



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 21, 2021 – 02:13 PM EDT

PDB ID : 5S4S
Title : Tubulin-Z240297434-complex
Authors : Muehlethaler, T.; Gioia, D.; Protá, A.E.; Sharpe, M.E.; Cavalli, A.; Steinmetz, M.O.
Deposited on : 2020-11-08
Resolution : 2.35 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.20
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.20

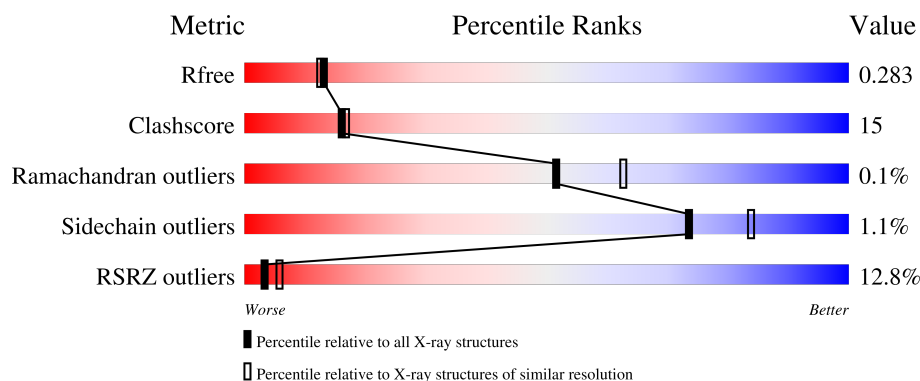
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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}	130704	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

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	<div> <div>8%</div> <div>69%</div> <div>28%</div> <div>.</div> </div>
1	C	451	<div> <div>7%</div> <div>74%</div> <div>24%</div> <div>.</div> </div>
2	B	445	<div> <div>11%</div> <div>61%</div> <div>33%</div> <div>5%</div> </div>
2	D	445	<div> <div>13%</div> <div>67%</div> <div>29%</div> <div>.</div> </div>
3	E	143	<div> <div>23%</div> <div>67%</div> <div>15%</div> <div>.</div> <div>16%</div> </div>

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Mol	Chain	Length	Quality of chain
4	F	384	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	CA	A	503	-	-	-	X

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 17863 atoms, of which 40 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	438	Total	C	N	O	S	0	0	0
			3424	2167	582	653	22			
1	C	440	Total	C	N	O	S	0	1	0
			3443	2178	585	657	23			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	421	Total	C	N	O	S	4	1	0
			3326	2091	569	639	27			
2	D	431	Total	C	N	O	S	7	0	0
			3368	2113	575	653	27			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	120	Total	C	N	O	S	0	0	0
			993	613	180	195	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	350	Total	C	N	O	S	0	0	0
			2865	1835	493	523	14			

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 (three-letter code: 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 (three-letter code: MG) (formula: Mg).

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

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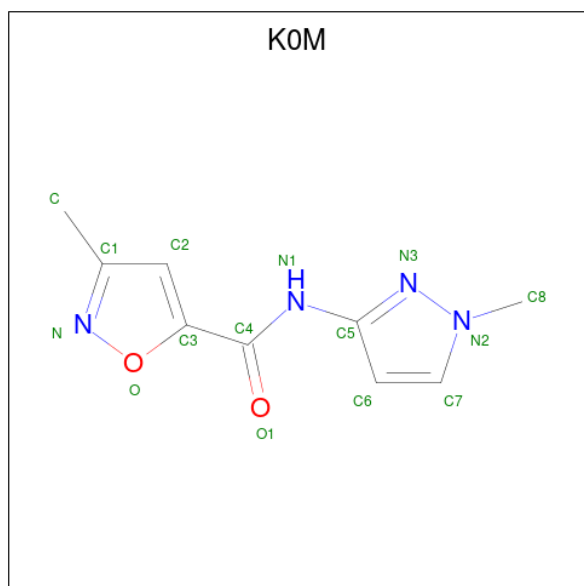
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	F	1	Total	Mg	0	0
			1	1		

- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

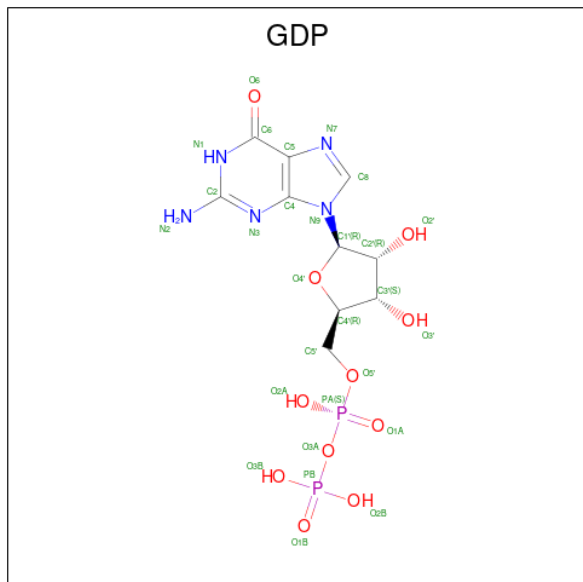
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Ca	0	0
			1	1		
7	B	1	Total	Ca	0	0
			1	1		
7	C	1	Total	Ca	0	0
			1	1		

- Molecule 8 is 3-methyl-N-(1-methyl-1H-pyrazol-3-yl)-1,2-oxazole-5-carboxamide (three-letter code: KOM) (formula: C₉H₁₀N₄O₂) (labeled as "Ligand of Interest" by depositor).



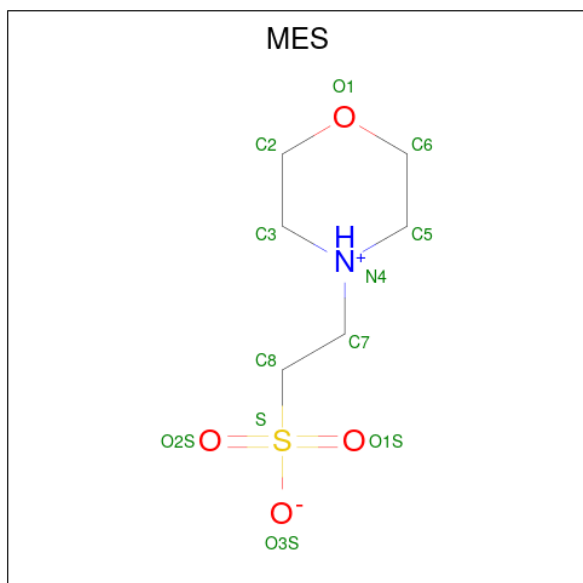
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	A	1	Total	C	H	N	O	0	0
			25	9	10	4	2		
8	B	1	Total	C	H	N	O	0	0
			25	9	10	4	2		
8	D	1	Total	C	H	N	O	0	0
			25	9	10	4	2		
8	D	1	Total	C	H	N	O	0	0
			25	9	10	4	2		

- Molecule 9 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



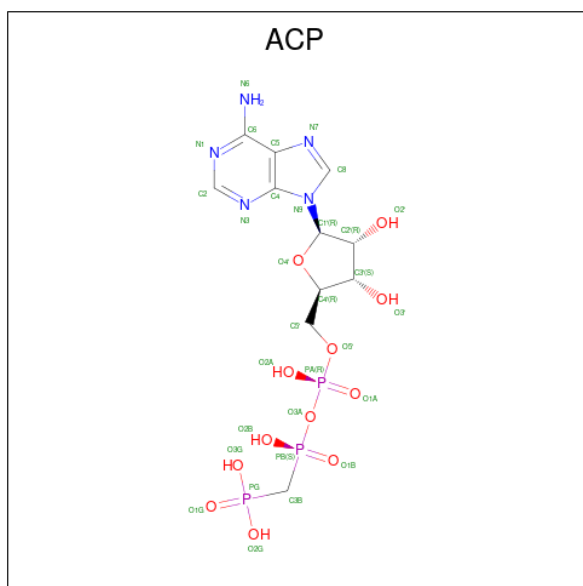
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	B	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
9	D	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- Molecule 10 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



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

- Molecule 11 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (three-letter code: 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		

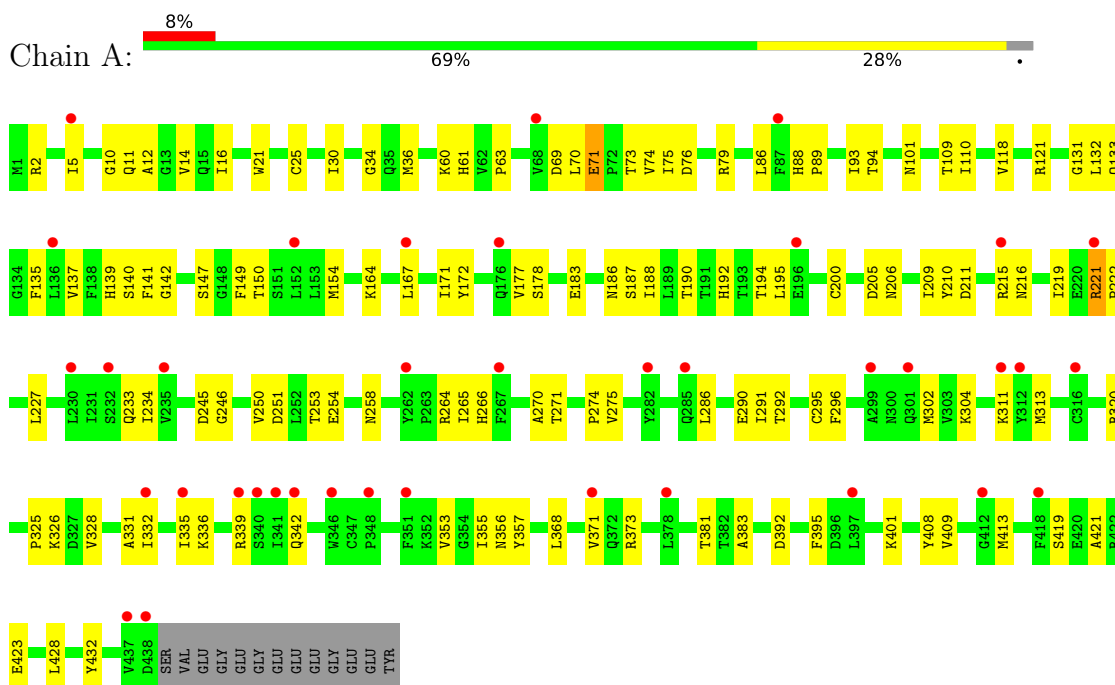
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	9	Total	O	0	0
			9	9		
12	B	32	Total	O	0	0
			32	32		
12	C	113	Total	O	0	0
			113	113		
12	D	17	Total	O	0	0
			17	17		
12	E	2	Total	O	0	0
			2	2		

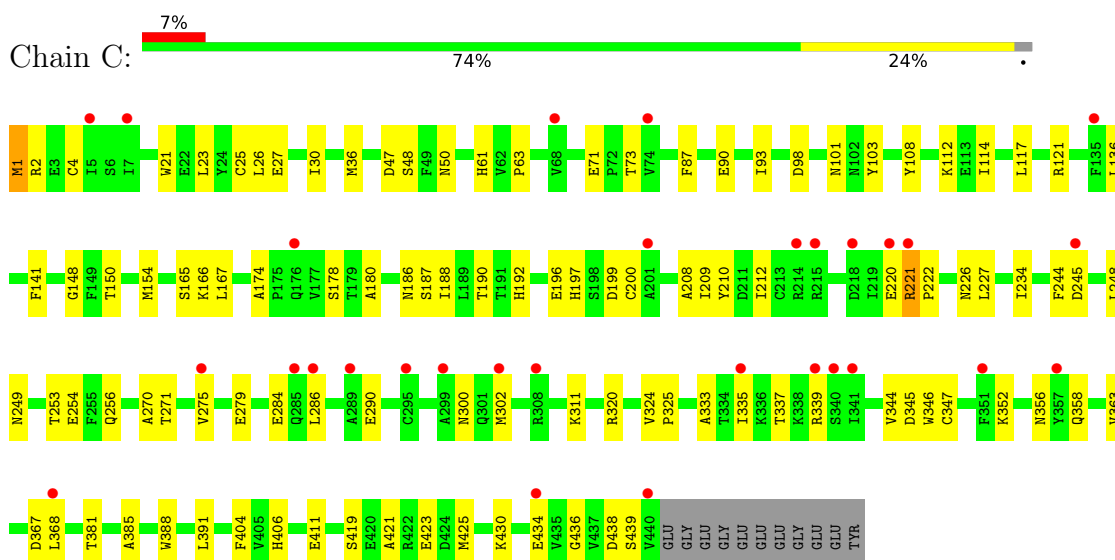
3 Residue-property plots [i](#)

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.

