIS:CD2	2:D:21:TRP:HE1	2.35	0.44
2:B:158:ARG:HD2	9:B:502:MES:H32	1.99	0.44
1:C:188:ILE:HG13	1:C:425:MET:HG3	2.00	0.44
2:B:231:VAL:O	2:B:235:MET:HG3	2.18	0.44
2:D:93:VAL:CG1	2:D:114:LEU:HD11	2.45	0.44
2:D:112:ALA:O	2:D:115:VAL:HG12	2.18	0.44
2:D:141:LEU:HD11	2:D:170:SER:HB3	1.99	0.44
4:F:206:LEU:CD2	4:F:353[B]:VAL:HG13	2.47	0.44
1:A:252:LEU:O	1:A:255:PHE:HB2	2.17	0.44
4:F:221:LEU:HB2	4:F:262:MET:HB3	1.99	0.44
4:F:358:VAL:HG13	4:F:359:PHE:CD2	2.53	0.44
2:B:115:VAL:HG13	2:B:116:ASP:N	2.33	0.44
2:B:146:GLY:O	2:B:150:GLY:HA3	2.18	0.44
2:D:150:GLY:O	2:D:154:ILE:HG13	2.18	0.44
1:A:28:HIS:O	1:A:36:MET:HE3	2.17	0.44
2:B:334:ASN:O	2:B:338:LYS:HB2	2.17	0.44
2:B:360:PRO:HG2	2:B:371:LEU:HB2	2.00	0.44
4:F:206:LEU:HD23	4:F:353[B]:VAL:CG1	2.48	0.44
2:B:7:ILE:O	2:B:137:LEU:HD12	2.17	0.43
1:C:71:GLU:HG2	1:C:72:PRO:N	2.32	0.43
1:A:22:GLU:HG3	1:A:83:TYR:CE1	2.53	0.43
1:A:83:TYR:HB3	1:A:86:LEU:HD22	1.99	0.43
1:A:3:GLU:O	1:A:133:GLN:HG3	2.18	0.43
2:D:215:ARG:HG2	2:D:215:ARG:HH11	1.83	0.43
2:D:303:ALA:O	2:D:305:CYS:N	2.51	0.43
2:D:403:ALA:HB1	2:D:404:PHE:CD2	2.53	0.43
4:F:71:LEU:O	4:F:332:VAL:HB	2.19	0.43
2:D:146:GLY:N	8:D:501:GDP:O2B	2.43	0.43
2:D:178:SER:HB2	8:D:501:GDP:O2'	2.18	0.43
4:F:169:LEU:HD21	4:F:182:ILE:HD12	2.01	0.43
2:B:48:ARG:NH1	2:B:245:PRO:HA	2.33	0.43
4:F:191:LEU:HD22	4:F:196:HIS:CE1	2.54	0.43
1:A:7:ILE:HG23	1:A:66[A]:VAL:HG13	2.00	0.43
1:A:161:TYR:HB3	1:A:164:LYS:HG2	2.01	0.43
2:B:28:HIS:HB3	2:B:49:ILE:HD12	1.98	0.43
1:C:276:ILE:HD11	1:C:371:VAL:HG13	2.01	0.43
1:C:276:ILE:HG22	1:C:280:LYS:HD3	2.00	0.43
2:D:385:GLN:HB2	2:D:429:VAL:HG13	1.99	0.43
4:F:55:GLU:HA	4:F:56:PRO:HD3	1.90	0.43
1:A:115:ILE:O	1:A:119:LEU:HG	2.19	0.43
1:A:163:LYS:C	1:A:164:LYS:HD3	2.44	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:38:GLY:HA3	2:B:45:GLN:OE1	2.18	0.43
4:F:347:CYS:HA	4:F:350:ILE:HD12	2.01	0.43
1:A:233:GLN:NE2	1:A:361:THR:O	2.47	0.43
2:B:295:MET:HE1	2:B:317:ALA:HB1	2.00	0.43
2:D:287:THR:HB	2:D:289:PRO:HD2	2.00	0.43
1:C:274:PRO:HG2	1:C:371:VAL:HG11	2.00	0.42
2:D:101:ASN:HD22	2:D:180:THR:HG21	1.84	0.42
4:F:94:PHE:HA	4:F:95:PRO:HD3	1.89	0.42
1:A:329:ASN:HD21	3:E:8:VAL:HG21	1.83	0.42
1:A:352:LYS:HE3	3:E:21:GLU:OE1	2.19	0.42
2:B:22:GLU:HG3	2:B:83:PHE:CD1	2.54	0.42
4:F:37:PHE:CZ	4:F:40:MET:HE3	2.54	0.42
2:B:1:MET:CB	2:B:2:ARG:HA	2.48	0.42
1:C:317:LEU:C	1:C:318:LEU:HD12	2.43	0.42
2:D:21:TRP:CZ3	2:D:63:PRO:HB3	2.54	0.42
2:D:153:LEU:O	2:D:157:ILE:HG13	2.19	0.42
4:F:217:ARG:NH2	4:F:374:ILE:HG22	2.34	0.42
1:A:90:GLU:O	1:A:121:ARG:HD2	2.18	0.42
1:C:265:ILE:HG23	1:C:432:TYR:CE1	2.54	0.42
2:D:295:MET:CG	2:D:377:PHE:HB2	2.49	0.42
4:F:341:LYS:H	4:F:341:LYS:HG2	1.55	0.42
1:A:406:HIS:CE1	2:B:263:PRO:HD3	2.54	0.42
2:B:31:ASP:OD1	2:B:35:SER:N	2.48	0.42
2:D:291:LEU:HD22	2:D:375:ALA:HB3	2.02	0.42
1:A:83:TYR:O	1:A:86:LEU:HB2	2.19	0.42
2:D:107:HIS:O	2:D:152:LEU:HD22	2.20	0.42
2:D:271:GLY:N	2:D:377:PHE:O	2.53	0.42
3:E:92:ASN:O	3:E:96:MET:HG3	2.19	0.42
4:F:70:LYS:O	4:F:76:SER:HB3	2.19	0.42
1:A:419:SER:O	1:A:423:GLU:HG3	2.19	0.42
1:C:295[B]:CYS:SG	1:C:375:VAL:HG13	2.59	0.42
2:D:1:MET:HG3	2:D:2:ARG:N	2.35	0.42
2:D:9:ALA:HA	2:D:68:VAL:O	2.19	0.42
2:D:209:LEU:CB	2:D:227:LEU:HD22	2.49	0.42
1:A:121:ARG:HD3	1:A:121:ARG:HA	1.87	0.42
4:F:191:LEU:N	4:F:191:LEU:HD12	2.34	0.42
4:F:267:PHE:CZ	4:F:271[A]:LEU:HD11	2.55	0.42
2:B:3:GLU:HB3	2:B:64:ARG:NH1	2.35	0.41
4:F:296:MET:SD	4:F:380:HIS:HB2	2.60	0.41
4:F:307:LEU:HD23	4:F:307:LEU:HA	1.83	0.41
1:A:336:LYS:HA	1:A:336:LYS:HD2	1.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:398:MET:HE2	2:B:398:MET:HB3	1.94	0.41
2:D:118:VAL:HG11	2:D:153:LEU:HD11	2.01	0.41
4:F:21:LEU:O	4:F:27:TRP:HB2	2.20	0.41
1:A:217:LEU:HD11	1:A:368:LEU:HD21	2.01	0.41
2:B:7:ILE:O	2:B:137:LEU:HA	2.20	0.41
2:B:297:ASP:OD1	2:B:298:SER:N	2.53	0.41
2:D:369:ARG:HA	2:D:370:GLY:HA2	1.61	0.41
1:C:413:MET:HE2	1:C:413:MET:HB3	1.90	0.41
3:E:136:ASN:O	3:E:140:LYS:HB2	2.20	0.41
2:D:115:VAL:HG21	2:D:152:LEU:HG	2.02	0.41
2:D:335:VAL:O	2:D:339:ASN:HB2	2.19	0.41
4:F:49:PHE:HA	4:F:52:LEU:HD13	2.01	0.41
1:C:209:ILE:HD11	1:C:302:MET:SD	2.61	0.41
1:C:211:ASP:OD2	1:C:304:LYS:HE3	2.20	0.41
2:D:295:MET:HG3	2:D:377:PHE:HB2	2.01	0.41
4:F:346:LEU:O	4:F:350:ILE:HG13	2.19	0.41
1:A:344:VAL:CG2	1:A:347:CYS:HB2	2.47	0.41
2:B:180:THR:HG22	2:B:182:VAL:H	1.85	0.41
2:B:296:PHE:CD2	2:B:335:VAL:HG11	2.56	0.41
2:D:312:TYR:CE1	2:D:377:PHE:HZ	2.38	0.41
4:F:6:VAL:HG22	4:F:29:ARG:NH2	2.35	0.41
4:F:137:ARG:C	4:F:137:ARG:HD2	2.45	0.41
2:D:274:PRO:HB3	2:D:286:LEU:HD11	2.01	0.41
4:F:299:GLU:N	4:F:300:PRO:CD	2.84	0.41
4:F:341:LYS:HE3	4:F:341:LYS:HB3	1.93	0.41
1:A:305:CYS:O	1:A:307:PRO:HD3	2.21	0.41
2:B:385:GLN:HG3	2:B:386:GLU:N	2.35	0.41
2:B:395:PHE:CE1	2:B:422:GLU:HB2	2.56	0.41
1:C:164:LYS:HE2	1:C:164:LYS:HB2	1.94	0.41
2:D:146:GLY:O	2:D:150:GLY:HA3	2.21	0.41
3:E:80:ARG:O	3:E:84:GLN:HB2	2.21	0.41
4:F:205:VAL:HG21	4:F:291:ILE:HD12	2.02	0.41
4:F:206:LEU:HD23	4:F:353[B]:VAL:HG11	2.02	0.41
1:A:96:LYS:O	2:B:1:MET:HE1	2.21	0.41
2:B:401:ARG:HD3	1:C:346:TRP:CD2	2.56	0.41
1:A:79:ARG:HH22	1:A:94:THR:HG21	1.85	0.40
2:B:1:MET:HB2	2:B:2:ARG:HA	2.03	0.40
1:C:253:THR:HG23	1:C:254:GLU:N	2.34	0.40
1:C:325:PRO:HA	10:C:503:71E:FAQ	2.11	0.40
2:D:413:MET:HE2	2:D:413:MET:HB3	1.89	0.40
1:C:250:VAL:HG13	1:C:254:GLU:OE1	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:30:ILE:HD12	2:D:30:ILE:O	2.21	0.40
2:D:183:GLU:HB2	2:D:184:PRO:HD3	2.03	0.40
2:D:408:TYR:O	2:D:413:MET:HB2	2.21	0.40
4:F:206:LEU:CD2	4:F:353[B]:VAL:CG1	3.00	0.40
2:B:371:LEU:O	2:B:372:LYS:HB2	2.21	0.40
2:D:39:ASP:N	2:D:45:GLN:OE1	2.55	0.40
2:D:194:LEU:HD22	2:D:198:THR:HG21	2.03	0.40
2:D:212:ILE:O	2:D:216:THR:HB	2.21	0.40
4:F:263:PHE:CE2	4:F:341:LYS:HG3	2.56	0.40
4:F:307:LEU:HD22	4:F:308:HIS:CE1	2.57	0.40
1:A:88:HIS:HB2	1:A:89:PRO:HD2	2.03	0.40
1:A:223:THR:CG2	1:A:224:TYR:N	2.84	0.40
1:A:395:PHE:C	1:A:395:PHE:CD1	2.99	0.40
1:C:440:VAL:O	1:C:440:VAL:HG12	2.22	0.40
4:F:135:TYR:CE1	4:F:145:ASN:HB3	2.56	0.40
4:F:317:PHE:HB3	4:F:319:PHE:CE2	2.57	0.40
1:A:10:GLY:O	1:A:14:VAL:HG23	2.22	0.40
1:A:217:LEU:CD2	1:A:368:LEU:HD23	2.46	0.40
1:C:328:VAL:HG11	1:C:353:VAL:HG11	2.03	0.40
2:D:99:ALA:O	2:D:102:ASN:HB3	2.22	0.40
4:F:4:PHE:HA	4:F:39:LEU:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	441/451 (98%)	422 (96%)	19 (4%)	0	100	100
1	C	440/451 (98%)	424 (96%)	16 (4%)	0	100	100
2	B	415/445 (93%)	398 (96%)	17 (4%)	0	100	100
2	D	420/445 (94%)	399 (95%)	20 (5%)	1 (0%)	43	58

