



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 11:41 AM UTC

PDB ID : 5S4S / pdb_00005s4s
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 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

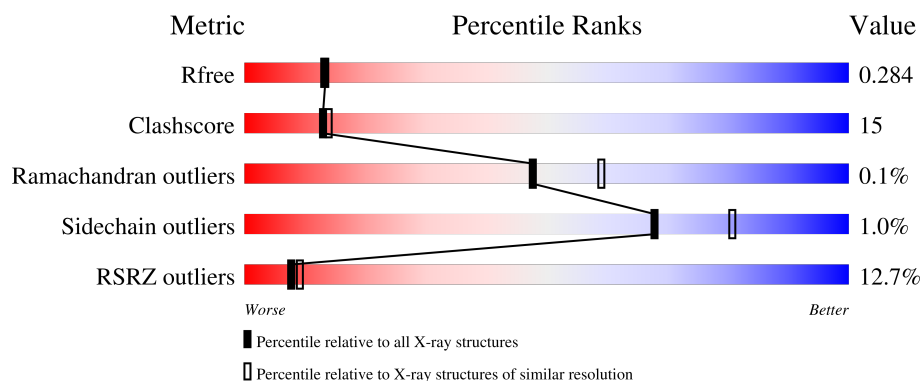
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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}	180053	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (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	9% 68% 29% .
1	C	451	8% 73% 24% .
2	B	445	13% 61% 33% 5% .
2	D	445	15% 66% 31% .
3	E	143	18% 67% 16% . 16%

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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: red (14%), green (65%), yellow (26%), and grey (9%). The percentages are labeled below the bar segments.

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 (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



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

- 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		
6	D	1	Total	Mg	0	0
			1	1		

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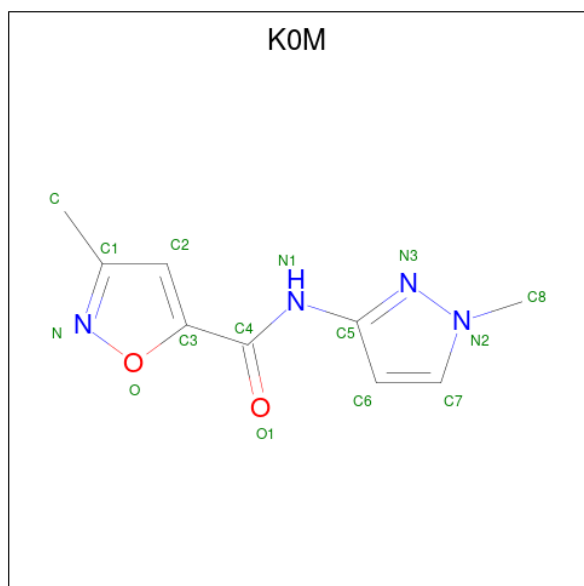
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	F	1	Total	Mg	0	0
			1	1		

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

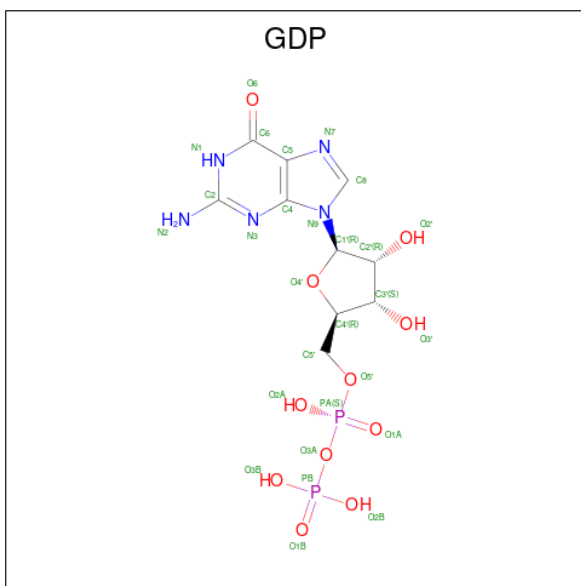
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Ca	0	0
			1	1		
7	B	1	Total	Ca	0	0
			1	1		
7	C	1	Total	Ca	0	0
			1	1		

- Molecule 8 is 3-methyl-N-(1-methyl-1H-pyrazol-3-yl)-1,2-oxazole-5-carboxamide (CCD ID: K0M) (formula: C₉H₁₀N₄O₂) (labeled as "Ligand of Interest" by depositor).



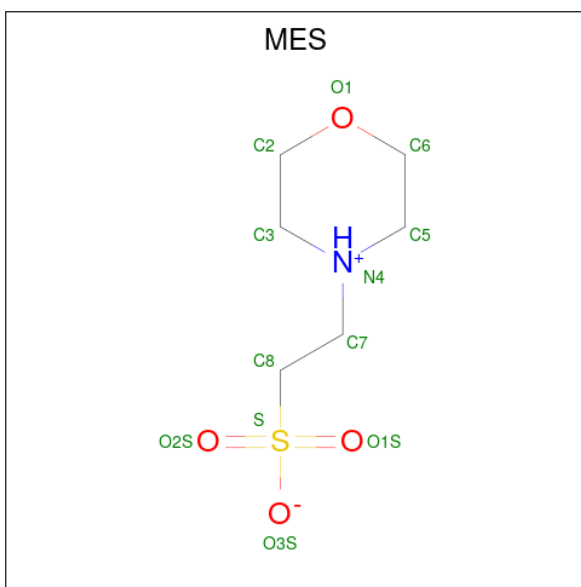
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	A	1	Total	C	H	N	O	0	0
			25	9	10	4	2		
8	B	1	Total	C	H	N	O	0	0
			25	9	10	4	2		
8	D	1	Total	C	H	N	O	0	0
			25	9	10	4	2		
8	D	1	Total	C	H	N	O	0	0
			25	9	10	4	2		

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



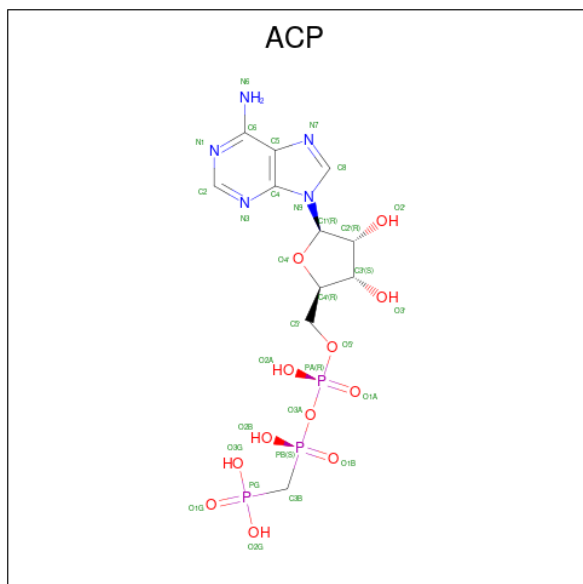
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	B	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
9	D	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- Molecule 10 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: 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 (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		

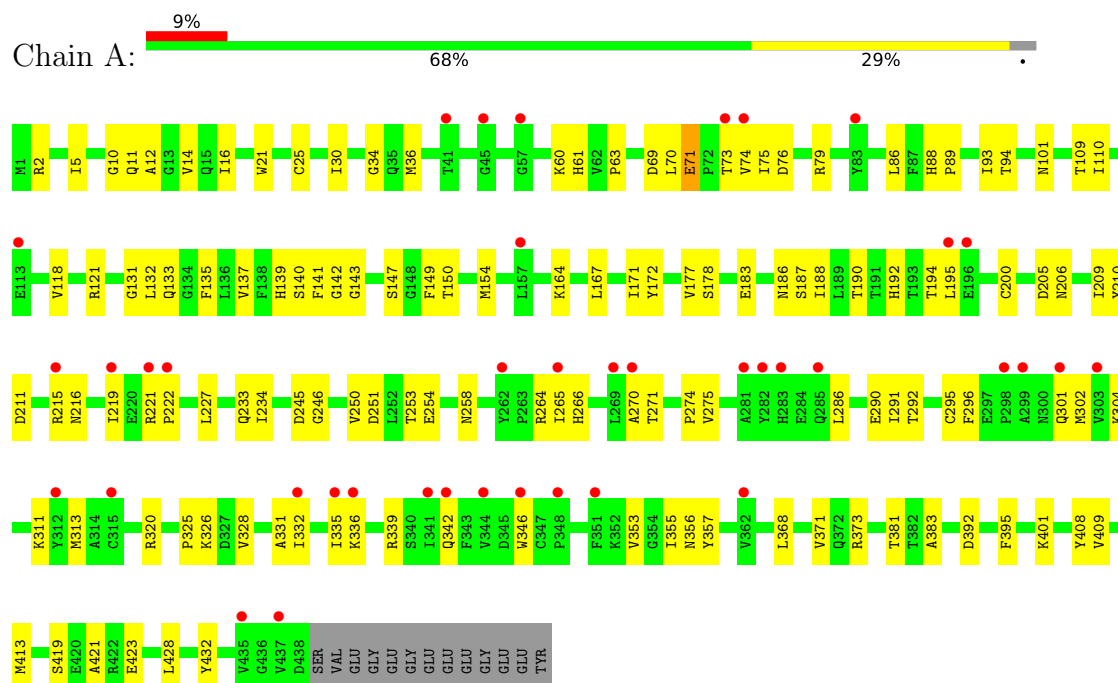
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	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		

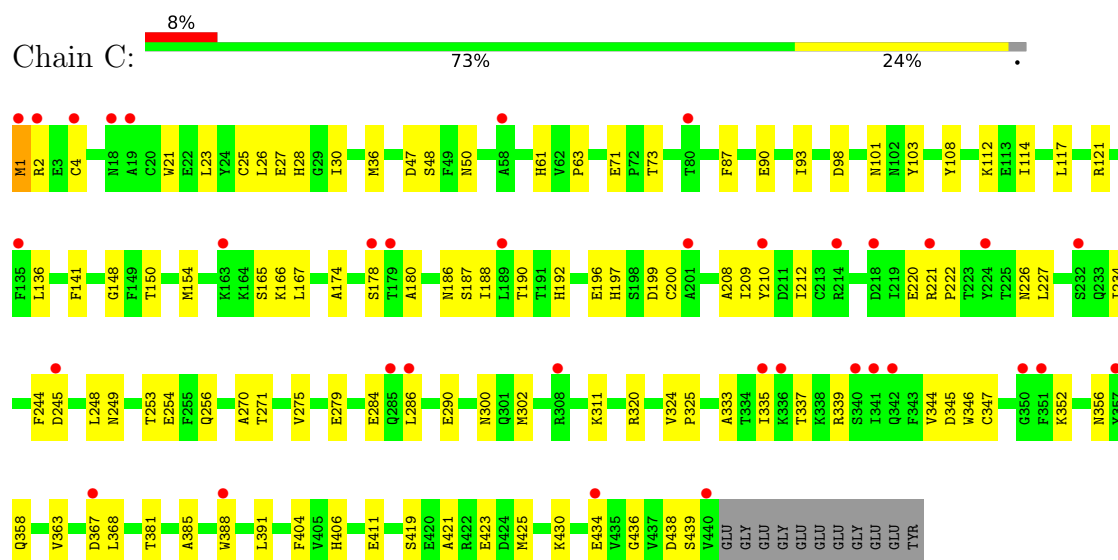
3 Residue-property plots

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.

