



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 06:12 AM UTC

PDB ID : 5S4N / pdb_00005s4n
Title : Tubulin-Z285782452-complex
Authors : Muehlethaler, T.; Gioia, D.; Protá, A.E.; Sharpe, M.E.; Cavalli, A.; Steinmetz, M.O.
Deposited on : 2020-11-08
Resolution : 2.53 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

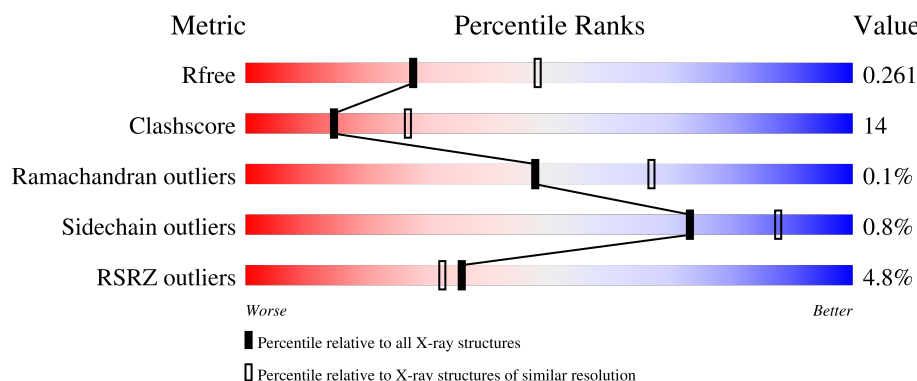
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.53 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7383 (2.54-2.50)
Clashscore	190562	8079 (2.54-2.50)
Ramachandran outliers	187476	7944 (2.54-2.50)
Sidechain outliers	187428	7946 (2.54-2.50)
RSRZ outliers	180081	7387 (2.54-2.50)

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

Mol	Chain	Length	Quality of chain
1	A	451	4% 69% 28% ..
1	C	451	4% 73% 25% .
2	B	445	4% 63% 32% .
2	D	445	4% 67% 29% .
3	E	143	8% 68% 17% 14%

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Mol	Chain	Length	Quality of chain			
			6%	64%	26%	9%
4	F	384				

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 17930 atoms, of which 44 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	425	Total	C	N	O	S	1	1	0
			3359	2109	577	646	27			
2	D	431	Total	C	N	O	S	5	0	0
			3368	2113	575	653	27			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	123	Total	C	N	O	S	0	0	0
			1014	625	183	201	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

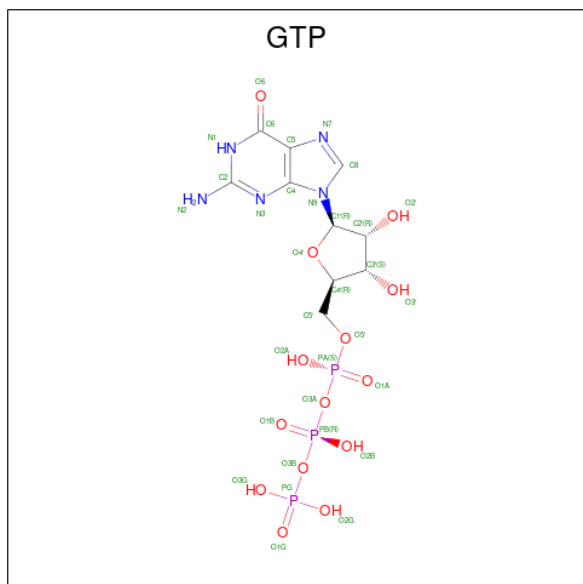
- Molecule 4 is a protein called Tubulin-Tyrosine Ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	349	Total	C	N	O	S	0	0	0
			2853	1830	489	520	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	C	N	O	P	0	0
			32	10	5	14	3		
5	C	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

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

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

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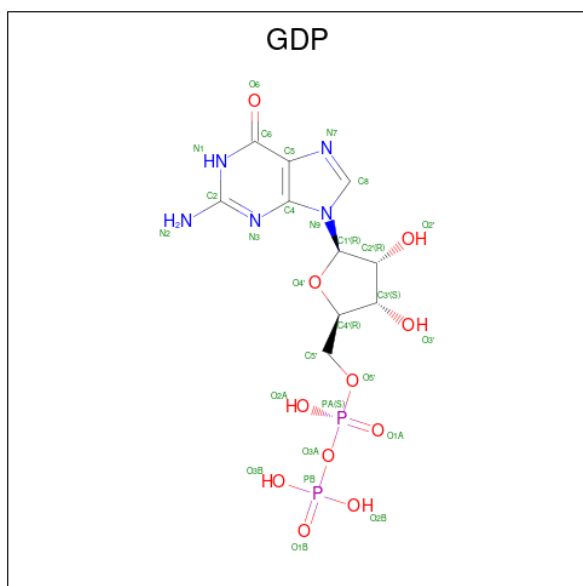
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	F	1	Total	Mg	0	0
			1	1		

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

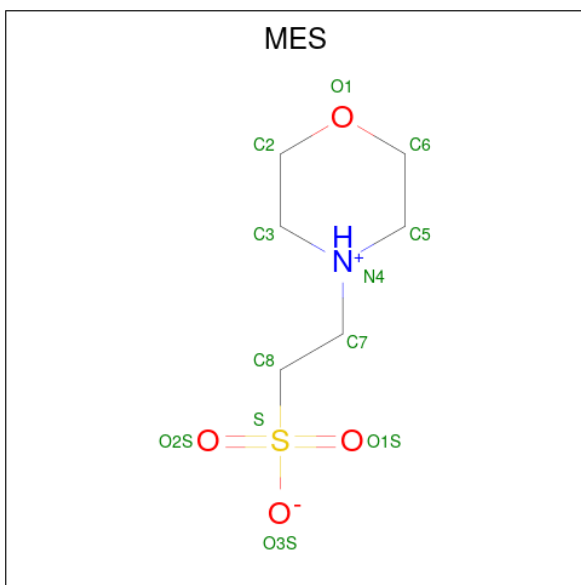
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Ca	0	0
			1	1		
7	B	1	Total	Ca	0	0
			1	1		
7	C	1	Total	Ca	0	0
			1	1		
7	E	1	Total	Ca	0	0
			1	1		

- Molecule 8 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



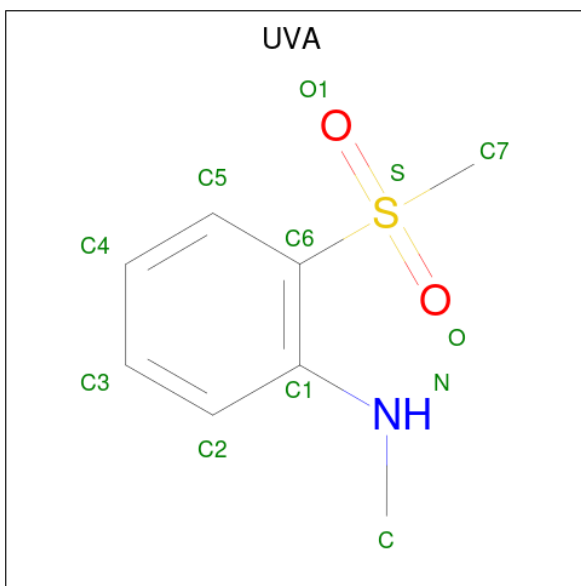
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	B	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
8	D	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- Molecule 9 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: C₆H₁₃NO₄S).



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

- Molecule 10 is N-methyl-2-(methylsulfonyl)aniline (CCD ID: UVA) (formula: $C_8H_{11}NO_2S$) (labeled as "Ligand of Interest" by depositor).



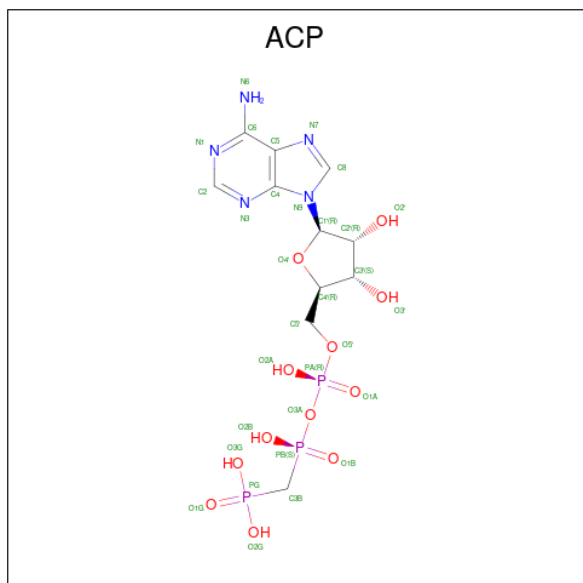
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
10	B	1	Total	C	H	N	O	S	0	0
			23	8	11	1	2	1		
10	B	1	Total	C	H	N	O	S	0	0
			23	8	11	1	2	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	B	1	Total	C	H	N	O	S	
			23	8	11	1	2	1	0
10	D	1	Total	C	H	N	O	S	
			23	8	11	1	2	1	0

- 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		
			31	11	5	12	3	0	0

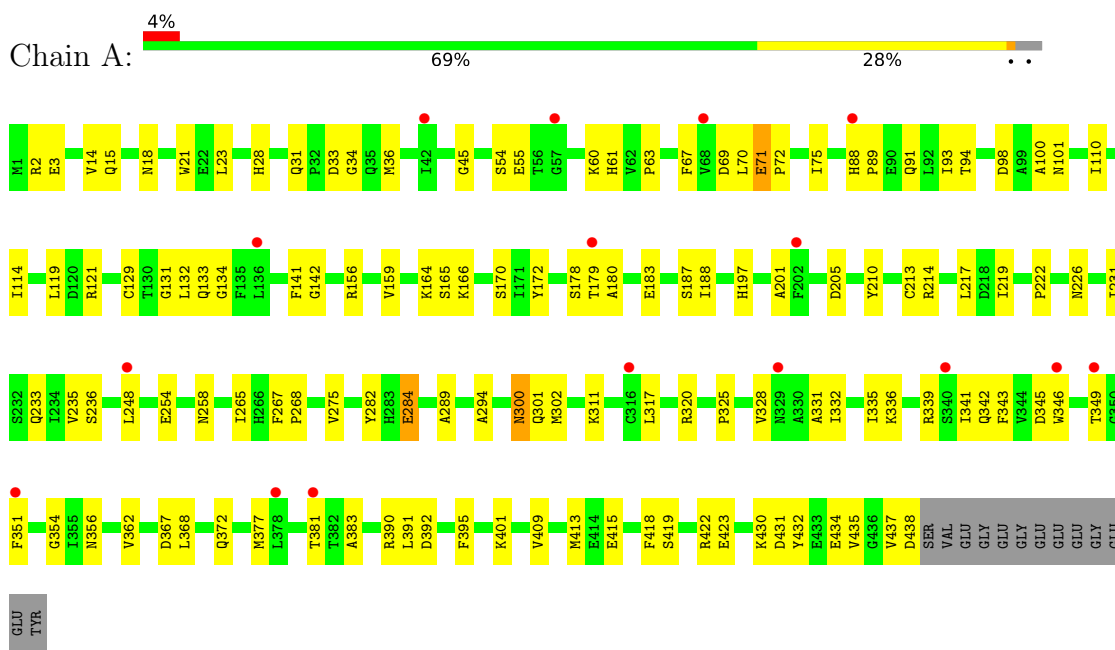
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	31	Total	O		
			31	31	0	0
12	B	44	Total	O		
			44	44	0	0
12	C	108	Total	O		
			108	108	0	0
12	D	12	Total	O		
			12	12	0	0
12	E	9	Total	O		
			9	9	0	0
12	F	1	Total	O		
			1	1	0	0

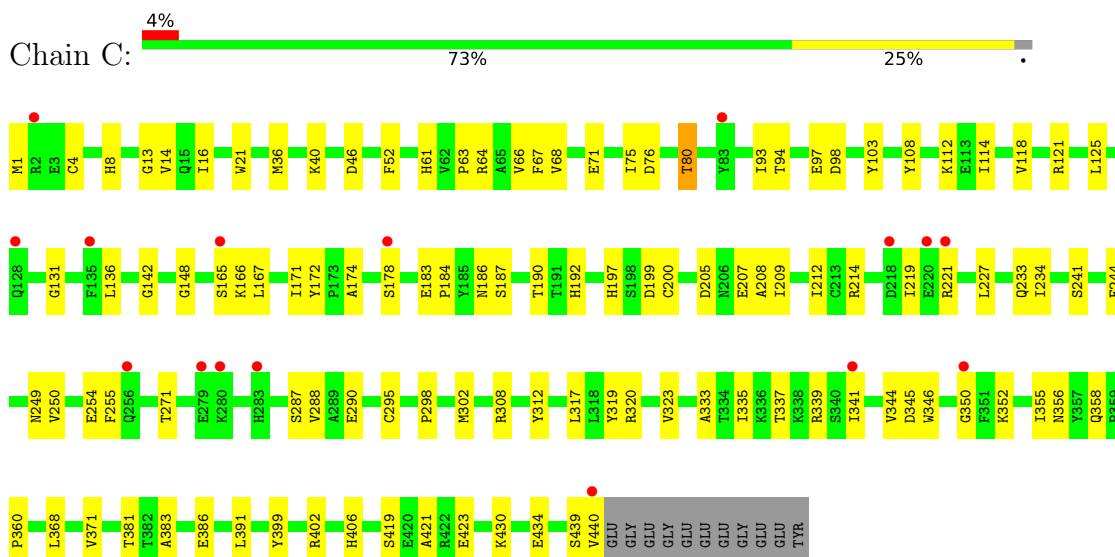
3 Residue-property plots [i](#)

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.