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	E	112/143 (78%)	110 (98%)	2 (2%)	0	100	100
4	F	285/384 (74%)	267 (94%)	18 (6%)	0	100	100
All	All	2113/2319 (91%)	2020 (96%)	92 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	401	ARG

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	374/379 (99%)	369 (99%)	5 (1%)	61	80
1	C	375/379 (99%)	367 (98%)	8 (2%)	47	69
2	B	363/383 (95%)	354 (98%)	9 (2%)	42	64
2	D	367/383 (96%)	353 (96%)	14 (4%)	29	49
3	E	105/127 (83%)	104 (99%)	1 (1%)	68	84
4	F	272/342 (80%)	261 (96%)	11 (4%)	28	47
All	All	1856/1993 (93%)	1808 (97%)	48 (3%)	40	63

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	94	THR
1	A	253	THR
1	A	286	LEU
1	A	313	MET
1	A	381	THR
2	B	16	ILE
2	B	77	SER
2	B	172	MET
2	B	190	SER

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Mol	Chain	Res	Type
2	B	238	VAL
2	B	300	ASN
2	B	385	GLN
2	B	387	LEU
2	B	430	SER
1	C	68[A]	VAL
1	C	68[B]	VAL
1	C	71	GLU
1	C	257	THR
1	C	271	THR
1	C	276	ILE
1	C	326	LYS
1	C	339	ARG
2	D	40	SER
2	D	62	VAL
2	D	67	LEU
2	D	133	GLN
2	D	168	THR
2	D	181	VAL
2	D	190	SER
2	D	201	THR
2	D	286	LEU
2	D	291	LEU
2	D	325	MET
2	D	331	GLN
2	D	402	LYS
2	D	424	ASN
3	E	116	LEU
4	F	6	VAL
4	F	13	VAL
4	F	28	LYS
4	F	125	THR
4	F	171	ASP
4	F	196	HIS
4	F	257	GLU
4	F	307	LEU
4	F	331	GLU
4	F	341	LYS
4	F	343	TYR