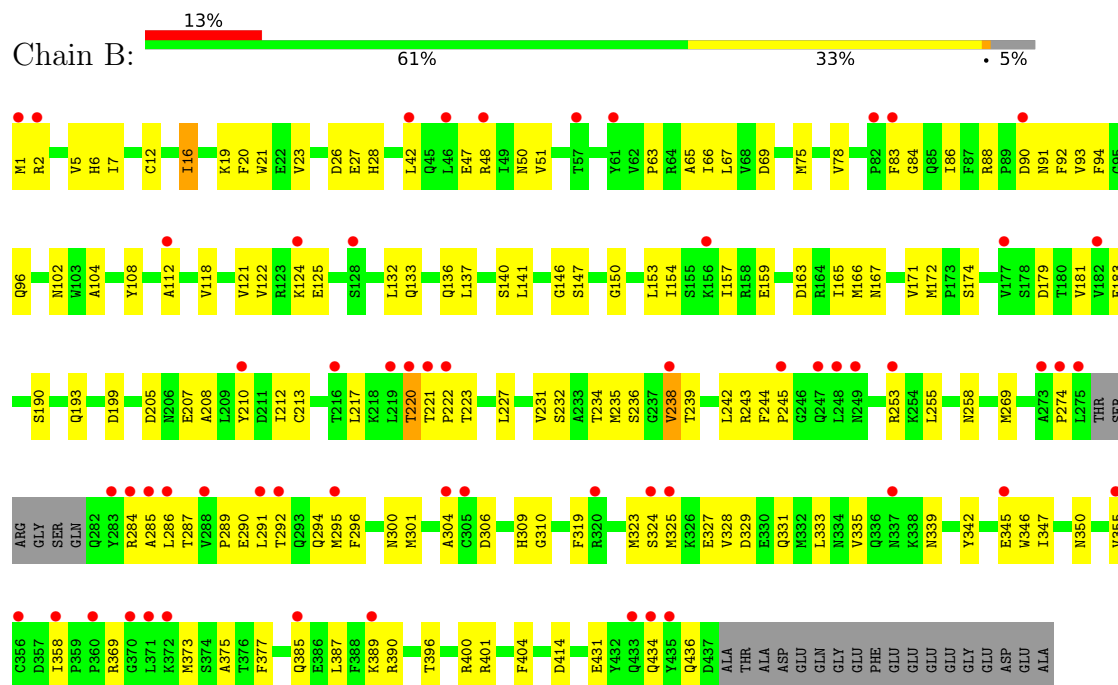
• Molecule 1: Tubulin alpha-1B chain



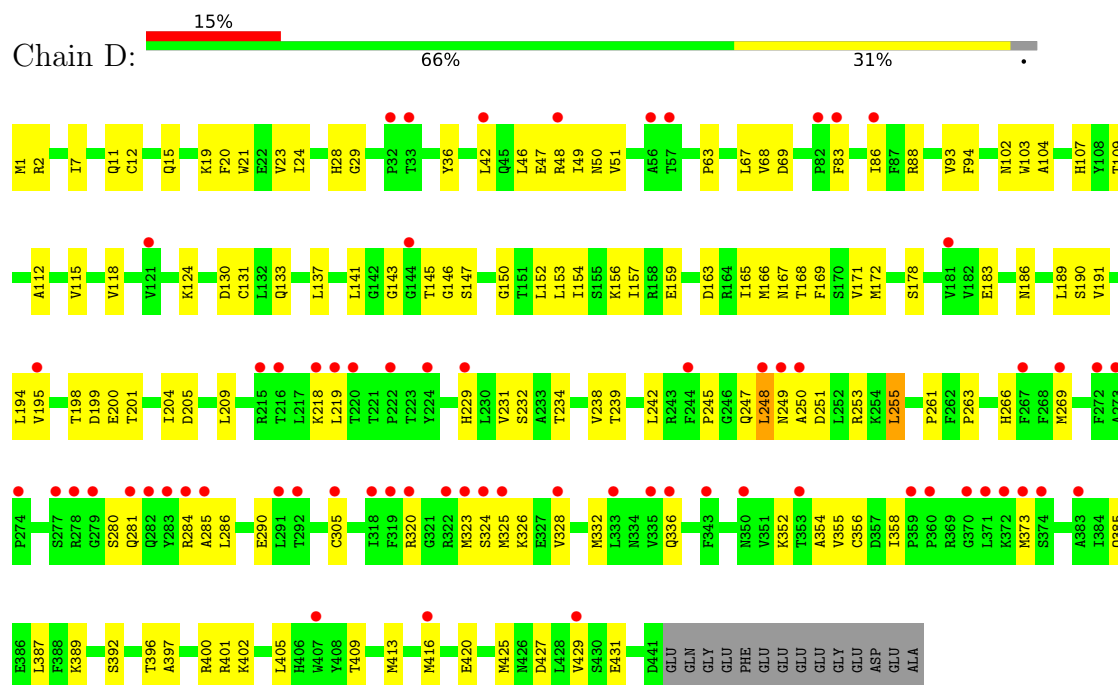
• Molecule 1: Tubulin alpha-1B chain



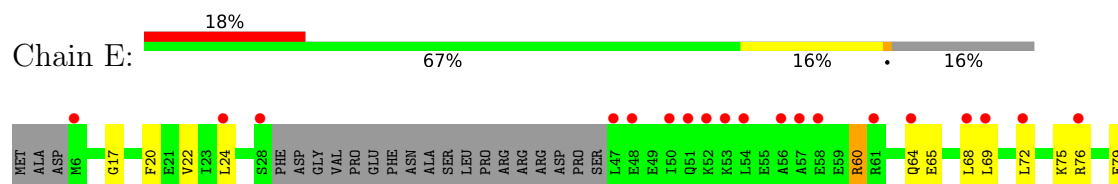
• Molecule 2: Tubulin beta-2B chain

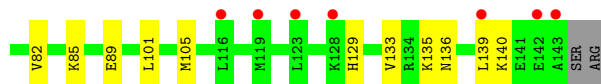


• Molecule 2: Tubulin beta-2B chain

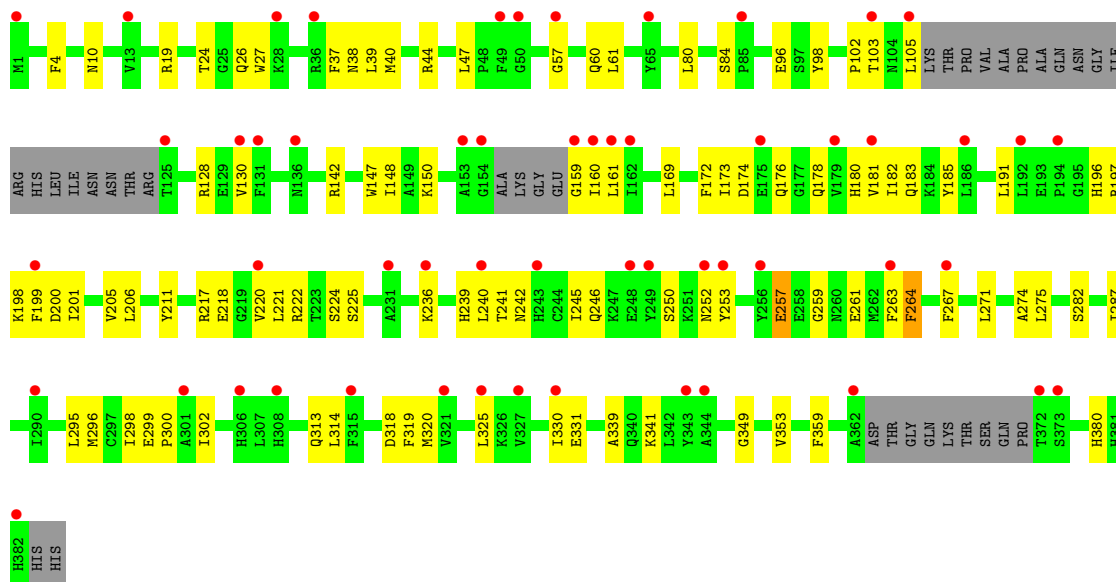


• Molecule 3: Stathmin-4





● 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 86.68 – 2.35	Depositor EDS
% Data completeness (in resolution range)	99.0 (86.68-2.35) 99.0 (86.68-2.35)	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 0.246 , 0.284	Depositor DCC
R_{free} test set	6075 reflections (4.83%)	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)	0.32 , 45.7	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: MES, GTP, ACP, MG, K0M, GDP, CA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.11	0/3502	0.28	0/4754
1	C	0.13	0/3521	0.31	0/4780
2	B	0.13	0/3400	0.30	0/4603
2	D	0.11	0/3442	0.28	0/4664
3	E	0.11	0/1000	0.24	0/1325
4	F	0.10	0/2931	0.28	0/3960
All	All	0.12	0/17796	0.29	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	103	0
1	C	3443	0	3352	86	1
2	B	3326	0	3202	138	0
2	D	3368	0	3236	116	0
3	E	993	0	1013	21	0
4	F	2865	0	2826	79	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	520	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 (520) 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
1:C:234:ILE:HG12	1:C:302:MET:HE2	1.60	0.81
2:D:172:MET:HG3	2:D:387:LEU:HD11	1.62	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	0.78
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
1:A:408:TYR:HB3	1:A:413:MET:HE2	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
2:B:325:MET:HE2	2:B:355:VAL:HG21	1.68	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
4:F:198:LYS:HE3	4:F:320:MET:HE1	1.73	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
2:D:269:MET:HE2	2:D:305:CYS:HB2	1.74	0.67
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
2:B:75:MET:HE3	2:B:92:PHE:CD2	2.33	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
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
4:F:159:GLY:C	4:F:160:ILE:HD12	2.24	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:B:147:SER:HG	2:B:190:SER:HG	1.48	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
2:B:75:MET:HE3	2:B:92:PHE:HD2	1.65	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
1:A:12:ALA:HB3	1:A:140:SER:HB3	1.82	0.61
2:D:392:SER:HB2	2:D:425:MET:HE3	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:265:ILE:HG21	1:A:313:MET:HE1	1.82	0.60
1:C:249:ASN:OD1	1:C:356:ASN:ND2	2.35	0.60
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:D:1:MET:HE2	2:D:50:ASN:HB2	1.86	0.57
1:A:93:ILE:HD11	1:A:121:ARG:HG3	1.85	0.57
1:A:381:THR:HG22	1:A:383:ALA:H	1.70	0.57
2:D:198:THR:HG1	2:D:266:HIS:HE2	1.52	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:A:302:MET:N	1:A:302:MET:HE2	2.20	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
4:F:37:PHE:CZ	4:F:40:MET:HE3	2.41	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
2:D:218:LYS:C	2:D:219:LEU:HD23	2.31	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
4:F:211:TYR:OH	4:F:295:LEU:O	2.25	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
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
1:C:28:HIS:O	1:C:36:MET:HE3	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: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:D:323:MET:HE2	2:D:373:MET:HG2	1.92	0.52
2:B:310:GLY:HA2	2:B:436:GLN:NE2	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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: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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:323:MET:HE2	2:B:373:MET:HE2	1.94	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
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
2:D:245:PRO:HA	2:D:249:ASN:CG	2.38	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
4:F:198:LYS:HE3	4:F:320:MET:CE	2.42	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
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:1:MET:HE2	2:D:50:ASN:CB	2.44	0.47
2:D:396:THR:O	2:D:400:ARG:HG2	2.14	0.47
2:B:295:MET:HE1	2:B:319:PHE:CZ	2.50	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:221:ARG:HD3	1:C:221:ARG:C	2.40	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
2:B:20:PHE:CD1	2:B:235:MET:HE2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:387:LEU:HD23	2:D:387:LEU:C	2.39	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
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:48:ARG:NH1	2:B:242:LEU:C	2.75	0.45
4:F:199:PHE:CE1	4:F:221:LEU:HD23	2.51	0.45
1:A:143:GLY:O	1:A:147:SER:OG	2.31	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
2:B:75:MET:CE	2:B:92:PHE:HD2	2.28	0.45
1:C:286:LEU:H	1:C:286:LEU:HD12	1.80	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
1:A:301:GLN:C	1:A:302:MET:HE2	2.42	0.45
2:B:235:MET:O	2:B:239:THR:HG23	2.17	0.45
2:B:124:LYS:HD3	2:B:124:LYS:C	2.42	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
2:D:124:LYS:C	2:D:124:LYS:HD3	2.42	0.44
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