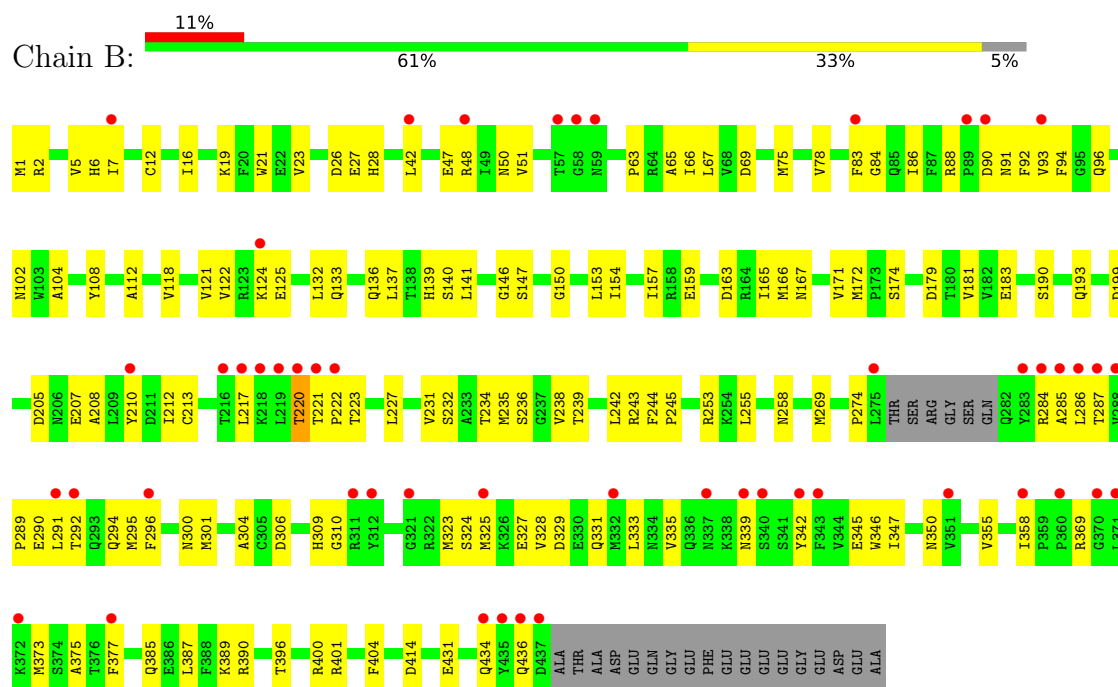
- Molecule 1: Tubulin alpha-1B chain



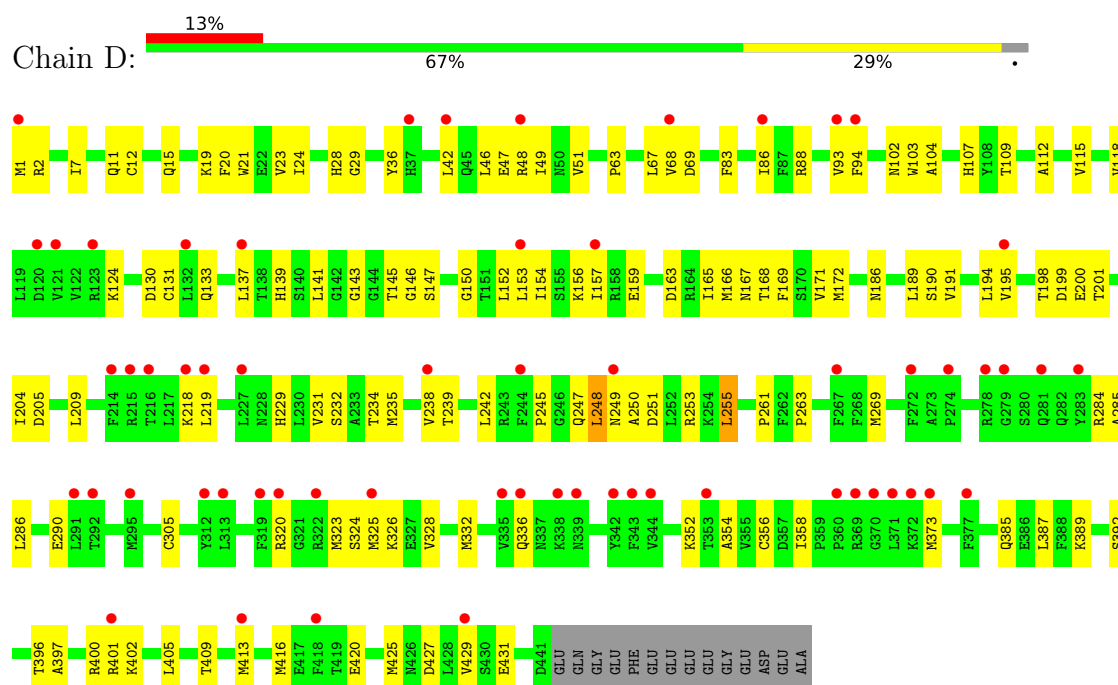
- Molecule 1: Tubulin alpha-1B chain



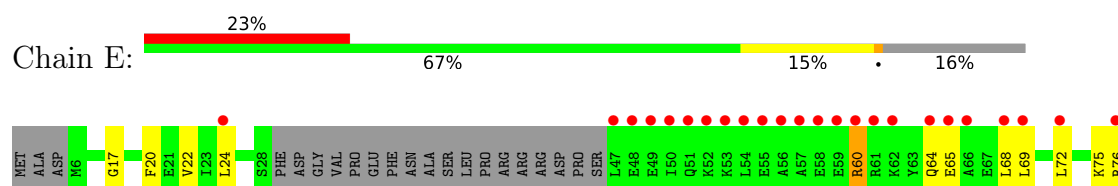
• Molecule 2: Tubulin beta-2B chain

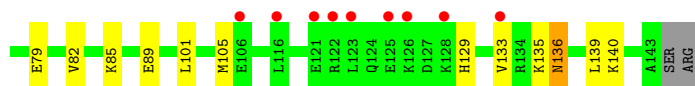


• Molecule 2: Tubulin beta-2B chain

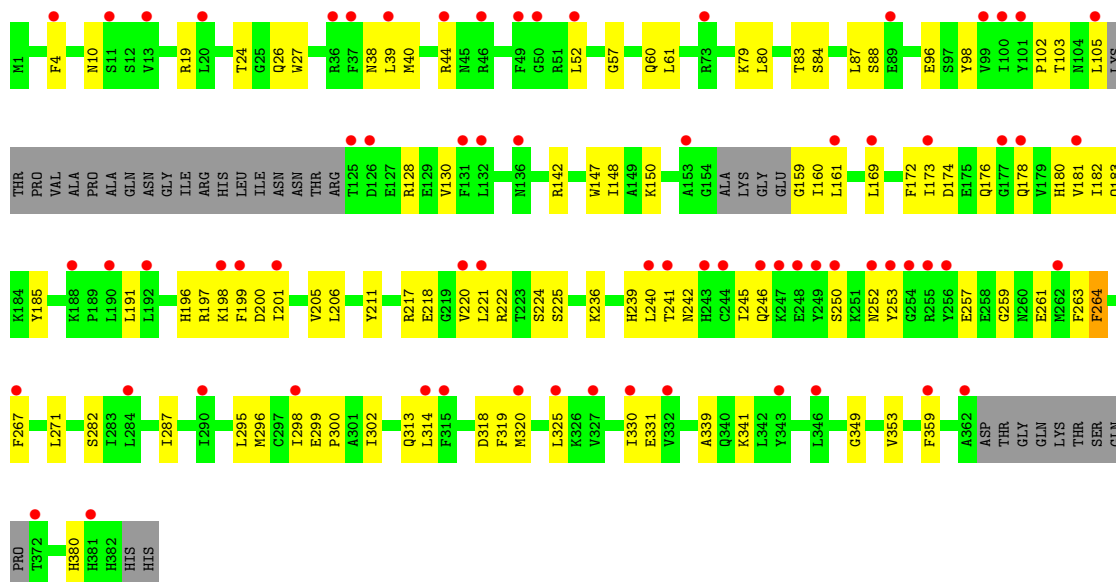


• Molecule 3: Stathmin-4





● 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	105.55Å 164.17Å 173.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	86.68 – 2.35 90.15 – 2.35	Depositor EDS
% Data completeness (in resolution range)	99.0 (86.68-2.35) 99.0 (90.15-2.35)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.10 (at 2.34Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.244 , 0.284 0.244 , 0.283	Depositor DCC
R_{free} test set	6075 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	59.6	Xtriage
Anisotropy	0.479	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 48.0	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	0.94	EDS
Total number of atoms	17863	wwPDB-VP
Average B, all atoms (Å ²)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.50% 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: ACP, GTP, CA, MG, GDP, MES, KOM

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	0.26	0/3502	0.42	0/4754
1	C	0.26	0/3521	0.42	0/4780
2	B	0.26	0/3400	0.42	0/4603
2	D	0.25	0/3442	0.41	0/4664
3	E	0.24	0/1000	0.34	0/1325
4	F	0.24	0/2931	0.40	0/3960
All	All	0.25	0/17796	0.41	0/24086

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	3424	0	3335	100	0
1	C	3443	0	3352	84	1
2	B	3326	0	3202	133	0
2	D	3368	0	3236	108	0
3	E	993	0	1013	21	0
4	F	2865	0	2826	80	0
5	A	32	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
6	D	1	0	0	0	0
6	F	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	A	15	10	0	0	0
8	B	15	10	0	0	0
8	D	30	20	0	3	0
9	B	28	0	12	1	0
9	D	28	0	12	3	0
10	B	12	0	12	3	0
11	F	31	0	14	5	0
12	A	9	0	0	1	0
12	B	32	0	0	3	1
12	C	113	0	0	4	0
12	D	17	0	0	1	0
12	E	2	0	0	0	0
All	All	17823	40	17038	503	1

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 15.