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

Mol	Chain	Res	Type
1	A	11	GLN
1	A	31	GLN
1	A	35	GLN
1	A	50	ASN
1	A	300	ASN
1	A	329	ASN
1	A	393	HIS
2	B	6	HIS
2	B	15	GLN
2	B	136	GLN
2	B	193	GLN
2	B	249	ASN
2	B	349	ASN
2	B	424	ASN
2	B	433	GLN
1	C	15	GLN
1	C	88	HIS
1	C	233	GLN
1	C	285	GLN
1	C	300	ASN
1	C	393	HIS
2	D	8	GLN
2	D	101	ASN
2	D	192	HIS
2	D	197	ASN
2	D	247	GLN
2	D	331	GLN
2	D	339	ASN
2	D	424	ASN
4	F	26	GLN
4	F	333	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 4 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
9	MES	B	502	-	12,12,12	2.40	1 (8%)	15,16,16	1.29	1 (6%)
11	ACP	F	401	-	31,33,33	2.14	11 (35%)	47,52,52	1.84	10 (21%)
8	GDP	D	501	-	29,30,30	1.18	3 (10%)	45,47,47	1.71	6 (13%)
5	GTP	C	501	6	33,34,34	0.93	1 (3%)	50,54,54	1.50	9 (18%)
10	71E	C	503	-	49,53,53	3.07	22 (44%)	64,83,83	2.30	24 (37%)
5	GTP	A	501	6	33,34,34	0.96	1 (3%)	50,54,54	1.61	9 (18%)
8	GDP	B	501	-	29,30,30	1.14	2 (6%)	45,47,47	1.69	7 (15%)

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
9	MES	B	502	-	-	5/6/14/14	0/1/1/1
11	ACP	F	401	-	-	7/19/38/38	0/3/3/3
8	GDP	D	501	-	-	2/16/32/32	0/3/3/3
5	GTP	C	501	6	-	7/22/38/38	0/3/3/3
10	71E	C	503	-	-	7/43/72/72	0/6/7/7
5	GTP	A	501	6	-	8/22/38/38	0/3/3/3
8	GDP	B	501	-	-	5/16/32/32	0/3/3/3

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	502	MES	C8-S	-8.03	1.66	1.77
10	C	503	71E	CD1-CAF	7.03	1.49	1.39
10	C	503	71E	CAP-CAL	6.74	1.49	1.39
10	C	503	71E	CBC-CBH	6.19	1.53	1.45
10	C	503	71E	C-NAV	5.60	1.46	1.34
11	F	401	ACP	PG-O1G	5.52	1.61	1.50
10	C	503	71E	CAE-CAF	-5.41	1.31	1.38
10	C	503	71E	CAM-CAK	5.32	1.48	1.39
10	C	503	71E	CAZ-NBD	5.30	1.38	1.29
10	C	503	71E	CBO-N	5.29	1.45	1.34
10	C	503	71E	CAD-CAE	5.02	1.49	1.39
11	F	401	ACP	C5-C4	4.80	1.47	1.39
10	C	503	71E	CAN-CAO	4.77	1.46	1.37
11	F	401	ACP	PB-O1B	4.24	1.61	1.51
10	C	503	71E	CBM-CBK	4.08	1.53	1.50
10	C	503	71E	CAK-NAJ	4.03	1.46	1.39
10	C	503	71E	CD2-CG	3.74	1.46	1.38
10	C	503	71E	CAP-CAO	3.47	1.43	1.37
10	C	503	71E	CAK-CAL	-3.38	1.35	1.39
11	F	401	ACP	PB-O2B	-3.25	1.48	1.56
8	B	501	GDP	C5-C4	3.16	1.47	1.38
8	D	501	GDP	C5-C4	3.15	1.47	1.38
11	F	401	ACP	PB-O3A	2.99	1.61	1.58
11	F	401	ACP	PG-O2G	-2.96	1.48	1.55
10	C	503	71E	CAD-CD2	2.95	1.43	1.38
11	F	401	ACP	PG-O3G	2.92	1.61	1.55
11	F	401	ACP	C5-C6	2.86	1.48	1.41
10	C	503	71E	CAI-CAF	2.70	1.55	1.52
10	C	503	71E	CBH-NBL	2.69	1.37	1.30
8	B	501	GDP	C6-N1	-2.51	1.34	1.38
11	F	401	ACP	C8-N7	2.40	1.36	1.31
8	D	501	GDP	C6-N1	-2.37	1.34	1.38
10	C	503	71E	OAG-CAE	2.28	1.41	1.37
10	C	503	71E	CAN-CAM	2.23	1.42	1.38
10	C	503	71E	CBJ-CBK	2.22	1.39	1.34
11	F	401	ACP	C5-N7	-2.21	1.35	1.39
10	C	503	71E	OBI-CBH	2.20	1.39	1.35
5	C	501	GTP	C2-N3	2.12	1.38	1.33
8	D	501	GDP	C5-N7	-2.11	1.34	1.39
11	F	401	ACP	PA-O3A	2.05	1.61	1.59
5	A	501	GTP	PB-O3B	2.01	1.61	1.59