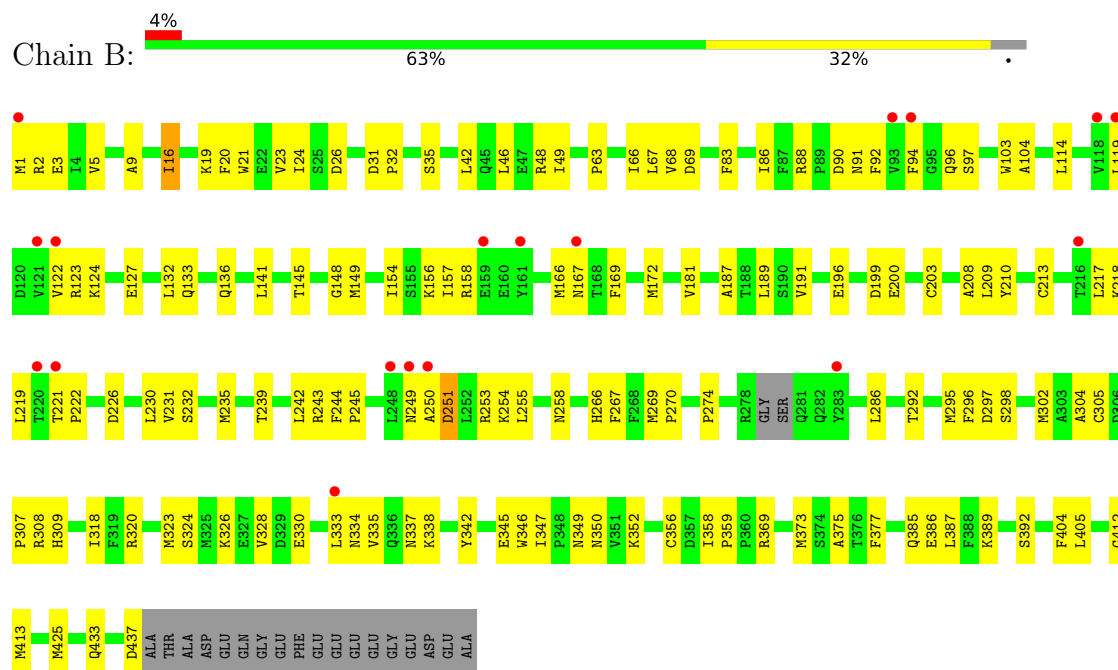
- Molecule 1: Tubulin alpha-1B chain



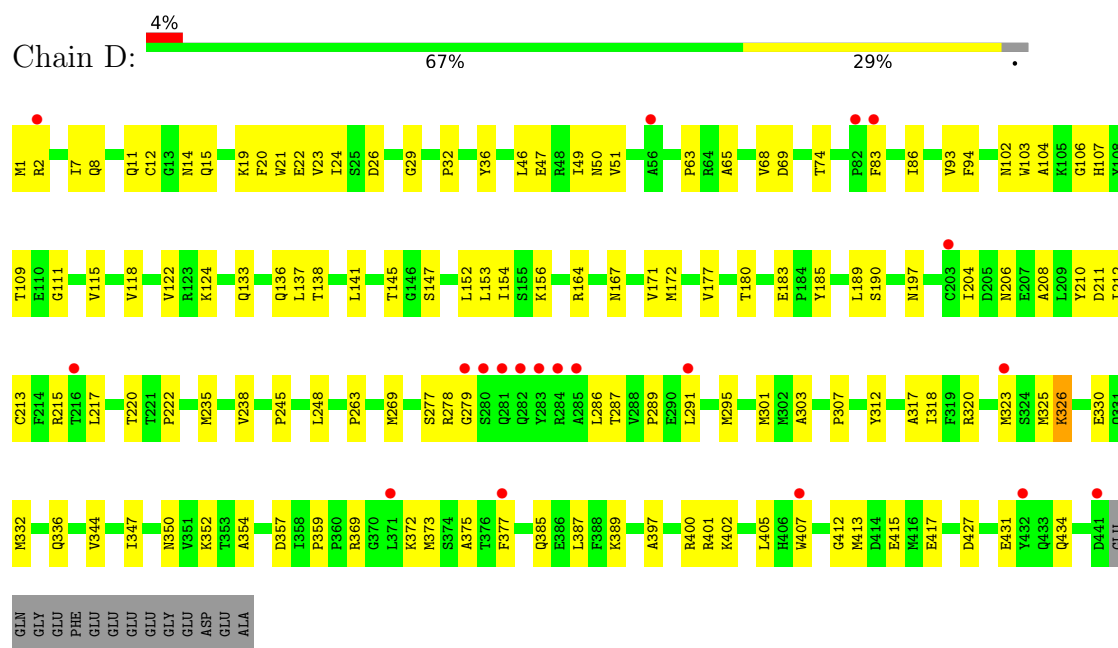
- Molecule 1: Tubulin alpha-1B chain



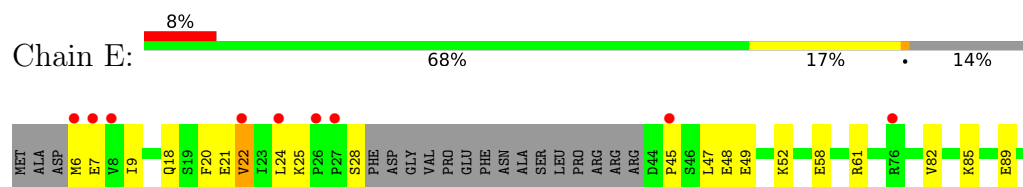
• Molecule 2: Tubulin beta-2B chain



• Molecule 2: Tubulin beta-2B chain

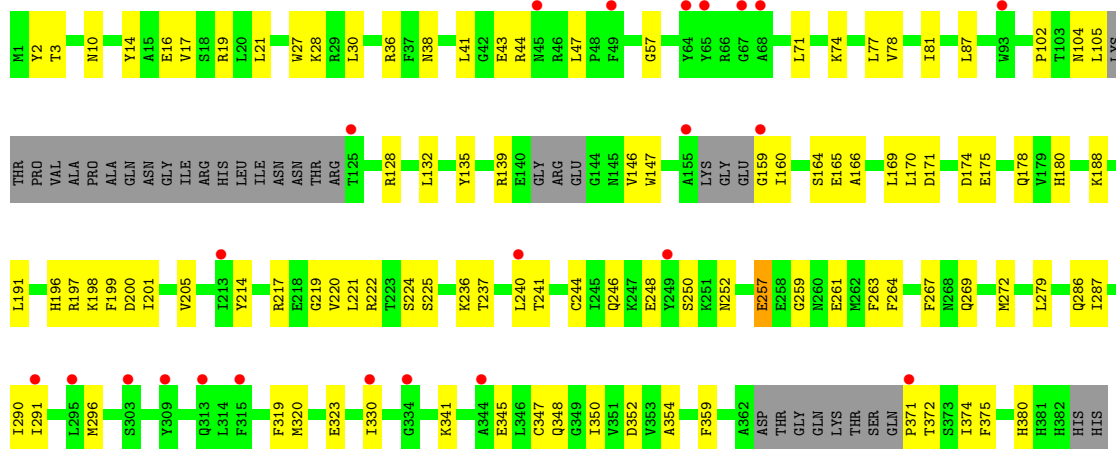


• Molecule 3: Stathmin-4





● 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	105.26Å 158.63Å 179.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	90.81 – 2.53 90.81 – 2.53	Depositor EDS
% Data completeness (in resolution range)	99.5 (90.81-2.53) 99.5 (90.81-2.53)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.23 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.216 , 0.258 0.221 , 0.261	Depositor DCC
R_{free} test set	5070 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	70.5	Xtriage
Anisotropy	0.397	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 56.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	17930	wwPDB-VP
Average B, all atoms (Å ²)	91.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.65% 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: UVA, GDP, GTP, MES, MG, CA, ACP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.11	0/3502	0.28	0/4754
1	C	0.12	0/3521	0.30	0/4780
2	B	0.12	0/3433	0.29	0/4647
2	D	0.12	0/3442	0.29	0/4664
3	E	0.10	0/1022	0.22	0/1356
4	F	0.09	0/2919	0.28	0/3944
All	All	0.12	0/17839	0.28	0/24145

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	3334	108	0
1	C	3443	0	3352	83	0
2	B	3359	0	3235	114	0
2	D	3368	0	3236	101	1
3	E	1014	0	1029	23	1
4	F	2853	0	2816	82	0
5	A	32	0	12	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	32	0	12	0	0
6	A	1	0	0	0	0
6	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
7	E	1	0	0	0	0
8	B	28	0	12	1	0
8	D	28	0	12	2	0
9	B	12	0	12	1	0
10	B	36	33	0	0	0
10	D	12	11	0	0	0
11	F	31	0	14	3	0
12	A	31	0	0	6	0
12	B	44	0	0	3	0
12	C	108	0	0	3	0
12	D	12	0	0	1	0
12	E	9	0	0	1	0
12	F	1	0	0	0	0
All	All	17886	44	17076	488	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 14.