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:65:ALA:C	2:B:66:ILE:HG13	2.43	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:103:TRP:HB2	2:D:186:ASN:OD1	2.19	0.43
2:D:280:SER:O	2:D:281:GLN:C	2.61	0.43
2:B:102:ASN:OD1	2:B:104:ALA:N	2.52	0.43
4:F:19:ARG:HD2	4:F:19:ARG:C	2.43	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:D:323:MET:HE2	2:D:373:MET:CG	2.48	0.43
4:F:253:TYR:CZ	4:F:259:GLY:HA2	2.54	0.43
1:A:346:TRP:CD1	1:A:346:TRP:H	2.36	0.43
2:B:213:CYS:HA	2:B:217:LEU:HB2	2.00	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
1:C:271:THR:HG23	1:C:300:ASN:C	2.43	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
2:D:68:VAL:HA	2:D:93:VAL:O	2.19	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
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:269:MET:HE2	2:B:301:MET:SD	2.60	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
2:D:178:SER:OG	2:D:183:GLU:OE2	2.33	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:D:325:MET:HE2	2:D:355:VAL:HG21	2.02	0.41
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
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
2:D:269:MET:HE1	2:D:305:CYS:HB2	2.00	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
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
4:F:47:LEU:C	4:F:47:LEU:HD23	2.46	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
2:B:310:GLY:HA2	2:B:436:GLN:CD	2.46	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
4:F:274:ALA:C	4:F:275:LEU:HD22	2.46	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
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
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 symmetry 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%)	43	52
1	C	439/451 (97%)	427 (97%)	12 (3%)	0	100	100
2	B	418/445 (94%)	401 (96%)	16 (4%)	1 (0%)	43	52
2	D	429/445 (96%)	409 (95%)	19 (4%)	1 (0%)	43	52

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	48	59

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 ⓘ

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%)	366 (99%)	3 (1%)	73	84
1	C	372/379 (98%)	369 (99%)	3 (1%)	73	84
2	B	364/383 (95%)	361 (99%)	3 (1%)	73	84
2	D	368/383 (96%)	363 (99%)	5 (1%)	59	73
3	E	107/127 (84%)	106 (99%)	1 (1%)	70	82
4	F	314/342 (92%)	311 (99%)	3 (1%)	68	81
All	All	1894/1993 (95%)	1876 (99%)	18 (1%)	68	81

All (18) 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
2	B	16	ILE
2	B	238	VAL
2	B	255	LEU
1	C	1	MET

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Mol	Chain	Res	Type
1	C	284	GLU
1	C	381	THR
2	D	159	GLU
2	D	229	HIS
2	D	247	GLN
2	D	248	LEU
2	D	255	LEU
3	E	60	ARG
4	F	142	ARG
4	F	257	GLU
4	F	264	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	88	HIS
1	A	283	HIS
1	A	301	GLN
2	B	15	GLN
2	B	133	GLN
2	B	167	ASN
2	B	192	HIS
2	B	193	GLN
2	B	258	ASN
2	B	294	GLN
2	B	434	GLN
1	C	15	GLN
1	C	85	GLN
1	C	101	ASN
1	C	256	GLN
1	C	285	GLN
1	C	393	HIS
2	D	6	HIS
2	D	37	HIS
2	D	133	GLN
2	D	136	GLN
2	D	167	ASN
2	D	249	ASN
2	D	331	GLN
2	D	339	ASN
3	E	136	ASN
4	F	178	GLN

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Mol	Chain	Res	Type
4	F	180	HIS
4	F	196	HIS
4	F	242	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 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	$\# Z > 2$
5	GTP	C	501	6	33,34,34	1.04	4 (12%)	50,54,54	1.57	9 (18%)
8	K0M	D	503	-	16,16,16	0.66	0	15,22,22	0.78	1 (6%)
8	K0M	D	504	-	16,16,16	0.67	0	15,22,22	0.82	1 (6%)
11	ACP	F	401	6	31,33,33	1.67	8 (25%)	47,52,52	1.88	9 (19%)
9	GDP	B	501	6	29,30,30	1.13	2 (6%)	45,47,47	1.74	7 (15%)
5	GTP	A	501	6	33,34,34	1.08	4 (12%)	50,54,54	1.59	9 (18%)
8	K0M	A	504	-	16,16,16	0.68	0	15,22,22	0.77	1 (6%)
10	MES	B	504	-	12,12,12	2.29	1 (8%)	15,16,16	1.86	4 (26%)
9	GDP	D	501	6	29,30,30	1.20	4 (13%)	45,47,47	1.75	5 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	K0M	B	505	-	16,16,16	0.66	0	15,22,22	0.81	1 (6%)

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
5	GTP	C	501	6	-	7/22/38/38	0/3/3/3
8	K0M	D	503	-	-	0/8/8/8	0/2/2/2
8	K0M	D	504	-	-	0/8/8/8	0/2/2/2
11	ACP	F	401	6	-	12/19/38/38	0/3/3/3
9	GDP	B	501	6	-	3/16/32/32	0/3/3/3
5	GTP	A	501	6	-	7/22/38/38	0/3/3/3
8	K0M	A	504	-	-	0/8/8/8	0/2/2/2
10	MES	B	504	-	-	4/6/14/14	0/1/1/1
9	GDP	D	501	6	-	6/16/32/32	0/3/3/3
8	K0M	B	505	-	-	0/8/8/8	0/2/2/2

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	504	MES	C8-S	-7.64	1.66	1.77
11	F	401	ACP	C5-C4	4.77	1.47	1.39
9	D	501	GDP	C5-C4	3.15	1.47	1.38
9	B	501	GDP	C5-C4	3.08	1.47	1.38
11	F	401	ACP	PG-O3G	3.04	1.61	1.55
11	F	401	ACP	PG-O2G	2.96	1.61	1.55
5	A	501	GTP	PB-O3B	2.76	1.62	1.59
11	F	401	ACP	PB-O3A	2.72	1.61	1.58
11	F	401	ACP	C5-C6	2.68	1.48	1.41
5	C	501	GTP	PA-O3A	2.48	1.62	1.59
9	D	501	GDP	C6-N1	-2.47	1.34	1.38
9	B	501	GDP	C6-N1	-2.38	1.34	1.38
5	A	501	GTP	PB-O3A	2.35	1.62	1.59
11	F	401	ACP	C8-N7	2.32	1.36	1.31
11	F	401	ACP	C5-N7	-2.29	1.34	1.39
5	A	501	GTP	PA-O3A	2.25	1.61	1.59
9	D	501	GDP	PA-O3A	2.24	1.61	1.59
5	A	501	GTP	C2-N3	2.19	1.38	1.33
11	F	401	ACP	PB-O2B	2.14	1.61	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	501	GTP	PB-O3A	2.14	1.61	1.59
9	D	501	GDP	C5-N7	-2.10	1.34	1.39
5	C	501	GTP	C2-N3	2.09	1.38	1.33
5	C	501	GTP	PB-O3B	2.03	1.61	1.59