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	C	503	71E	OBA-CAZ-NBD	-6.82	106.97	114.14
10	C	503	71E	CAZ-OBA-CBB	6.54	111.81	105.11
8	D	501	GDP	C5-C4-N3	-6.12	118.66	128.39
11	F	401	ACP	C5-C4-N3	-6.04	118.39	126.72
8	B	501	GDP	C5-C4-N3	-5.66	119.39	128.39
5	A	501	GTP	C2-N3-C4	4.99	120.89	112.30
5	A	501	GTP	C5-C4-N3	-4.95	120.50	128.39
8	B	501	GDP	C2-N3-C4	4.93	120.79	112.30
8	D	501	GDP	C2-N3-C4	4.88	120.71	112.30
10	C	503	71E	OBI-CBH-NBL	-4.75	108.43	114.12
11	F	401	ACP	N3-C4-N9	4.67	135.12	127.17
8	D	501	GDP	N9-C4-N3	4.65	135.25	125.95
5	C	501	GTP	C5-C4-N3	-4.48	121.26	128.39
10	C	503	71E	CG-CB-CA	-4.41	101.63	113.36
10	C	503	71E	CAF-CAI-CBB	-4.34	99.98	111.01
10	C	503	71E	CAL-CAI-CAF	4.21	121.55	112.48
5	C	501	GTP	C2-N3-C4	4.19	119.51	112.30
8	B	501	GDP	N9-C4-N3	4.14	134.22	125.95
10	C	503	71E	CBC-NBD-CAZ	4.04	107.87	104.35
11	F	401	ACP	C2-N3-C4	3.73	120.95	111.83
11	F	401	ACP	C4-C5-N7	-3.65	106.40	110.58
10	C	503	71E	CAD-CAE-CAF	-3.64	118.74	122.83
11	F	401	ACP	PB-O3A-PA	-3.60	120.61	132.37
8	B	501	GDP	C6-C5-N7	3.59	136.83	130.29
10	C	503	71E	CAX-CAZ-NBD	3.29	133.66	129.02
10	C	503	71E	CBP-CBO-N	3.21	120.57	116.22
10	C	503	71E	CBJ-OBI-CBH	3.18	107.24	104.33
11	F	401	ACP	N3-C2-N1	-3.09	123.90	128.58
10	C	503	71E	OAG-CAE-CAD	3.02	129.80	123.85
10	C	503	71E	CAZ-CAX-NAV	-3.02	103.94	108.54
8	D	501	GDP	C6-C5-N7	3.02	135.79	130.29
5	A	501	GTP	N9-C4-N3	3.00	131.96	125.95
5	C	501	GTP	N9-C4-N3	2.97	131.90	125.95
5	A	501	GTP	C2-N1-C6	-2.83	119.98	125.11
5	C	501	GTP	N9-C8-N7	-2.76	108.29	113.40
5	A	501	GTP	N9-C8-N7	-2.63	108.53	113.40
11	F	401	ACP	C5-N7-C8	2.62	107.57	103.45
8	B	501	GDP	C4-C5-N7	-2.61	106.53	110.67
10	C	503	71E	CA-C-NAV	2.58	122.12	116.63
5	C	501	GTP	C2-N1-C6	-2.50	120.58	125.11
5	A	501	GTP	C5-C6-N1	2.50	119.61	113.25
9	B	502	MES	C5-N4-C3	2.48	114.19	108.84
5	C	501	GTP	C8-N7-C5	2.46	108.64	104.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	D	501	GDP	C4-C5-N7	-2.45	106.78	110.67
5	A	501	GTP	C8-N7-C5	2.45	108.62	104.26
5	A	501	GTP	O6-C6-C5	-2.44	120.10	126.53
11	F	401	ACP	C4-N9-C8	2.41	108.27	105.74
10	C	503	71E	CAH-CAI-CBB	2.40	117.11	112.07
5	A	501	GTP	O2A-PA-O3A	2.39	113.73	107.27
10	C	503	71E	CB-CG-CD2	2.38	125.33	120.90
5	C	501	GTP	C5-C6-N1	2.34	119.20	113.25
10	C	503	71E	C-CA-N	-2.33	104.82	111.11
11	F	401	ACP	C3'-C2'-C1'	2.32	105.85	101.46
10	C	503	71E	O-C-NAV	-2.30	118.83	122.96
5	C	501	GTP	O6-C6-C5	-2.26	120.57	126.53
5	C	501	GTP	O2A-PA-O3A	2.26	113.37	107.27
10	C	503	71E	CBC-CBH-NBL	-2.22	122.18	128.16
10	C	503	71E	CAK-NAJ-CAH	-2.22	106.19	109.83
8	D	501	GDP	O6-C6-C5	-2.10	120.99	126.53
11	F	401	ACP	C6-C5-N7	2.10	136.13	132.09
10	C	503	71E	CB-CA-N	2.05	115.08	110.83
8	B	501	GDP	O6-C6-C5	-2.05	121.13	126.53
8	B	501	GDP	O2B-PB-O3A	2.04	111.48	104.64
10	C	503	71E	CBM-CBK-NBL	2.04	124.60	119.34
10	C	503	71E	OAG-CAE-CAF	-2.03	111.46	113.29
10	C	503	71E	CBE-CAY-CAX	-2.01	105.59	109.71

There are no chirality outliers.

All (41) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	501	GTP	PB-O3B-PG-O2G
5	A	501	GTP	C5'-O5'-PA-O3A
5	A	501	GTP	C5'-O5'-PA-O1A
5	A	501	GTP	C5'-O5'-PA-O2A
5	C	501	GTP	C5'-O5'-PA-O3A
5	C	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O2A
8	B	501	GDP	C5'-O5'-PA-O3A
8	B	501	GDP	C5'-O5'-PA-O1A
8	B	501	GDP	C5'-O5'-PA-O2A
9	B	502	MES	C7-C8-S-O2S
10	C	503	71E	CAY-CAX-CAZ-OBA
10	C	503	71E	N-CBO-CBP-OBS
10	C	503	71E	N-CBO-CBP-CBR

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Mol	Chain	Res	Type	Atoms
10	C	503	71E	OBQ-CBO-CBP-OBS
10	C	503	71E	OBQ-CBO-CBP-CBR
11	F	401	ACP	PG-C3B-PB-O1B
11	F	401	ACP	PG-C3B-PB-O2B
11	F	401	ACP	C5'-O5'-PA-O1A
11	F	401	ACP	O4'-C4'-C5'-O5'
11	F	401	ACP	C3'-C4'-C5'-O5'
9	B	502	MES	C7-C8-S-O3S
9	B	502	MES	C8-C7-N4-C3
9	B	502	MES	C7-C8-S-O1S
10	C	503	71E	NAV-CAX-CAZ-OBA
10	C	503	71E	NAV-CAX-CAZ-NBD
11	F	401	ACP	PG-C3B-PB-O3A
11	F	401	ACP	PB-O3A-PA-O2A
9	B	502	MES	C8-C7-N4-C5
8	B	501	GDP	PB-O3A-PA-O2A
5	C	501	GTP	C4'-C5'-O5'-PA
5	A	501	GTP	PB-O3B-PG-O1G
5	A	501	GTP	PB-O3B-PG-O3G
5	C	501	GTP	PB-O3B-PG-O2G
5	A	501	GTP	PB-O3A-PA-O1A
5	A	501	GTP	PB-O3A-PA-O2A
5	C	501	GTP	PB-O3A-PA-O1A
5	C	501	GTP	PB-O3A-PA-O2A
8	B	501	GDP	PB-O3A-PA-O1A
8	D	501	GDP	PB-O3A-PA-O1A
8	D	501	GDP	PB-O3A-PA-O2A