All (503) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:93:ILE:HD11	1:C:121:ARG:HG3	1.49	0.94
2:B:274:PRO:HB3	2:B:286:LEU:HD22	1.47	0.94
4:F:102:PRO:HG2	4:F:105:LEU:HD13	1.52	0.91
4:F:236:LYS:HB3	4:F:240:LEU:HD13	1.55	0.88
1:C:209:ILE:HG22	1:C:227:LEU:HD22	1.56	0.86
1:A:336:LYS:HG3	3:E:24:LEU:HD13	1.60	0.84
2:B:309:HIS:O	2:B:436:GLN:NE2	2.12	0.82
2:D:172:MET:HG3	2:D:387:LEU:HD11	1.62	0.81
1:C:234:ILE:HG12	1:C:302:MET:HE2	1.60	0.81
2:B:48:ARG:CZ	2:B:51:VAL:HG21	2.10	0.81
2:B:23:VAL:HG21	2:B:232:SER:HB3	1.63	0.81
2:D:385:GLN:HB2	2:D:429:VAL:HG13	1.63	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:LEU:O	1:A:164:LYS:NZ	2.16	0.78
2:B:253[A]:ARG:NH1	10:B:504:MES:O3S	2.16	0.78
1:A:211:ASP:OD2	1:A:304:LYS:NZ	2.15	0.77
1:C:335:ILE:HG23	1:C:339:ARG:HG3	1.66	0.76
1:A:335:ILE:HG23	1:A:339:ARG:HG3	1.68	0.76
1:C:209:ILE:HD11	1:C:302:MET:HE3	1.68	0.75
2:B:284:ARG:NH2	2:B:290:GLU:OE2	2.19	0.74
2:D:1:MET:N	2:D:130:ASP:OD2	2.18	0.74
4:F:197:ARG:NH1	4:F:257:GLU:OE2	2.21	0.73
2:B:96:GLN:HB3	1:C:1:MET:HG2	1.69	0.73
1:A:209:ILE:HG22	1:A:227:LEU:HD22	1.72	0.72
2:D:165:ILE:HG22	2:D:167:ASN:ND2	2.06	0.71
1:C:221:ARG:HG3	2:D:325:MET:HG2	1.73	0.70
2:B:208:ALA:HB2	2:B:304:ALA:HB2	1.73	0.70
4:F:10:ASN:HB2	4:F:44:ARG:HH22	1.57	0.70
2:D:324:SER:O	2:D:328:VAL:HG23	1.92	0.70
2:D:332:MET:O	2:D:336:GLN:HG3	1.92	0.70
2:B:5:VAL:HG23	2:B:132:LEU:HD11	1.73	0.69
2:B:48:ARG:HD3	2:B:242:LEU:O	1.91	0.69
1:A:274:PRO:HG2	1:A:371:VAL:HG11	1.75	0.69
1:C:209:ILE:HD11	1:C:302:MET:CE	2.23	0.69
2:D:147:SER:HB2	2:D:190:SER:OG	1.92	0.69
2:B:221:THR:HG21	1:C:325:PRO:HB2	1.75	0.69
5:C:501:GTP:O1G	12:C:601:HOH:O	2.11	0.69
2:D:402:LYS:HB3	2:D:405:LEU:HD12	1.75	0.69
2:B:48:ARG:NH1	2:B:51:VAL:HG21	2.08	0.68
1:A:75:ILE:HD12	1:A:94:THR:HG22	1.76	0.68
2:B:1:MET:HA	2:B:50:ASN:HD21	1.59	0.68
4:F:128:ARG:NH2	4:F:174:ASP:OD1	2.26	0.68
1:A:210:TYR:CE1	1:A:222:PRO:HD2	2.29	0.68
1:A:211:ASP:HB3	1:A:215:ARG:NH2	2.09	0.67
2:B:154:ILE:HG23	2:B:166:MET:HG2	1.76	0.67
2:B:172:MET:HG3	2:B:387:LEU:HD11	1.75	0.67
2:D:141:LEU:HA	2:D:147:SER:HB3	1.76	0.67
2:D:269:MET:CE	2:D:305:CYS:HB2	2.25	0.66
1:C:430:LYS:HE2	1:C:434:GLU:OE2	1.93	0.66
2:D:83:PHE:O	2:D:86:ILE:HG22	1.95	0.66
2:B:295:MET:HG3	2:B:377:PHE:HB2	1.77	0.66
2:B:345:GLU:OE1	2:B:345:GLU:N	2.23	0.65
1:A:291:ILE:HD13	1:A:373:ARG:HG3	1.78	0.65
2:D:245:PRO:HA	2:D:249:ASN:OD1	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:331:GLU:OE2	11:F:401:ACP:O3G	2.14	0.65
2:B:21:TRP:CZ3	2:B:63:PRO:HB3	2.32	0.65
2:B:274:PRO:HB3	2:B:286:LEU:CD2	2.24	0.65
1:C:254:GLU:HG2	1:C:352:LYS:HE2	1.78	0.65
1:C:93:ILE:HG22	1:C:114:ILE:HD11	1.79	0.64
1:C:4[A]:CYS:SG	1:C:136:LEU:HG	2.38	0.64
1:C:21:TRP:CZ3	1:C:63:PRO:HB3	2.32	0.64
2:D:431:GLU:OE1	12:D:601:HOH:O	2.15	0.64
1:A:233:GLN:HG3	1:A:368:LEU:CD1	2.28	0.63
2:D:251:ASP:O	2:D:255:LEU:HD22	1.98	0.63
3:E:72:LEU:O	3:E:76:ARG:HG2	1.98	0.63
3:E:129:HIS:O	3:E:133:VAL:HG23	1.97	0.63
4:F:173:ILE:HG23	4:F:180:HIS:HB2	1.80	0.63
2:B:147:SER:HG	2:B:190:SER:HG	1.47	0.63
1:C:26:LEU:CD1	1:C:363:VAL:HG22	2.29	0.63
3:E:136:ASN:ND2	3:E:140:LYS:HE3	2.14	0.63
2:B:244:PHE:CE1	2:B:358:ILE:HD12	2.34	0.62
2:D:19:LYS:O	2:D:23:VAL:HG23	1.98	0.62
2:D:154:ILE:HG23	2:D:166:MET:HG2	1.81	0.62
4:F:220:VAL:HG11	4:F:339:ALA:HB2	1.81	0.62
2:D:409:THR:HA	2:D:413:MET:O	2.00	0.62
2:B:48:ARG:HH12	2:B:51:VAL:HG11	1.64	0.61
2:B:294:GLN:HE21	2:B:300:ASN:HD21	1.47	0.61
1:C:166:LYS:HE2	1:C:197:HIS:O	2.00	0.61
4:F:39:LEU:HD12	4:F:61:LEU:O	2.00	0.61
3:E:135:LYS:O	3:E:139:LEU:HG	2.01	0.61
2:D:191:VAL:O	2:D:195:VAL:HG23	2.00	0.61
2:B:193:GLN:HB3	12:B:607:HOH:O	1.99	0.61
2:D:269:MET:HE2	2:D:305:CYS:HB2	1.80	0.61
1:A:12:ALA:HB3	1:A:140:SER:HB3	1.82	0.61
2:D:112:ALA:O	2:D:115:VAL:HG12	2.00	0.60
4:F:200:ASP:OD1	4:F:222:ARG:HB2	2.01	0.60
4:F:282:SER:HB2	4:F:325:LEU:HD13	1.83	0.60
2:B:48:ARG:NH2	2:B:133:GLN:HE22	1.99	0.60
2:D:234:THR:O	2:D:238:VAL:HG13	2.00	0.60
1:A:12:ALA:CB	1:A:140:SER:HB3	2.32	0.60
1:C:187:SER:HB3	1:C:391:LEU:HD21	1.83	0.60
1:C:196:GLU:HG2	12:C:622:HOH:O	2.00	0.60
2:D:427:ASP:O	2:D:431:GLU:HG3	2.00	0.60
2:D:21:TRP:CZ3	2:D:63:PRO:HB3	2.36	0.60
1:C:249:ASN:OD1	1:C:356:ASN:ND2	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:324:VAL:HG22	12:C:604:HOH:O	2.02	0.60
2:D:107:HIS:O	2:D:152:LEU:HD22	2.01	0.60
2:B:1:MET:HA	2:B:50:ASN:ND2	2.16	0.60
1:C:210:TYR:CE1	1:C:222:PRO:HD2	2.37	0.60
2:D:2:ARG:HB2	2:D:133:GLN:HE21	1.66	0.60
2:D:416:MET:O	2:D:420:GLU:HG3	2.02	0.59
4:F:191:LEU:HA	4:F:197:ARG:O	2.02	0.59
1:A:254:GLU:HG2	1:A:258:ASN:ND2	2.17	0.59
1:C:320:ARG:HA	1:C:356:ASN:O	2.02	0.59
1:A:16:ILE:CD1	1:A:171:ILE:HD11	2.33	0.59
1:A:357:TYR:CZ	3:E:17:GLY:HA2	2.37	0.59
2:D:21:TRP:CE3	2:D:63:PRO:HB3	2.36	0.59
1:A:36:MET:HB3	1:A:61:HIS:CE1	2.38	0.59
1:C:333:ALA:O	1:C:337:THR:HG23	2.03	0.59
2:D:204:ILE:HG21	2:D:231:VAL:HG22	1.85	0.59
1:A:250:VAL:HG12	1:A:254:GLU:OE1	2.02	0.58
1:A:320:ARG:NH1	12:A:604:HOH:O	2.36	0.58
1:C:26:LEU:HD11	1:C:363:VAL:HG22	1.84	0.58
1:C:234:ILE:HG12	1:C:302:MET:CE	2.31	0.58
4:F:38:ASN:O	4:F:60:GLN:HA	2.03	0.58
1:C:275:VAL:HG13	1:C:368:LEU:HD21	1.85	0.58
2:B:157:ILE:HG21	2:B:166:MET:HE1	1.86	0.58
3:E:60:ARG:O	3:E:64:GLN:HG3	2.02	0.58
2:D:93:VAL:HG11	2:D:118:VAL:HG22	1.83	0.58
4:F:241:THR:OG1	11:F:401:ACP:O3'	2.07	0.58
2:B:48:ARG:NH1	2:B:242:LEU:O	2.37	0.58
2:D:141:LEU:HD22	2:D:190:SER:HB3	1.86	0.58
2:D:248:LEU:HD22	2:D:354:ALA:HB1	1.86	0.58
2:D:137:LEU:HB3	2:D:168:THR:HG22	1.86	0.57
2:D:167:ASN:OD1	2:D:200:GLU:HG3	2.03	0.57
4:F:150:LYS:HB3	4:F:160:ILE:HG13	1.86	0.57
1:A:188:ILE:HD12	1:A:395:PHE:HB2	1.87	0.57
2:B:141:LEU:HD12	2:B:172:MET:SD	2.44	0.57
4:F:242:ASN:HD22	4:F:245:ILE:HD12	1.70	0.57
2:B:88:ARG:HH11	2:B:90:ASP:HB2	1.69	0.57
2:B:27:GLU:OE2	2:B:236:SER:OG	2.19	0.57
2:D:397:ALA:O	2:D:401:ARG:NH1	2.38	0.57
1:A:335:ILE:CG2	1:A:339:ARG:HG3	2.34	0.57
2:B:69:ASP:O	2:B:94:PHE:HA	2.05	0.57
4:F:159:GLY:C	4:F:160:ILE:HD12	2.24	0.57
1:A:93:ILE:HD11	1:A:121:ARG:HG3	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:381:THR:HG22	1:A:383:ALA:H	1.70	0.57
2:D:205:ASP:O	2:D:209:LEU:HG	2.04	0.57
1:A:292:THR:HG22	1:A:335:ILE:CD1	2.35	0.56
1:A:325:PRO:HB3	3:E:20:PHE:CE1	2.40	0.56
1:C:226:ASN:ND2	1:C:367:ASP:OD2	2.38	0.56
2:D:165:ILE:HG22	2:D:167:ASN:HD21	1.69	0.56
3:E:136:ASN:O	3:E:140:LYS:HG2	2.06	0.56
4:F:102:PRO:HG2	4:F:105:LEU:CD1	2.31	0.56
4:F:242:ASN:HD22	4:F:245:ILE:CD1	2.18	0.56
4:F:267:PHE:CZ	4:F:271:LEU:HD21	2.40	0.56
2:B:75:MET:HE3	2:B:92:PHE:CD2	2.40	0.56
2:D:2:ARG:HB3	2:D:133:GLN:CG	2.34	0.56
2:B:306:ASP:HB3	2:B:309:HIS:ND1	2.21	0.56
1:C:1:MET:O	1:C:2:ARG:HB2	2.06	0.56
2:B:78:VAL:O	2:B:84:GLY:HA3	2.05	0.56
2:B:83:PHE:O	2:B:86:ILE:HG22	2.06	0.56
2:D:171:VAL:HA	2:D:204:ILE:O	2.05	0.56
1:C:48:SER:OG	1:C:245:ASP:HB2	2.06	0.56
1:C:220:GLU:HB3	2:D:326:LYS:HD2	1.87	0.56
1:C:271:THR:HG23	1:C:300:ASN:O	2.05	0.56
1:A:188:ILE:HD12	1:A:395:PHE:CD2	2.41	0.56
2:D:284:ARG:O	2:D:285:ALA:HB3	2.06	0.55
1:C:411:GLU:OE2	12:C:602:HOH:O	2.18	0.55
2:B:118:VAL:HG11	2:B:153:LEU:HD11	1.87	0.55
2:B:2:ARG:HB2	2:B:133:GLN:HE21	1.71	0.55
2:D:218:LYS:O	2:D:219:LEU:HD23	2.07	0.55
1:C:419:SER:O	1:C:423:GLU:HG3	2.06	0.55
4:F:98:TYR:CE1	4:F:130:VAL:HG12	2.42	0.55
1:A:265:ILE:HG21	1:A:313:MET:HE1	1.88	0.55
4:F:24:THR:O	4:F:26:GLN:HG3	2.07	0.55
1:C:244:PHE:CD1	1:C:358:GLN:HG2	2.42	0.54
1:C:101:ASN:ND2	1:C:180:ALA:HB2	2.22	0.54
3:E:68:LEU:O	3:E:72:LEU:HG	2.08	0.54
4:F:299:GLU:HB3	4:F:300:PRO:HD3	1.89	0.54
2:B:210:TYR:CE2	2:B:222:PRO:HD2	2.42	0.54
1:C:174:ALA:O	1:C:178:SER:HB3	2.08	0.54
1:A:34:GLY:O	1:A:61:HIS:N	2.38	0.54
2:D:143:GLY:O	2:D:186:ASN:ND2	2.41	0.54
3:E:85:LYS:O	3:E:89:GLU:HG3	2.07	0.54
2:B:174:SER:CB	2:B:207:GLU:HB2	2.37	0.54
2:D:2:ARG:CB	2:D:133:GLN:HE21	2.20	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:246:GLN:O	4:F:250:SER:HB3	2.07	0.54
4:F:267:PHE:CE2	4:F:271:LEU:HD11	2.42	0.54
2:B:88:ARG:NH1	2:B:90:ASP:HB2	2.23	0.54
2:B:108:TYR:CG	3:E:82:VAL:HG11	2.42	0.54
1:A:401:LYS:HG3	2:B:346:TRP:CD2	2.42	0.54
2:B:165:ILE:HA	2:B:199:ASP:OD2	2.08	0.54
4:F:10:ASN:CB	4:F:44:ARG:HH22	2.20	0.54
4:F:150:LYS:NZ	11:F:401:ACP:N7	2.55	0.54
1:A:21:TRP:CZ3	1:A:63:PRO:HB3	2.43	0.54
2:B:163:ASP:O	2:B:253[A]:ARG:NH2	2.40	0.54
2:B:174:SER:OG	2:B:207:GLU:HB2	2.08	0.53
2:D:152:LEU:O	2:D:156:LYS:HG2	2.07	0.53
2:D:69:ASP:O	2:D:94:PHE:HA	2.08	0.53
1:A:25:CYS:SG	1:A:86:LEU:HD11	2.49	0.53
2:B:2:ARG:O	2:B:51:VAL:HG22	2.09	0.53
2:D:146:GLY:O	2:D:150:GLY:HA3	2.09	0.53
1:A:142:GLY:HA3	1:A:183:GLU:HG2	1.91	0.53
2:B:159:GLU:HB2	3:E:72:LEU:HD13	1.90	0.53
2:B:47:GLU:HG2	2:B:245:PRO:HG3	1.90	0.53
1:A:2:ARG:HB2	1:A:133:GLN:HE21	1.73	0.52
1:A:188:ILE:HD12	1:A:395:PHE:CB	2.39	0.52
1:A:141:PHE:HB3	1:A:187:SER:OG	2.09	0.52
4:F:225:SER:HG	4:F:250:SER:HG	1.56	0.52
4:F:267:PHE:O	4:F:271:LEU:HG	2.09	0.52
1:C:186:ASN:O	1:C:190:THR:HG22	2.09	0.52
1:C:253:THR:O	1:C:256:GLN:HB2	2.08	0.52
2:B:208:ALA:O	2:B:212:ILE:HG13	2.09	0.52
2:B:295:MET:CG	2:B:377:PHE:HB2	2.38	0.52
2:B:310:GLY:HA2	2:B:436:GLN:NE2	2.25	0.52
2:D:245:PRO:HA	2:D:249:ASN:HD21	1.75	0.52
2:B:2:ARG:HB3	2:B:133:GLN:HG3	1.92	0.52
2:D:242:LEU:HD23	2:D:250:ALA:O	2.10	0.52
1:C:47:ASP:O	1:C:50:ASN:HB2	2.09	0.52
1:C:141:PHE:HB3	1:C:187:SER:OG	2.09	0.52
2:D:397:ALA:HA	2:D:400:ARG:CZ	2.39	0.52
4:F:176:GLN:HB3	4:F:178:GLN:NE2	2.25	0.52
1:C:93:ILE:HD11	1:C:121:ARG:CG	2.31	0.52
2:D:165:ILE:HA	2:D:199:ASP:OD2	2.10	0.52
2:B:2:ARG:CB	2:B:133:GLN:HE21	2.23	0.52
3:E:76:ARG:NH2	3:E:79:GLU:OE2	2.37	0.51
1:A:270:ALA:HB3	1:A:302:MET:CG	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:16:ILE:HD12	2:B:171:VAL:HG21	1.92	0.51
2:B:88:ARG:NH1	2:B:90:ASP:OD2	2.43	0.51
2:B:205:ASP:OD2	2:B:390:ARG:NH2	2.43	0.51
2:B:385:GLN:O	2:B:389:LYS:HG3	2.11	0.51
4:F:206:LEU:HD12	4:F:313:GLN:O	2.11	0.51
2:D:218:LYS:C	2:D:219:LEU:HD23	2.31	0.51
2:B:2:ARG:HB3	2:B:133:GLN:CG	2.40	0.51
2:B:286:LEU:HA	2:B:290:GLU:OE1	2.10	0.51
2:D:165:ILE:CG2	2:D:167:ASN:HD21	2.24	0.51
1:C:221:ARG:HG3	2:D:325:MET:CG	2.38	0.51
2:D:153:LEU:O	2:D:157:ILE:HG13	2.11	0.51
4:F:349:GLY:O	4:F:353:VAL:HG22	2.11	0.51
1:A:265:ILE:HG23	1:A:432:TYR:CZ	2.46	0.51
1:C:209:ILE:HG22	1:C:227:LEU:CD2	2.33	0.51
4:F:103:THR:HG23	4:F:128:ARG:NH2	2.26	0.51
1:A:336:LYS:CG	3:E:24:LEU:HD13	2.38	0.51
1:A:177:VAL:HG21	1:A:206:ASN:HB3	1.91	0.50
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.29	0.50
2:B:75:MET:HE3	2:B:92:PHE:HD2	1.75	0.50
2:B:157:ILE:HG21	2:B:166:MET:CE	2.40	0.50
2:D:103:TRP:CE3	2:D:189:LEU:HD13	2.46	0.50
2:D:204:ILE:HG22	2:D:209:LEU:HD11	1.94	0.50
1:A:271:THR:CG2	1:A:295:CYS:HA	2.41	0.50
1:C:221:ARG:NH1	1:C:222:PRO:O	2.44	0.50
4:F:198:LYS:HE3	4:F:320:MET:CE	2.42	0.50
2:B:292:THR:HG22	2:B:335:VAL:HG21	1.92	0.50
4:F:318:ASP:OD2	11:F:401:ACP:O2G	2.30	0.50
2:B:47:GLU:HG2	2:B:245:PRO:CB	2.42	0.50
2:B:136:GLN:HA	2:B:167:ASN:O	2.11	0.50
1:C:71:GLU:HG2	1:C:98:ASP:HB3	1.92	0.50
4:F:40:MET:HE3	4:F:52:LEU:HD21	1.94	0.50
1:C:404:PHE:CD1	2:D:261:PRO:HA	2.46	0.50
2:D:28:HIS:HB3	2:D:49:ILE:HD13	1.93	0.50