All (488) 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:A:381:THR:HG22	1:A:383:ALA:H	1.28	0.97
4:F:10:ASN:HB2	4:F:44:ARG:HH22	1.30	0.96
2:D:323:MET:HE2	2:D:373:MET:HG2	1.51	0.91
4:F:236:LYS:HB3	4:F:240:LEU:HD13	1.52	0.89
4:F:269:GLN:HA	4:F:272:MET:HE2	1.55	0.88
4:F:102:PRO:HG2	4:F:105:LEU:HD13	1.56	0.86
2:D:397:ALA:O	2:D:401:ARG:NH1	2.14	0.81
2:D:1:MET:HE2	2:D:50:ASN:HB2	1.63	0.81
2:D:47:GLU:HG2	2:D:245:PRO:HG3	1.62	0.80
1:A:226:ASN:ND2	1:A:367:ASP:OD2	2.16	0.78
2:B:208:ALA:HB2	2:B:304:ALA:HB2	1.64	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:167:ASN:OD1	2:B:200:GLU:HB2	1.82	0.78
2:D:295:MET:HE2	2:D:377:PHE:HB2	1.66	0.76
2:B:96:GLN:HB3	1:C:1:MET:HE2	1.68	0.76
1:C:430:LYS:HE2	1:C:434:GLU:OE2	1.88	0.74
4:F:348:GLN:NE2	4:F:352:ASP:OD1	2.21	0.73
4:F:146:VAL:HG22	4:F:164:SER:HB3	1.72	0.72
2:B:23:VAL:HG21	2:B:232:SER:HB3	1.72	0.72
1:C:254:GLU:HG2	1:C:352:LYS:HE2	1.72	0.72
4:F:197:ARG:NH1	4:F:257:GLU:OE2	2.19	0.72
2:B:218:LYS:O	2:B:219:LEU:HD23	1.89	0.71
4:F:128:ARG:NH2	4:F:174:ASP:OD1	2.23	0.70
1:A:172:TYR:HB3	1:A:205:ASP:HA	1.72	0.70
1:A:336:LYS:HD2	1:A:341:ILE:HD12	1.72	0.70
2:B:16:ILE:HD13	2:B:231:VAL:HG11	1.73	0.70
2:B:83:PHE:O	2:B:86:ILE:HG22	1.92	0.70
2:D:136:GLN:HA	2:D:167:ASN:O	1.92	0.70
4:F:102:PRO:HG2	4:F:105:LEU:CD1	2.21	0.69
1:C:178:SER:OG	2:D:352:LYS:NZ	2.25	0.69
1:C:76:ASP:O	1:C:80:THR:HG22	1.93	0.68
2:B:253[A]:ARG:NH1	9:B:504:MES:O3S	2.26	0.68
1:C:93:ILE:HG22	1:C:114:ILE:HD11	1.74	0.68
1:A:332:ILE:HG21	1:A:351:PHE:CZ	2.29	0.68
2:D:434:GLN:OE1	12:D:601:HOH:O	2.11	0.68
2:B:274:PRO:HB3	2:B:286:LEU:HD22	1.75	0.67
2:D:83:PHE:O	2:D:86:ILE:HG22	1.94	0.67
2:D:347:ILE:HG22	2:D:350:ASN:HB3	1.77	0.66
1:A:300:ASN:OD1	12:A:601:HOH:O	2.14	0.66
2:D:208:ALA:O	2:D:212:ILE:HG13	1.96	0.66
2:B:337:ASN:OD1	4:F:36:ARG:HD3	1.96	0.66
1:C:234:ILE:HG12	1:C:302:MET:HE2	1.76	0.66
2:D:152:LEU:O	2:D:156:LYS:HG2	1.95	0.65
2:D:172:MET:HG3	2:D:387:LEU:HD11	1.78	0.65
1:A:142:GLY:HA3	1:A:183:GLU:OE2	1.97	0.65
2:B:145:THR:HB	8:B:501:GDP:O2B	1.97	0.64
2:D:269:MET:HG3	2:D:303:ALA:HB3	1.79	0.64
2:D:217:LEU:HA	2:D:277:SER:HB3	1.80	0.64
1:C:172:TYR:HB3	1:C:205:ASP:HA	1.80	0.64
4:F:14:TYR:HB3	4:F:41:LEU:HD13	1.80	0.63
1:C:241:SER:HA	1:C:249:ASN:OD1	1.98	0.63
2:D:21:TRP:CZ3	2:D:63:PRO:HB3	2.34	0.63
4:F:205:VAL:HG21	4:F:291:ILE:HD13	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:159:GLY:C	4:F:160:ILE:HD12	2.23	0.63
1:A:419:SER:O	1:A:423:GLU:HG3	1.98	0.63
4:F:188:LYS:HD3	4:F:323:GLU:OE2	1.99	0.63
2:B:69:ASP:O	2:B:94:PHE:HA	1.99	0.63
1:C:298:PRO:HG2	1:C:308:ARG:NH2	2.14	0.62
2:B:2:ARG:HB2	2:B:133:GLN:CG	2.29	0.62
4:F:246:GLN:O	4:F:250:SER:HB3	1.98	0.62
1:A:179:THR:HA	2:B:352:LYS:HD2	1.80	0.62
1:A:362:VAL:HG22	12:A:607:HOH:O	2.00	0.62
1:A:2:ARG:HB2	1:A:133:GLN:HE21	1.65	0.62
1:A:28:HIS:O	1:A:36:MET:HE3	2.00	0.62
2:D:248:LEU:HD23	2:D:354:ALA:HB2	1.80	0.62
1:C:350:GLY:O	12:C:601:HOH:O	2.15	0.62
4:F:237:THR:O	4:F:246:GLN:NE2	2.32	0.62
2:B:210:TYR:HE1	2:B:221:THR:HA	1.64	0.61
2:D:69:ASP:O	2:D:94:PHE:HA	1.99	0.61
2:D:2:ARG:HB3	2:D:133:GLN:HG2	1.82	0.61
2:D:397:ALA:HA	2:D:400:ARG:NH1	2.15	0.61
1:A:210:TYR:CE1	1:A:222:PRO:HD2	2.36	0.61
1:A:335:ILE:HG23	1:A:339:ARG:HG3	1.80	0.61
2:B:292:THR:HG22	2:B:335:VAL:HG21	1.83	0.61
2:D:22:GLU:HG2	2:D:83:PHE:CD1	2.36	0.61
4:F:371:PRO:HA	4:F:372:THR:C	2.25	0.61
2:B:269:MET:HE1	2:B:307:PRO:HG3	1.82	0.61
1:C:221:ARG:NH2	2:D:325:MET:HE2	2.16	0.61
1:C:75:ILE:HD12	1:C:94:THR:HG22	1.82	0.61
2:D:220:THR:O	2:D:222:PRO:HD3	2.00	0.61
2:B:295:MET:SD	2:B:375:ALA:HB1	2.41	0.61
2:B:172:MET:HG3	2:B:387:LEU:HD11	1.82	0.61
1:C:174:ALA:O	1:C:178:SER:HB3	2.01	0.61
2:D:295:MET:CE	2:D:377:PHE:HB2	2.30	0.60
2:B:231:VAL:O	2:B:235:MET:HG3	2.02	0.60
1:C:320:ARG:HA	1:C:356:ASN:O	2.02	0.60
2:B:67:LEU:HD22	2:B:92:PHE:CE2	2.37	0.60
2:B:347:ILE:HG22	2:B:350:ASN:HB3	1.84	0.60
2:D:141:LEU:HD12	2:D:172:MET:SD	2.41	0.60
4:F:71:LEU:HD12	4:F:77:LEU:HD13	1.84	0.59
2:D:145:THR:HB	8:D:501:GDP:O2B	2.02	0.59
2:D:147:SER:HB2	2:D:190:SER:OG	2.03	0.59
4:F:2:TYR:CE1	4:F:359:PHE:HB3	2.37	0.59
4:F:236:LYS:HB3	4:F:240:LEU:CD1	2.27	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:333:ALA:O	1:C:337:THR:HG23	2.03	0.59
2:D:19:LYS:O	2:D:23:VAL:HG23	2.03	0.59
2:D:102:ASN:ND2	2:D:407:TRP:HB3	2.18	0.59
2:B:213:CYS:HB3	2:B:222:PRO:HG3	1.85	0.58
1:A:233:GLN:HG3	1:A:368:LEU:CD1	2.34	0.58
4:F:147:TRP:HB2	4:F:169:LEU:HD11	1.85	0.58
1:A:166:LYS:HE2	1:A:197:HIS:O	2.04	0.58
2:B:242:LEU:HD23	2:B:250:ALA:HB1	1.85	0.58
1:A:265:ILE:HG23	1:A:432:TYR:CE1	2.39	0.58
1:A:36:MET:HB3	1:A:61:HIS:CE1	2.38	0.58
2:B:88:ARG:HD3	2:B:91:ASN:OD1	2.04	0.58
4:F:201:ILE:HG12	4:F:221:LEU:HG	1.86	0.58
1:A:93:ILE:HD11	1:A:121:ARG:HG3	1.86	0.57
4:F:371:PRO:HA	4:F:372:THR:HB	1.86	0.57
1:C:4[A]:CYS:SG	1:C:136:LEU:HG	2.43	0.57
2:D:180:THR:O	2:D:183:GLU:HG3	2.04	0.57
2:D:291:LEU:HG	2:D:375:ALA:HB2	1.84	0.57
2:B:123:ARG:O	2:B:127:GLU:HG3	2.05	0.57
2:B:200:GLU:OE2	2:B:255:LEU:HG	2.04	0.57
1:A:88:HIS:HB2	1:A:89:PRO:HD2	1.87	0.57
1:C:21:TRP:CZ3	1:C:63:PRO:HB3	2.39	0.57
4:F:286:GLN:O	4:F:290:ILE:HG13	2.05	0.57
4:F:371:PRO:CA	4:F:372:THR:HB	2.34	0.57
2:D:171:VAL:HA	2:D:204:ILE:O	2.05	0.57
4:F:198:LYS:HG2	4:F:199:PHE:H	1.69	0.57
2:B:46:LEU:HA	2:B:49:ILE:HB	1.86	0.57
4:F:371:PRO:HA	4:F:372:THR:O	2.05	0.56
2:B:136:GLN:HA	2:B:167:ASN:O	2.04	0.56
2:D:20:PHE:CZ	2:D:24:ILE:HD13	2.40	0.56
1:A:3:GLU:OE1	1:A:129:CYS:HB3	2.06	0.56
2:B:324:SER:O	2:B:328:VAL:HG23	2.05	0.56
2:B:305:CYS:O	2:B:307:PRO:HD3	2.05	0.56
1:A:349:THR:HB	3:E:25:LYS:HB3	1.87	0.56
1:A:346:TRP:HZ2	1:A:435:VAL:HG13	1.70	0.56
1:C:312:TYR:CD2	1:C:341:ILE:HG23	2.40	0.56
2:D:21:TRP:CE3	2:D:63:PRO:HB3	2.39	0.56
2:D:332:MET:O	2:D:336:GLN:HG3	2.05	0.56
1:A:254:GLU:HG2	1:A:258:ASN:ND2	2.20	0.56
1:C:214:ARG:HG2	1:C:219:ILE:O	2.06	0.56
2:D:1:MET:HG3	2:D:50:ASN:HB2	1.88	0.56
2:B:244:PHE:CD1	2:B:358:ILE:HD12	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:141:LEU:HD12	2:B:172:MET:SD	2.46	0.55
2:D:1:MET:HE2	2:D:50:ASN:CB	2.34	0.55
1:A:45:GLY:HA3	12:A:620:HOH:O	2.06	0.55
1:A:180:ALA:HB3	1:A:183:GLU:HG3	1.87	0.55
1:A:213:CYS:O	1:A:217:LEU:HB2	2.07	0.55
1:C:221:ARG:HH21	2:D:325:MET:HE2	1.72	0.55
4:F:199:PHE:HA	4:F:241:THR:HG21	1.89	0.55
4:F:320:MET:HG3	4:F:330:ILE:HD11	1.89	0.55
1:C:142:GLY:HA3	1:C:183:GLU:OE1	2.06	0.55
4:F:191:LEU:HD13	4:F:196:HIS:CD2	2.42	0.55
2:B:119:LEU:HD11	2:B:156:LYS:HB3	1.88	0.55
2:B:222:PRO:HB2	2:B:226:ASP:HB2	1.89	0.55
1:C:360:PRO:HG2	1:C:371:VAL:HG23	1.87	0.55
2:D:1:MET:CE	2:D:50:ASN:HB2	2.35	0.55
2:D:286:LEU:HD23	2:D:291:LEU:HD13	1.89	0.55
1:A:188:ILE:HD12	1:A:395:PHE:HB2	1.87	0.54
2:D:1:MET:HE1	2:D:51:VAL:HG23	1.89	0.54
2:D:8:GLN:NE2	2:D:14:ASN:HA	2.22	0.54
2:D:133:GLN:O	2:D:164:ARG:HD3	2.06	0.54
1:C:209:ILE:HG22	1:C:227:LEU:HD22	1.90	0.54
1:C:93:ILE:HD11	1:C:121:ARG:HG3	1.90	0.54
2:D:301:MET:HE3	2:D:307:PRO:HG3	1.88	0.54
1:A:14:VAL:HG13	1:A:67:PHE:HD2	1.73	0.54
2:D:141:LEU:HD22	2:D:190:SER:HB3	1.90	0.54
2:B:297:ASP:OD1	2:B:298:SER:N	2.41	0.54
2:B:308:ARG:HA	2:B:342:TYR:CE1	2.43	0.54
4:F:241:THR:OG1	11:F:401:ACP:O3'	2.22	0.54
4:F:269:GLN:HA	4:F:272:MET:CE	2.34	0.54
2:D:387:LEU:HD23	2:D:387:LEU:C	2.32	0.54
4:F:214:TYR:HB3	4:F:375:PHE:HB3	1.88	0.54
1:A:141:PHE:HB3	1:A:187:SER:OG	2.08	0.54
4:F:128:ARG:NH1	4:F:170:LEU:HD22	2.23	0.54
2:B:42:LEU:H	2:B:42:LEU:HD12	1.73	0.53
3:E:85:LYS:NZ	12:E:301:HOH:O	2.32	0.53
1:C:165:SER:HA	1:C:199:ASP:OD2	2.08	0.53
1:C:312:TYR:CE2	1:C:341:ILE:HG23	2.43	0.53
4:F:147:TRP:HB2	4:F:169:LEU:CD1	2.39	0.53
1:A:98:ASP:HB2	5:A:501:GTP:O2G	2.08	0.53
2:B:19:LYS:O	2:B:23:VAL:HG23	2.09	0.53
4:F:3:THR:HA	4:F:28:LYS:O	2.08	0.53
2:B:2:ARG:NH1	2:B:249:ASN:O	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:210:TYR:CE1	2:D:222:PRO:HG2	2.43	0.53
2:B:114:LEU:HD23	2:B:149:MET:HE1	1.90	0.52
1:C:187:SER:HB3	1:C:391:LEU:HD21	1.91	0.52
4:F:200:ASP:OD1	4:F:222:ARG:HB2	2.08	0.52
4:F:205:VAL:CG2	4:F:291:ILE:HD13	2.39	0.52
1:A:100:ALA:HA	2:B:254:LYS:HG3	1.92	0.52
1:A:317:LEU:HD23	1:A:377:MET:HG3	1.91	0.52
4:F:267:PHE:CE2	4:F:279:LEU:HD13	2.45	0.52
1:A:284:GLU:CD	1:A:284:GLU:H	2.17	0.52
1:A:311:LYS:HA	1:A:342:GLN:O	2.09	0.52
1:C:71:GLU:HG2	1:C:98:ASP:HB3	1.91	0.52
1:C:319:TYR:HB2	1:C:355:ILE:HG12	1.91	0.52
2:D:7:ILE:O	2:D:137:LEU:HD12	2.09	0.52
4:F:217:ARG:NH2	4:F:374:ILE:HA	2.24	0.52
1:A:231:ILE:O	1:A:235:VAL:HG23	2.10	0.52
1:A:328:VAL:O	1:A:332:ILE:HG12	2.08	0.52
2:D:427:ASP:O	2:D:431:GLU:HG3	2.09	0.52
2:B:97:SER:N	12:B:603:HOH:O	2.42	0.52
2:B:203:CYS:SG	2:B:267:PHE:HB3	2.49	0.52
1:C:208:ALA:O	1:C:212:ILE:HG13	2.10	0.52
2:D:124:LYS:C	2:D:124:LYS:HD3	2.35	0.52
2:B:318:ILE:N	2:B:318:ILE:HD12	2.25	0.52
4:F:171:ASP:O	4:F:175:GLU:HG3	2.10	0.52
1:C:1:MET:HE3	1:C:131:GLY:HA3	1.92	0.52
2:D:46:LEU:HA	2:D:49:ILE:HB	1.92	0.52
4:F:17:VAL:O	4:F:21:LEU:HG	2.10	0.52
1:C:172:TYR:CE1	1:C:391:LEU:HD22	2.45	0.51
2:D:326:LYS:O	2:D:330:GLU:HG3	2.09	0.51
2:B:250:ALA:O	2:B:251:ASP:HB3	2.09	0.51
11:F:401:ACP:O3G	11:F:401:ACP:O1B	2.28	0.51
2:D:141:LEU:HD22	2:D:190:SER:CB	2.40	0.51
2:B:295:MET:CG	2:B:377:PHE:HB2	2.41	0.51
1:C:209:ILE:HD11	1:C:302:MET:CE	2.39	0.51
2:B:66:ILE:HD12	2:B:122:VAL:HG22	1.93	0.51
1:C:178:SER:HB2	1:C:183:GLU:OE2	2.11	0.51
1:C:66:VAL:HG23	1:C:125:LEU:HD11	1.93	0.51
1:A:75:ILE:HB	1:A:94:THR:CG2	2.41	0.51
2:D:15:GLN:NE2	2:D:74:THR:HG23	2.26	0.51
3:E:45:PRO:HA	3:E:49:GLU:OE1	2.10	0.51
1:A:302:MET:N	1:A:302:MET:HE2	2.26	0.50
1:A:372:GLN:OE1	1:A:372:GLN:HA	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:88:ARG:NH1	2:B:90:ASP:HB2	2.25	0.50
1:C:221:ARG:HG3	2:D:325:MET:HG2	1.92	0.50
4:F:10:ASN:CB	4:F:44:ARG:HH22	2.13	0.50
2:D:2:ARG:O	2:D:133:GLN:NE2	2.34	0.50
1:A:75:ILE:HD12	1:A:94:THR:CG2	2.42	0.50
1:A:349:THR:O	1:A:349:THR:HG22	2.11	0.50
1:C:234:ILE:HD12	1:C:234:ILE:N	2.27	0.50
2:B:349:ASN:O	2:B:352:LYS:HE2	2.12	0.50
4:F:287:ILE:HG23	4:F:319:PHE:CZ	2.46	0.50
1:A:141:PHE:CE1	1:A:170:SER:HB3	2.47	0.50
4:F:10:ASN:HB2	4:F:44:ARG:NH2	2.14	0.50
1:A:294:ALA:O	1:A:300:ASN:ND2	2.45	0.50
2:D:177:VAL:HG21	2:D:206:ASN:HB3	1.94	0.50
1:A:69:ASP:O	1:A:94:THR:HA	2.12	0.49
1:A:98:ASP:OD1	1:A:100:ALA:N	2.42	0.49
4:F:198:LYS:O	4:F:199:PHE:HB3	2.11	0.49
1:A:142:GLY:CA	1:A:183:GLU:HG2	2.42	0.49
1:A:325:PRO:HB3	3:E:20:PHE:CE2	2.47	0.49
2:B:209:LEU:HD21	2:B:302:MET:HG3	1.93	0.49
1:C:192:HIS:CG	1:C:421:ALA:HA	2.47	0.49
2:D:1:MET:HG3	2:D:50:ASN:CB	2.42	0.49
2:B:187:ALA:O	2:B:191:VAL:HG23	2.12	0.49
3:E:47:LEU:HD12	3:E:47:LEU:O	2.13	0.49
2:B:199:ASP:O	2:B:266:HIS:HB2	2.13	0.49
2:B:239:THR:O	2:B:243:ARG:HG3	2.12	0.49
2:B:1:MET:HB3	2:B:3:GLU:OE2	2.13	0.49
1:A:31:GLN:HB2	1:A:33:ASP:OD1	2.13	0.49