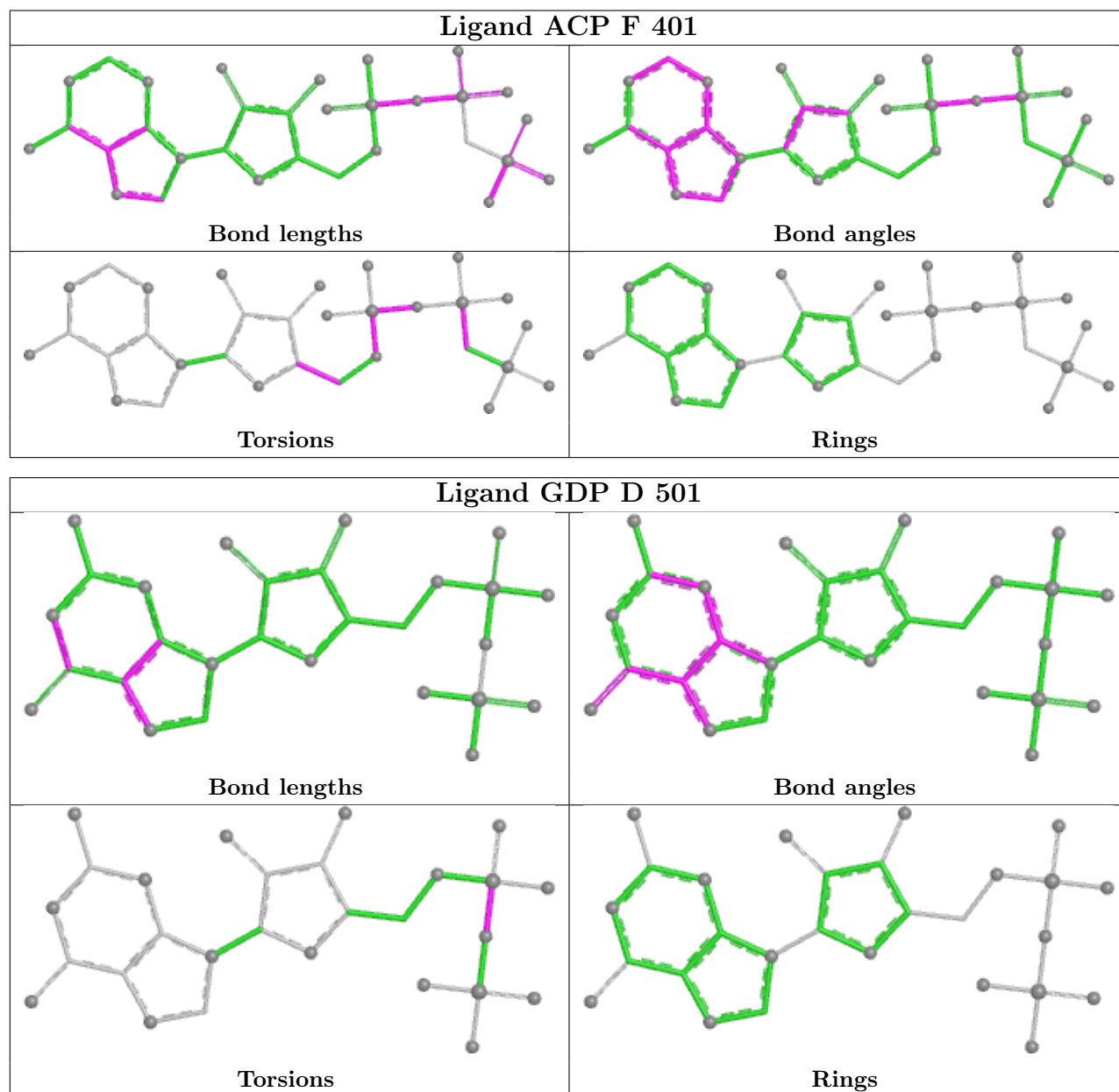
There are no ring outliers.

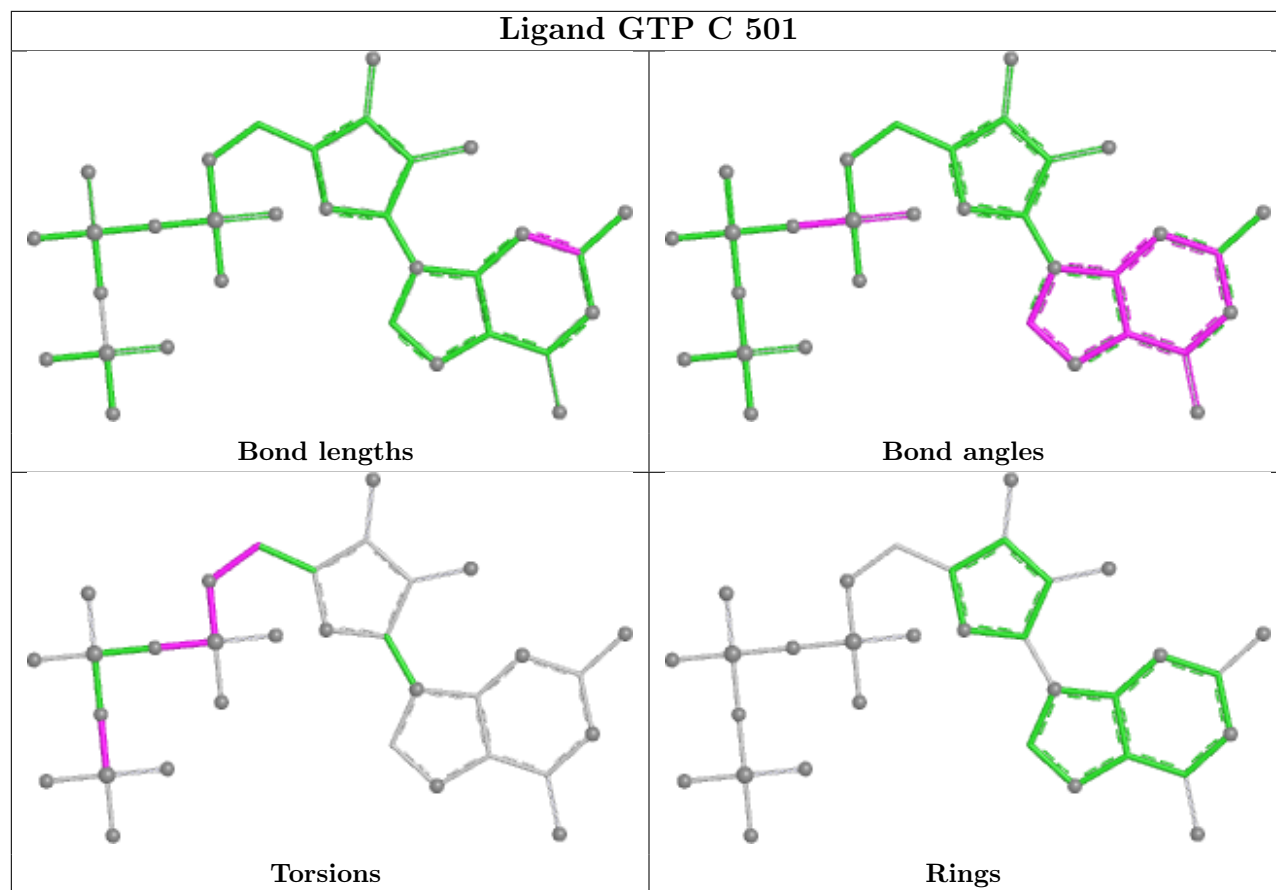
5 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	B	502	MES	1	0
11	F	401	ACP	1	0
8	D	501	GDP	5	0
5	C	501	GTP	1	0
10	C	503	71E	2	0

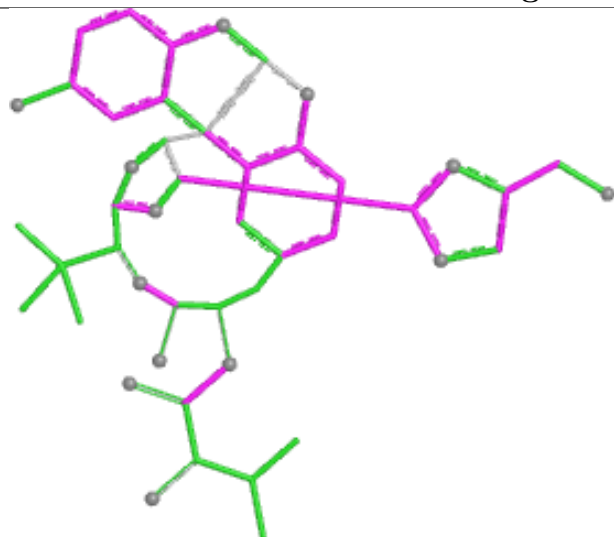
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