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	D	501	GDP	C5-C4-N3	-6.26	118.42	128.39
9	B	501	GDP	C5-C4-N3	-5.96	118.91	128.39
11	F	401	ACP	C5-C4-N3	-5.86	118.65	126.72
9	D	501	GDP	C2-N3-C4	5.08	121.05	112.30
9	B	501	GDP	C2-N3-C4	5.04	120.98	112.30
5	A	501	GTP	C5-C4-N3	-5.03	120.38	128.39
5	C	501	GTP	C5-C4-N3	-4.99	120.44	128.39
5	C	501	GTP	C2-N3-C4	4.66	120.33	112.30
11	F	401	ACP	N3-C4-N9	4.63	135.04	127.17
9	D	501	GDP	N9-C4-N3	4.59	135.13	125.95
5	A	501	GTP	C2-N3-C4	4.52	120.09	112.30
9	B	501	GDP	N9-C4-N3	4.33	134.62	125.95
11	F	401	ACP	PB-O3A-PA	-3.99	119.36	132.37
10	B	504	MES	C5-N4-C3	3.86	117.16	108.84
11	F	401	ACP	C2-N3-C4	3.61	120.66	111.83
9	B	501	GDP	C6-C5-N7	3.55	136.75	130.29
11	F	401	ACP	C4-C5-N7	-3.50	106.58	110.58
5	A	501	GTP	N9-C4-N3	3.37	132.69	125.95
9	D	501	GDP	C6-C5-N7	3.20	136.12	130.29
5	C	501	GTP	N9-C4-N3	3.19	132.34	125.95
11	F	401	ACP	N3-C2-N1	-3.08	123.92	128.58
10	B	504	MES	C6-C5-N4	-2.95	105.64	110.12
5	A	501	GTP	C2-N1-C6	-2.87	119.90	125.11
9	B	501	GDP	C4-C5-N7	-2.74	106.33	110.67
5	C	501	GTP	C2-N1-C6	-2.74	120.15	125.11
11	F	401	ACP	C3'-C2'-C1'	2.67	106.51	101.46
5	A	501	GTP	N9-C8-N7	-2.65	108.48	113.40
9	D	501	GDP	C4-C5-N7	-2.64	106.48	110.67
11	F	401	ACP	C4-N9-C8	2.58	108.44	105.74
5	A	501	GTP	O6-C6-C5	-2.54	119.81	126.53
11	F	401	ACP	C5-N7-C8	2.53	107.42	103.45
5	C	501	GTP	C8-N7-C5	2.51	108.74	104.26
5	C	501	GTP	N9-C8-N7	-2.51	108.75	113.40
5	A	501	GTP	C8-N7-C5	2.50	108.72	104.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	501	GTP	O6-C6-C5	-2.41	120.18	126.53
5	C	501	GTP	O2B-PB-O3A	2.40	113.76	107.27
5	A	501	GTP	C5-C6-N1	2.35	119.23	113.25
5	C	501	GTP	C5-C6-N1	2.34	119.20	113.25
8	D	504	K0M	O-C3-C2	-2.29	108.35	109.86
5	A	501	GTP	O3G-PG-O3B	2.27	112.26	104.64
10	B	504	MES	C7-N4-C5	2.27	117.30	111.24
10	B	504	MES	O1S-S-C8	2.16	109.99	106.73
9	B	501	GDP	O2B-PB-O3A	2.07	111.58	104.64
8	A	504	K0M	O-C3-C2	-2.07	108.50	109.86
9	B	501	GDP	O6-C6-C5	-2.06	121.11	126.53
8	D	503	K0M	O-C3-C2	-2.05	108.51	109.86
8	B	505	K0M	O-C3-C2	-2.03	108.52	109.86

There are no chirality outliers.

All (39) 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
9	B	501	GDP	C5'-O5'-PA-O3A
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	C5'-O5'-PA-O3A
11	F	401	ACP	O4'-C4'-C5'-O5'
11	F	401	ACP	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
10	B	504	MES	C7-C8-S-O3S
10	B	504	MES	C7-C8-S-O1S
10	B	504	MES	C7-C8-S-O2S
9	D	501	GDP	C5'-O5'-PA-O1A
11	F	401	ACP	PG-C3B-PB-O2B
11	F	401	ACP	C5'-O5'-PA-O2A
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	PB-O3A-PA-O2A
5	C	501	GTP	PB-O3A-PA-O2A
5	A	501	GTP	PB-O3A-PA-O1A

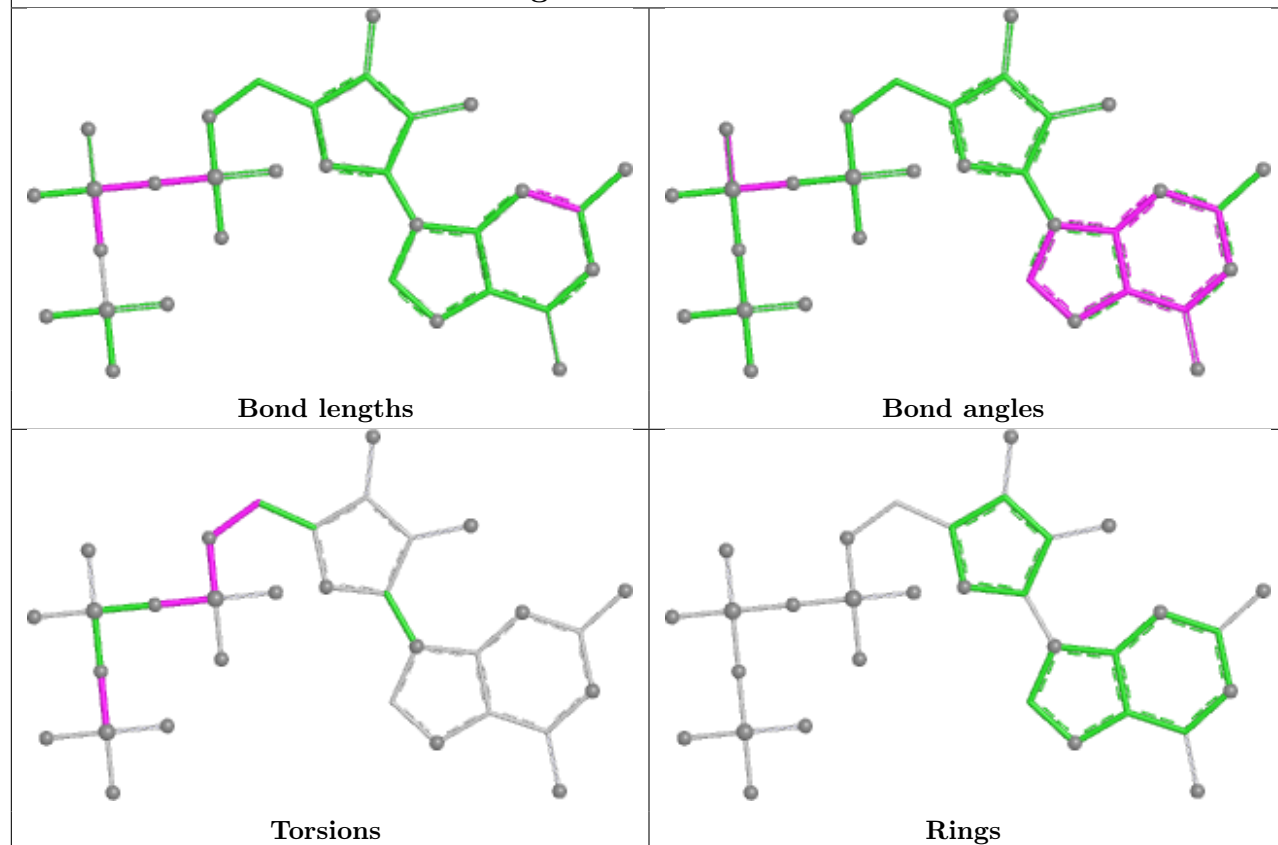
There are no ring outliers.

6 monomers are involved in 16 short contacts:

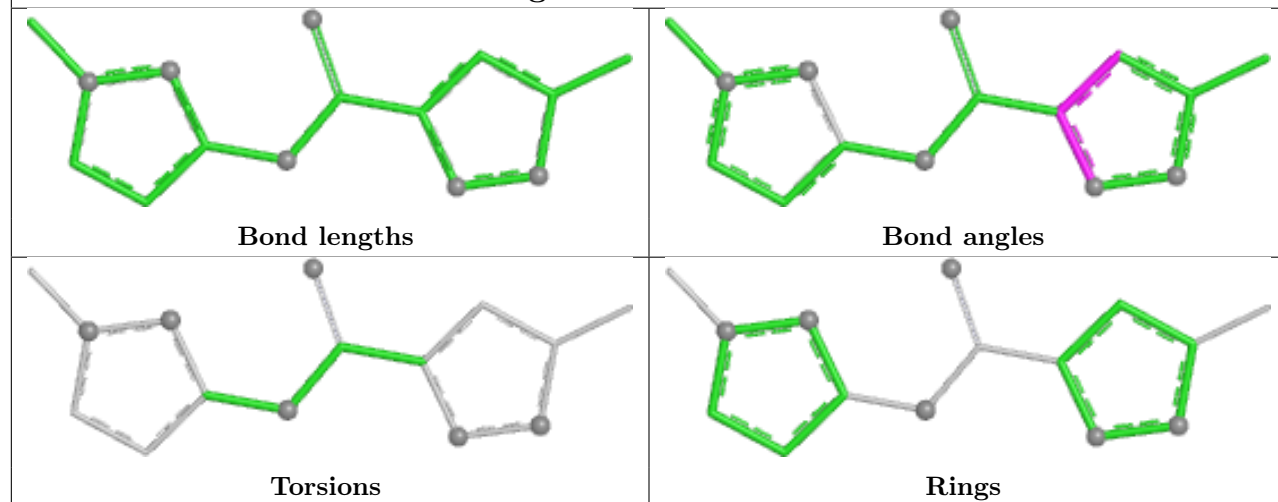
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	501	GTP	1	0
8	D	503	K0M	3	0
11	F	401	ACP	5	0
9	B	501	GDP	1	0
10	B	504	MES	3	0
9	D	501	GDP	3	0