4:F:3:THR:HB	4:F:30:LEU:HD11	1.95	0.49
2:B:21:TRP:CZ3	2:B:63:PRO:HB3	2.48	0.49
1:C:36:MET:HB3	1:C:61:HIS:CE1	2.47	0.49
1:A:188:ILE:HD12	1:A:395:PHE:CB	2.43	0.48
1:C:250:VAL:HG11	1:C:352:LYS:HE3	1.94	0.48
1:C:419:SER:O	1:C:423:GLU:HG3	2.12	0.48
1:A:2:ARG:HB3	1:A:131:GLY:O	2.13	0.48
2:B:213:CYS:CB	2:B:222:PRO:HG3	2.43	0.48
2:B:31:ASP:HB2	2:B:32:PRO:HD2	1.95	0.48
2:B:181:VAL:HG21	2:B:404:PHE:CZ	2.48	0.48
2:D:213:CYS:HA	2:D:217:LEU:HB2	1.95	0.48
2:D:287:THR:HB	2:D:289:PRO:HD2	1.95	0.48
3:E:137:LYS:HE2	3:E:141:GLU:OE2	2.14	0.48
4:F:259:GLY:O	4:F:261:GLU:HG3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:ALA:O	1:A:268:PRO:HD2	2.14	0.48
1:A:15:GLN:O	1:A:18:ASN:HB2	2.13	0.48
2:B:2:ARG:HB2	2:B:133:GLN:HG3	1.95	0.48
2:B:31:ASP:HB2	2:B:32:PRO:CD	2.44	0.48
1:C:287:SER:OG	1:C:290:GLU:HG3	2.14	0.48
2:D:295:MET:SD	2:D:375:ALA:HB1	2.53	0.48
2:B:114:LEU:O	2:B:114:LEU:HG	2.12	0.48
4:F:178:GLN:HE21	4:F:180:HIS:HE1	1.61	0.48
1:A:21:TRP:CZ3	1:A:63:PRO:HB3	2.48	0.48
1:A:75:ILE:HB	1:A:94:THR:HG21	1.96	0.48
2:D:2:ARG:HB3	2:D:133:GLN:CG	2.43	0.48
2:B:67:LEU:N	2:B:67:LEU:HD12	2.29	0.47
2:B:230:LEU:HB3	2:B:302:MET:CE	2.43	0.47
2:B:345:GLU:OE1	2:B:345:GLU:N	2.38	0.47
2:B:31:ASP:OD1	2:B:35:SER:N	2.47	0.47
1:A:159:VAL:HG11	3:E:47:LEU:HB2	1.95	0.47
3:E:7:GLU:O	3:E:22:VAL:HA	2.14	0.47
1:A:395:PHE:CD1	1:A:422:ARG:HD3	2.50	0.47
2:B:169:PHE:CD1	2:B:235:MET:HE3	2.50	0.47
1:C:21:TRP:CH2	1:C:63:PRO:HB3	2.50	0.47
1:C:233:GLN:HG3	1:C:368:LEU:CD1	2.44	0.47
1:A:71:GLU:HG2	1:A:72:PRO:HD2	1.97	0.47
2:B:2:ARG:HB2	2:B:133:GLN:HE21	1.80	0.47
4:F:222:ARG:O	4:F:241:THR:HB	2.15	0.47
2:B:5:VAL:HG23	2:B:132:LEU:CD1	2.45	0.47
2:D:413:MET:HE3	2:D:417:GLU:CD	2.39	0.47
4:F:220:VAL:HG12	4:F:263:PHE:CD1	2.50	0.47
1:A:75:ILE:HD12	1:A:94:THR:HG22	1.96	0.47
1:A:233:GLN:HG3	1:A:368:LEU:HD12	1.96	0.47
2:B:124:LYS:HD3	2:B:124:LYS:C	2.40	0.47
1:C:344:VAL:HG21	1:C:346:TRP:CE2	2.50	0.47
2:D:115:VAL:HG23	2:D:153:LEU:HD23	1.97	0.47
4:F:217:ARG:NH2	4:F:374:ILE:HG22	2.30	0.47
1:A:301:GLN:C	1:A:302:MET:HE2	2.40	0.46
2:B:119:LEU:HD11	2:B:156:LYS:CB	2.44	0.46
1:C:108:TYR:O	1:C:112:LYS:HG2	2.15	0.46
1:A:187:SER:CB	1:A:391:LEU:HD21	2.45	0.46
2:B:296:PHE:CD2	2:B:335:VAL:HG11	2.50	0.46
2:B:320:ARG:O	2:B:373:MET:HA	2.15	0.46
1:A:401:LYS:HG3	2:B:346:TRP:CE3	2.50	0.46
3:E:128:LYS:O	3:E:128:LYS:HD3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:81:ILE:HA	4:F:87:LEU:HD12	1.98	0.46
1:A:54:SER:O	1:A:61:HIS:HA	2.15	0.46
2:B:103:TRP:CE3	2:B:189:LEU:HD13	2.49	0.46
2:B:157:ILE:HG21	2:B:166:MET:HE1	1.97	0.46
2:B:154:ILE:HG23	2:B:166:MET:HG2	1.98	0.46
2:D:318:ILE:N	2:D:318:ILE:HD12	2.31	0.46
2:D:32:PRO:HA	2:D:83:PHE:CD2	2.50	0.46
2:D:277:SER:O	2:D:279:GLY:N	2.48	0.46
1:A:142:GLY:HA3	1:A:183:GLU:HG2	1.97	0.46
1:C:383:ALA:O	1:C:386:GLU:HG3	2.16	0.46
1:A:430:LYS:HE2	1:A:434:GLU:OE2	2.15	0.46
2:B:83:PHE:HA	12:B:601:HOH:O	2.14	0.46
2:B:244:PHE:HB3	2:B:245:PRO:HD2	1.98	0.46
1:C:271:THR:HG21	1:C:295:CYS:O	2.16	0.46
1:C:345:ASP:OD2	1:C:439:SER:N	2.42	0.46
2:D:104:ALA:HB2	2:D:413:MET:SD	2.56	0.46
1:A:34:GLY:HA3	1:A:60:LYS:HG3	1.97	0.45
1:A:201:ALA:HB3	1:A:267:PHE:CD1	2.52	0.45
1:C:288:VAL:HG22	1:C:323:VAL:HG22	1.98	0.45
2:D:29:GLY:O	2:D:36:TYR:HA	2.17	0.45
2:D:211:ASP:O	2:D:215:ARG:HB2	2.15	0.45
1:C:80:THR:O	1:C:80:THR:OG1	2.31	0.45
4:F:16:GLU:OE2	4:F:19:ARG:NH2	2.48	0.45
2:B:295:MET:HG2	2:B:377:PHE:HB2	1.97	0.45
1:C:66:VAL:HG23	1:C:125:LEU:CD1	2.46	0.45
1:C:249:ASN:OD1	1:C:356:ASN:ND2	2.42	0.45
1:A:335:ILE:HG23	1:A:339:ARG:CG	2.45	0.45
2:B:104:ALA:HB2	2:B:413:MET:SD	2.56	0.45
1:A:188:ILE:HD11	1:A:392:ASP:HA	1.98	0.45
3:E:48:GLU:HG2	3:E:52:LYS:HE3	1.98	0.45
2:D:115:VAL:HG23	2:D:153:LEU:CD2	2.47	0.45
2:D:385:GLN:O	2:D:389:LYS:HG3	2.17	0.45
4:F:160:ILE:HD12	4:F:160:ILE:N	2.32	0.45
4:F:296:MET:SD	4:F:380:HIS:HB2	2.57	0.45
1:A:343:PHE:CD1	1:A:349:THR:HG23	2.51	0.45
2:D:1:MET:HE2	2:D:50:ASN:C	2.42	0.45
4:F:19:ARG:HD2	4:F:19:ARG:C	2.42	0.45
2:B:26:ASP:OD1	2:B:369:ARG:NH2	2.50	0.45
2:B:96:GLN:CB	1:C:1:MET:HE2	2.43	0.45
1:C:68:VAL:HG11	1:C:118:VAL:HG21	1.98	0.45
1:C:335:ILE:HG23	1:C:339:ARG:HG3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:199:PHE:CA	4:F:241:THR:HG21	2.47	0.45
1:C:399:TYR:O	1:C:402:ARG:NH1	2.45	0.45
4:F:178:GLN:NE2	4:F:180:HIS:HE1	2.15	0.45
1:A:88:HIS:CE1	1:A:91:GLN:HG3	2.52	0.45
2:B:210:TYR:OH	2:B:221:THR:HG22	2.17	0.45
2:B:213:CYS:HA	2:B:217:LEU:HB2	1.98	0.45
1:C:166:LYS:HE2	1:C:197:HIS:O	2.17	0.45
2:D:402:LYS:HE2	2:D:415:GLU:OE1	2.17	0.45
1:A:213:CYS:HA	1:A:217:LEU:HD12	1.99	0.44
4:F:241:THR:HG1	11:F:401:ACP:HO3'	1.56	0.44
1:A:325:PRO:HD3	3:E:18:GLN:NE2	2.32	0.44
2:B:270:PRO:HG2	2:B:302:MET:HB2	1.97	0.44
3:E:9:ILE:HG12	3:E:21:GLU:O	2.18	0.44
1:A:248:LEU:HD23	1:A:354:GLY:HA3	2.00	0.44
2:B:20:PHE:CZ	2:B:24:ILE:HD13	2.53	0.44
1:C:14:VAL:HG13	1:C:67:PHE:HD2	1.83	0.44
1:C:234:ILE:HD12	1:C:234:ILE:H	1.80	0.44
2:D:141:LEU:HA	2:D:147:SER:HB3	1.99	0.44
2:D:154:ILE:HG22	2:D:197:ASN:HB3	1.97	0.44
1:A:409:VAL:HA	1:A:413:MET:O	2.17	0.44
2:B:347:ILE:CG2	2:B:350:ASN:HB3	2.47	0.44
2:D:12:CYS:HB2	8:D:501:GDP:C8	2.52	0.44
2:D:402:LYS:HB3	2:D:405:LEU:HD12	1.99	0.44
2:B:158:ARG:NH1	2:B:196:GLU:O	2.51	0.44
1:A:55:GLU:HA	1:A:60:LYS:O	2.17	0.44
2:B:309:HIS:ND1	2:B:386:GLU:OE2	2.47	0.44
4:F:135:TYR:CZ	4:F:166:ALA:HB2	2.53	0.44
1:A:265:ILE:HG23	1:A:432:TYR:CZ	2.51	0.44
1:C:46:ASP:N	1:C:46:ASP:OD1	2.49	0.44
1:C:255:PHE:CE1	1:C:352:LYS:HG2	2.53	0.44
1:C:423:GLU:HB3	12:C:658:HOH:O	2.17	0.44
2:B:334:ASN:O	2:B:338:LYS:HG3	2.18	0.43
2:B:385:GLN:OE1	2:B:389:LYS:HE3	2.18	0.43
4:F:16:GLU:HB3	4:F:347:CYS:SG	2.58	0.43
2:B:218:LYS:C	2:B:219:LEU:HD23	2.42	0.43
1:A:356:ASN:HB2	12:A:628:HOH:O	2.17	0.43
2:B:2:ARG:HB2	2:B:133:GLN:NE2	2.32	0.43
2:B:209:LEU:CD2	2:B:302:MET:HG3	2.48	0.43
1:A:345:ASP:O	3:E:28:SER:HB2	2.19	0.43
1:A:346:TRP:HZ2	1:A:435:VAL:CG1	2.31	0.43
4:F:341:LYS:HG2	4:F:341:LYS:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:LEU:HD22	1:A:110:ILE:CG2	2.48	0.43
1:A:431:ASP:O	1:A:435:VAL:HG23	2.19	0.43
2:B:5:VAL:HG23	2:B:132:LEU:HD13	2.00	0.43
2:B:412:GLY:C	3:E:82:VAL:HG13	2.43	0.43
1:C:16:ILE:HD11	1:C:171:ILE:HD11	2.00	0.43
1:C:40:LYS:HG2	12:C:669:HOH:O	2.19	0.43
1:C:174:ALA:CB	1:C:207:GLU:HB2	2.48	0.43
4:F:38:ASN:HB3	4:F:359:PHE:CE1	2.54	0.43
1:A:3:GLU:O	1:A:132:LEU:HD12	2.19	0.43
1:C:103:TYR:CE2	1:C:148:GLY:HA2	2.54	0.43
2:D:21:TRP:CZ2	2:D:65:ALA:HB2	2.52	0.43
2:D:326:LYS:NZ	2:D:326:LYS:HB3	2.34	0.43
1:A:15:GLN:NE2	5:A:501:GTP:O6	2.49	0.43
1:A:430:LYS:O	1:A:434:GLU:HG3	2.18	0.43
1:C:174:ALA:HB1	1:C:207:GLU:HB2	2.01	0.43
2:D:109:THR:HG21	3:E:137:LYS:NZ	2.33	0.43
4:F:139:ARG:NH2	4:F:165:GLU:OE1	2.51	0.43
2:D:118:VAL:O	2:D:122:VAL:HG23	2.18	0.43
3:E:85:LYS:NZ	3:E:89:GLU:OE2	2.41	0.43
1:A:390:ARG:NH2	12:A:610:HOH:O	2.52	0.42
2:B:333:LEU:HD13	4:F:57:GLY:HA3	2.00	0.42
1:A:275:VAL:HG13	1:A:368:LEU:CD2	2.50	0.42
2:B:392:SER:HB2	2:B:425:MET:CE	2.49	0.42
4:F:225:SER:HB2	4:F:252:ASN:O	2.19	0.42
2:D:107:HIS:O	2:D:152:LEU:HD22	2.19	0.42
2:D:220:THR:C	2:D:222:PRO:HD3	2.44	0.42
4:F:217:ARG:NH1	4:F:345:GLU:OE2	2.53	0.42
1:A:289:ALA:HA	1:A:331:ALA:CB	2.49	0.42
1:A:415:GLU:O	1:A:418:PHE:HB2	2.19	0.42
2:D:2:ARG:C	2:D:133:GLN:HE21	2.22	0.42
3:E:48:GLU:CG	3:E:52:LYS:HE3	2.49	0.42
1:A:164:LYS:HE2	12:A:631:HOH:O	2.20	0.42
1:A:180:ALA:CB	1:A:183:GLU:HG3	2.49	0.42
1:C:97:GLU:HG3	2:D:2:ARG:NH2	2.34	0.42
2:D:312:TYR:O	2:D:344:VAL:HG22	2.20	0.42
4:F:220:VAL:HG12	4:F:263:PHE:CE1	2.54	0.42
4:F:244:CYS:O	4:F:248:GLU:HB2	2.19	0.42
1:A:23:LEU:HD23	1:A:236:SER:HB2	2.01	0.42
1:A:345:ASP:HB3	3:E:28:SER:HB2	2.02	0.42
2:D:1:MET:SD	2:D:50:ASN:HB2	2.59	0.42
2:D:106:GLY:O	2:D:111:GLY:HA3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:320:ARG:O	2:D:373:MET:HA	2.20	0.42
4:F:197:ARG:HB2	4:F:224:SER:O	2.19	0.42
4:F:240:LEU:HD12	4:F:240:LEU:N	2.35	0.42
1:C:16:ILE:CD1	1:C:171:ILE:HD11	2.50	0.42
1:C:136:LEU:HD23	1:C:167:LEU:HB2	2.02	0.42
2:D:68:VAL:HA	2:D:93:VAL:O	2.20	0.42
1:A:214:ARG:HG2	1:A:219:ILE:O	2.19	0.41
1:A:332:ILE:HG21	1:A:351:PHE:CE2	2.55	0.41
1:C:8:HIS:HB3	1:C:13:GLY:O	2.20	0.41
2:D:11:GLN:O	2:D:15:GLN:HG2	2.20	0.41
2:D:138:THR:HG21	2:D:235:MET:HE1	2.02	0.41
2:D:291:LEU:HG	2:D:375:ALA:CB	2.50	0.41
4:F:372:THR:O	4:F:372:THR:HG22	2.20	0.41
1:A:381:THR:HG22	1:A:383:ALA:N	2.13	0.41
1:A:437:VAL:HG12	1:A:438:ASP:N	2.36	0.41
1:C:167:LEU:HA	1:C:200:CYS:O	2.20	0.41
1:C:244:PHE:CD1	1:C:358:GLN:HG2	2.55	0.41
4:F:47:LEU:C	4:F:47:LEU:HD23	2.44	0.41
4:F:350:ILE:O	4:F:354:ALA:HB3	2.20	0.41
1:A:187:SER:HB3	1:A:391:LEU:HD21	2.01	0.41
2:B:103:TRP:CD1	2:B:148:GLY:HA2	2.54	0.41
1:C:103:TYR:CD2	1:C:148:GLY:HA2	2.54	0.41
2:B:320:ARG:HB3	2:B:359:PRO:HA	2.03	0.41
1:C:183:GLU:N	1:C:184:PRO:CD	2.84	0.41
1:A:320:ARG:HA	1:A:356:ASN:O	2.20	0.41
2:B:323:MET:HB3	2:B:373:MET:HE2	2.02	0.41
2:B:392:SER:HB2	2:B:425:MET:HE3	2.02	0.41
2:B:405:LEU:HD23	2:B:405:LEU:HA	1.88	0.41
1:C:52:PHE:O	1:C:64:ARG:HG3	2.21	0.41
1:C:440:VAL:HG12	1:C:440:VAL:O	2.20	0.41
2:D:103:TRP:CE3	2:D:189:LEU:HD13	2.56	0.41
2:D:317:ALA:C	2:D:318:ILE:HD12	2.45	0.41
1:A:101:ASN:HD22	2:B:258:ASN:HD21	1.68	0.41
1:A:119:LEU:HD11	1:A:156:ARG:HB3	2.03	0.41
2:B:320:ARG:HA	2:B:356:CYS:O	2.20	0.41
4:F:132:LEU:HD21	4:F:170:LEU:HD11	2.02	0.41
1:A:134:GLY:HA3	1:A:165:SER:O	2.20	0.41
2:D:185:TYR:O	2:D:189:LEU:HG	2.21	0.41
4:F:74:LYS:O	4:F:78:VAL:HG23	2.20	0.41
4:F:219:GLY:HA3	4:F:264:PHE:CZ	2.56	0.41
1:A:14:VAL:HG13	1:A:67:PHE:CD2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:244:PHE:CE1	2:B:358:ILE:HD12	2.56	0.41
2:B:433:GLN:OE1	2:B:433:GLN:HA	2.20	0.41
1:A:114:ILE:O	1:A:114:ILE:HG12	2.21	0.41
1:A:178:SER:OG	1:A:183:GLU:OE1	2.09	0.41
2:D:1:MET:CG	2:D:50:ASN:HB2	2.51	0.41
3:E:92:ASN:O	3:E:96:MET:HG2	2.20	0.41
2:B:48:ARG:HH22	2:B:250:ALA:HB3	1.85	0.40
2:B:307:PRO:C	2:B:309:HIS:H	2.29	0.40
2:B:326:LYS:O	2:B:330:GLU:HG3	2.21	0.40
2:B:387:LEU:HD23	2:B:387:LEU:C	2.46	0.40
2:D:412:GLY:C	3:E:133:VAL:HG13	2.46	0.40
4:F:2:TYR:HB2	4:F:27:TRP:CD2	2.56	0.40
4:F:217:ARG:HH22	4:F:374:ILE:HG22	1.86	0.40
1:A:317:LEU:CD2	1:A:377:MET:HG3	2.51	0.40
2:B:42:LEU:HD12	2:B:42:LEU:N	2.34	0.40
12:B:619:HOH:O	1:C:254:GLU:HA	2.20	0.40
1:C:317:LEU:HB3	1:C:319:TYR:CE1	2.56	0.40
1:C:406:HIS:CG	2:D:263:PRO:HD3	2.56	0.40
3:E:6:MET:SD	3:E:24:LEU:HD23	2.61	0.40
3:E:58:GLU:HA	3:E:61:ARG:NH2	2.36	0.40
1:A:349:THR:O	3:E:24:LEU:HB2	2.22	0.40
1:C:186:ASN:O	1:C:190:THR:HG22	2.21	0.40
2:D:357:ASP:O	2:D:359:PRO:HD3	2.22	0.40
2:B:9:ALA:HA	2:B:68:VAL:O	2.22	0.40
4:F:2:TYR:CD1	4:F:359:PHE:HB3	2.56	0.40
4:F:104:ASN:C	4:F:105:LEU:HD12	2.47	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)
2:D:372:LYS:NZ	3:E:58:GLU:OE2[4_455]	2.11	0.09