2:D:12:CYS:HB2	9:D:501:GDP:C8	2.47	0.49
2:B:327:GLU:O	2:B:331:GLN:HG2	2.12	0.49
4:F:225:SER:OG	4:F:250:SER:OG	2.30	0.49
1:A:2:ARG:HB3	1:A:131:GLY:O	2.12	0.49
2:B:42:LEU:HB2	2:B:358:ILE:HD11	1.94	0.49
2:D:11:GLN:O	2:D:15:GLN:HG2	2.12	0.49
2:D:194:LEU:HD22	2:D:198:THR:HG21	1.95	0.49
1:A:76:ASP:OD1	1:A:79:ARG:NH1	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:328:VAL:HG11	1:A:353:VAL:HG11	1.93	0.49
2:D:163:ASP:O	2:D:253:ARG:NH2	2.43	0.49
4:F:178:GLN:HE21	4:F:180:HIS:HE1	1.61	0.49
1:A:335:ILE:O	1:A:339:ARG:HB2	2.13	0.49
1:C:344:VAL:HG23	1:C:347:CYS:HB3	1.95	0.49
1:A:101:ASN:HD22	2:B:258:ASN:HD21	1.59	0.49
1:A:245:ASP:OD1	1:A:246:GLY:N	2.46	0.49
2:B:47:GLU:HG2	2:B:245:PRO:HB3	1.94	0.49
2:D:239:THR:HG22	8:D:503:K0M:C	2.43	0.49
1:C:21:TRP:CH2	1:C:63:PRO:HB3	2.48	0.49
2:D:11:GLN:N	9:D:501:GDP:O3B	2.28	0.49
2:D:36:TYR:CD2	2:D:46:LEU:HD11	2.48	0.49
2:D:245:PRO:HA	2:D:249:ASN:ND2	2.27	0.49
2:B:12:CYS:HB2	9:B:501:GDP:C8	2.48	0.48
4:F:147:TRP:HB2	4:F:169:LEU:CD1	2.42	0.48
4:F:148:ILE:HD11	4:F:160:ILE:HG21	1.95	0.48
1:A:71:GLU:OE2	1:A:73:THR:OG1	2.30	0.48
1:A:292:THR:HG22	1:A:335:ILE:HD12	1.94	0.48
2:D:23:VAL:HG21	2:D:232:SER:HB2	1.95	0.48
2:D:248:LEU:HB2	2:D:249:ASN:H	1.51	0.48
1:A:328:VAL:O	1:A:332:ILE:HG13	2.13	0.48
2:D:145:THR:N	9:D:501:GDP:O2B	2.46	0.48
2:B:42:LEU:H	2:B:42:LEU:HD12	1.79	0.48
2:D:29:GLY:O	2:D:36:TYR:HA	2.13	0.48
4:F:205:VAL:O	4:F:314:LEU:HD12	2.13	0.48
1:A:331:ALA:O	1:A:335:ILE:HG13	2.13	0.48
1:C:165:SER:HA	1:C:199:ASP:OD2	2.14	0.48
2:D:397:ALA:HA	2:D:400:ARG:NH1	2.29	0.48
2:B:324:SER:O	2:B:328:VAL:HG23	2.14	0.48
2:B:5:VAL:HG23	2:B:132:LEU:CD1	2.43	0.48
2:B:291:LEU:HD11	2:B:373:MET:HG3	1.96	0.48
4:F:173:ILE:HD11	4:F:182:ILE:HD11	1.96	0.48
4:F:320:MET:HG3	4:F:330:ILE:HD11	1.96	0.48
1:A:271:THR:HG21	1:A:295:CYS:HA	1.95	0.48
1:C:108:TYR:O	1:C:112:LYS:HG2	2.14	0.48
1:C:311:LYS:HD2	1:C:436:GLY:O	2.14	0.48
1:C:406:HIS:CG	2:D:263:PRO:HD3	2.48	0.48
2:B:339:ASN:HB3	2:B:342:TYR:HD2	1.78	0.48
1:A:16:ILE:HD11	1:A:171:ILE:HD11	1.96	0.47
2:B:23:VAL:CG2	2:B:232:SER:HB3	2.41	0.47
1:C:311:LYS:NZ	1:C:438:ASP:OD1	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:150:LYS:HZ3	11:F:401:ACP:C8	2.27	0.47
4:F:217:ARG:HG3	4:F:218:GLU:N	2.28	0.47
2:B:333:LEU:HD11	4:F:57:GLY:HA3	1.96	0.47
1:C:187:SER:CB	1:C:391:LEU:HD21	2.44	0.47
2:D:269:MET:HE1	2:D:305:CYS:HB2	1.94	0.47
2:D:396:THR:O	2:D:400:ARG:HG2	2.14	0.47
1:C:71:GLU:OE1	1:C:73:THR:HG23	2.14	0.47
1:C:209:ILE:CG2	1:C:227:LEU:HD22	2.36	0.47
2:D:20:PHE:CZ	2:D:24:ILE:HD13	2.49	0.47
2:D:286:LEU:HD12	2:D:290:GLU:OE1	2.13	0.47
4:F:98:TYR:HE1	4:F:130:VAL:HG12	1.79	0.47
1:C:36:MET:HB3	1:C:61:HIS:CE1	2.49	0.47
1:A:192:HIS:CG	1:A:421:ALA:HA	2.49	0.47
1:A:221:ARG:HG3	2:B:325:MET:SD	2.55	0.47
1:C:254:GLU:HG2	1:C:352:LYS:CE	2.44	0.47
1:A:141:PHE:O	1:A:147:SER:HB3	2.15	0.47
2:B:401:ARG:HG3	1:C:346:TRP:CD1	2.49	0.47
2:B:431:GLU:O	2:B:434:GLN:HG2	2.14	0.47
1:C:90:GLU:HB3	1:C:121:ARG:HD2	1.96	0.47
1:A:167:LEU:HG	1:A:200:CYS:HB3	1.97	0.47
2:B:12:CYS:HB3	2:B:140:SER:HB3	1.97	0.47
1:C:178:SER:OG	2:D:352:LYS:NZ	2.39	0.47
3:E:75:LYS:O	3:E:79:GLU:HG3	2.14	0.47
2:D:48:ARG:HG2	2:D:51:VAL:CG2	2.45	0.46
1:A:270:ALA:HB3	1:A:302:MET:HG3	1.96	0.46
1:A:296:PHE:CE2	1:A:335:ILE:HG21	2.50	0.46
2:B:7:ILE:O	2:B:137:LEU:HA	2.14	0.46
1:C:208:ALA:O	1:C:212:ILE:HG13	2.15	0.46
4:F:201:ILE:HG12	4:F:221:LEU:HG	1.97	0.46
1:A:34:GLY:HA3	1:A:60:LYS:HG3	1.97	0.46
2:B:269:MET:HE2	2:B:301:MET:SD	2.55	0.46
1:A:234:ILE:HD12	1:A:234:ILE:N	2.30	0.46
2:B:181:VAL:HG21	2:B:404:PHE:CZ	2.51	0.46
2:D:88:ARG:NH2	2:D:124:LYS:HE3	2.31	0.46
4:F:287:ILE:HG23	4:F:319:PHE:CE2	2.50	0.46
2:B:48:ARG:NH1	2:B:51:VAL:HG11	2.30	0.46
2:B:414:ASP:HB3	12:B:627:HOH:O	2.15	0.46
1:A:194:THR:O	1:A:194:THR:HG22	2.16	0.46
1:A:265:ILE:HG23	1:A:432:TYR:CE1	2.49	0.46
4:F:19:ARG:HD2	4:F:19:ARG:O	2.16	0.46
1:A:88:HIS:CD2	1:A:89:PRO:HD2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:419:SER:O	1:A:423:GLU:HG3	2.16	0.46
2:D:2:ARG:HA	2:D:131:CYS:O	2.16	0.46
2:D:204:ILE:CG2	2:D:231:VAL:HG22	2.46	0.46
2:B:75:MET:CE	2:B:92:PHE:HD2	2.28	0.45
4:F:199:PHE:CE1	4:F:221:LEU:HD23	2.51	0.45
1:A:188:ILE:HD11	1:A:392:ASP:HA	1.99	0.45
2:B:16:ILE:CD1	2:B:171:VAL:HG21	2.46	0.45
4:F:161:LEU:HD22	4:F:172:PHE:HB2	1.97	0.45
2:B:112:ALA:HB1	12:B:628:HOH:O	2.15	0.45
2:B:199:ASP:OD1	10:B:504:MES:H62	2.15	0.45
1:C:192:HIS:CD2	1:C:421:ALA:HA	2.52	0.45
1:A:188:ILE:HD12	1:A:395:PHE:CG	2.51	0.45
1:C:286:LEU:H	1:C:286:LEU:HD12	1.80	0.45
1:A:408:TYR:HB3	1:A:413:MET:HE2	1.98	0.45
2:B:253[A]:ARG:NH1	10:B:504:MES:S	2.75	0.45
2:B:329:ASP:O	2:B:333:LEU:HG	2.16	0.45
1:C:188:ILE:HG13	1:C:425:MET:HG3	1.98	0.45
4:F:199:PHE:CD1	4:F:221:LEU:HD23	2.51	0.45
2:B:235:MET:O	2:B:239:THR:HG23	2.17	0.45
2:B:347:ILE:HG22	2:B:350:ASN:HB3	1.99	0.45
2:D:67:LEU:N	2:D:67:LEU:HD12	2.31	0.45
1:A:11:GLN:HG3	1:A:74:VAL:HG21	1.98	0.45
2:B:65:ALA:O	2:B:91:ASN:ND2	2.37	0.45
2:D:320:ARG:HA	2:D:356:CYS:O	2.17	0.44
4:F:211:TYR:OH	4:F:295:LEU:O	2.25	0.44
2:B:234:THR:O	2:B:238:VAL:HG13	2.17	0.44
1:C:63:PRO:HG2	1:C:87:PHE:CE1	2.52	0.44
4:F:80:LEU:HD12	4:F:84:SER:OG	2.17	0.44
4:F:185:TYR:OH	4:F:239:HIS:HB3	2.17	0.44
4:F:259:GLY:O	4:F:261:GLU:HG3	2.17	0.44
2:D:245:PRO:HA	2:D:249:ASN:CG	2.38	0.44
2:D:385:GLN:O	2:D:389:LYS:HG3	2.18	0.44
2:B:19:LYS:O	2:B:23:VAL:HG23	2.18	0.44
2:B:401:ARG:HG3	1:C:346:TRP:CG	2.52	0.44
1:A:320:ARG:HA	1:A:356:ASN:O	2.17	0.44
1:C:26:LEU:HD12	1:C:363:VAL:HG22	1.99	0.44
1:C:103:TYR:CD2	1:C:148:GLY:HA2	2.53	0.44
2:D:47:GLU:OE1	2:D:47:GLU:HA	2.17	0.44
2:D:255:LEU:HG	8:D:503:K0M:C5	2.46	0.44
1:A:70:LEU:HD22	1:A:110:ILE:HG22	2.00	0.44
2:B:296:PHE:CD2	2:B:335:VAL:HG11	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:102:ASN:OD1	2:D:104:ALA:HB3	2.18	0.44
2:B:125:GLU:HA	2:B:125:GLU:OE1	2.18	0.44
2:B:295:MET:SD	2:B:375:ALA:HB1	2.58	0.44
1:C:23:LEU:O	1:C:27:GLU:HG3	2.18	0.44
4:F:225:SER:O	4:F:252:ASN:HB2	2.18	0.44
1:A:195:LEU:HD12	1:A:266:HIS:CE1	2.53	0.43
1:A:286:LEU:HA	1:A:290:GLU:OE1	2.18	0.43
2:D:7:ILE:O	2:D:137:LEU:HA	2.17	0.43
4:F:79:LYS:O	4:F:83:THR:OG1	2.29	0.43
1:A:2:ARG:CB	1:A:133:GLN:HG3	2.48	0.43
2:B:220:THR:O	2:B:222:PRO:HD3	2.18	0.43
1:A:251:ASP:OD1	1:A:253:THR:HB	2.18	0.43
1:C:270:ALA:O	1:C:302:MET:HG2	2.18	0.43
4:F:38:ASN:HB3	4:F:359:PHE:CE1	2.53	0.43
1:A:118:VAL:HG21	1:A:149:PHE:HZ	1.83	0.43
1:A:172:TYR:HB3	1:A:205:ASP:HA	2.00	0.43
2:B:47:GLU:CB	2:B:245:PRO:HG3	2.48	0.43
2:B:294:GLN:HB3	2:B:300:ASN:ND2	2.33	0.43
1:A:10:GLY:O	1:A:14:VAL:HG23	2.18	0.43
2:D:20:PHE:CD1	2:D:235:MET:HE2	2.53	0.43
2:D:103:TRP:HB2	2:D:186:ASN:OD1	2.19	0.43
2:B:102:ASN:OD1	2:B:104:ALA:N	2.52	0.43
4:F:96:GLU:O	4:F:183:GLN:HA	2.18	0.43
1:A:216:ASN:HB3	1:A:275:VAL:O	2.19	0.43
2:B:28:HIS:NE2	2:B:243:ARG:HB3	2.34	0.43
1:C:385:ALA:HA	1:C:388:TRP:CD1	2.53	0.43
3:E:22:VAL:HG13	3:E:22:VAL:O	2.19	0.43
1:A:137:VAL:HG21	1:A:154:MET:SD	2.59	0.43
2:B:93:VAL:HG21	2:B:121:VAL:HG21	2.00	0.43
2:B:163:ASP:O	2:B:253[B]:ARG:NH1	2.51	0.43
4:F:253:TYR:CZ	4:F:259:GLY:HA2	2.54	0.43
2:B:213:CYS:HA	2:B:217:LEU:HB2	2.00	0.43
4:F:198:LYS:HE3	4:F:320:MET:HE1	1.99	0.43
4:F:341:LYS:HG2	4:F:341:LYS:O	2.19	0.43
1:A:69:ASP:O	1:A:94:THR:HA	2.19	0.43
2:B:223:THR:O	2:B:227:LEU:HD13	2.18	0.43
2:D:46:LEU:HA	2:D:49:ILE:HB	2.01	0.43
4:F:263:PHE:CE1	4:F:341:LYS:HE2	2.53	0.43
1:A:355:ILE:O	3:E:17:GLY:HA3	2.18	0.42
2:B:67:LEU:N	2:B:67:LEU:HD12	2.34	0.42
1:C:345:ASP:OD2	1:C:439:SER:N	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:68:VAL:HA	2:D:93:VAL:O	2.19	0.42
4:F:87:LEU:O	4:F:88:SER:OG	2.31	0.42
1:C:221:ARG:HD3	1:C:221:ARG:C	2.40	0.42
1:C:286:LEU:HA	1:C:290:GLU:OE1	2.19	0.42
4:F:4:PHE:HD1	4:F:27:TRP:HE3	1.68	0.42
2:B:208:ALA:HB2	2:B:304:ALA:CB	2.47	0.42
2:D:387:LEU:HD23	2:D:387:LEU:C	2.39	0.42
4:F:296:MET:SD	4:F:380:HIS:HB2	2.59	0.42
1:A:186:ASN:O	1:A:190:THR:HG22	2.20	0.42
2:D:392:SER:HB2	2:D:425:MET:CE	2.48	0.42
3:E:101:LEU:O	3:E:105:MET:HG2	2.20	0.42
4:F:148:ILE:O	4:F:182:ILE:HA	2.19	0.42
4:F:191:LEU:HD12	4:F:196:HIS:CE1	2.54	0.42
2:B:284:ARG:HG2	2:B:285:ALA:O	2.20	0.42
1:A:25:CYS:HB3	1:A:30:ILE:O	2.19	0.42
1:A:34:GLY:O	1:A:60:LYS:HA	2.19	0.42
2:B:26:ASP:OD2	2:B:369:ARG:HB2	2.19	0.42
2:B:287:THR:HB	2:B:289:PRO:HD2	2.00	0.42
2:D:48:ARG:HG2	2:D:51:VAL:HG23	2.02	0.42
1:A:93:ILE:CD1	1:A:121:ARG:HG3	2.49	0.42
1:A:401:LYS:HG3	2:B:346:TRP:CE3	2.54	0.42
1:A:408:TYR:HB3	1:A:413:MET:CE	2.48	0.42
2:B:21:TRP:CE3	2:B:63:PRO:HB3	2.54	0.42
1:C:167:LEU:N	1:C:167:LEU:HD12	2.34	0.42
1:A:210:TYR:CZ	1:A:222:PRO:HD2	2.54	0.42
2:B:48:ARG:HH22	2:B:133:GLN:HE22	1.64	0.42
2:B:323:MET:HB3	2:B:373:MET:CE	2.50	0.42
2:D:141:LEU:HD12	2:D:172:MET:SD	2.60	0.42
1:C:21:TRP:CE3	1:C:63:PRO:HB3	2.54	0.42
2:D:154:ILE:HG23	2:D:166:MET:CG	2.49	0.42
4:F:197:ARG:HB2	4:F:224:SER:O	2.20	0.42
1:A:275:VAL:HG13	1:A:368:LEU:HD21	2.01	0.42
4:F:264:PHE:HD1	4:F:264:PHE:HA	1.73	0.41
2:D:194:LEU:HD13	2:D:201:THR:HG21	2.02	0.41
4:F:320:MET:HB3	4:F:320:MET:HE3	1.93	0.41
2:D:242:LEU:HD11	8:D:503:K0M:C2	2.50	0.41
1:A:142:GLY:CA	1:A:183:GLU:HG2	2.51	0.41
4:F:176:GLN:HG3	4:F:180:HIS:CE1	2.54	0.41
4:F:263:PHE:CZ	4:F:341:LYS:HE2	2.55	0.41
1:C:25:CYS:HB3	1:C:30:ILE:O	2.20	0.41
2:D:42:LEU:HB2	2:D:358:ILE:HD11	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:LEU:HD22	1:A:110:ILE:CG2	2.51	0.41
1:A:264:ARG:HH21	1:A:428:LEU:HA	1.85	0.41
2:B:67:LEU:HD22	2:B:92:PHE:CE2	2.56	0.41
1:A:409:VAL:HA	1:A:413:MET:O	2.21	0.41
2:B:47:GLU:HG2	2:B:245:PRO:CG	2.51	0.41
2:B:231:VAL:O	2:B:235:MET:HG3	2.20	0.41
1:C:221:ARG:HG3	2:D:325:MET:SD	2.60	0.41
1:C:345:ASP:OD1	1:C:346:TRP:N	2.54	0.41
2:B:12:CYS:CB	2:B:140:SER:HB3	2.51	0.41
2:B:21:TRP:CH2	2:B:63:PRO:HB3	2.55	0.41
2:B:48:ARG:NH1	2:B:242:LEU:C	2.75	0.41
2:B:66:ILE:HD13	2:B:122:VAL:HG22	2.03	0.41
2:B:179:ASP:N	2:B:183:GLU:OE2	2.46	0.41
1:C:167:LEU:HA	1:C:200:CYS:O	2.21	0.41
3:E:65:GLU:O	3:E:69:LEU:HG	2.21	0.41
4:F:39:LEU:HA	4:F:61:LEU:O	2.20	0.41
2:B:146:GLY:O	2:B:150:GLY:HA3	2.21	0.41
2:B:396:THR:O	2:B:400:ARG:HG2	2.20	0.41
4:F:298:ILE:O	4:F:302:ILE:HG12	2.21	0.41
1:A:21:TRP:CE3	1:A:63:PRO:HB3	2.55	0.40
1:C:117:LEU:HD11	1:C:121:ARG:NH2	2.37	0.40
2:D:137:LEU:HD23	2:D:154:ILE:HD11	2.02	0.40
2:D:323:MET:HE1	2:D:373:MET:CG	2.52	0.40
4:F:173:ILE:CG2	4:F:180:HIS:HB2	2.50	0.40
4:F:220:VAL:HG12	4:F:263:PHE:CE1	2.56	0.40
1:A:233:GLN:HG3	1:A:368:LEU:HD12	2.02	0.40
1:A:311:LYS:HA	1:A:342:GLN:O	2.21	0.40
2:B:108:TYR:CD2	3:E:82:VAL:HG11	2.56	0.40
1:A:5:ILE:HB	1:A:135:PHE:CD1	2.57	0.40
1:A:139:HIS:CD2	1:A:150:THR:HG21	2.56	0.40
1:A:286:LEU:O	1:A:373:ARG:NH1	2.49	0.40
4:F:150:LYS:O	4:F:181:VAL:HG22	2.22	0.40
2:B:325:MET:HE2	2:B:355:VAL:HG21	2.03	0.40
1:C:150:THR:O	1:C:154:MET:HG2	2.22	0.40
2:D:2:ARG:HB3	2:D:133:GLN:HG2	2.02	0.40
2:D:169:PHE:HE2	2:D:238:VAL:HG21	1.87	0.40
2:D:284:ARG:O	2:D:285:ALA:CB	2.69	0.40
1:A:326:LYS:HB3	1:A:326:LYS:HE2	1.83	0.40
2:B:124:LYS:C	2:B:124:LYS:HD3	2.42	0.40
1:C:248:LEU:HD13	1:C:325:PRO:HG3	2.04	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:279:GLU:OE2	12:B:628:HOH:O[4_455]	1.99	0.21