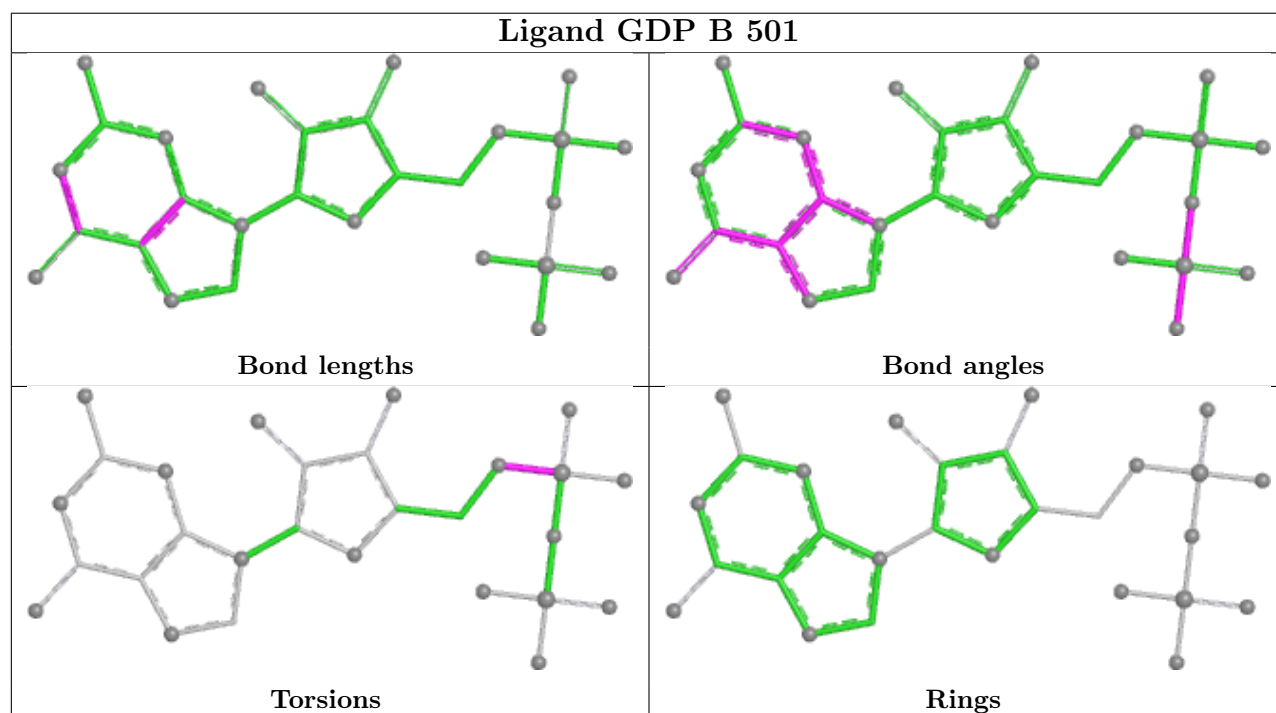
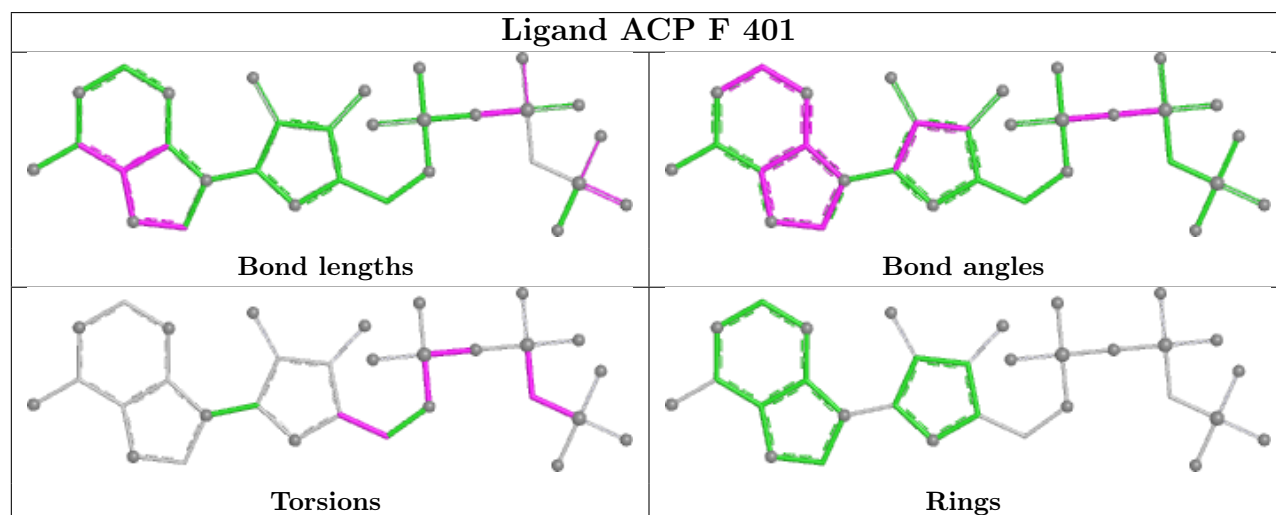
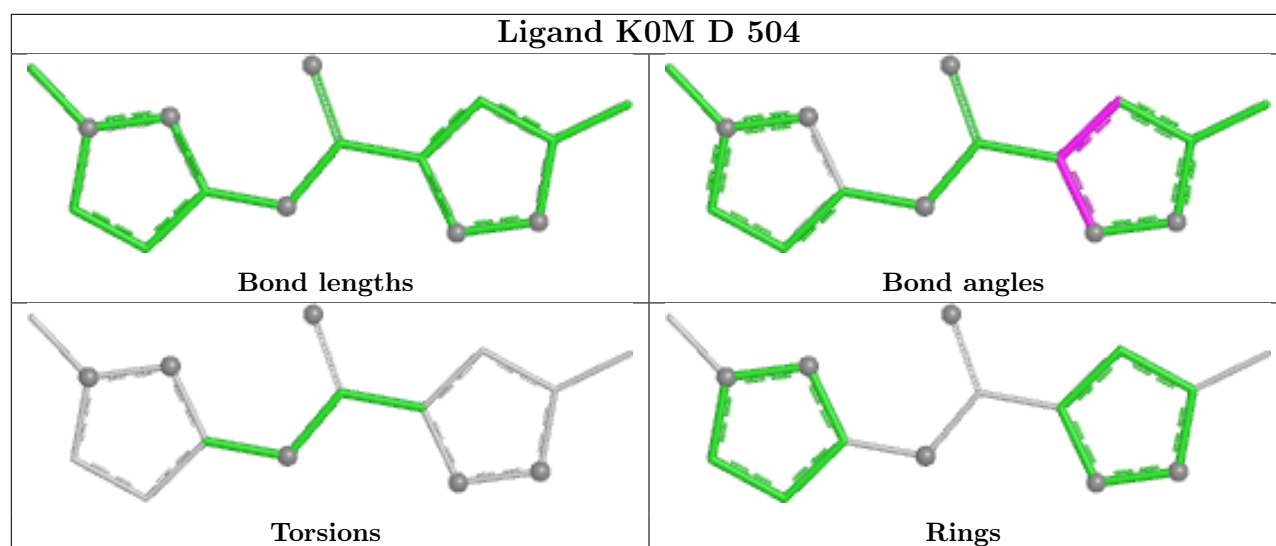
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