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%)	419 (96%)	17 (4%)	0	100	100
1	C	439/451 (97%)	425 (97%)	14 (3%)	0	100	100
2	B	422/445 (95%)	400 (95%)	21 (5%)	1 (0%)	43	62
2	D	429/445 (96%)	409 (95%)	19 (4%)	1 (0%)	43	62
3	E	119/143 (83%)	118 (99%)	1 (1%)	0	100	100
4	F	339/384 (88%)	322 (95%)	17 (5%)	0	100	100
All	All	2184/2319 (94%)	2093 (96%)	89 (4%)	2 (0%)	48	67

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	278	ARG
2	B	251	ASP

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%)	365 (99%)	4 (1%)	65	83
1	C	372/379 (98%)	370 (100%)	2 (0%)	81	91
2	B	368/383 (96%)	366 (100%)	2 (0%)	81	91
2	D	368/383 (96%)	364 (99%)	4 (1%)	65	83
3	E	110/127 (87%)	108 (98%)	2 (2%)	51	75
4	F	313/342 (92%)	311 (99%)	2 (1%)	78	90
All	All	1900/1993 (95%)	1884 (99%)	16 (1%)	73	88

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	GLU
1	A	282	TYR
1	A	284	GLU
1	A	300	ASN
2	B	16	ILE
2	B	437	ASP
1	C	80	THR
1	C	381	THR
2	D	26	ASP
2	D	238	VAL
2	D	326	LYS
2	D	369	ARG
3	E	22	VAL
3	E	128	LYS
4	F	43	GLU
4	F	257	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	GLN
1	A	88	HIS
1	A	101	ASN
1	A	283	HIS
1	A	285	GLN
1	A	309	HIS
1	A	342	GLN
1	C	133	GLN
1	C	283	HIS
1	C	329	ASN
2	D	349	ASN
3	E	12	ASN
3	E	71	HIS
4	F	180	HIS
4	F	183	GLN
4	F	306	HIS
4	F	333	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [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 19 ligands modelled in this entry, 9 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$
8	GDP	D	501	6	29,30,30	1.16	3 (10%)	45,47,47	1.76	6 (13%)
8	GDP	B	501	6	29,30,30	1.17	3 (10%)	45,47,47	1.70	7 (15%)
10	UVA	B	506	-	12,12,12	0.33	0	17,17,17	0.92	1 (5%)
10	UVA	D	503	-	12,12,12	0.27	0	17,17,17	0.90	1 (5%)
5	GTP	C	501	6	33,34,34	1.00	3 (9%)	50,54,54	1.51	8 (16%)
9	MES	B	504	-	12,12,12	2.34	1 (8%)	15,16,16	1.91	4 (26%)
10	UVA	B	507	-	12,12,12	0.31	0	17,17,17	0.88	1 (5%)
11	ACP	F	401	6	31,33,33	1.66	8 (25%)	47,52,52	1.89	10 (21%)
10	UVA	B	505	-	12,12,12	0.29	0	17,17,17	0.87	1 (5%)
5	GTP	A	501	6	33,34,34	1.00	3 (9%)	50,54,54	1.55	8 (16%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	GDP	D	501	6	-	2/16/32/32	0/3/3/3
8	GDP	B	501	6	-	2/16/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	UVA	B	506	-	-	0/8/8/8	0/1/1/1
10	UVA	D	503	-	-	0/8/8/8	0/1/1/1
5	GTP	C	501	6	-	8/22/38/38	0/3/3/3
9	MES	B	504	-	-	4/6/14/14	0/1/1/1
10	UVA	B	507	-	-	0/8/8/8	0/1/1/1
11	ACP	F	401	6	-	10/19/38/38	0/3/3/3
10	UVA	B	505	-	-	0/8/8/8	0/1/1/1
5	GTP	A	501	6	-	5/22/38/38	0/3/3/3

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	504	MES	C8-S	-7.83	1.66	1.77
11	F	401	ACP	C5-C4	4.72	1.47	1.39
8	B	501	GDP	C5-C4	3.19	1.47	1.38
8	D	501	GDP	C5-C4	3.09	1.47	1.38
11	F	401	ACP	PG-O2G	3.00	1.61	1.55
11	F	401	ACP	PG-O3G	2.90	1.61	1.55
11	F	401	ACP	C5-C6	2.73	1.48	1.41
11	F	401	ACP	PB-O3A	2.63	1.61	1.58
8	D	501	GDP	C6-N1	-2.49	1.34	1.38
5	C	501	GTP	PA-O3A	2.40	1.62	1.59
8	B	501	GDP	C6-N1	-2.33	1.34	1.38
5	A	501	GTP	PA-O3A	2.32	1.62	1.59
11	F	401	ACP	C8-N7	2.31	1.36	1.31
8	B	501	GDP	C5-N7	-2.25	1.34	1.39
5	C	501	GTP	C2-N3	2.21	1.38	1.33
11	F	401	ACP	C5-N7	-2.19	1.35	1.39
11	F	401	ACP	PB-O2B	2.18	1.61	1.56
8	D	501	GDP	C5-N7	-2.17	1.34	1.39
5	A	501	GTP	PB-O3B	2.16	1.61	1.59
5	A	501	GTP	C2-N3	2.07	1.38	1.33
5	C	501	GTP	PB-O3A	2.03	1.61	1.59

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	D	501	GDP	C5-C4-N3	-6.14	118.62	128.39
8	B	501	GDP	C5-C4-N3	-5.99	118.86	128.39
11	F	401	ACP	C5-C4-N3	-5.82	118.71	126.72
8	D	501	GDP	C2-N3-C4	4.96	120.85	112.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	501	GDP	C2-N3-C4	4.95	120.83	112.30
5	A	501	GTP	C5-C4-N3	-4.86	120.66	128.39
5	C	501	GTP	C5-C4-N3	-4.80	120.75	128.39
11	F	401	ACP	N3-C4-N9	4.67	135.10	127.17
5	A	501	GTP	C2-N3-C4	4.62	120.25	112.30
8	D	501	GDP	N9-C4-N3	4.57	135.08	125.95
8	B	501	GDP	N9-C4-N3	4.53	135.02	125.95
5	C	501	GTP	C2-N3-C4	4.43	119.93	112.30
11	F	401	ACP	PB-O3A-PA	-4.03	119.23	132.37
9	B	504	MES	C5-N4-C3	3.75	116.92	108.84
11	F	401	ACP	C2-N3-C4	3.68	120.81	111.83
11	F	401	ACP	C4-C5-N7	-3.42	106.68	110.58
9	B	504	MES	C6-C5-N4	-3.40	104.96	110.12
8	B	501	GDP	C6-C5-N7	3.32	136.33	130.29
11	F	401	ACP	N3-C2-N1	-3.21	123.72	128.58
8	D	501	GDP	C6-C5-N7	3.20	136.11	130.29
5	C	501	GTP	N9-C4-N3	3.07	132.10	125.95
5	A	501	GTP	N9-C4-N3	2.95	131.85	125.95
5	A	501	GTP	C2-N1-C6	-2.85	119.95	125.11
5	C	501	GTP	C2-N1-C6	-2.83	119.98	125.11
5	C	501	GTP	N9-C8-N7	-2.73	108.34	113.40
11	F	401	ACP	C4-N9-C8	2.72	108.59	105.74
10	D	503	UVA	C6-C1-N	-2.68	119.60	122.18
5	A	501	GTP	N9-C8-N7	-2.68	108.43	113.40
8	D	501	GDP	C4-C5-N7	-2.65	106.47	110.67
10	B	505	UVA	C6-C1-N	-2.65	119.63	122.18
10	B	506	UVA	C6-C1-N	-2.65	119.63	122.18
8	B	501	GDP	C4-C5-N7	-2.63	106.50	110.67
11	F	401	ACP	C3'-C2'-C1'	2.59	106.36	101.46
5	C	501	GTP	C8-N7-C5	2.54	108.79	104.26
5	A	501	GTP	C8-N7-C5	2.53	108.77	104.26
11	F	401	ACP	C5-N7-C8	2.51	107.39	103.45
10	B	507	UVA	C6-C1-N	-2.45	119.82	122.18
5	A	501	GTP	C5-C6-N1	2.43	119.45	113.25
5	C	501	GTP	C5-C6-N1	2.41	119.40	113.25
5	C	501	GTP	O6-C6-C5	-2.38	120.25	126.53
9	B	504	MES	C7-N4-C5	2.27	117.28	111.24
9	B	504	MES	O1S-S-C8	2.17	110.01	106.73
5	A	501	GTP	O6-C6-C5	-2.16	120.84	126.53
8	D	501	GDP	O6-C6-C5	-2.10	121.00	126.53
8	B	501	GDP	O6-C6-C5	-2.09	121.01	126.53
8	B	501	GDP	C8-N7-C5	2.01	107.84	104.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	F	401	ACP	C6-C5-N7	2.01	135.97	132.09

There are no chirality outliers.

All (31) torsion outliers are listed below:

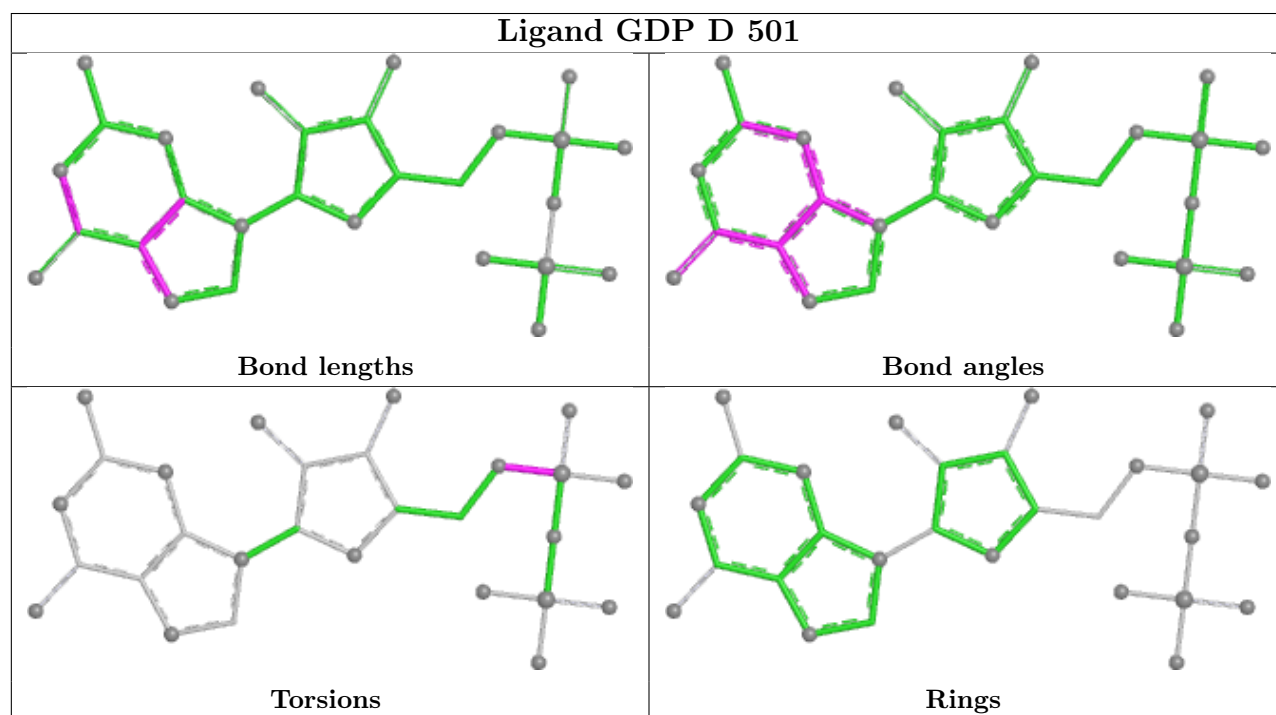
Mol	Chain	Res	Type	Atoms
5	A	501	GTP	PB-O3B-PG-O2G
5	A	501	GTP	C5'-O5'-PA-O3A
5	A	501	GTP	C5'-O5'-PA-O1A
5	A	501	GTP	C5'-O5'-PA-O2A
5	C	501	GTP	C5'-O5'-PA-O3A
5	C	501	GTP	C5'-O5'-PA-O1A
8	B	501	GDP	C5'-O5'-PA-O3A
8	B	501	GDP	C5'-O5'-PA-O2A
8	D	501	GDP	C5'-O5'-PA-O3A
8	D	501	GDP	C5'-O5'-PA-O2A
9	B	504	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-O2B
11	F	401	ACP	PG-C3B-PB-O3A
11	F	401	ACP	C5'-O5'-PA-O1A
11	F	401	ACP	C5'-O5'-PA-O2A
11	F	401	ACP	C5'-O5'-PA-O3A
9	B	504	MES	C7-C8-S-O3S
9	B	504	MES	C7-C8-S-O1S
9	B	504	MES	C7-C8-S-O2S
5	C	501	GTP	C5'-O5'-PA-O2A
5	C	501	GTP	PB-O3A-PA-O2A
5	C	501	GTP	PB-O3B-PG-O1G
5	A	501	GTP	PB-O3A-PA-O2A
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	C	501	GTP	PB-O3A-PA-O1A

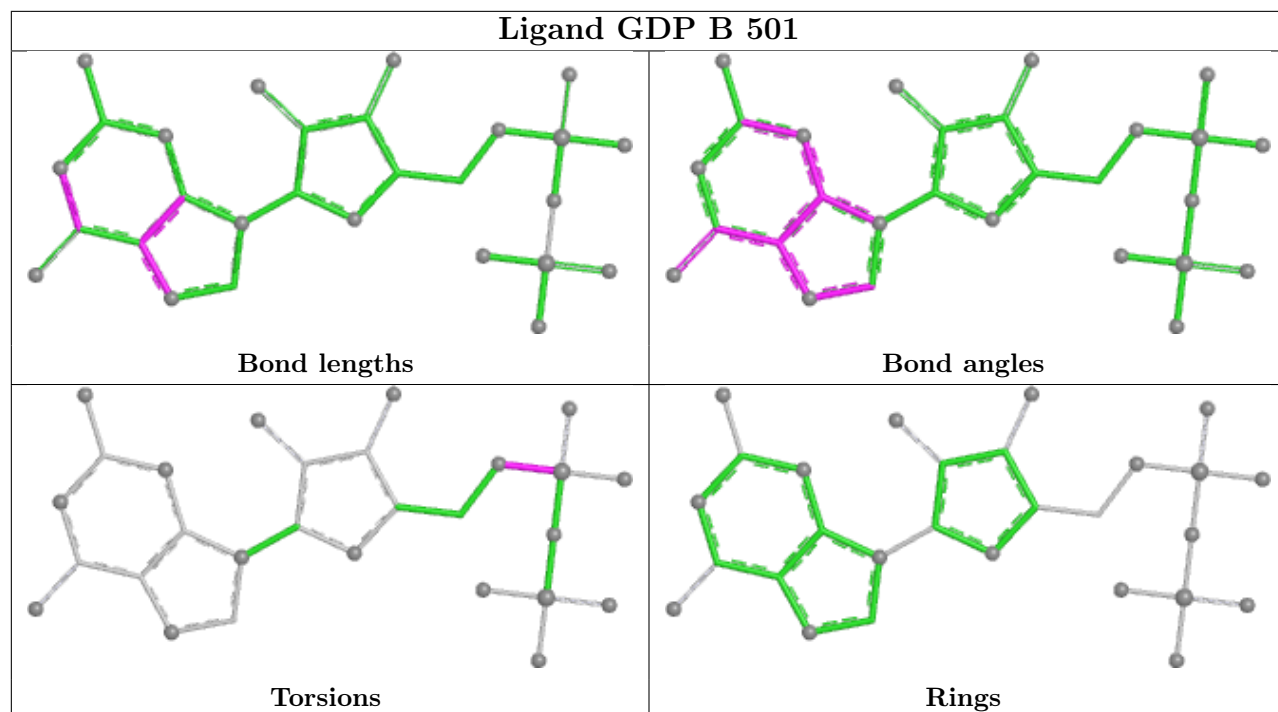
There are no ring outliers.