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	436/451 (97%)	417 (96%)	18 (4%)	1 (0%)	47	56
1	C	439/451 (97%)	427 (97%)	12 (3%)	0	100	100
2	B	418/445 (94%)	401 (96%)	16 (4%)	1 (0%)	47	56
2	D	429/445 (96%)	409 (95%)	19 (4%)	1 (0%)	47	56
3	E	116/143 (81%)	115 (99%)	1 (1%)	0	100	100
4	F	342/384 (89%)	322 (94%)	20 (6%)	0	100	100
All	All	2180/2319 (94%)	2091 (96%)	86 (4%)	3 (0%)	51	63

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	220	THR
1	A	109	THR
2	D	109	THR

5.3.2 Protein sidechains [i](#)

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	369/379 (97%)	365 (99%)	4 (1%)	73	84
1	C	372/379 (98%)	368 (99%)	4 (1%)	73	84
2	B	364/383 (95%)	362 (100%)	2 (0%)	88	94
2	D	368/383 (96%)	362 (98%)	6 (2%)	62	75
3	E	107/127 (84%)	105 (98%)	2 (2%)	57	68
4	F	314/342 (92%)	312 (99%)	2 (1%)	86	93
All	All	1894/1993 (95%)	1874 (99%)	20 (1%)	73	84

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	GLU
1	A	178	SER
1	A	219	ILE
1	A	221	ARG
2	B	139	HIS
2	B	255	LEU
1	C	1	MET
1	C	221	ARG
1	C	284	GLU
1	C	381	THR
2	D	139	HIS
2	D	159	GLU
2	D	229	HIS
2	D	247	GLN
2	D	248	LEU
2	D	255	LEU
3	E	60	ARG
3	E	136	ASN
4	F	142	ARG
4	F	264	PHE

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

Mol	Chain	Res	Type
1	A	88	HIS
1	A	101	ASN
1	A	258	ASN
1	A	283	HIS
2	B	133	GLN

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Mol	Chain	Res	Type
2	B	167	ASN
2	B	294	GLN
2	B	300	ASN
1	C	11	GLN
1	C	101	ASN
1	C	285	GLN
2	D	37	HIS
2	D	167	ASN
2	D	247	GLN
2	D	249	ASN
3	E	136	ASN
4	F	178	GLN
4	F	180	HIS
4	F	229	ASN
4	F	242	ASN
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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 8 are monoatomic - leaving 10 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	GDP	D	501	6	24,30,30	1.19	2 (8%)	31,47,47	1.91	8 (25%)
5	GTP	A	501	6	26,34,34	1.00	1 (3%)	33,54,54	1.73	7 (21%)
5	GTP	C	501	6	26,34,34	1.00	1 (3%)	33,54,54	1.75	6 (18%)
10	MES	B	504	-	12,12,12	2.24	1 (8%)	14,16,16	1.94	5 (35%)
8	K0M	D	503	-	10,16,16	0.74	0	12,22,22	0.74	0
8	K0M	D	504	-	10,16,16	0.75	0	12,22,22	0.71	0
9	GDP	B	501	6	24,30,30	1.20	2 (8%)	31,47,47	1.92	8 (25%)
8	K0M	B	505	-	10,16,16	0.75	0	12,22,22	0.74	0
8	K0M	A	504	-	10,16,16	0.74	0	12,22,22	0.71	0
11	ACP	F	401	6	27,33,33	1.39	5 (18%)	32,52,52	1.51	4 (12%)

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	GDP	D	501	6	-	6/12/32/32	0/3/3/3
5	GTP	A	501	6	-	6/18/38/38	0/3/3/3
5	GTP	C	501	6	-	7/18/38/38	0/3/3/3
10	MES	B	504	-	-	4/6/14/14	0/1/1/1
8	K0M	D	503	-	-	0/3/8/8	0/2/2/2
8	K0M	D	504	-	-	0/3/8/8	0/2/2/2
9	GDP	B	501	6	-	3/12/32/32	0/3/3/3
8	K0M	B	505	-	-	0/3/8/8	0/2/2/2
8	K0M	A	504	-	-	0/3/8/8	0/2/2/2
11	ACP	F	401	6	-	11/15/38/38	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	504	MES	C8-S	-7.48	1.66	1.77
9	D	501	GDP	C6-C5	4.20	1.48	1.41
9	B	501	GDP	C6-C5	4.15	1.48	1.41
5	A	501	GTP	C6-N1	3.25	1.38	1.33
5	C	501	GTP	C6-N1	3.20	1.38	1.33
11	F	401	ACP	PG-O3G	2.99	1.61	1.54
11	F	401	ACP	PG-O2G	2.91	1.61	1.54
11	F	401	ACP	PB-O3A	2.75	1.61	1.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	F	401	ACP	C5-C4	2.52	1.47	1.40
9	D	501	GDP	C5-C4	2.45	1.47	1.40
9	B	501	GDP	C5-C4	2.37	1.47	1.40
11	F	401	ACP	PB-O2B	2.23	1.61	1.56

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	501	GTP	N3-C2-N1	-5.31	120.14	127.22
5	A	501	GTP	N3-C2-N1	-5.16	120.34	127.22
9	D	501	GDP	C2-N3-C4	4.98	121.05	115.36
9	B	501	GDP	C2-N3-C4	4.92	120.98	115.36
5	C	501	GTP	C2-N3-C4	4.36	120.33	115.36
11	F	401	ACP	PA-O3A-PB	-4.16	119.36	132.56
5	A	501	GTP	C2-N3-C4	4.14	120.09	115.36
9	B	501	GDP	C6-C5-C4	-4.06	116.92	120.80
9	B	501	GDP	C6-N1-C2	4.03	122.33	115.93
9	D	501	GDP	C6-N1-C2	4.03	122.33	115.93
9	D	501	GDP	C5-C6-N1	-4.01	117.95	123.43
9	B	501	GDP	C5-C6-N1	-3.87	118.13	123.43
10	B	504	MES	C5-N4-C3	3.70	117.16	108.83
11	F	401	ACP	C3'-C2'-C1'	3.67	106.51	100.98
9	D	501	GDP	C6-C5-C4	-3.57	117.39	120.80
9	B	501	GDP	N3-C2-N1	-3.37	122.73	127.22
9	D	501	GDP	N3-C2-N1	-3.27	122.86	127.22
5	A	501	GTP	PB-O3B-PG	-3.14	122.04	132.83
5	C	501	GTP	C5-C6-N1	-3.10	119.20	123.43
5	A	501	GTP	C5-C6-N1	-3.07	119.23	123.43
11	F	401	ACP	N3-C2-N1	-3.04	123.92	128.68
9	B	501	GDP	C4-C5-N7	-2.95	106.33	109.40
10	B	504	MES	C6-C5-N4	-2.95	105.64	110.10
5	C	501	GTP	PB-O3B-PG	-2.93	122.78	132.83
9	D	501	GDP	PA-O3A-PB	-2.83	123.12	132.83
9	D	501	GDP	C4-C5-N7	-2.80	106.48	109.40
11	F	401	ACP	C4-C5-N7	-2.70	106.58	109.40
5	C	501	GTP	C6-N1-C2	2.65	120.15	115.93
9	B	501	GDP	PA-O3A-PB	-2.60	123.91	132.83
10	B	504	MES	O1S-S-C8	2.55	109.99	106.92
5	A	501	GTP	C6-N1-C2	2.50	119.90	115.93
5	A	501	GTP	PA-O3A-PB	-2.47	124.35	132.83
10	B	504	MES	C7-N4-C5	2.37	117.30	111.23
10	B	504	MES	O3S-S-C8	2.28	109.46	105.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	501	GTP	O3G-PG-O3B	2.27	112.26	104.64
5	C	501	GTP	PA-O3A-PB	-2.26	125.06	132.83
9	D	501	GDP	C3'-C2'-C1'	2.14	104.20	100.98
9	B	501	GDP	O2B-PB-O3A	2.07	111.58	104.64

There are no chirality outliers.

All (37) 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-O1A
5	A	501	GTP	C5'-O5'-PA-O2A
5	C	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O2A
9	B	501	GDP	C5'-O5'-PA-O1A
9	B	501	GDP	C5'-O5'-PA-O2A
9	D	501	GDP	PA-O3A-PB-O2B
9	D	501	GDP	PA-O3A-PB-O3B
9	D	501	GDP	C5'-O5'-PA-O3A
9	D	501	GDP	C5'-O5'-PA-O2A
10	B	504	MES	C8-C7-N4-C5
11	F	401	ACP	PB-C3B-PG-O1G
11	F	401	ACP	PB-C3B-PG-O2G
11	F	401	ACP	PB-C3B-PG-O3G
11	F	401	ACP	PG-C3B-PB-O1B
11	F	401	ACP	PG-C3B-PB-O3A
11	F	401	ACP	C5'-O5'-PA-O1A
11	F	401	ACP	C3'-C4'-C5'-O5'
11	F	401	ACP	O4'-C4'-C5'-O5'
10	B	504	MES	C7-C8-S-O3S
9	B	501	GDP	C5'-O5'-PA-O3A
11	F	401	ACP	C5'-O5'-PA-O3A
11	F	401	ACP	C5'-O5'-PA-O2A
10	B	504	MES	C7-C8-S-O1S
10	B	504	MES	C7-C8-S-O2S
5	A	501	GTP	C4'-C5'-O5'-PA
5	C	501	GTP	C4'-C5'-O5'-PA
9	D	501	GDP	PA-O3A-PB-O1B
5	C	501	GTP	PB-O3B-PG-O2G
5	C	501	GTP	PB-O3B-PG-O3G
11	F	401	ACP	PB-O3A-PA-O2A
5	A	501	GTP	C5'-O5'-PA-O3A

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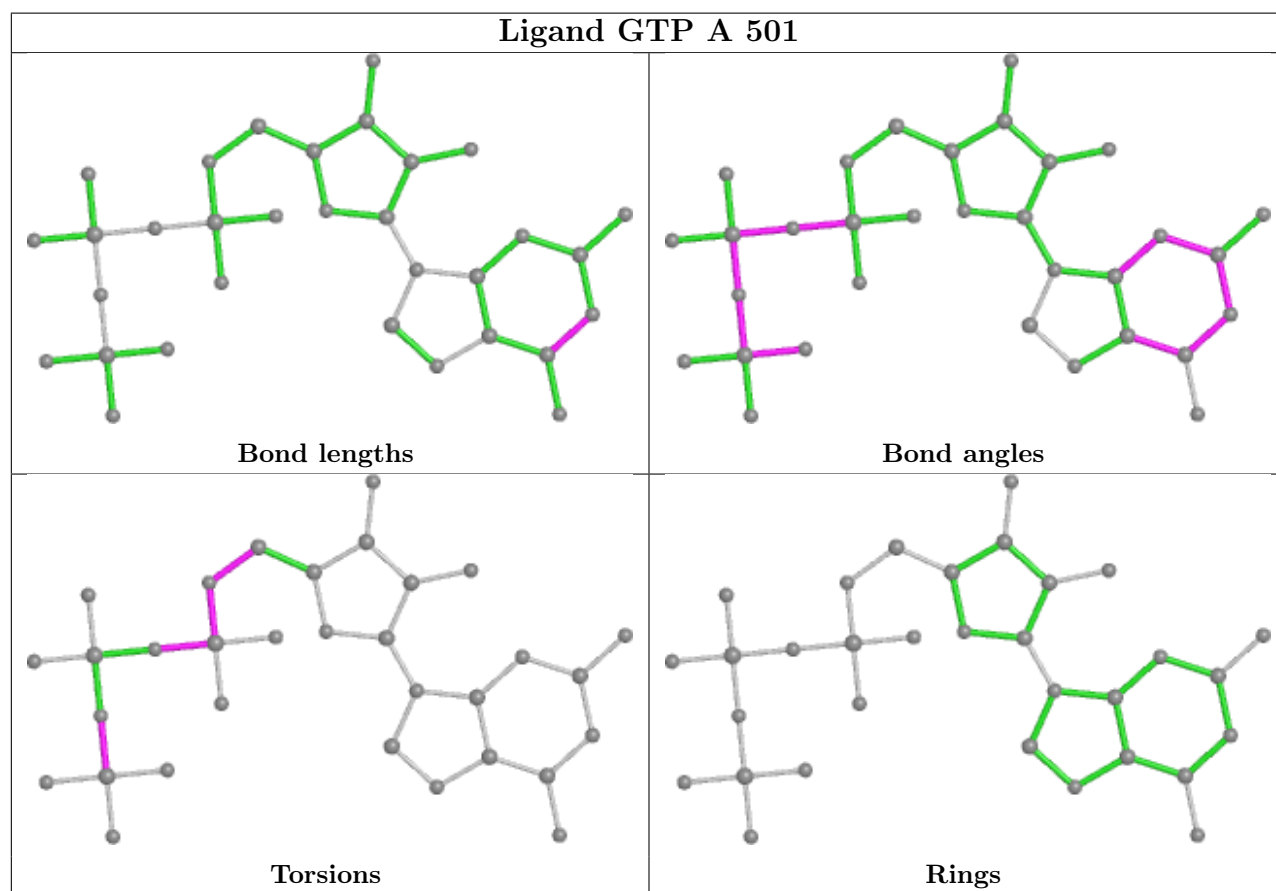
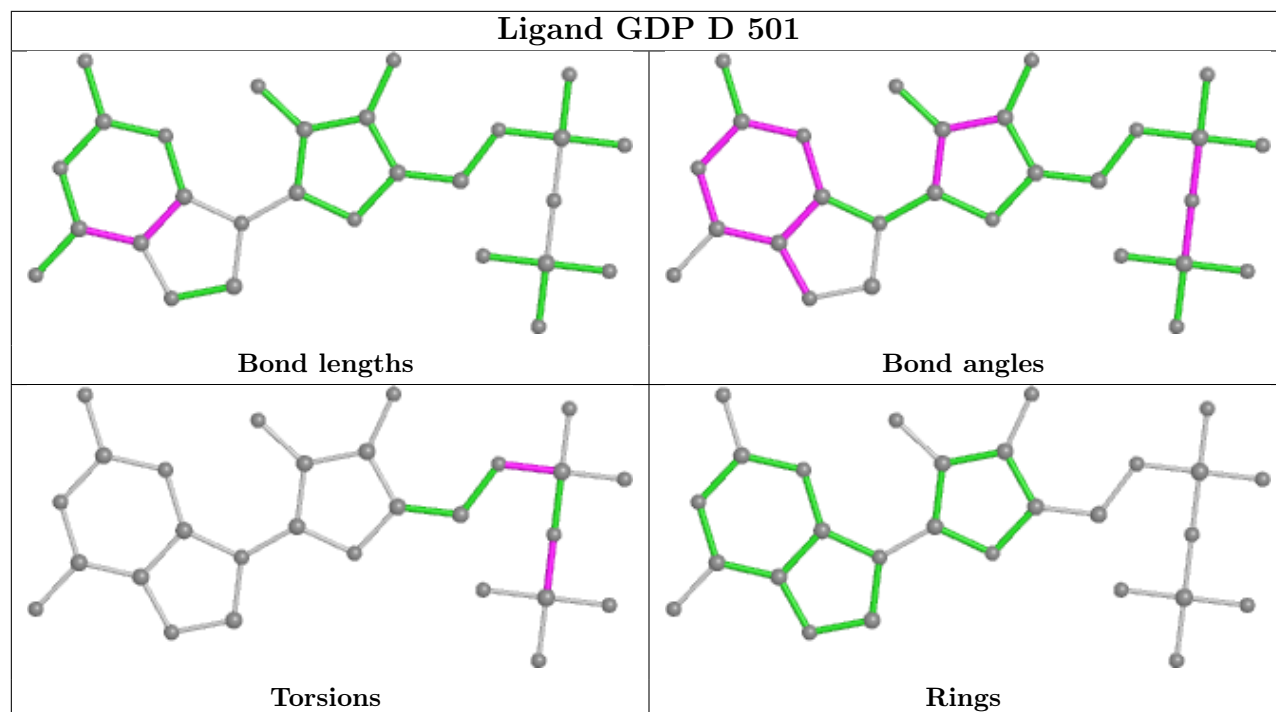
Mol	Chain	Res	Type	Atoms
5	C	501	GTP	C5'-O5'-PA-O3A
5	A	501	GTP	PB-O3A-PA-O2A
5	C	501	GTP	PB-O3A-PA-O2A
9	D	501	GDP	C5'-O5'-PA-O1A