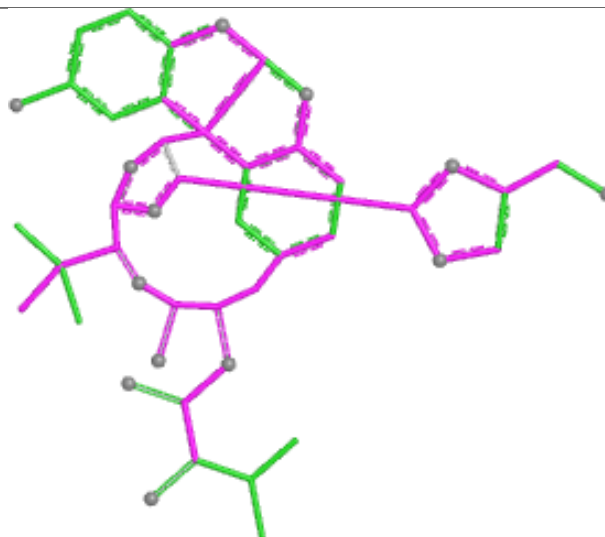




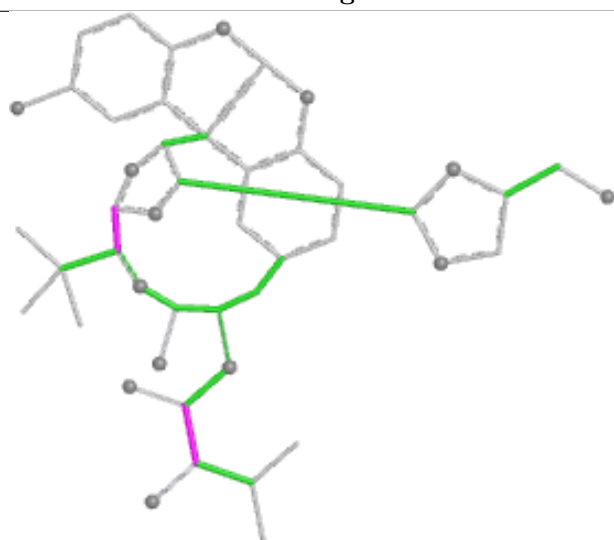
Ligand 71E C 503



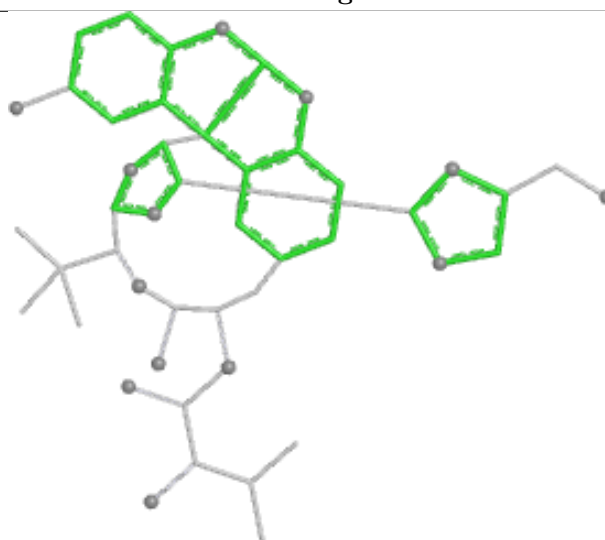
Bond lengths



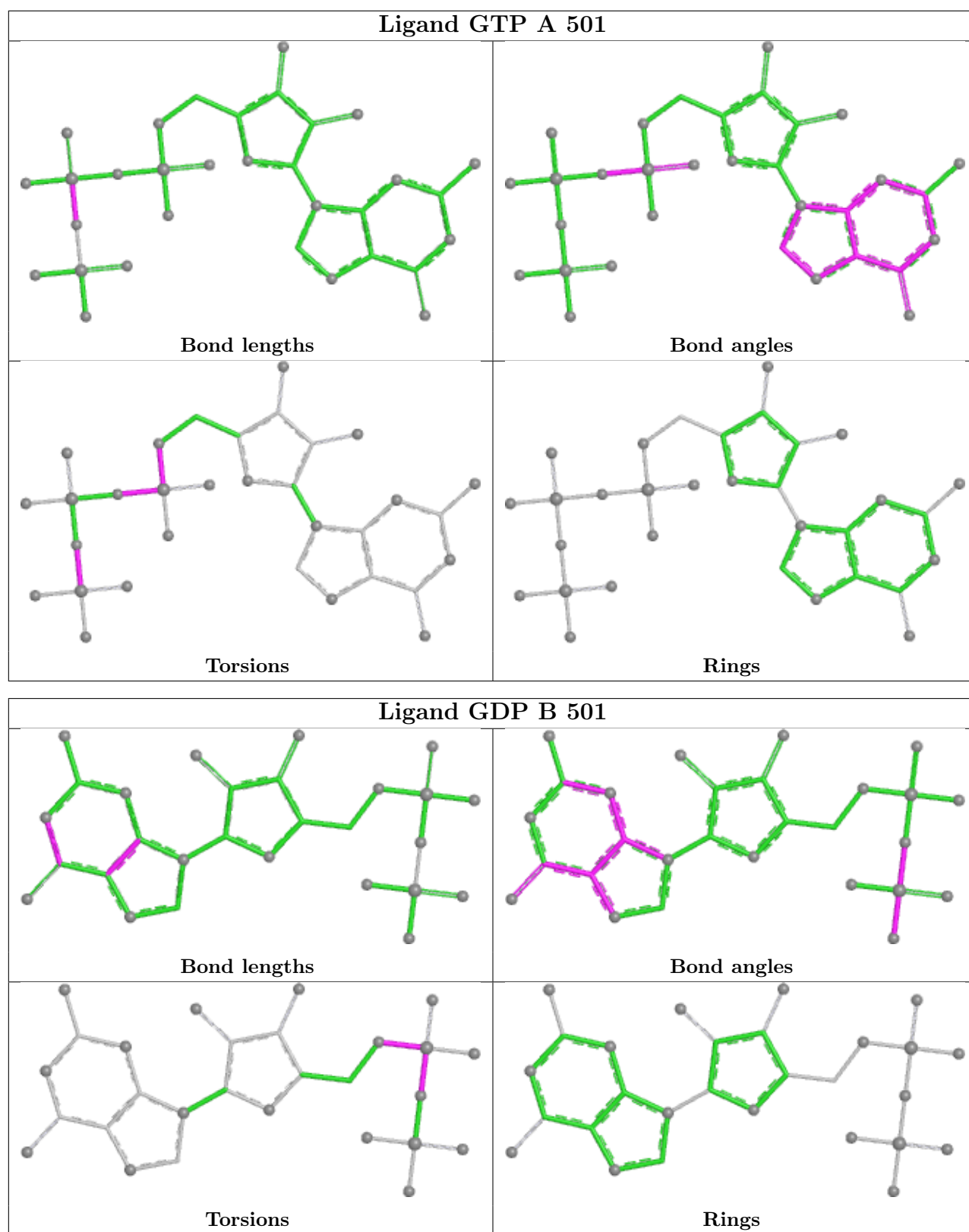
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	E	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	140:LYS	C	141:GLU	N	3.18