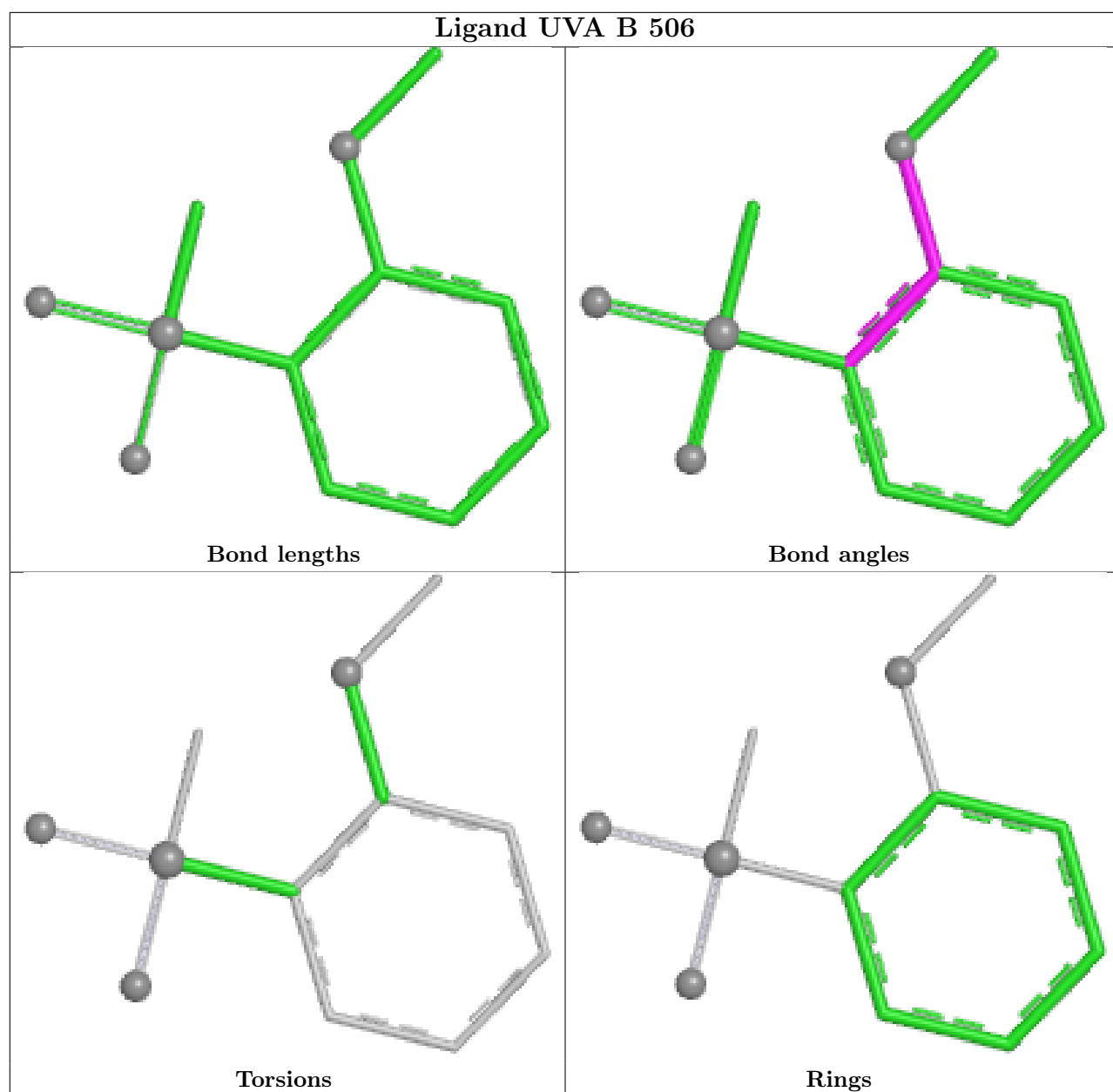
5 monomers are involved in 9 short contacts:

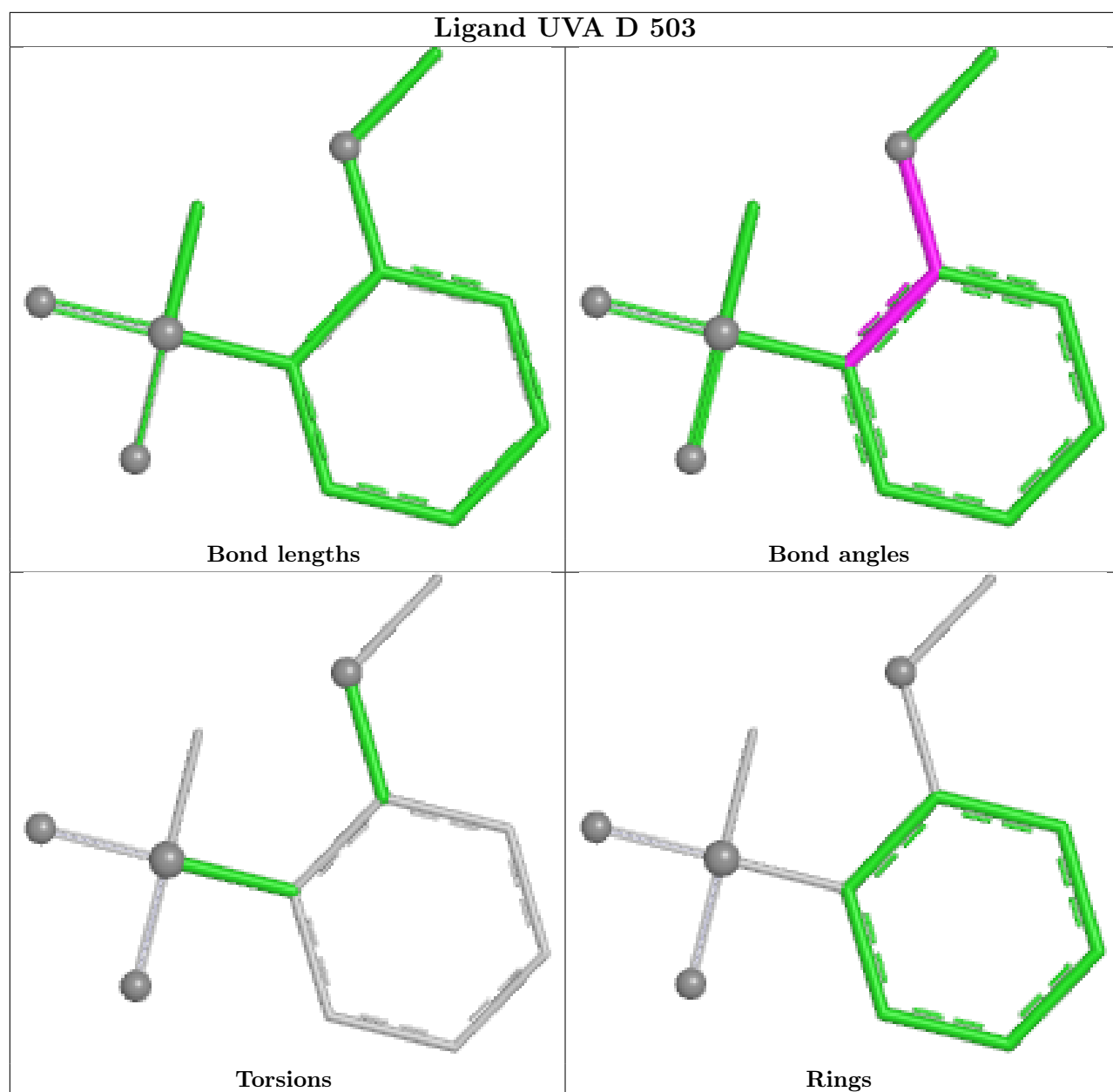
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	D	501	GDP	2	0
8	B	501	GDP	1	0
9	B	504	MES	1	0
11	F	401	ACP	3	0
5	A	501	GTP	2	0

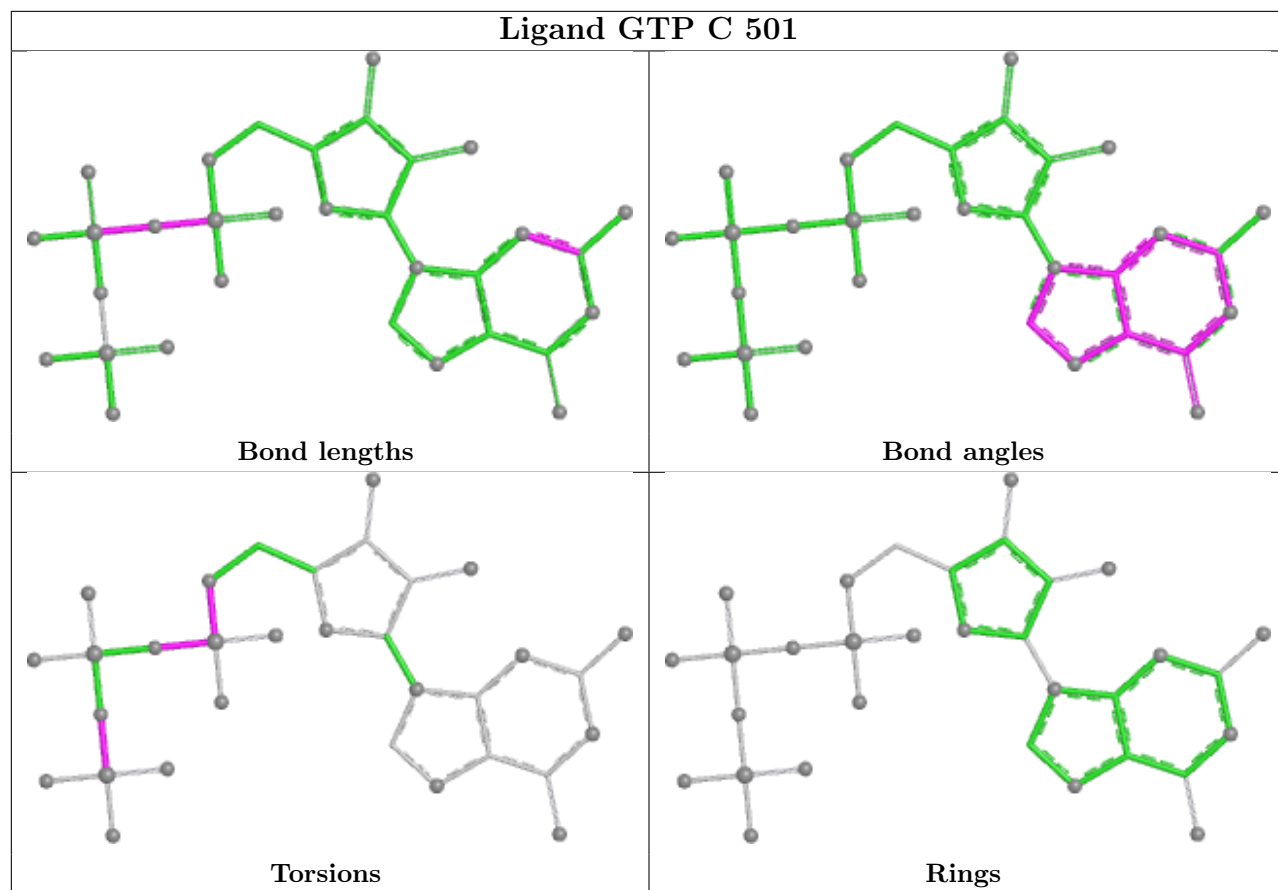
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