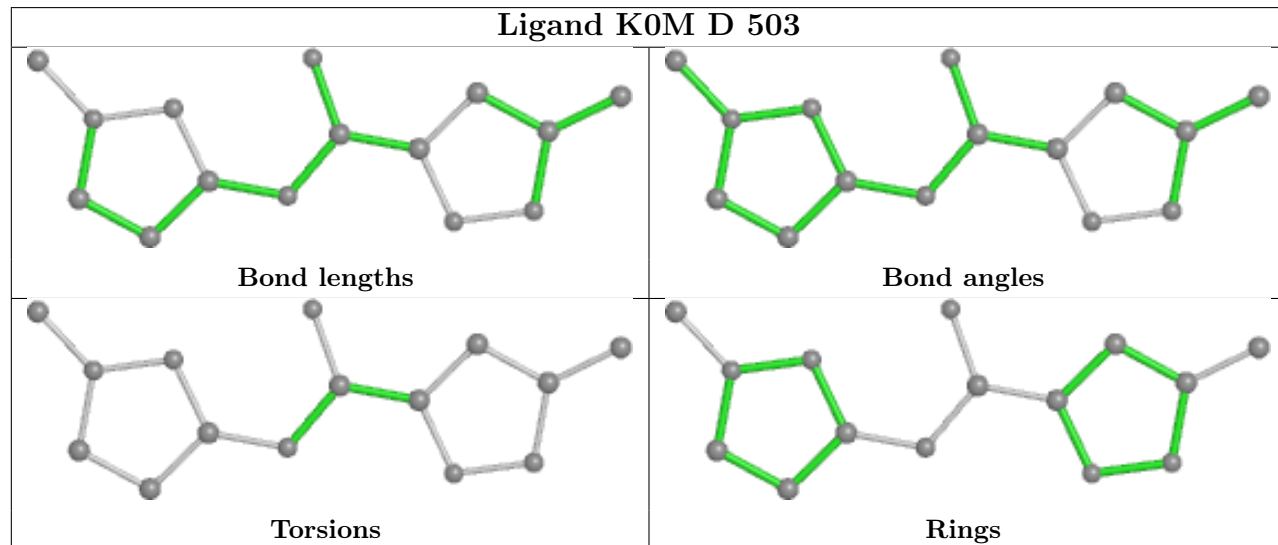
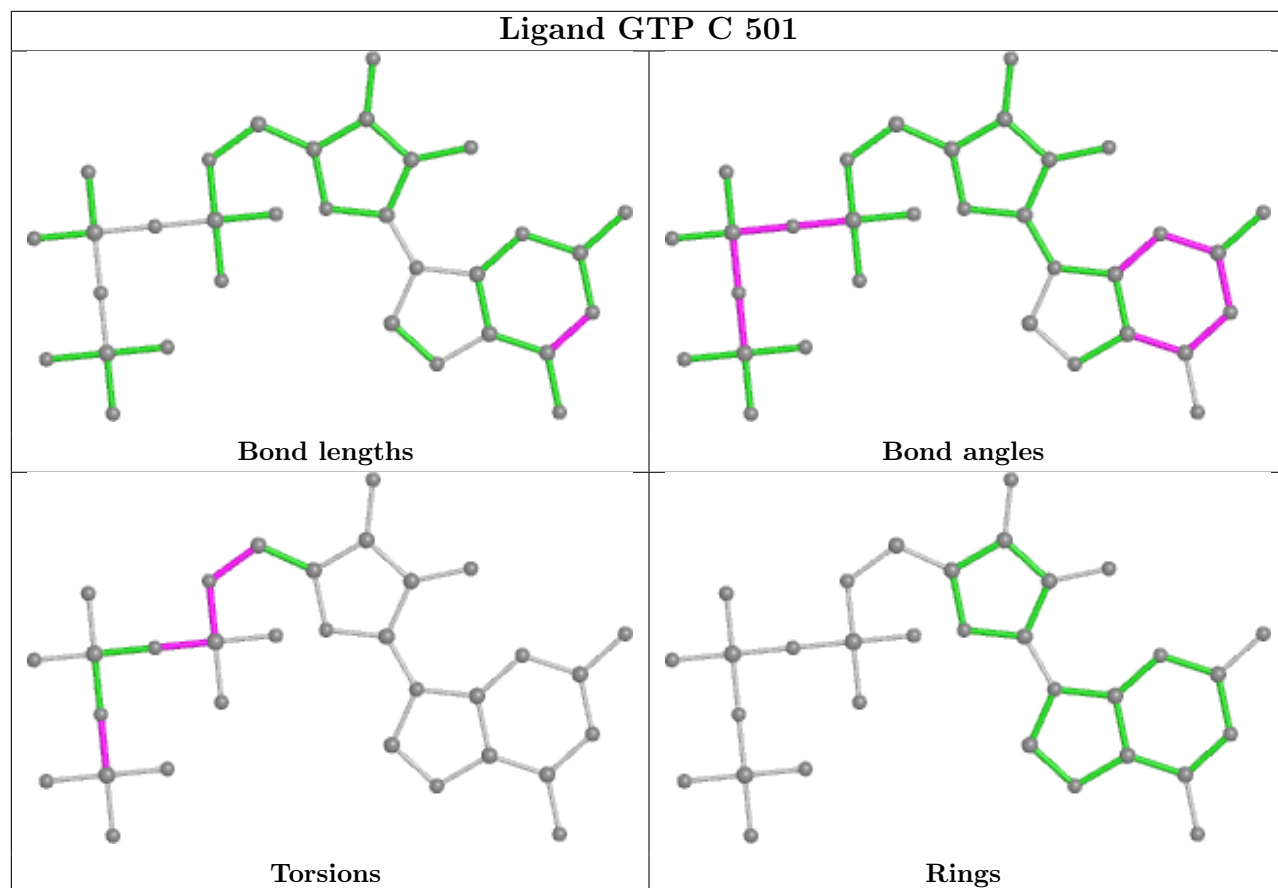
There are no ring outliers.

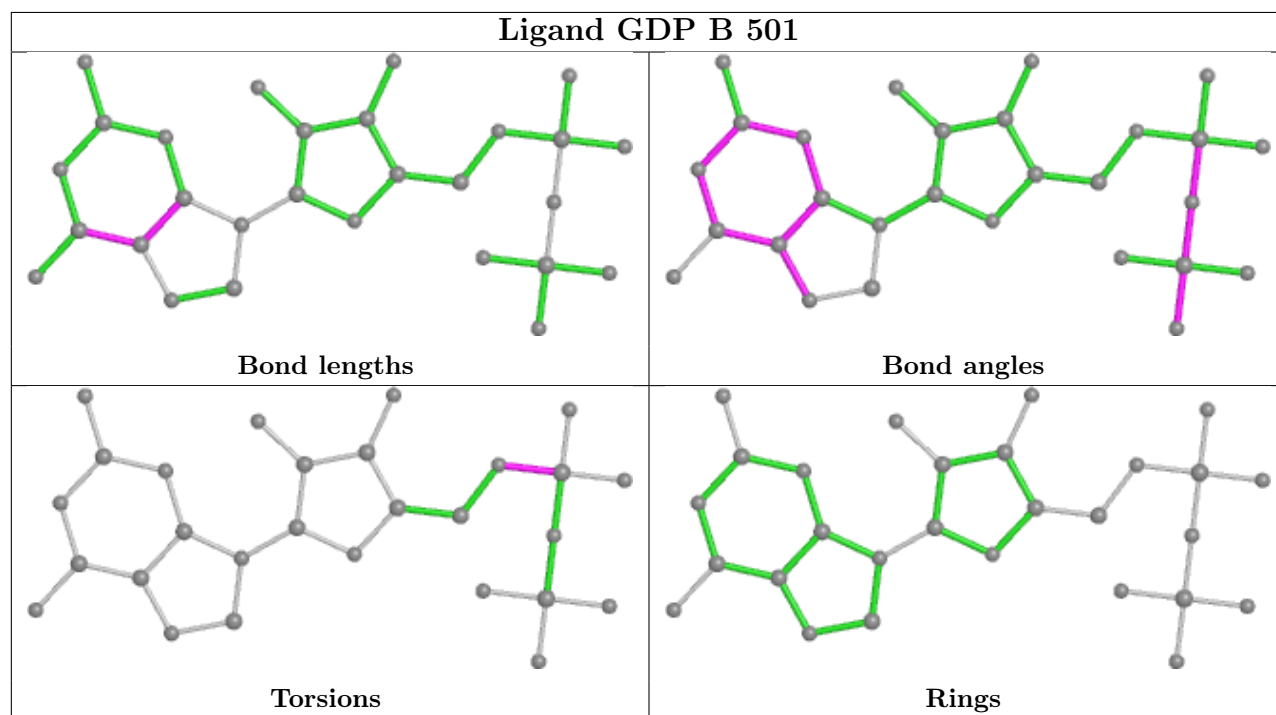
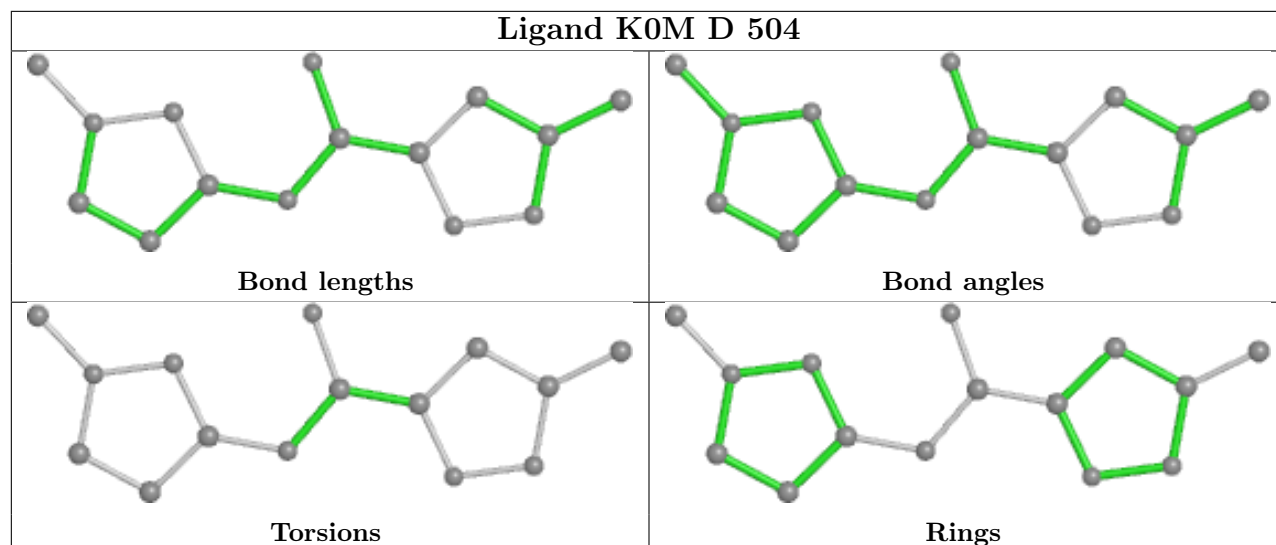
6 monomers are involved in 16 short contacts:

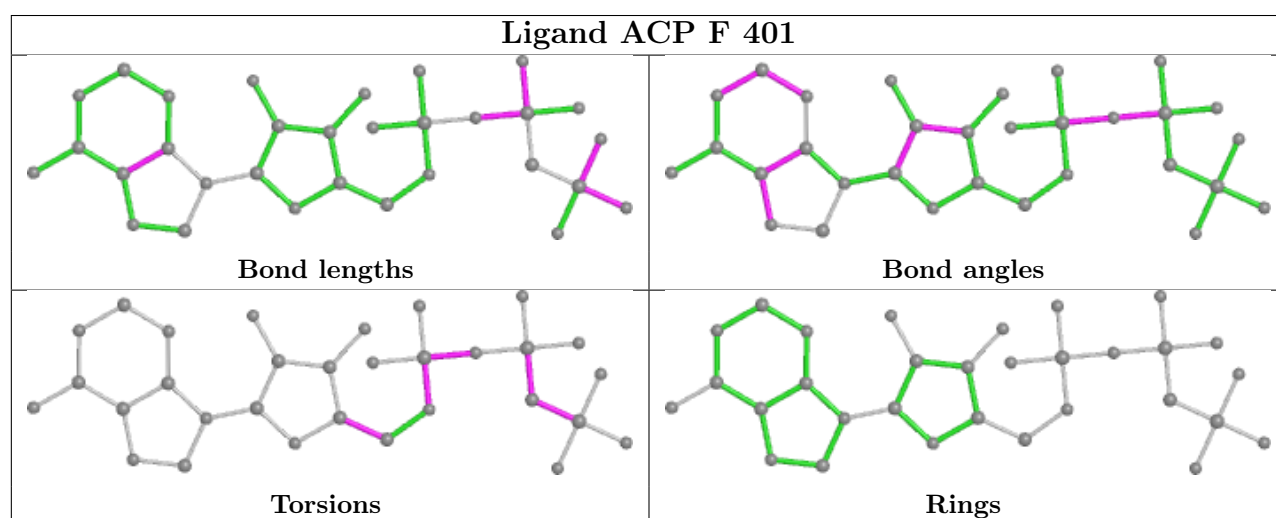
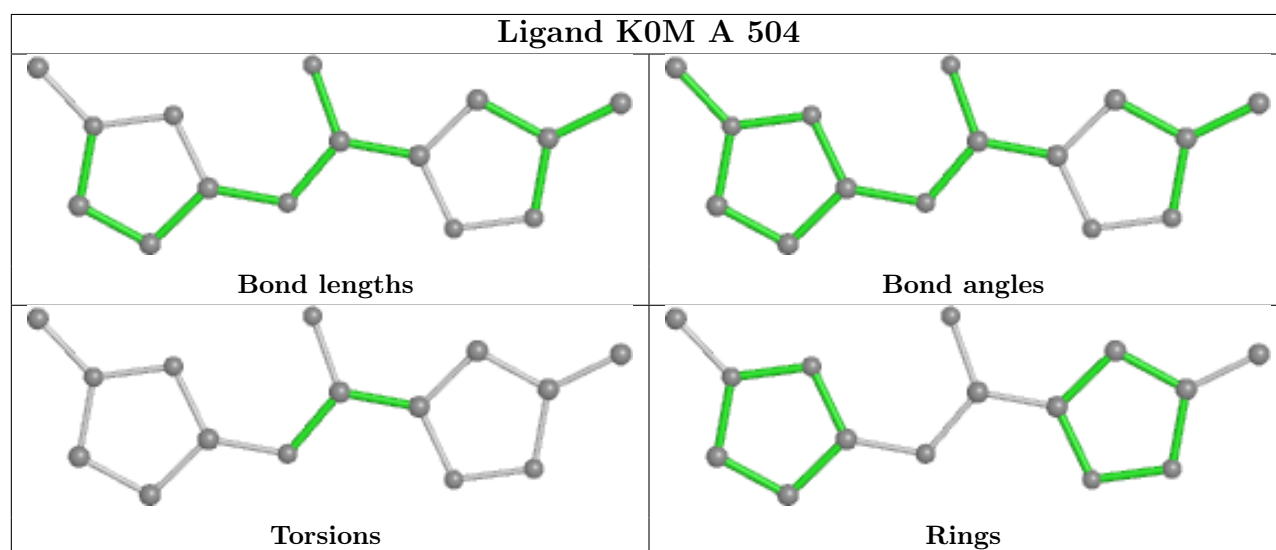
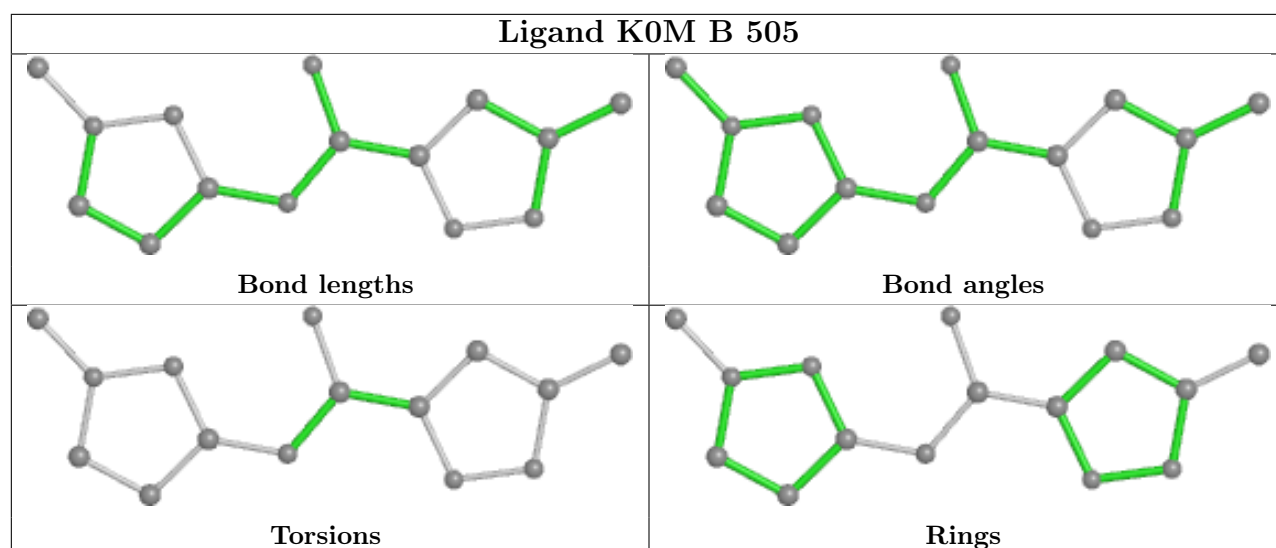
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	D	501	GDP	3	0
5	C	501	GTP	1	0
10	B	504	MES	3	0
8	D	503	K0M	3	0
9	B	501	GDP	1	0
11	F	401	ACP	5	0

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.









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

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	438/451 (97%)	0.70	38 (8%)	10 15	55, 70, 103, 143	0
1	C	440/451 (97%)	0.92	30 (6%)	17 25	53, 64, 90, 152	0
2	B	421/445 (94%)	0.94	50 (11%)	4 7	52, 68, 118, 193	5 (1%)
2	D	431/445 (96%)	0.91	60 (13%)	2 4	63, 87, 126, 168	6 (1%)
3	E	120/143 (83%)	1.73	33 (27%)	0 0	59, 89, 142, 189	0
4	F	350/384 (91%)	1.23	70 (20%)	1 2	68, 91, 143, 184	0
All	All	2200/2319 (94%)	0.97	281 (12%)	3 6	52, 76, 124, 193	11 (0%)

All (281) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	E	50	ILE	11.3
3	E	57	ALA	11.3
3	E	53	LYS	10.0
2	B	57	THR	8.0
2	B	283	TYR	8.0
3	E	49	GLU	7.8
3	E	68	LEU	7.4
3	E	48	GLU	7.4
4	F	105	LEU	7.3
4	F	253	TYR	7.2
4	F	177	GLY	7.0
3	E	54	LEU	6.9
2	B	285	ALA	6.6
2	D	335	VAL	6.5
2	B	48	ARG	6.4
4	F	247	LYS	6.2
4	F	249	TYR	5.5
3	E	64	GLN	5.4
4	F	248	GLU	5.4

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Mol	Chain	Res	Type	RSRZ
2	B	325	MET	5.3
1	C	340	SER	5.2
2	D	369	ARG	5.1
4	F	325	LEU	5.1
3	E	51	GLN	5.0
2	D	218	LYS	5.0
3	E	62	LYS	4.9
2	D	360	PRO	4.9
1	A	262	TYR	4.7
4	F	199	PHE	4.6
2	B	437	ASP	4.6
4	F	250	SER	4.6
4	F	49	PHE	4.5
4	F	267	PHE	4.5
3	E	126	LYS	4.4
3	E	123	LEU	4.4
2	B	284	ARG	4.4
2	D	373	MET	4.3
4	F	254	GLY	4.3
4	F	125	THR	4.3
3	E	55	GLU	4.2
1	C	285	GLN	4.2
4	F	240	LEU	4.1
3	E	61	ARG	4.1
1	A	335	ILE	4.1
2	D	42	LEU	4.1
2	B	436	GLN	4.0
4	F	201	ILE	4.0
1	A	351	PHE	4.0
2	D	94	PHE	4.0
4	F	46	ARG	3.9
2	B	291	LEU	3.9
2	B	286	LEU	3.9
4	F	243	HIS	3.9
4	F	256	TYR	3.9
2	B	83	PHE	3.9
2	D	272	PHE	3.8
4	F	36	ARG	3.8
2	D	370	GLY	3.8
2	D	322	ARG	3.8
1	A	215	ARG	3.8
4	F	315	PHE	3.7

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Mol	Chain	Res	Type	RSRZ
4	F	290	ILE	3.7
2	D	121	VAL	3.7
1	A	341	ILE	3.7
2	D	215	ARG	3.7
1	C	218	ASP	3.7
3	E	24	LEU	3.6
4	F	192	LEU	3.6
3	E	72	LEU	3.6
2	B	219	LEU	3.6
1	A	346	TRP	3.6
4	F	178	GLN	3.5
2	D	338	LYS	3.5
1	C	368	LEU	3.5
4	F	244	CYS	3.5
2	B	372	LYS	3.4
1	A	312	TYR	3.4
2	D	325	MET	3.4
2	D	429	VAL	3.4
4	F	173	ILE	3.4
1	A	437	VAL	3.3
1	C	221	ARG	3.3
4	F	181	VAL	3.3
2	B	371	LEU	3.3
2	D	278	ARG	3.3
2	D	214	PHE	3.3
1	A	418	PHE	3.3
2	D	320	ARG	3.3
2	D	319	PHE	3.2
2	B	321	GLY	3.2
3	E	76	ARG	3.2
2	D	244	PHE	3.2
1	C	440	VAL	3.2
2	B	288	VAL	3.2
4	F	20	LEU	3.2
2	D	279	GLY	3.1
4	F	37	PHE	3.1
3	E	66	ALA	3.1
2	D	137	LEU	3.1
1	C	68	VAL	3.1
1	A	282	TYR	3.1
4	F	372	THR	3.1
4	F	221	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
2	D	339	ASN	3.0
1	A	221	ARG	3.0
2	B	312	TYR	3.0
1	C	214	ARG	3.0
1	C	335	ILE	2.9
3	E	47	LEU	2.9
4	F	343	TYR	2.9
1	A	332	ILE	2.9
1	C	215	ARG	2.9
2	D	37	HIS	2.9
2	D	216	THR	2.9
1	C	245	ASP	2.9
1	A	342	GLN	2.9
2	D	249	ASN	2.9
4	F	330	ILE	2.9
2	B	218	LYS	2.9
2	D	342	TYR	2.9
3	E	59	GLU	2.9
2	D	267	PHE	2.9
2	D	291	LEU	2.9
1	A	196	GLU	2.8
2	B	220	THR	2.8
1	A	438	ASP	2.8
4	F	381	HIS	2.8
3	E	128	LYS	2.8
4	F	99	VAL	2.8
1	A	285	GLN	2.8
4	F	101	TYR	2.8
2	B	124	LYS	2.8
4	F	89	GLU	2.8
1	A	68	VAL	2.7
4	F	13	VAL	2.7
4	F	131	PHE	2.7
1	C	289	ALA	2.7
3	E	58	GLU	2.7
4	F	241	THR	2.7
4	F	246	GLN	2.7
2	D	283	TYR	2.7
2	D	313	LEU	2.7
2	D	86	ILE	2.7
4	F	255	ARG	2.7
2	D	401	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
3	E	125	GLU	2.6
1	C	357	TYR	2.6
4	F	52	LEU	2.6
4	F	359	PHE	2.6
4	F	100	ILE	2.6
4	F	327	VAL	2.6
4	F	362	ALA	2.6
4	F	39	LEU	2.6
4	F	320	MET	2.6
1	C	176	GLN	2.6
2	B	370	GLY	2.6
1	A	340	SER	2.6
3	E	69	LEU	2.6
4	F	190	LEU	2.6
2	B	311	ARG	2.5
2	D	418	PHE	2.5
2	D	336	GLN	2.5
2	B	342	TYR	2.5
2	B	358	ILE	2.5
2	D	157	ILE	2.5
1	A	397	LEU	2.5
1	C	302	MET	2.5
2	D	195	VAL	2.5
1	A	301	GLN	2.5
2	B	339	ASN	2.5
4	F	4	PHE	2.5
2	D	219	LEU	2.5
1	A	232	SER	2.5
2	B	275	LEU	2.5
2	D	1	MET	2.5
2	D	312	TYR	2.5
1	C	5	ILE	2.5
4	F	11	SER	2.4
2	B	434	GLN	2.4
2	B	340	SER	2.4
2	D	123	ARG	2.4
4	F	169	LEU	2.4
4	F	284	LEU	2.4
2	D	372	LYS	2.4
1	A	412	GLY	2.4
2	B	221	THR	2.4
4	F	50	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
3	E	121	GLU	2.4
1	A	87	PHE	2.4
2	B	337	ASN	2.4
2	D	353	THR	2.4
2	D	281	GLN	2.4
3	E	65	GLU	2.4
2	B	222	PRO	2.4
1	A	371	VAL	2.4
1	C	295	CYS	2.4
2	D	153	LEU	2.4
4	F	314	LEU	2.4
1	A	348	PRO	2.4
1	A	339	ARG	2.3
4	F	298	ILE	2.3
1	A	299	ALA	2.3
1	A	235	VAL	2.3
2	D	93	VAL	2.3
1	C	341	ILE	2.3
2	B	360	PRO	2.3
1	C	201	ALA	2.3
2	D	48	ARG	2.3
2	D	295	MET	2.3
2	B	296	PHE	2.3
4	F	220	VAL	2.3
2	B	7	ILE	2.3
2	D	274	PRO	2.3
1	A	311	LYS	2.3
1	C	339	ARG	2.3
3	E	56	ALA	2.3
1	A	152	LEU	2.3
2	D	292	THR	2.3
1	A	176	GLN	2.3
2	B	216	THR	2.3
1	C	308	ARG	2.3
1	C	351	PHE	2.3
1	C	286	LEU	2.2
2	B	59	ASN	2.2
4	F	198	LYS	2.2
4	F	126	ASP	2.2
1	A	5	ILE	2.2
1	C	299	ALA	2.2
1	A	167	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	230	LEU	2.2
4	F	262	MET	2.2
2	D	343	PHE	2.2
3	E	122	ARG	2.2
2	D	238	VAL	2.2
1	A	136	LEU	2.2
2	B	42	LEU	2.2
2	B	58	GLY	2.2
2	D	377	PHE	2.2
2	D	413	MET	2.2
2	B	435	TYR	2.2
4	F	332	VAL	2.2
2	B	343	PHE	2.2
3	E	52	LYS	2.2
2	B	217	LEU	2.2
1	C	220	GLU	2.2
4	F	44	ARG	2.1
1	A	316	CYS	2.1
4	F	73	ARG	2.1
1	C	275	VAL	2.1
3	E	133	VAL	2.1
2	B	287	THR	2.1
4	F	188	LYS	2.1
2	D	227	LEU	2.1
3	E	60	ARG	2.1
1	C	434	GLU	2.1
1	A	267	PHE	2.1
1	C	7	ILE	2.1
4	F	136	ASN	2.1
2	B	89	PRO	2.1
2	D	132	LEU	2.1
3	E	106	GLU	2.1
2	B	292	THR	2.1
2	B	210	TYR	2.1
1	A	378	LEU	2.1
3	E	116	LEU	2.1
2	B	332	MET	2.1
4	F	153	ALA	2.1
1	C	135	PHE	2.1
2	D	371	LEU	2.1
2	D	120	ASP	2.1
2	B	93	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
2	D	68	VAL	2.1
4	F	132	LEU	2.0
4	F	346	LEU	2.0
1	C	74	VAL	2.0
2	D	344	VAL	2.0
4	F	252	ASN	2.0
2	B	90	ASP	2.0
2	B	351	VAL	2.0
2	B	377	PHE	2.0
4	F	161	LEU	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 monosaccharides 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(Å ²)	Q<0.9
6	MG	F	402	1/1	0.03	0.17	114,114,114,114	0
7	CA	A	503	1/1	0.46	0.64	138,138,138,138	0
6	MG	C	502	1/1	0.81	0.20	69,69,69,69	0
11	ACP	F	401	31/31	0.88	0.12	86,108,118,125	0
10	MES	B	504	12/12	0.89	0.15	85,91,100,100	0
6	MG	D	502	1/1	0.89	0.14	80,80,80,80	0
8	K0M	D	503	15/15	0.92	0.24	67,74,89,89	25
8	K0M	D	504	15/15	0.92	0.18	68,82,108,108	0
6	MG	B	502	1/1	0.92	0.23	51,51,51,51	0
8	K0M	B	505	15/15	0.92	0.17	60,69,86,86	0
7	CA	C	503	1/1	0.93	0.16	73,73,73,73	0
7	CA	B	503	1/1	0.94	0.34	110,110,110,110	0
9	GDP	D	501	28/28	0.94	0.14	73,82,88,90	0