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	437/451 (96%)	0.04	4 (0%) 81 78	37, 74, 118, 168	6 (1%)
1	C	437/451 (96%)	-0.11	12 (2%) 56 52	33, 60, 93, 140	7 (1%)
2	B	417/445 (93%)	0.08	6 (1%) 73 69	35, 75, 133, 175	4 (0%)
2	D	422/445 (94%)	0.18	7 (1%) 69 65	47, 86, 128, 180	8 (1%)
3	E	117/143 (81%)	0.38	6 (5%) 33 30	62, 88, 129, 149	0
4	F	298/384 (77%)	0.41	10 (3%) 48 44	49, 104, 165, 195	5 (1%)
All	All	2128/2319 (91%)	0.11	45 (2%) 63 59	33, 79, 133, 195	30 (1%)

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	437	VAL	4.9
4	F	362	ALA	4.7
2	D	404	PHE	3.8
1	C	339	ARG	3.5
1	C	440	VAL	3.3
1	C	163	LYS	3.3
2	D	220	THR	3.3
4	F	125	THR	3.3
1	C	2	ARG	3.2
3	E	126	LYS	3.2
2	B	276	THR	3.1
4	F	102	PRO	3.0
1	C	365	GLY	2.9
4	F	149	ALA	2.8
2	D	246	GLY	2.7
4	F	162	ILE	2.7
4	F	170	LEU	2.7
1	A	75	ILE	2.6
2	B	117	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	255	PHE	2.6
2	D	276	THR	2.6
1	C	253	THR	2.5
4	F	372	THR	2.5
2	D	82	PRO	2.4
1	C	210	TYR	2.4
3	E	140	LYS	2.3
3	E	26	PRO	2.3
1	A	78	VAL	2.3
2	B	51	VAL	2.2
2	B	324	SER	2.2
4	F	319	PHE	2.2
2	D	122	VAL	2.2
4	F	181	VAL	2.2
1	A	163	LYS	2.2
1	C	128	GLN	2.2
1	C	283	HIS	2.1
1	C	357	TYR	2.1
3	E	22	VAL	2.1
1	C	250	VAL	2.1
2	D	407	TRP	2.0
3	E	44	ASP	2.0
3	E	47	LEU	2.0
2	B	156	LYS	2.0
2	B	1	MET	2.0
4	F	227	PRO	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

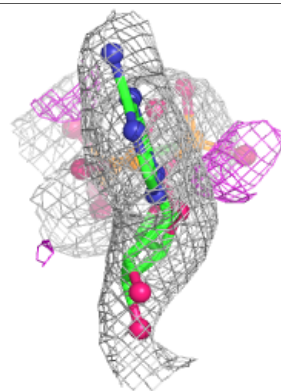
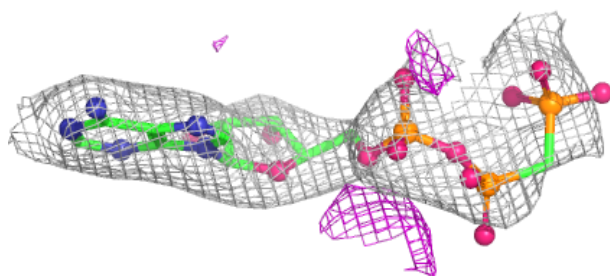
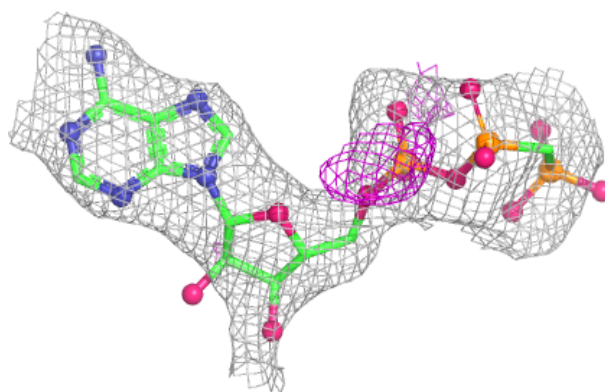
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
11	ACP	F	401	31/31	0.72	0.11	124,139,219,237	0
6	MG	B	503	1/1	0.78	0.19	84,84,84,84	0
9	MES	B	502	12/12	0.89	0.10	53,83,117,122	0
8	GDP	D	501	28/28	0.90	0.10	72,77,114,144	0
10	71E	C	503	47/47	0.95	0.07	36,58,79,91	0
6	MG	A	502	1/1	0.97	0.06	82,82,82,82	0
5	GTP	A	501	32/32	0.97	0.06	48,57,70,81	0
6	MG	C	502	1/1	0.97	0.09	47,47,47,47	0
7	CA	A	503	1/1	0.97	0.07	102,102,102,102	0
5	GTP	C	501	32/32	0.98	0.06	38,48,59,66	0
8	GDP	B	501	28/28	0.98	0.05	47,54,64,68	0

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

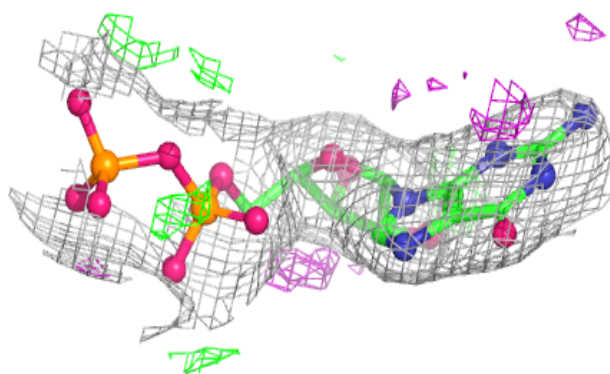
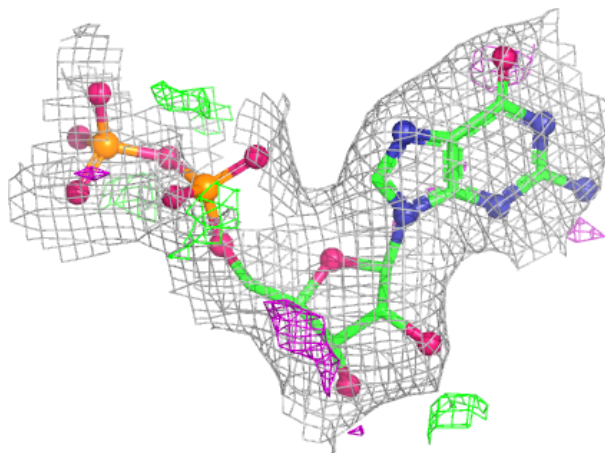
Electron density around ACP F 401:

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



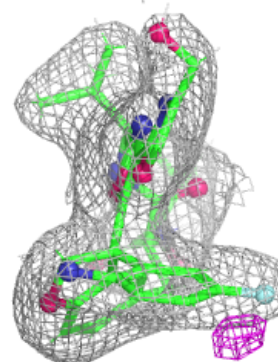
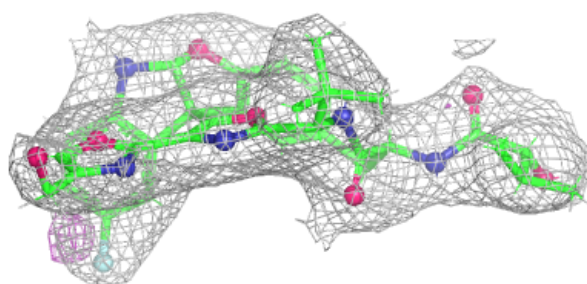
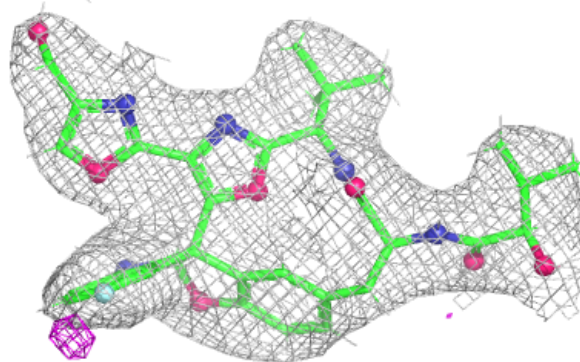
Electron density around GDP D 501:

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

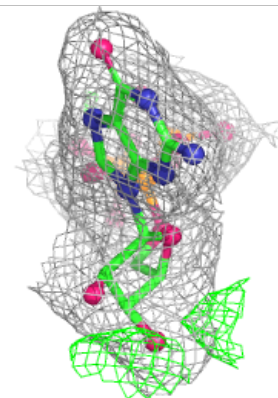
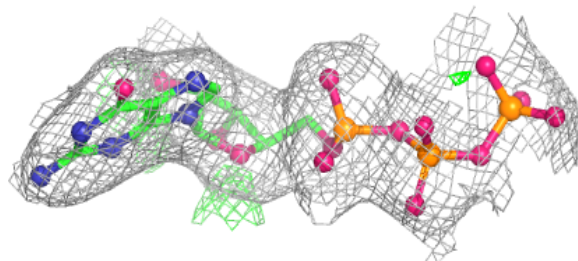
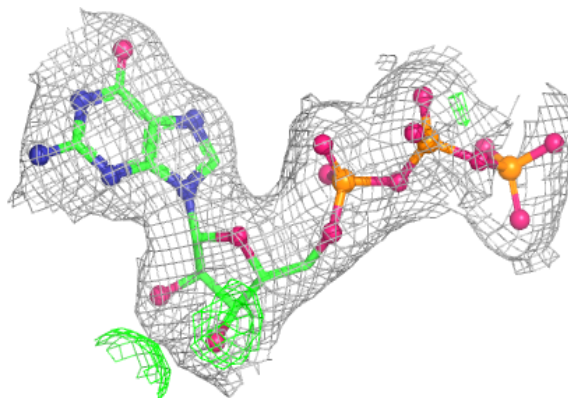


Electron density around 71E C 503:

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

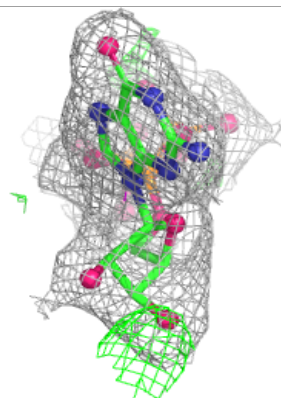
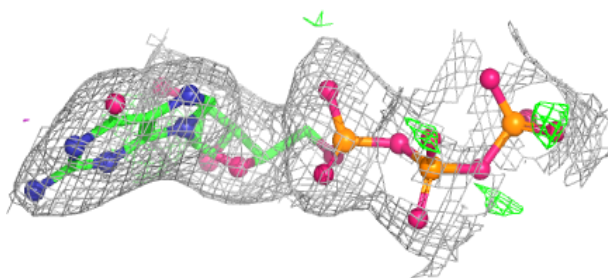
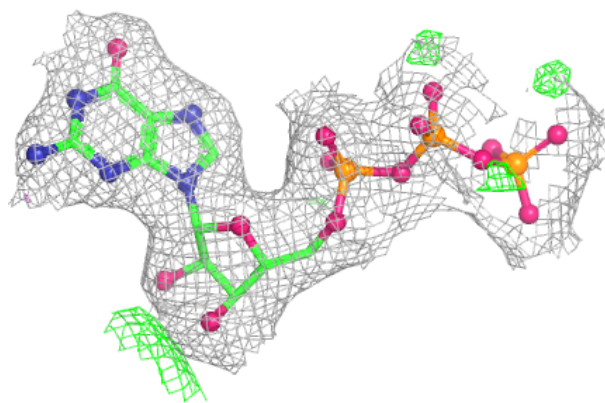
**Electron density around GTP A 501:**

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



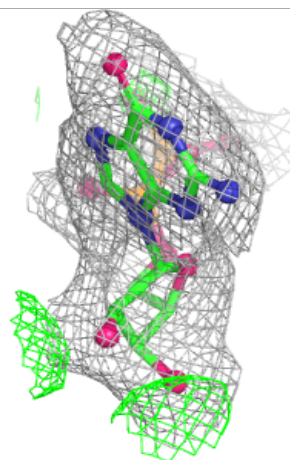
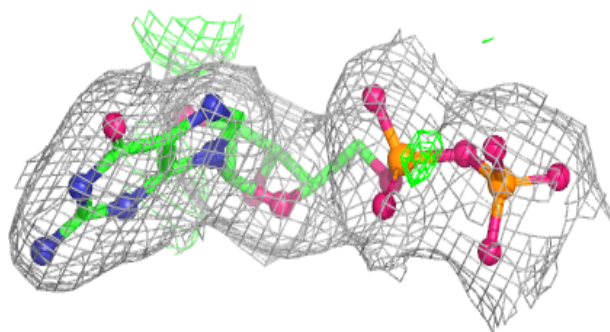
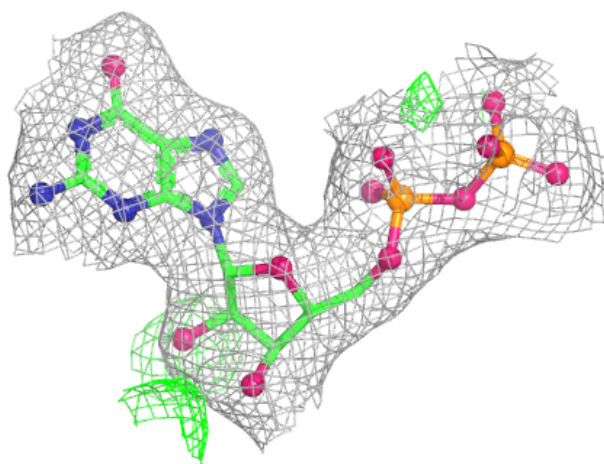
Electron density around GTP C 501:

$2mF_o-DF_c$ (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)



6.5 Other polymers [i](#)

There are no such residues in this entry.