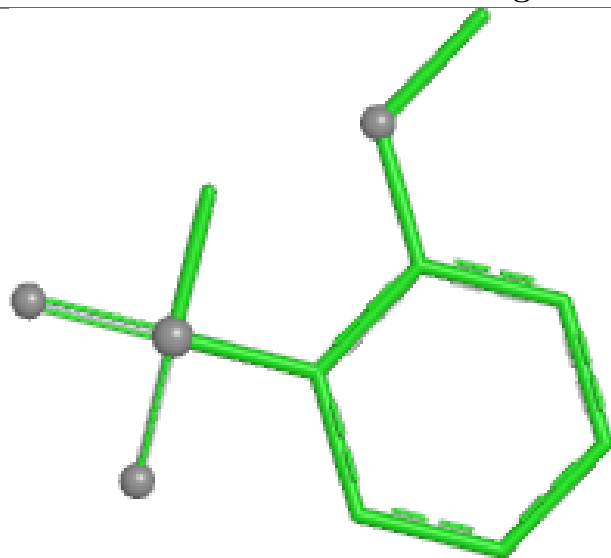




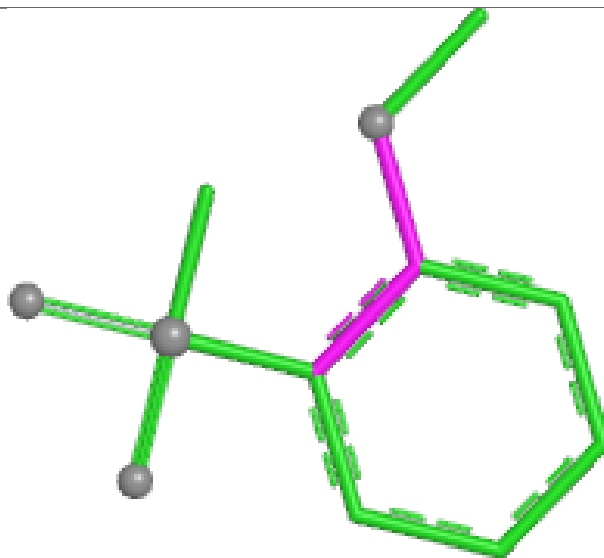




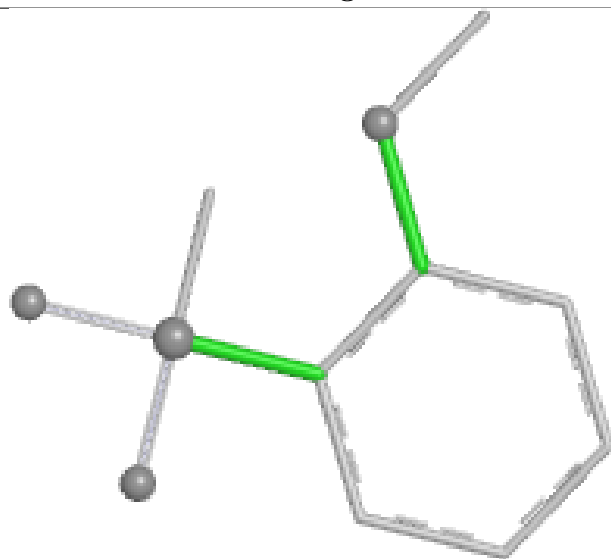
Ligand UVA B 507



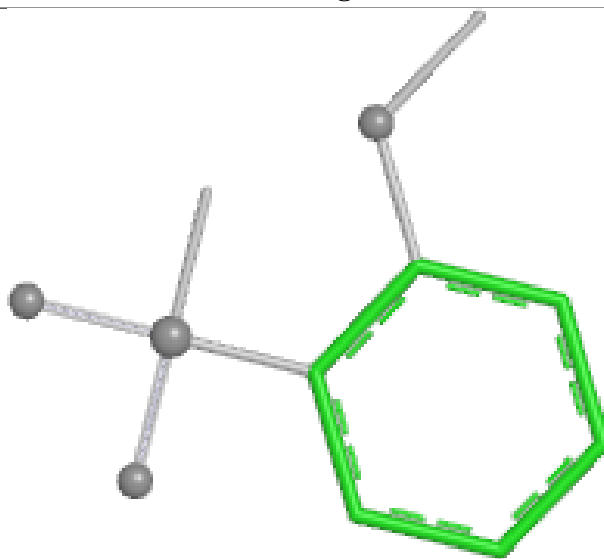
Bond lengths



Bond angles

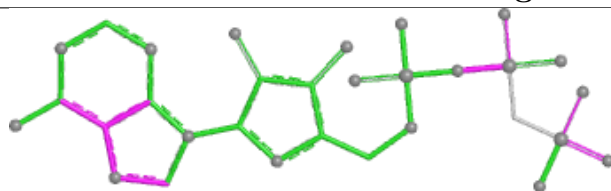


Torsions

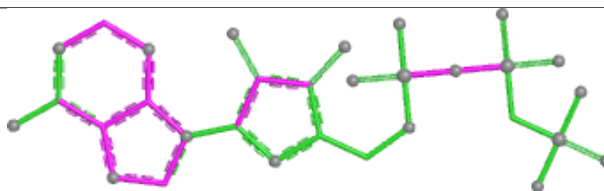


Rings

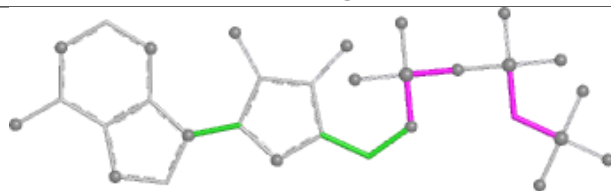
Ligand ACP F 401



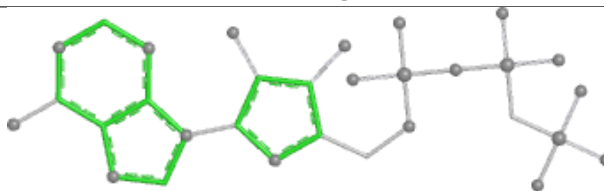
Bond lengths



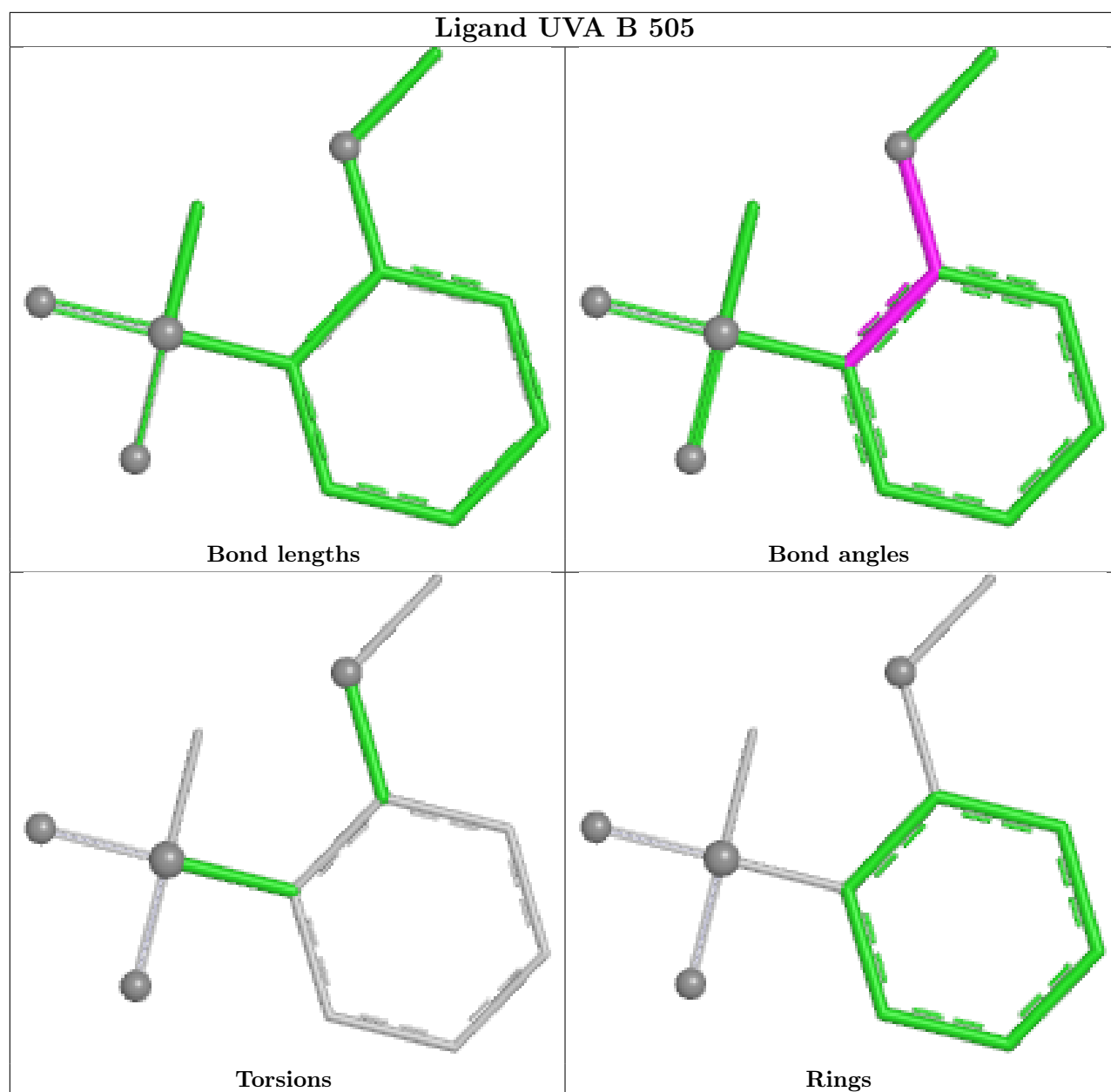
Bond angles

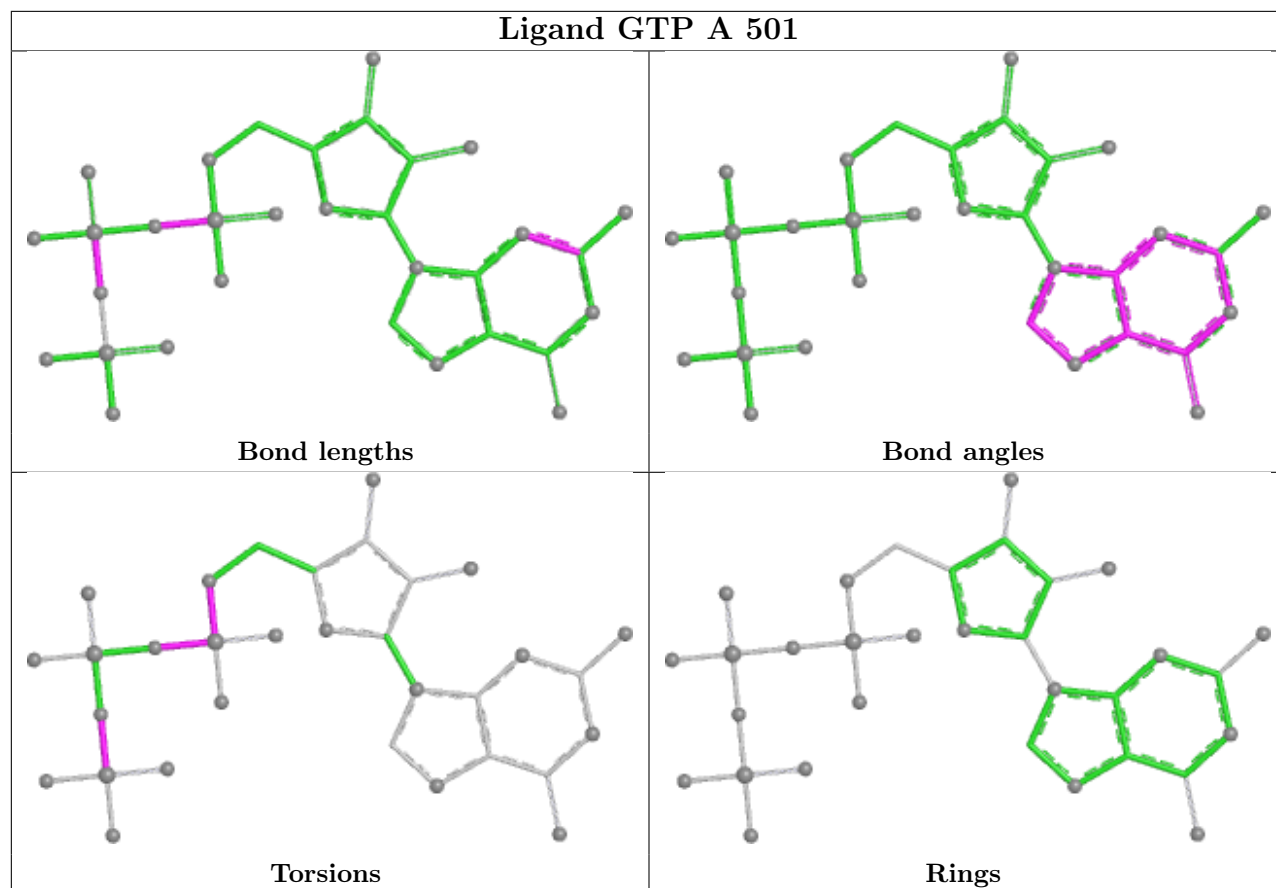


Torsions



Rings





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%)	0.47	16 (3%)	45	41	63, 82, 125, 204	0
1	C	440/451 (97%)	0.21	16 (3%)	46	42	37, 69, 100, 153	1 (0%)
2	B	425/445 (95%)	0.39	18 (4%)	40	37	39, 78, 125, 161	3 (0%)
2	D	431/445 (96%)	0.48	20 (4%)	37	34	65, 88, 129, 211	4 (0%)
3	E	123/143 (86%)	0.71	12 (9%)	13	11	71, 94, 144, 182	0
4	F	349/384 (90%)	0.74	23 (6%)	24	22	80, 119, 179, 213	0
All	All	2206/2319 (95%)	0.46	105 (4%)	35	32	37, 85, 147, 213	8 (0%)

All (105) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	155	ALA	5.5
2	B	249	ASN	5.4
3	E	24	LEU	5.1
2	B	248	LEU	4.4
2	B	250	ALA	4.2
3	E	143	ALA	4.1
4	F	159	GLY	4.0
2	B	121	VAL	3.9
4	F	344	ALA	3.8
4	F	315	PHE	3.7
4	F	371	PRO	3.7
1	C	350	GLY	3.3
1	C	128	GLN	3.3
2	B	221	THR	3.3
2	D	281	GLN	3.2
2	D	323	MET	3.2
1	A	179	THR	3.2
1	A	349	THR	3.2
2	B	220	THR	3.2

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Mol	Chain	Res	Type	RSRZ
4	F	330	ILE	3.2
4	F	313	GLN	3.2
1	C	135	PHE	3.2
2	D	82	PRO	3.1
2	B	119	LEU	3.1
1	A	340	SER	3.1
1	A	378	LEU	3.0
1	A	351	PHE	3.0
1	C	440	VAL	2.9
2	B	93	VAL	2.9
4	F	64	TYR	2.9
2	D	284	ARG	2.8
2	B	122	VAL	2.8
3	E	45	PRO	2.8
3	E	6	MET	2.8
2	B	283	TYR	2.7
2	D	283	TYR	2.7
2	D	203	CYS	2.7
2	D	407	TRP	2.7
3	E	26	PRO	2.7
3	E	116	LEU	2.7
3	E	7	GLU	2.7
4	F	45	ASN	2.6
4	F	295	LEU	2.6
2	D	279	GLY	2.6
1	A	329	ASN	2.6
2	D	282	GLN	2.6
1	A	42	ILE	2.6
3	E	22	VAL	2.6
4	F	49	PHE	2.6
1	C	221	ARG	2.5
1	A	346	TRP	2.5
1	C	218	ASP	2.5
4	F	68	ALA	2.5
1	A	316	CYS	2.5
4	F	240	LEU	2.4
1	A	202	PHE	2.4
1	A	68	VAL	2.4
2	B	216	THR	2.4
4	F	65	TYR	2.4
1	A	88	HIS	2.4
2	B	94	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
4	F	125	THR	2.4
2	D	280	SER	2.4
4	F	303	SER	2.4
2	D	291	LEU	2.4
1	A	381	THR	2.3
4	F	93	TRP	2.3
2	D	56	ALA	2.3
2	D	83	PHE	2.3
3	E	8	VAL	2.3
2	D	285	ALA	2.3
1	C	280	LYS	2.3
1	C	256	GLN	2.2
4	F	291	ILE	2.2
2	D	377	PHE	2.2
2	B	118	VAL	2.2
2	D	2	ARG	2.2
1	C	83	TYR	2.2
2	D	432	TYR	2.2
1	A	57	GLY	2.2
1	A	248	LEU	2.2
3	E	76	ARG	2.2
1	C	2	ARG	2.2
3	E	27	PRO	2.2
2	B	161	TYR	2.2
4	F	249	TYR	2.2
1	C	341	ILE	2.2
3	E	122	ARG	2.2
1	C	220	GLU	2.1
2	D	371	LEU	2.1
4	F	67	GLY	2.1
1	C	279	GLU	2.1
2	B	159	GLU	2.1
1	A	136	LEU	2.1
4	F	213	ILE	2.1
1	C	178	SER	2.1
2	B	167	ASN	2.1
4	F	334	GLY	2.1
2	D	441	ASP	2.1
4	F	309	TYR	2.1
1	C	165	SER	2.1
2	B	333	LEU	2.0
2	D	216	THR	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	283	HIS	2.0
2	B	1	MET	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

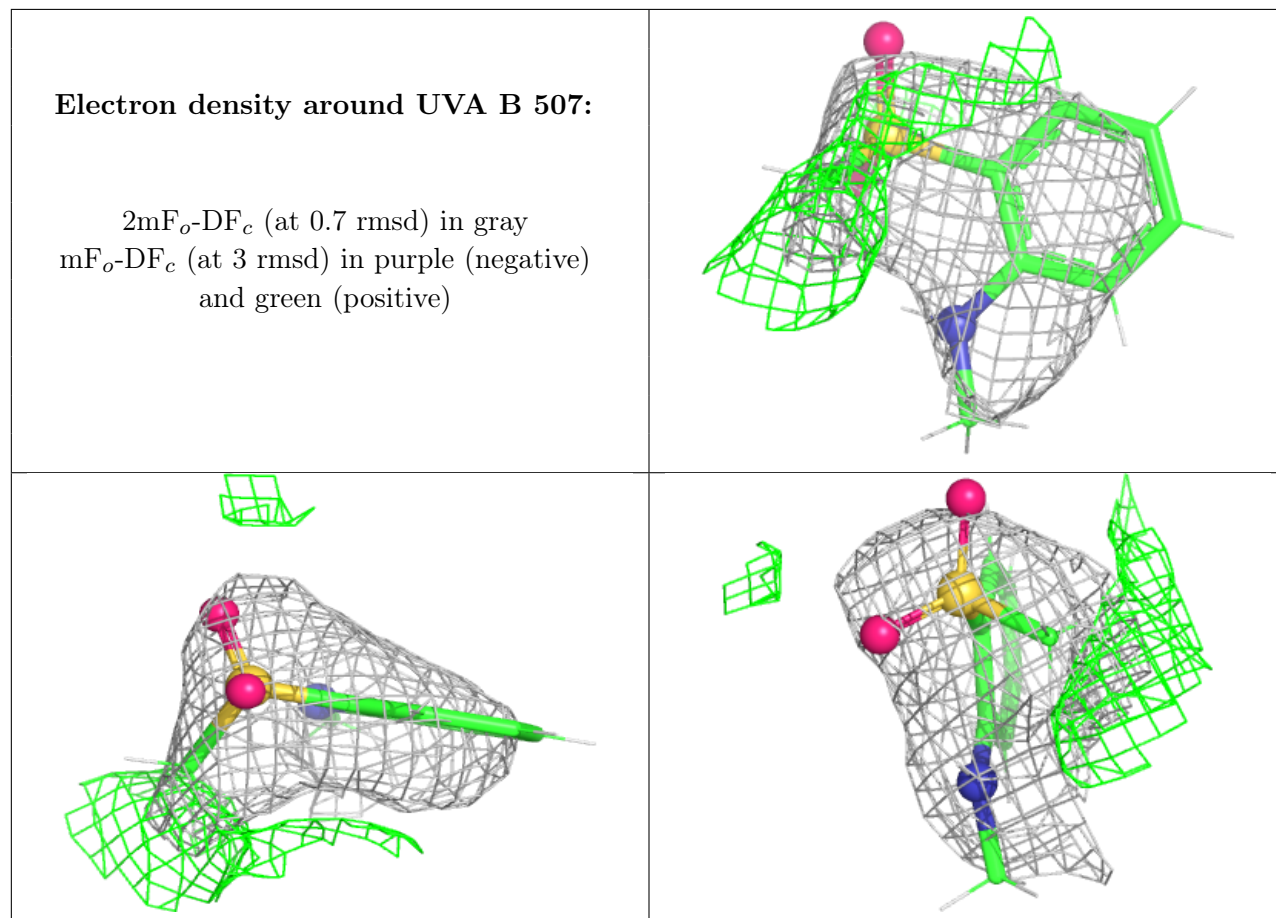
6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	CA	B	503	1/1	0.63	0.16	133,133,133,133	0
6	MG	D	502	1/1	0.73	0.10	92,92,92,92	0
10	UVA	B	507	12/12	0.77	0.24	91,110,122,126	23
9	MES	B	504	12/12	0.85	0.13	88,94,104,110	0
6	MG	A	502	1/1	0.87	0.11	69,69,69,69	0
11	ACP	F	401	31/31	0.88	0.09	115,125,134,138	0
10	UVA	D	503	12/12	0.92	0.10	75,86,103,104	0
10	UVA	B	506	12/12	0.92	0.11	66,80,97,97	0
8	GDP	D	501	28/28	0.93	0.09	77,85,92,97	0
6	MG	F	402	1/1	0.93	0.07	117,117,117,117	0
7	CA	E	201	1/1	0.95	0.07	100,100,100,100	0
5	GTP	A	501	32/32	0.96	0.07	59,65,71,76	0
6	MG	B	502	1/1	0.96	0.12	61,61,61,61	0
8	GDP	B	501	28/28	0.97	0.06	52,59,63,67	0
10	UVA	B	505	12/12	0.97	0.07	70,78,93,94	0
5	GTP	C	501	32/32	0.97	0.07	54,61,66,69	0
7	CA	C	503	1/1	0.99	0.02	92,92,92,92	0
7	CA	A	503	1/1	0.99	0.05	109,109,109,109	0
6	MG	C	502	1/1	1.00	0.04	61,61,61,61	0

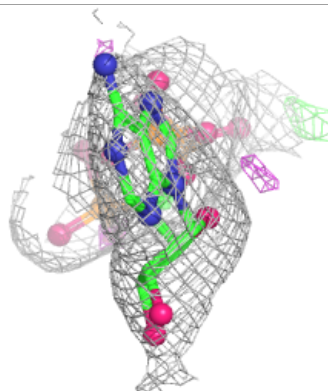
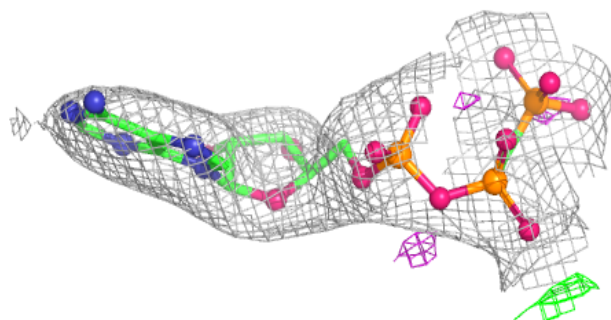
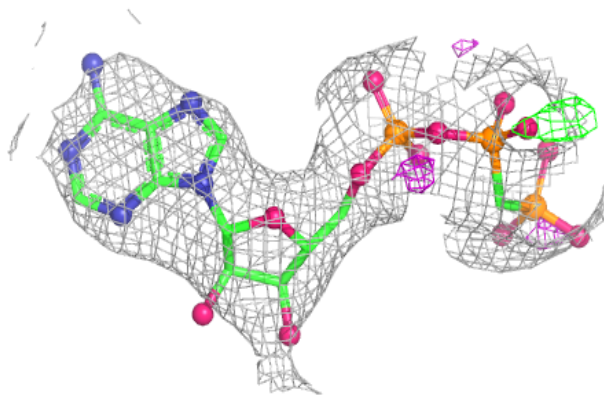
The following is a graphical depiction of the model fit to experimental electron density of all

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.