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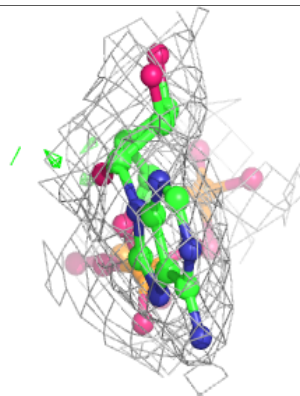
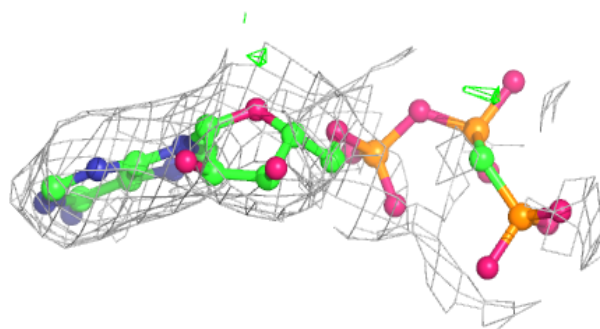
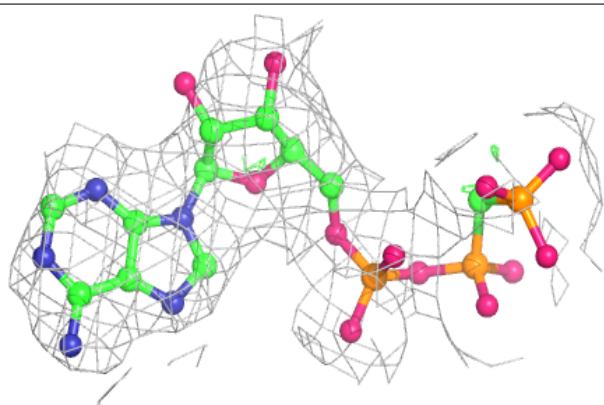
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	GTP	A	501	32/32	0.95	0.15	53,57,61,62	0
5	GTP	C	501	32/32	0.96	0.19	57,59,66,72	0
8	K0M	A	504	15/15	0.96	0.18	60,69,88,89	0
9	GDP	B	501	28/28	0.97	0.19	50,54,57,62	0
6	MG	A	502	1/1	0.97	0.12	56,56,56,56	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.

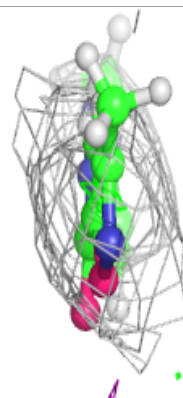
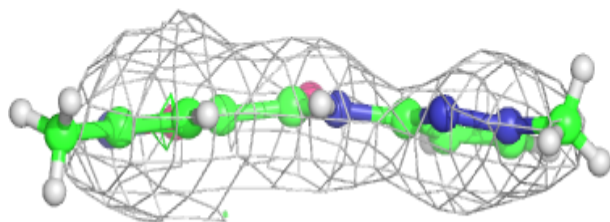
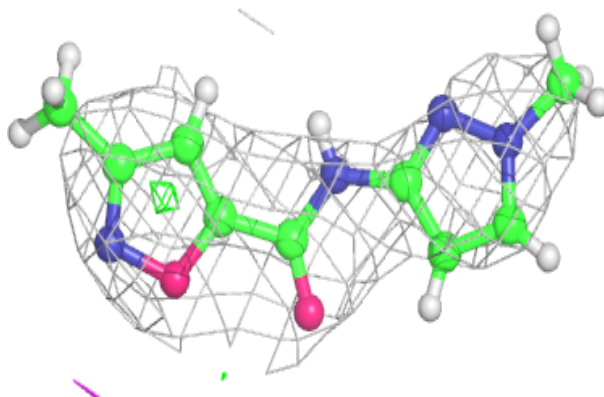
Electron density around ACP F 401:

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

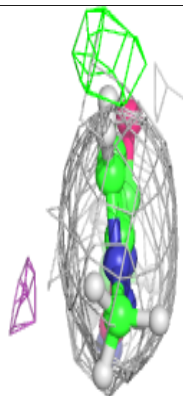
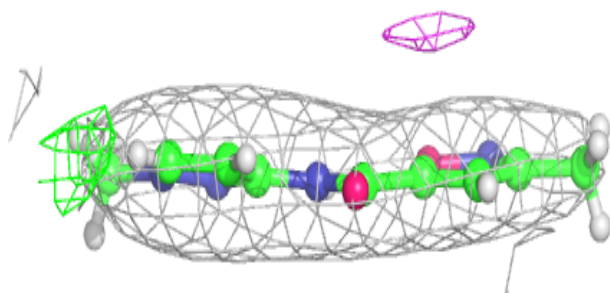
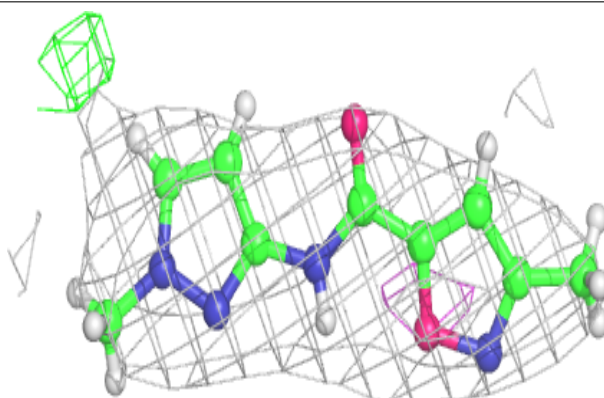


Electron density around K0M D 503:

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

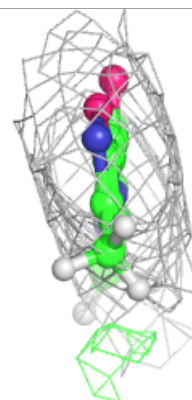
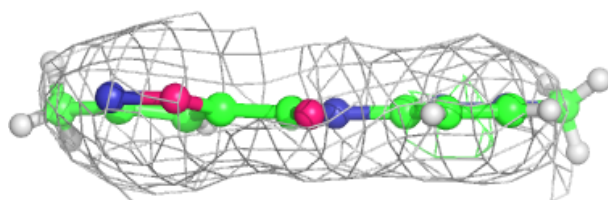
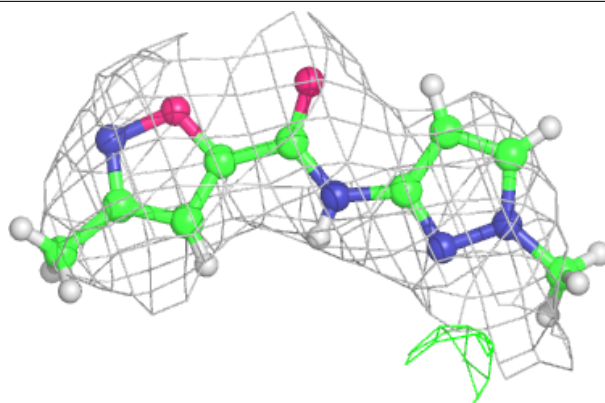
**Electron density around K0M D 504:**

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



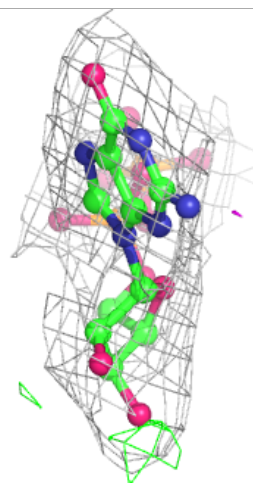
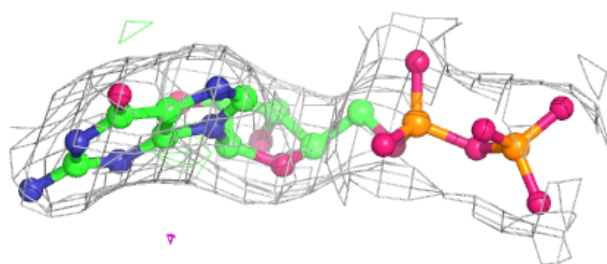
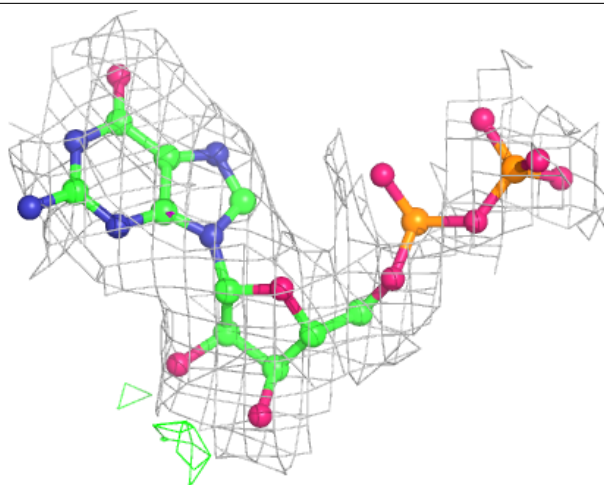
Electron density around K0M B 505:

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



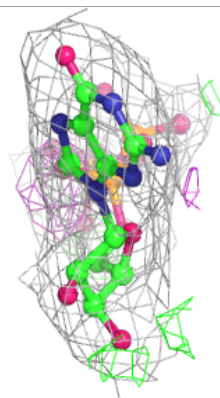
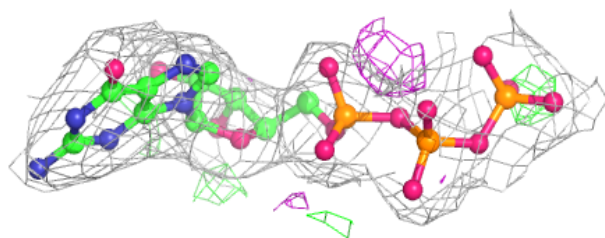
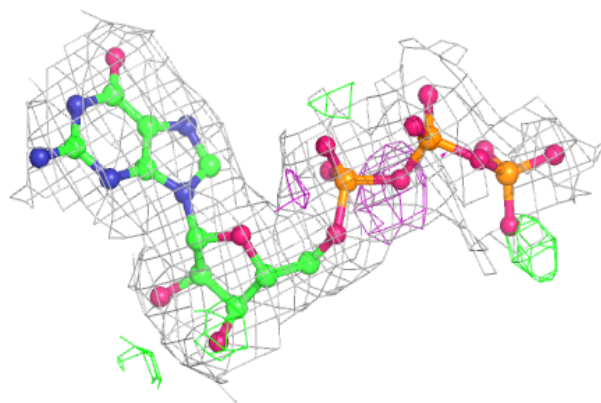
Electron density around GDP D 501:

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

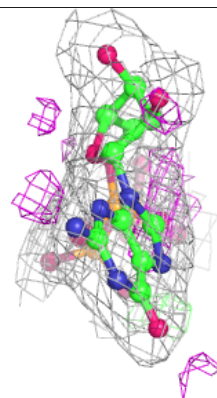
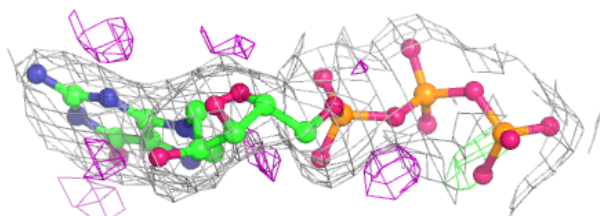
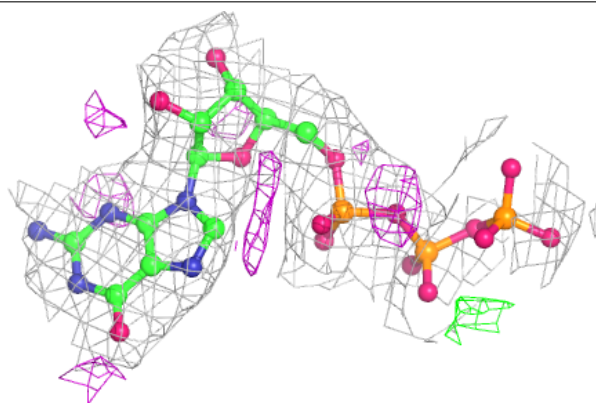


Electron density around GTP A 501:

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

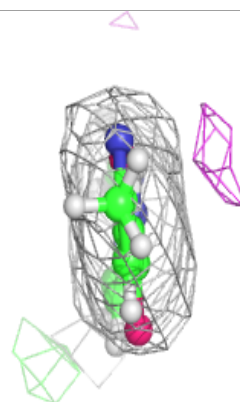
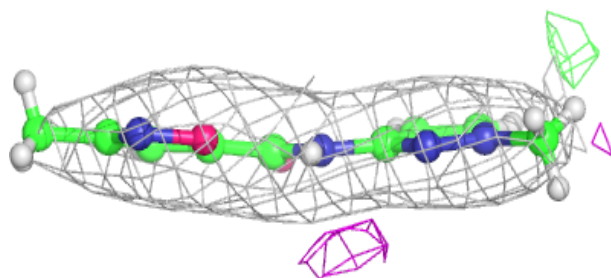
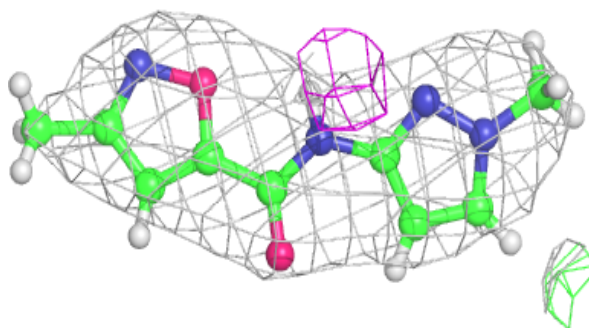
**Electron density around GTP C 501:**

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

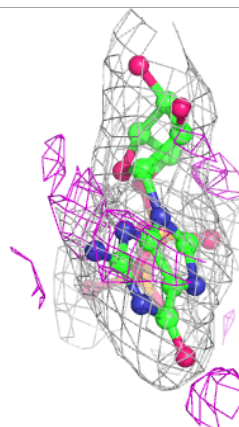
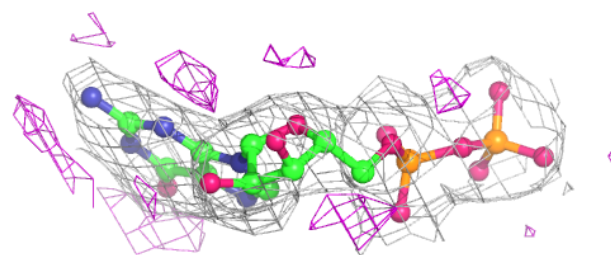
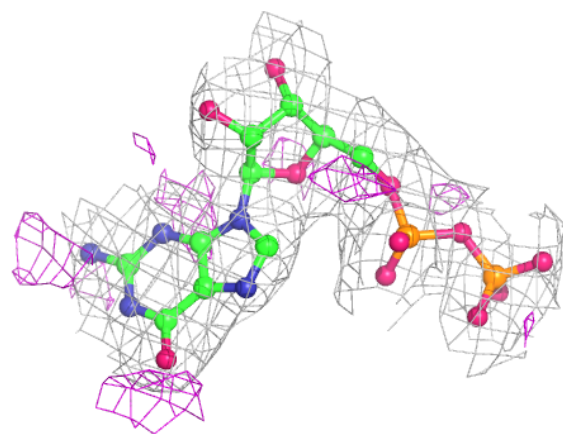


Electron density around K0M A 504:

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

**Electron density around 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.