Ligand GTP C 501

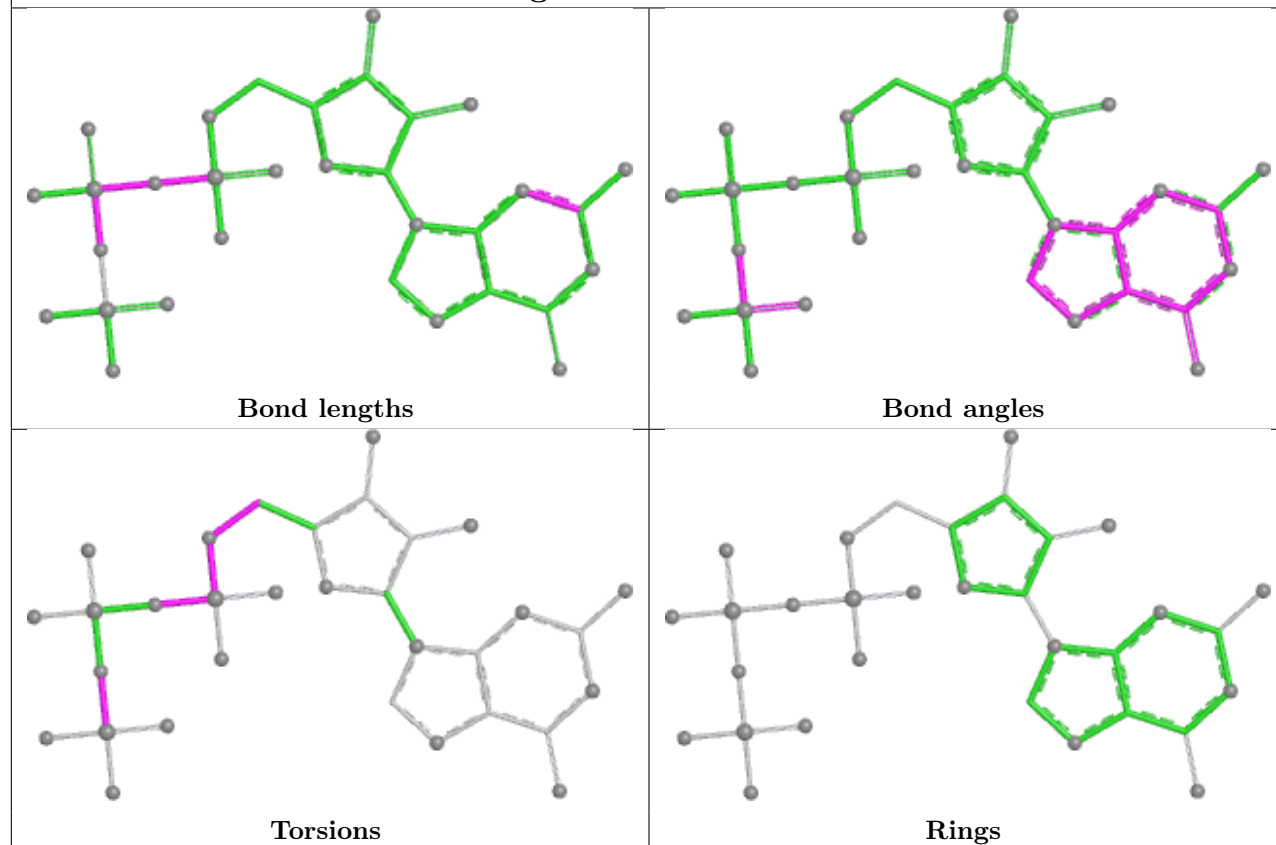


Ligand KOM D 503

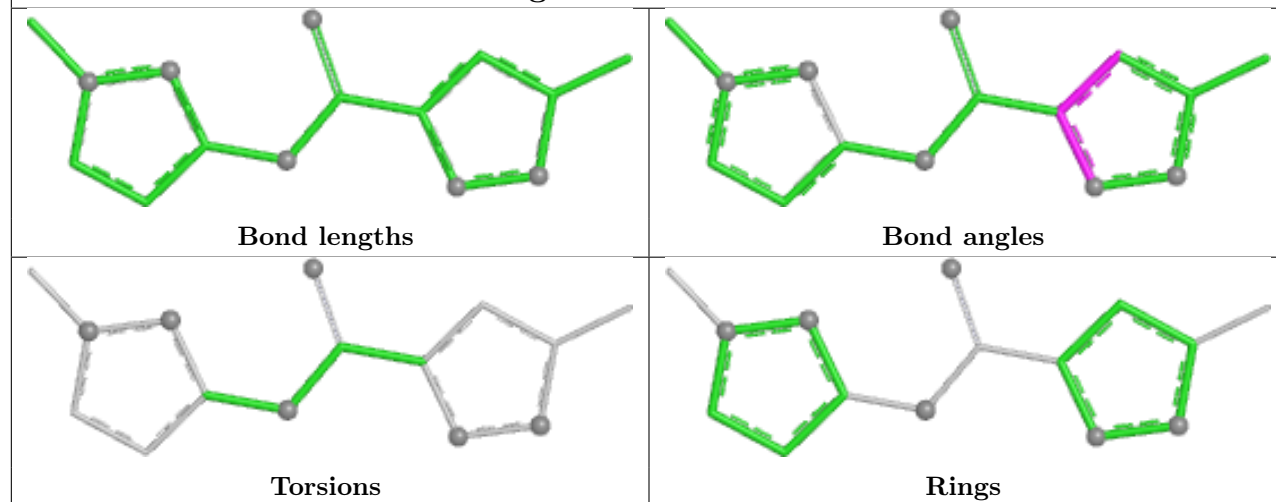


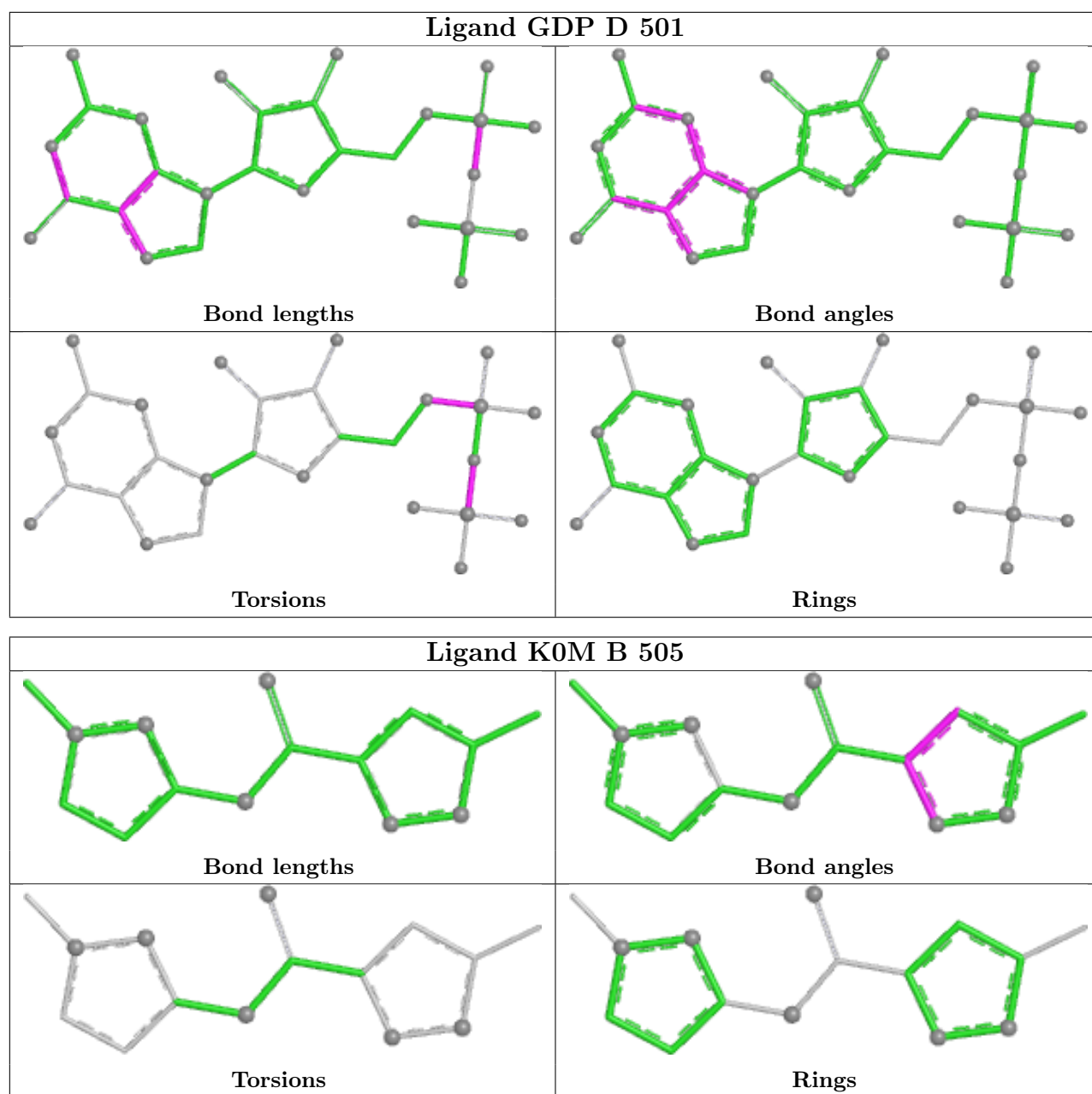


Ligand GTP A 501



Ligand KOM A 504





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%)	0.91	40 (9%) 15 17	55, 70, 103, 143	0
1	C	440/451 (97%)	0.79	35 (7%) 18 21	32, 64, 90, 152	1 (0%)
2	B	421/445 (94%)	1.02	58 (13%) 6 7	37, 68, 117, 193	6 (1%)
2	D	431/445 (96%)	1.25	66 (15%) 5 6	55, 87, 126, 168	5 (1%)
3	E	120/143 (83%)	1.43	26 (21%) 2 2	59, 89, 142, 189	0
4	F	350/384 (91%)	1.21	55 (15%) 5 5	68, 91, 143, 184	0
All	All	2200/2319 (94%)	1.05	280 (12%) 8 9	32, 76, 124, 193	12 (0%)

All (280) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	159	GLY	7.9
2	B	48	ARG	7.0
4	F	154	GLY	6.3
2	D	373	MET	5.3
3	E	143	ALA	5.2
2	B	283	TYR	5.0
1	C	340	SER	4.9
1	C	179	THR	4.9
2	B	220	THR	4.7
2	D	279	GLY	4.6
3	E	54	LEU	4.6
3	E	50	ILE	4.5
3	E	68	LEU	4.4
4	F	325	LEU	4.4
2	D	56	ALA	4.3
2	B	219	LEU	4.3
3	E	47	LEU	4.3
3	E	57	ALA	4.2
2	D	282	GLN	4.2

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Mol	Chain	Res	Type	RSRZ
2	D	284	ARG	4.1
4	F	160	ILE	4.0
4	F	231	ALA	4.0
2	D	370	GLY	4.0
2	B	83	PHE	3.9
4	F	49	PHE	3.9
2	B	275	LEU	3.9
2	B	356	CYS	3.8
2	D	57	THR	3.8
2	B	221	THR	3.8
3	E	72	LEU	3.8
2	D	283	TYR	3.7
4	F	161	LEU	3.7
1	A	362	VAL	3.7
2	D	216	THR	3.6
2	B	355	VAL	3.6
2	D	360	PRO	3.6
2	B	216	THR	3.5
1	C	440	VAL	3.5
1	C	221	ARG	3.5
2	B	1	MET	3.4
2	B	248	LEU	3.4
4	F	253	TYR	3.4
2	D	249	ASN	3.4
1	A	282	TYR	3.4
2	D	319	PHE	3.4
2	D	281	GLN	3.4
2	D	272	PHE	3.3
2	B	325	MET	3.3
1	C	2	ARG	3.3
3	E	69	LEU	3.3
2	B	90	ASP	3.2
2	B	249	ASN	3.2
1	C	434	GLU	3.2
3	E	53	LYS	3.2
1	C	285	GLN	3.2
2	D	195	VAL	3.2
4	F	105	LEU	3.2
4	F	162	ILE	3.2
2	B	57	THR	3.2
1	A	315	CYS	3.2
2	B	286	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	221	ARG	3.1
2	D	48	ARG	3.1
2	B	285	ALA	3.1
3	E	56	ALA	3.1
2	B	288	VAL	3.1
2	B	210	TYR	3.1
1	A	301	GLN	3.1
2	B	358	ILE	3.1
3	E	52	LYS	3.1
2	D	429	VAL	3.1
2	D	291	LEU	3.1
1	C	80	THR	3.1
1	C	58	ALA	3.1
2	D	250	ALA	3.1
2	D	42	LEU	3.1
2	D	407	TRP	3.1
2	B	128	SER	3.1
1	A	215	ARG	3.1
2	D	335	VAL	3.1
4	F	36	ARG	3.1
4	F	248	GLU	3.0
4	F	153	ALA	3.0
2	D	267	PHE	3.0
3	E	6	MET	3.0
1	A	312	TYR	3.0
1	C	341	ILE	3.0
1	A	73	THR	3.0
1	C	1	MET	3.0
2	D	219	LEU	3.0
4	F	179	VAL	3.0
2	D	278	ARG	3.0
1	A	45	GLY	3.0
2	B	370	GLY	3.0
1	A	351	PHE	2.9
1	A	437	VAL	2.9
2	D	274	PRO	2.9
1	A	435	VAL	2.9
2	B	182	VAL	2.9
1	C	218	ASP	2.9
1	A	269	LEU	2.9
1	A	285	GLN	2.9
2	B	273	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
4	F	220	VAL	2.9
2	D	305	CYS	2.9
1	C	232	SER	2.8
1	A	262	TYR	2.8
2	D	343	PHE	2.8
2	B	291	LEU	2.8
1	A	270	ALA	2.8
2	D	86	ILE	2.8
2	D	285	ALA	2.8
2	B	320	ARG	2.8
4	F	382	HIS	2.8
1	C	350	GLY	2.8
2	D	82	PRO	2.8
2	D	325	MET	2.8
4	F	199	PHE	2.8
2	D	121	VAL	2.8
4	F	252	ASN	2.7
2	D	144	GLY	2.7
2	B	371	LEU	2.7
2	D	248	LEU	2.7
1	C	201	ALA	2.7
2	D	383	ALA	2.7
2	D	292	THR	2.7
1	A	298	PRO	2.7
1	C	178	SER	2.7
2	B	82	PRO	2.7
2	D	323	MET	2.6
3	E	24	LEU	2.6
4	F	125	THR	2.6
4	F	373	SER	2.6
2	B	46	LEU	2.6
2	D	218	LYS	2.6
2	B	61	TYR	2.6
4	F	50	GLY	2.6
4	F	130	VAL	2.6
1	A	335	ILE	2.6
2	D	372	LYS	2.6
1	A	219	ILE	2.6
4	F	85	PRO	2.5
1	A	332	ILE	2.5
1	C	210	TYR	2.5
1	C	357	TYR	2.5