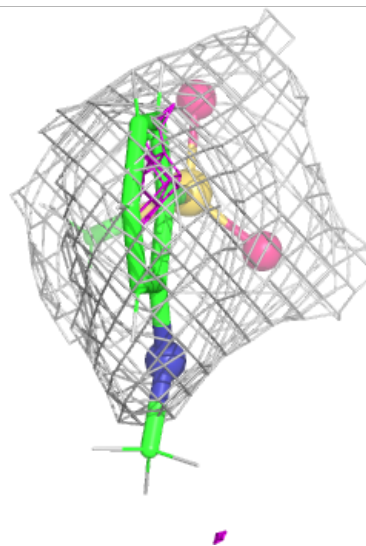
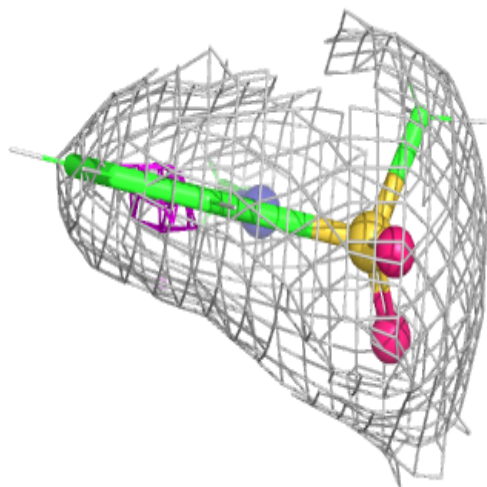
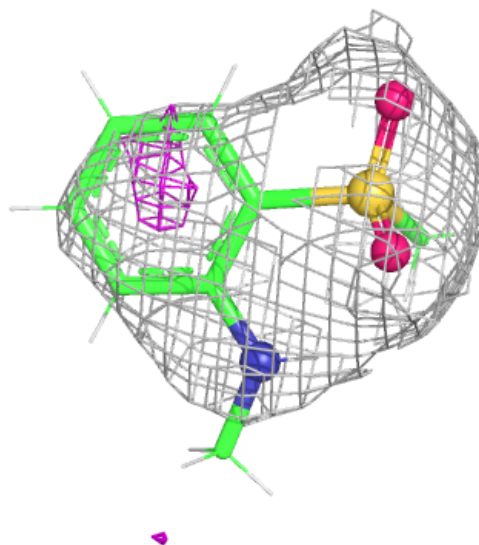
Electron density around ACP F 401:

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



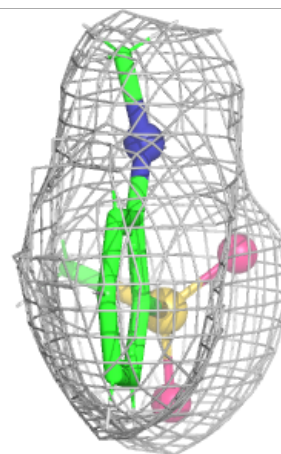
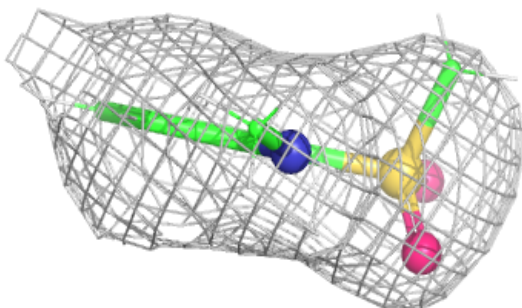
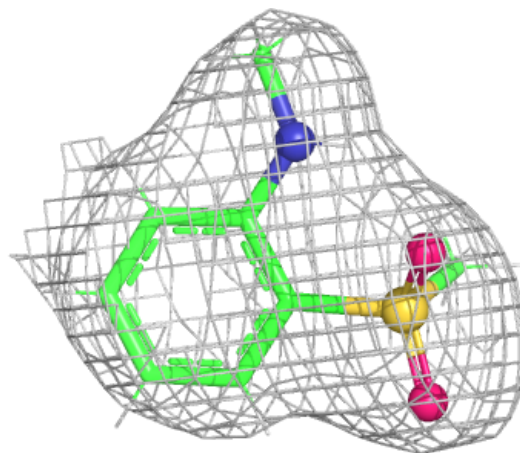
Electron density around UVA D 503:

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



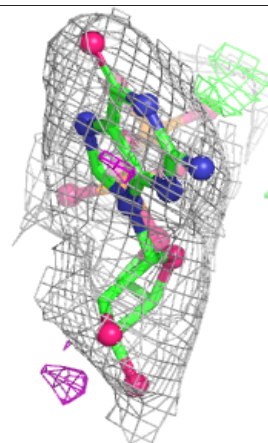
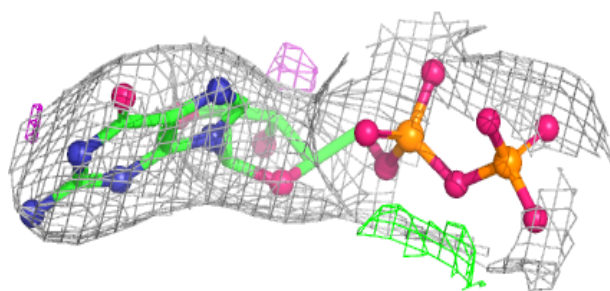
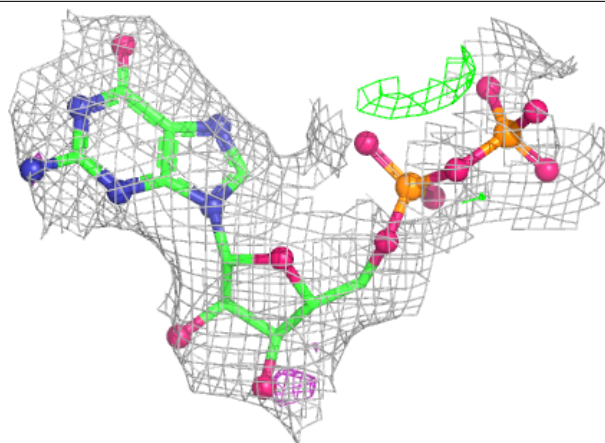
Electron density around UVA B 506:

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

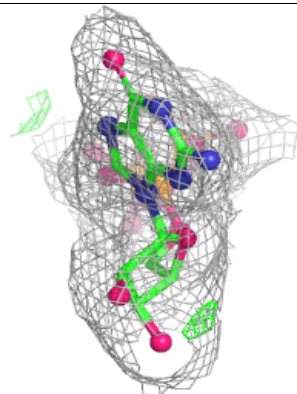
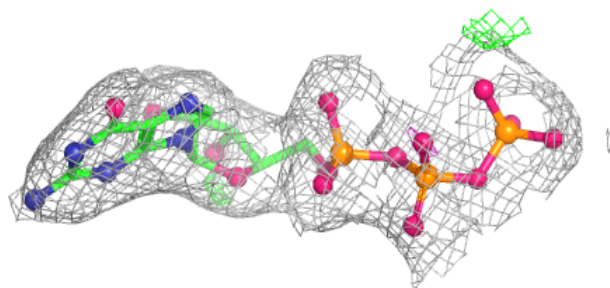
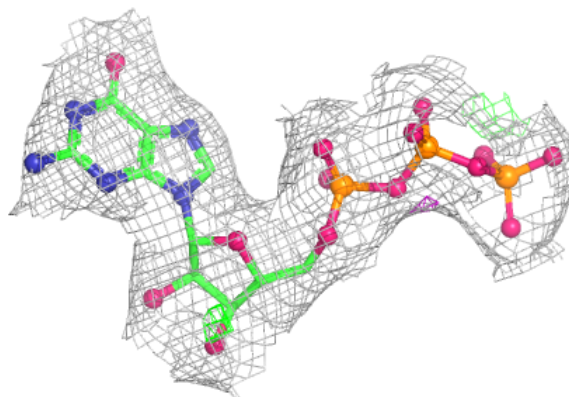


Electron density around GDP D 501:

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

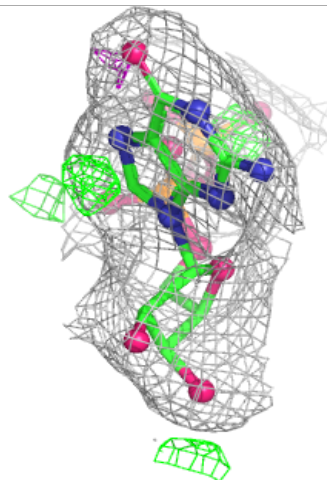
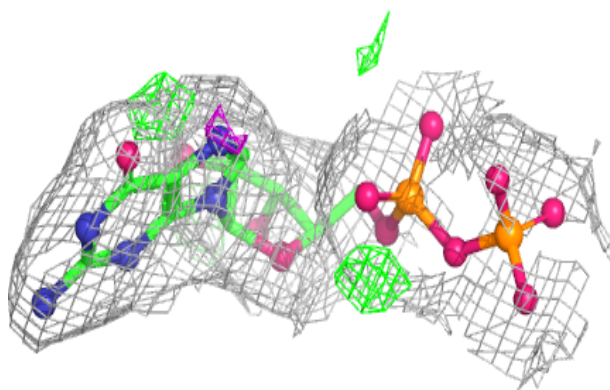
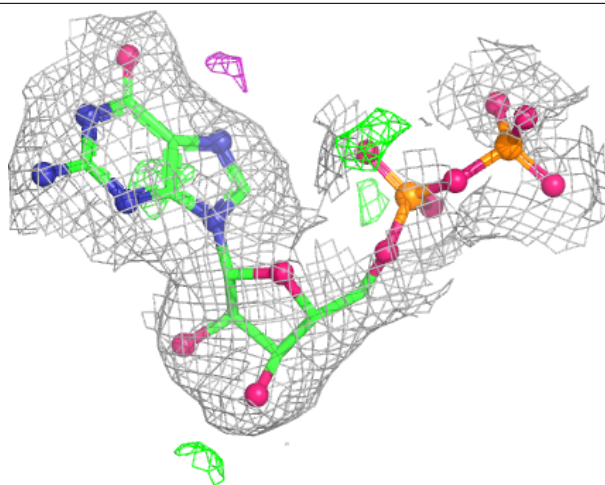
**Electron density around GTP A 501:**

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



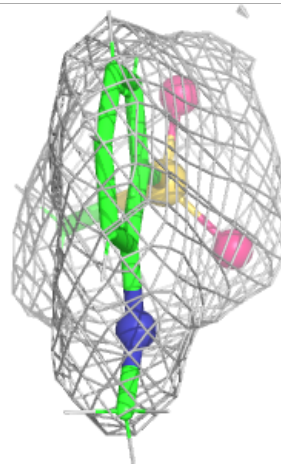
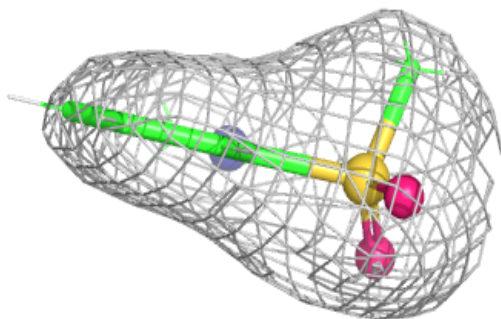
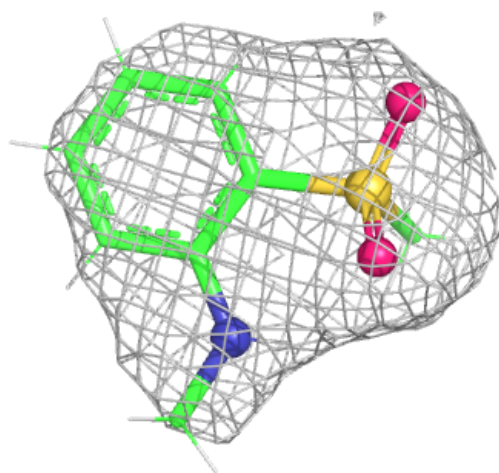
Electron density around GDP B 501:

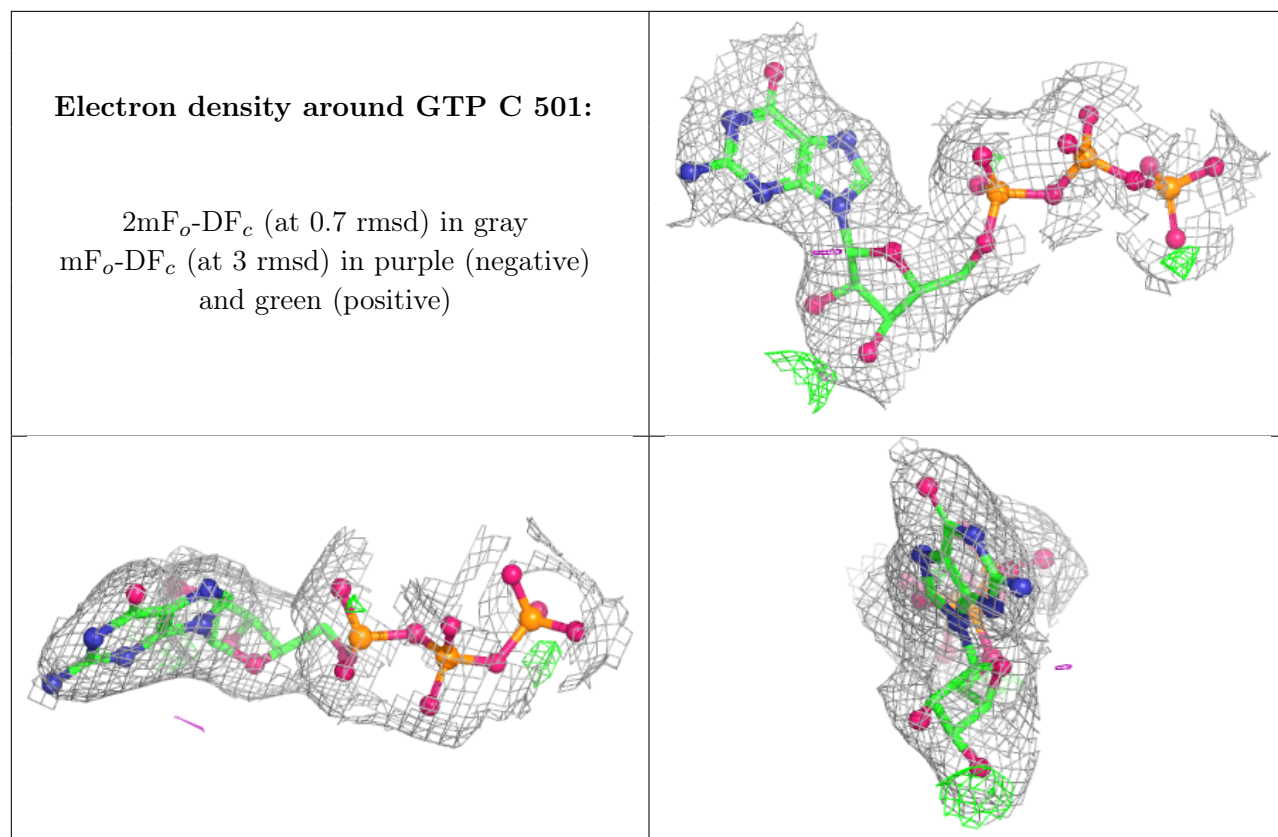
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around UVA 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.