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Mol	Chain	Res	Type	RSRZ
3	E	61	ARG	2.5
1	C	19	ALA	2.5
4	F	344	ALA	2.5
1	A	41	THR	2.5
2	D	83	PHE	2.5
2	B	247	GLN	2.5
4	F	181	VAL	2.5
1	A	83	TYR	2.5
2	B	360	PRO	2.5
1	C	286	LEU	2.5
3	E	116	LEU	2.5
4	F	1	MET	2.5
1	C	245	ASP	2.5
1	A	341	ILE	2.4
4	F	343	TYR	2.4
4	F	306	HIS	2.4
1	C	342	GLN	2.4
3	E	76	ARG	2.4
4	F	362	ALA	2.4
2	D	220	THR	2.4
2	D	374	SER	2.4
1	C	163	LYS	2.4
4	F	192	LEU	2.4
2	D	320	ARG	2.4
4	F	194	PRO	2.4
2	D	244	PHE	2.4
4	F	290	ILE	2.4
1	C	189	LEU	2.4
1	C	388	TRP	2.4
2	B	385	GLN	2.4
2	D	33	THR	2.4
2	D	322	ARG	2.4
3	E	58	GLU	2.4
1	A	299	ALA	2.3
2	D	416	MET	2.3
2	D	328	VAL	2.3
4	F	240	LEU	2.3
2	B	124	LYS	2.3
4	F	65	TYR	2.3
4	F	57	GLY	2.3
2	D	353	THR	2.3
4	F	243	HIS	2.3

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Mol	Chain	Res	Type	RSRZ
4	F	267	PHE	2.3
2	D	371	LEU	2.3
2	D	359	PRO	2.3
2	D	273	ALA	2.3
2	B	253[A]	ARG	2.3
2	B	324	SER	2.3
2	D	269	MET	2.3
2	B	2	ARG	2.3
4	F	249	TYR	2.3
1	C	135	PHE	2.2
1	C	351	PHE	2.2
2	D	333	LEU	2.2
4	F	315	PHE	2.2
4	F	327	VAL	2.3
1	C	4[A]	CYS	2.2
2	B	222	PRO	2.2
4	F	103	THR	2.2
2	D	277	SER	2.2
3	E	123	LEU	2.2
1	C	18	ASN	2.2
1	A	348	PRO	2.2
2	B	274	PRO	2.2
2	D	222	PRO	2.2
1	A	113	GLU	2.2
3	E	142	GLU	2.2
3	E	64	GLN	2.2
1	A	346	TRP	2.2
1	A	74	VAL	2.2
1	C	214	ARG	2.2
1	C	367	ASP	2.2
2	D	350	ASN	2.2
2	B	305	CYS	2.2
2	D	336	GLN	2.2
3	E	51	GLN	2.2
4	F	308	HIS	2.2
2	B	112	ALA	2.2
2	D	318	ILE	2.2
2	B	284	ARG	2.2
2	B	295	MET	2.2
2	B	245	PRO	2.2
2	D	32	PRO	2.2
2	B	345	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
4	F	175	GLU	2.2
4	F	236	LYS	2.2
1	A	342	GLN	2.2
2	B	433	GLN	2.2
2	D	229	HIS	2.2
2	B	292	THR	2.2
2	B	304	ALA	2.2
2	B	435	TYR	2.1
3	E	128	LYS	2.1
2	D	324	SER	2.1
1	C	308	ARG	2.1
2	D	224	TYR	2.1
1	A	195	LEU	2.1
1	A	265	ILE	2.1
1	C	336	LYS	2.1
2	B	42	LEU	2.1
2	B	337	ASN	2.1
2	B	177	VAL	2.1
4	F	13	VAL	2.1
4	F	263	PHE	2.1
1	A	57	GLY	2.1
2	B	156	LYS	2.1
2	B	389	LYS	2.1
3	E	119	MET	2.1
1	A	157	LEU	2.1
1	C	335	ILE	2.1
4	F	186	LEU	2.1
1	A	222	PRO	2.1
4	F	321	VAL	2.1
3	E	28	SER	2.1
1	A	281	ALA	2.1
2	B	372	LYS	2.1
4	F	301	ALA	2.1
1	A	196	GLU	2.1
1	A	283	HIS	2.1
4	F	136	ASN	2.1
1	C	224	TYR	2.1
4	F	256	TYR	2.1
1	A	303	VAL	2.1
2	B	238	VAL	2.1
1	A	336	LYS	2.0
3	E	48	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
2	B	434	GLN	2.0
1	A	344	VAL	2.0
2	D	181	VAL	2.0
4	F	131	PHE	2.0
4	F	372	THR	2.0
3	E	139	LEU	2.0
2	D	215	ARG	2.0
4	F	330	ILE	2.0
4	F	28	LYS	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(Å ²)	Q<0.9
6	MG	F	402	1/1	0.24	0.36	114,114,114,114	0
7	CA	A	503	1/1	0.53	0.10	138,138,138,138	0
10	MES	B	504	12/12	0.81	0.15	85,91,100,100	0
11	ACP	F	401	31/31	0.87	0.11	86,108,118,125	0
7	CA	B	503	1/1	0.89	0.21	110,110,110,110	0
8	K0M	D	504	15/15	0.90	0.14	68,82,108,108	0
6	MG	D	502	1/1	0.91	0.17	80,80,80,80	0
9	GDP	D	501	28/28	0.91	0.10	73,82,88,90	0
6	MG	C	502	1/1	0.92	0.11	69,69,69,69	0
8	K0M	A	504	15/15	0.94	0.10	60,69,88,89	0
8	K0M	B	505	15/15	0.94	0.09	60,69,86,86	0
5	GTP	A	501	32/32	0.94	0.08	53,57,61,62	0
9	GDP	B	501	28/28	0.95	0.08	50,54,57,62	0
8	K0M	D	503	15/15	0.95	0.13	67,74,89,89	25

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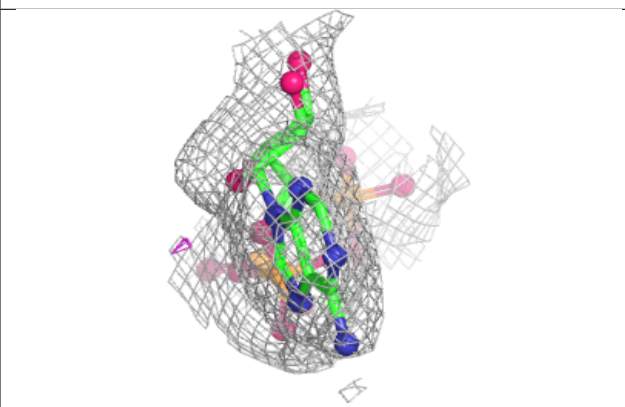
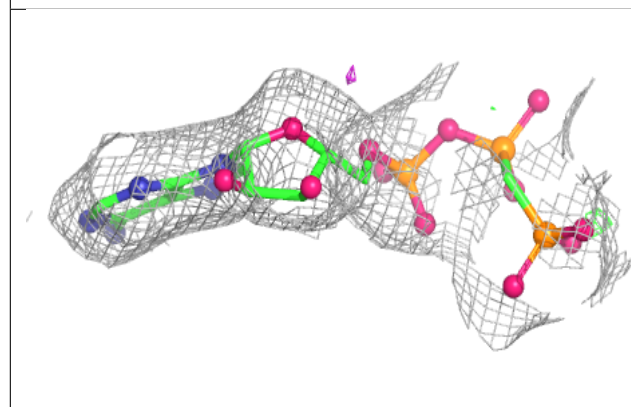
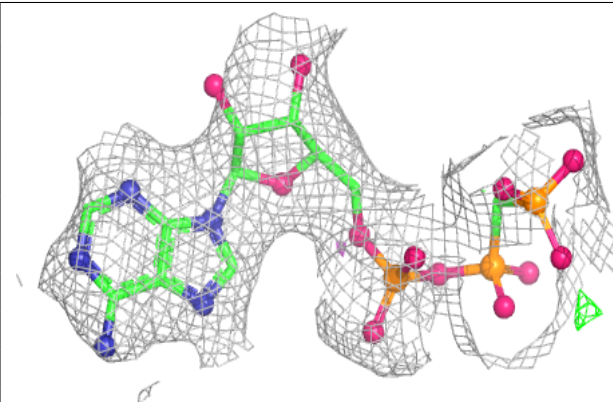
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	GTP	C	501	32/32	0.96	0.08	57,59,66,72	0
7	CA	C	503	1/1	0.98	0.04	73,73,73,73	0
6	MG	A	502	1/1	0.99	0.05	56,56,56,56	0
6	MG	B	502	1/1	0.99	0.10	51,51,51,51	0

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.

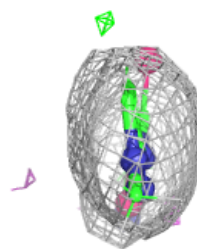
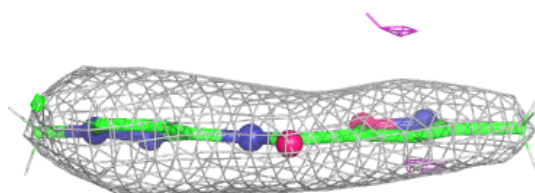
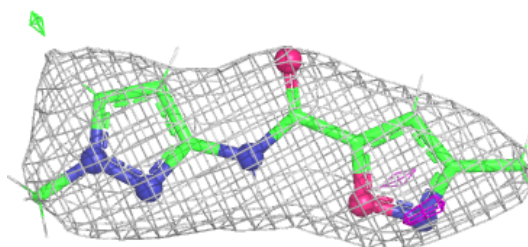
Electron density around ACP F 401:

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



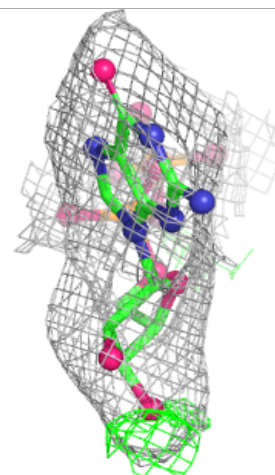
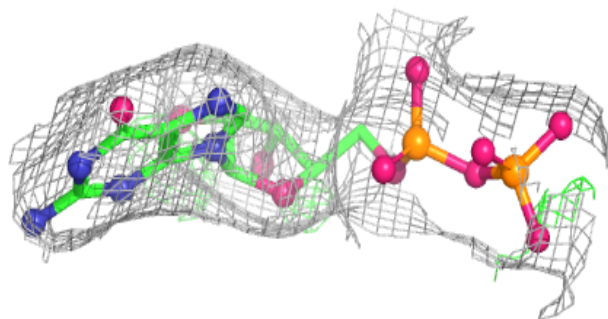
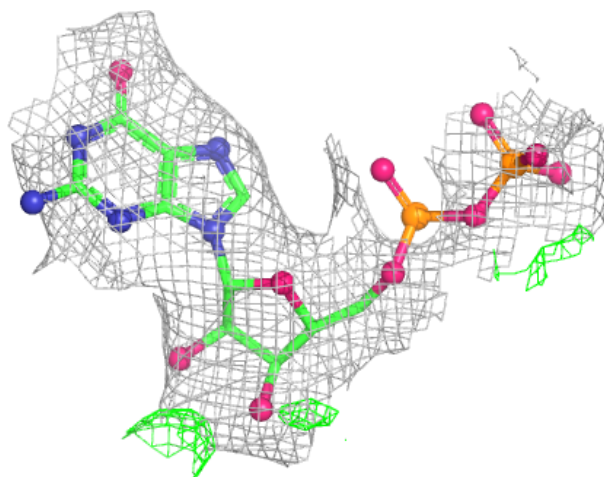
Electron density around K0M D 504:

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



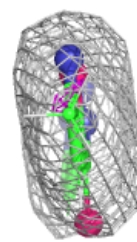
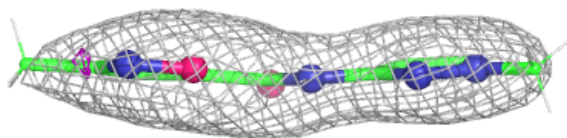
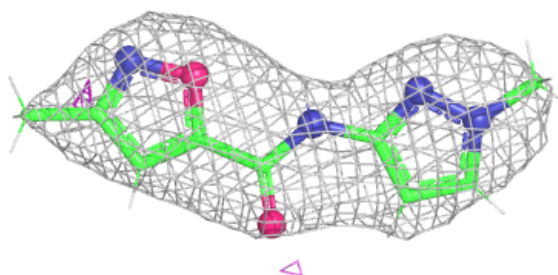
Electron density around GDP D 501:

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

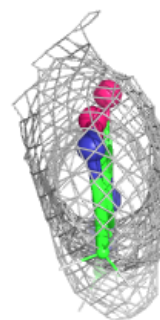
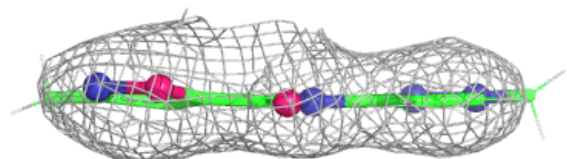
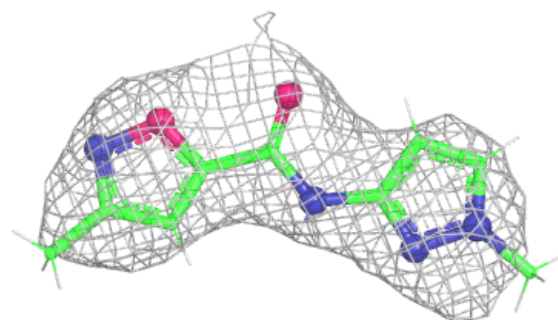


Electron density around K0M A 504:

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

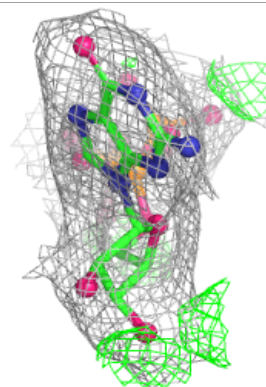
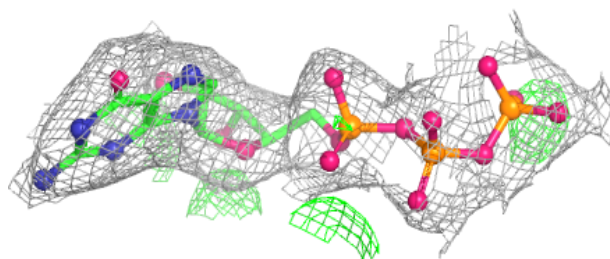
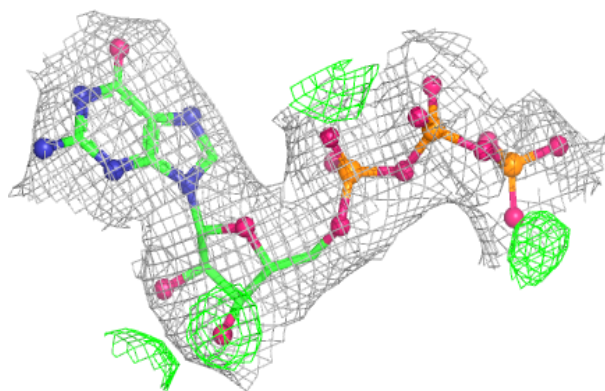
**Electron density around K0M B 505:**

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



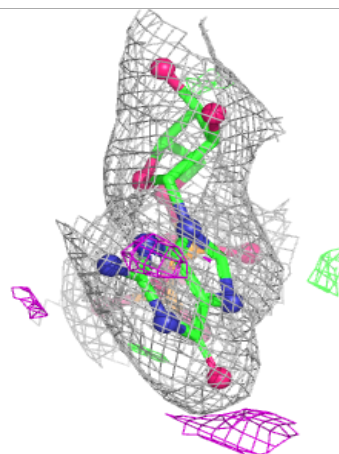
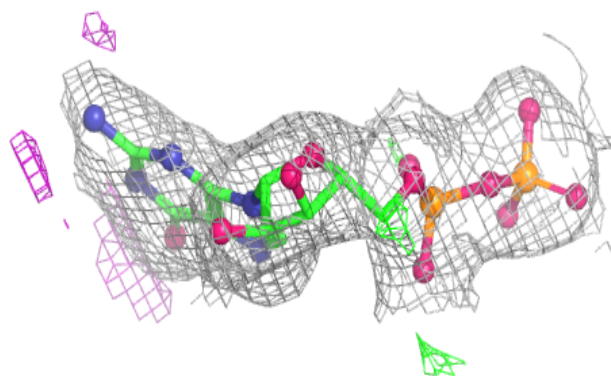
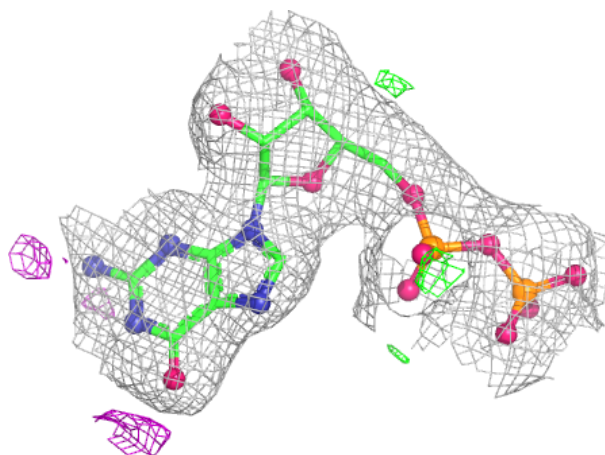
Electron density around GTP A 501:

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



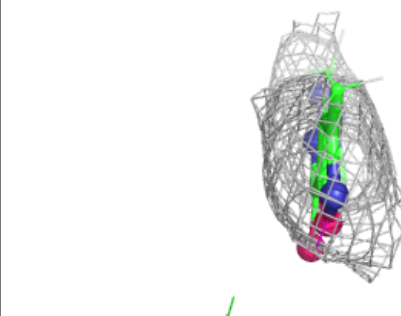
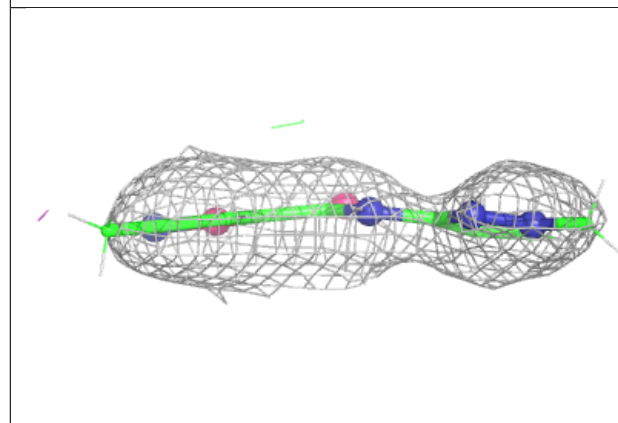
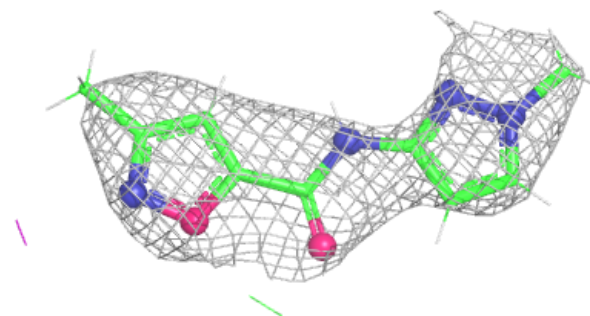
Electron density around GDP B 501:

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

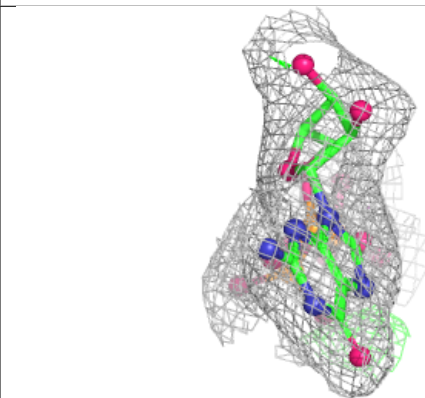
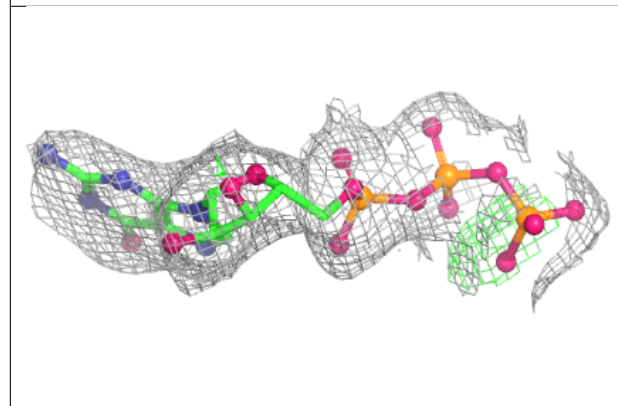
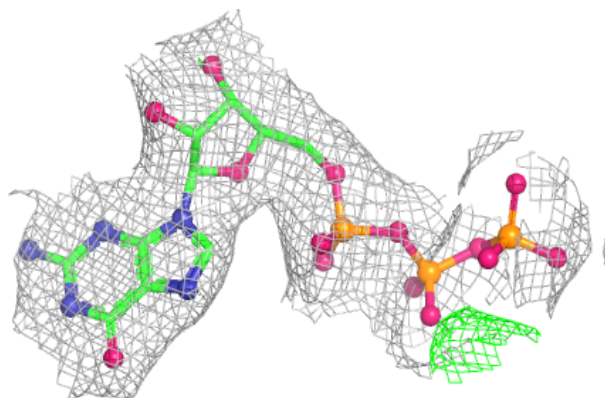


Electron density around K0M D 503:

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

**Electron density around GTP C 501:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.