



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2024 – 06:55 PM EST

PDB ID : 5S5N
Title : Tubulin-Z165170770-complex
Authors : Muehlethaler, T.; Gioia, D.; Prota, A.E.; Sharpe, M.E.; Cavalli, A.; Steinmetz, M.O.
Deposited on : 2020-11-08
Resolution : 2.90 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

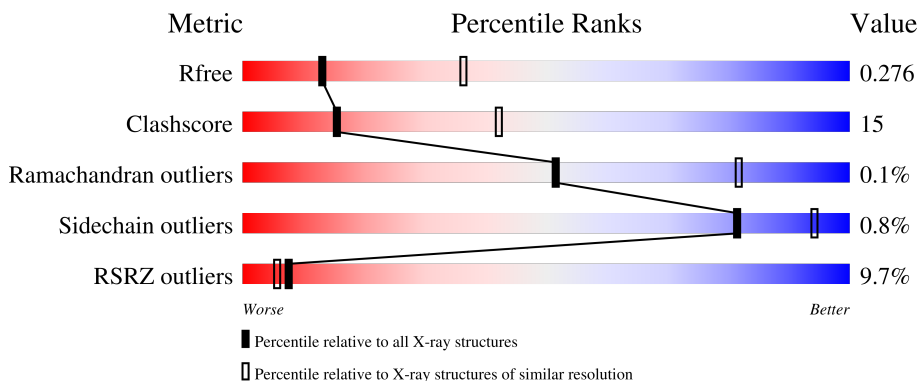
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 Å.

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



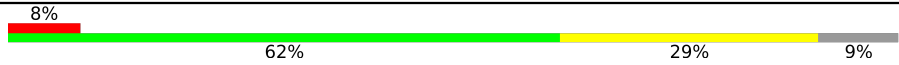
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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% (Poor fit) 69% (0-1 outliers) 28% (2-3 outliers) . (Not modelled)
1	C	451	8% (Poor fit) 69% (0-1 outliers) 29% (2-3 outliers) . (Not modelled)
2	B	445	7% (Poor fit) 62% (0-1 outliers) 33% (2-3 outliers) 5% (Not modelled)
2	D	445	15% (Poor fit) 63% (0-1 outliers) 33% (2-3 outliers) . (Not modelled)
3	E	143	8% (Poor fit) 68% (0-1 outliers) 17% (2-3 outliers) 15% (Not modelled)

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Mol	Chain	Length	Quality of chain
4	F	384	 <p>A horizontal bar chart representing the quality of chain. The bar is divided into four segments: a red segment on the left labeled '8%', a large green segment labeled '62%', a yellow segment labeled '29%', and a small grey segment on the far right labeled '9%'.</p>

2 Entry composition [i](#)

There are 12 unique types of molecules in this entry. The entry contains 17728 atoms, of which 20 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
			Total	C	N	O	S			
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
			Total	C	N	O	S			
2	B	422	Total	C	N	O	S	2	0	0
			3324	2090	567	640	27			
2	D	425	Total	C	N	O	S	6	1	0
			3354	2108	572	647	27			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	E	122	Total	C	N	O	S	0	0	0
			1008	622	182	199	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

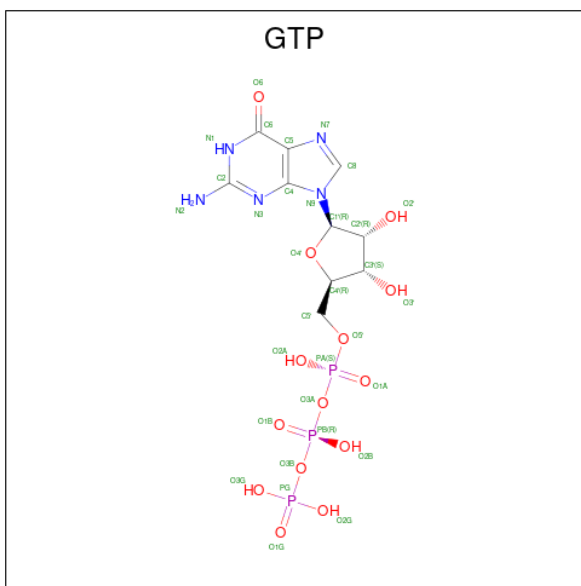
- Molecule 4 is a protein called Tubulin-Tyrosine Ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	F	350	Total	C	N	O	S	0	0	0
			2863	1834	493	522	14			

There are 6 discrepancies between the modelled and reference sequences:

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

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



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

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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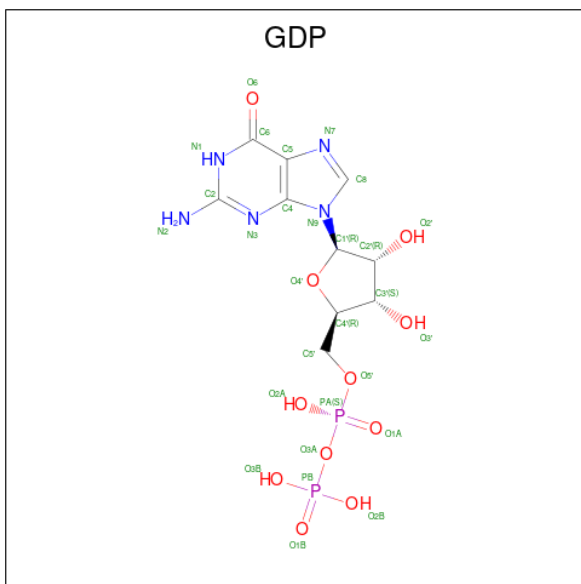
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	F	1	Total	Mg	0	0
			1	1		

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

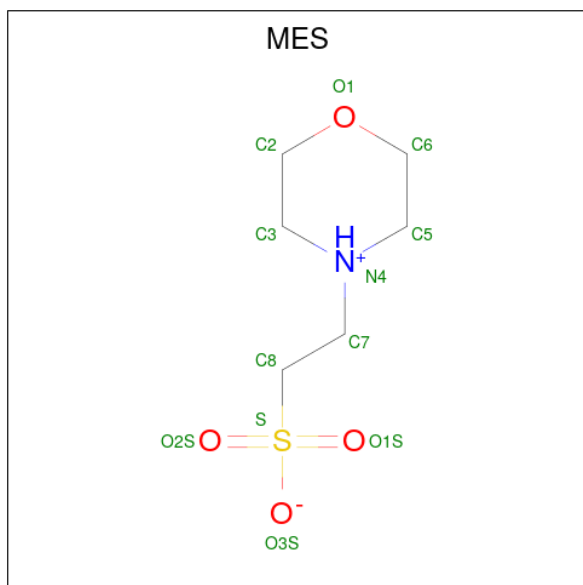
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Ca	0	0
			1	1		
7	B	1	Total	Ca	0	0
			1	1		
7	C	1	Total	Ca	0	0
			1	1		
7	E	1	Total	Ca	0	0
			1	1		

- Molecule 8 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



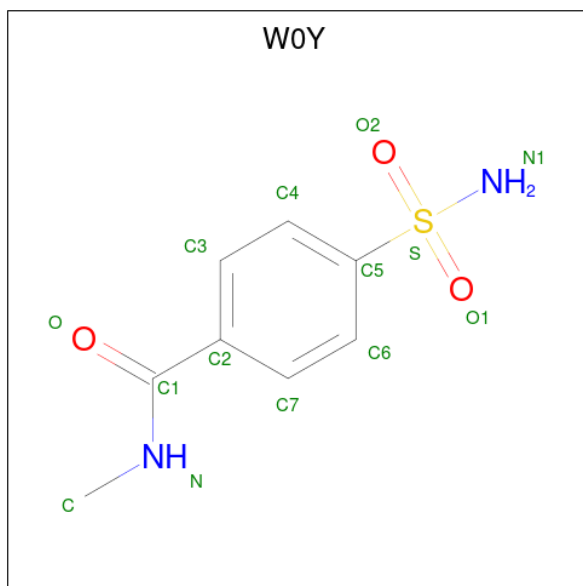
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
8	B	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
8	D	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- Molecule 9 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C₆H₁₃NO₄S).



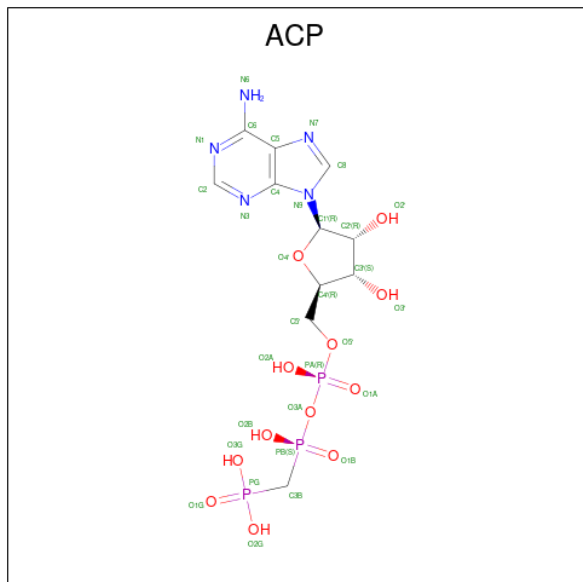
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
9	B	1	12	6	1	4	1	0	0

- Molecule 10 is N-methyl-4-sulfamoylbenzamide (three-letter code: W0Y) (formula: $C_8H_{10}N_2O_3S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	H	N	O			S
10	B	1	24	8	10	2	3	1	0	0
10	C	1	24	8	10	2	3	1	0	0

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
11	F	1	31	11	5	12	3	0	0

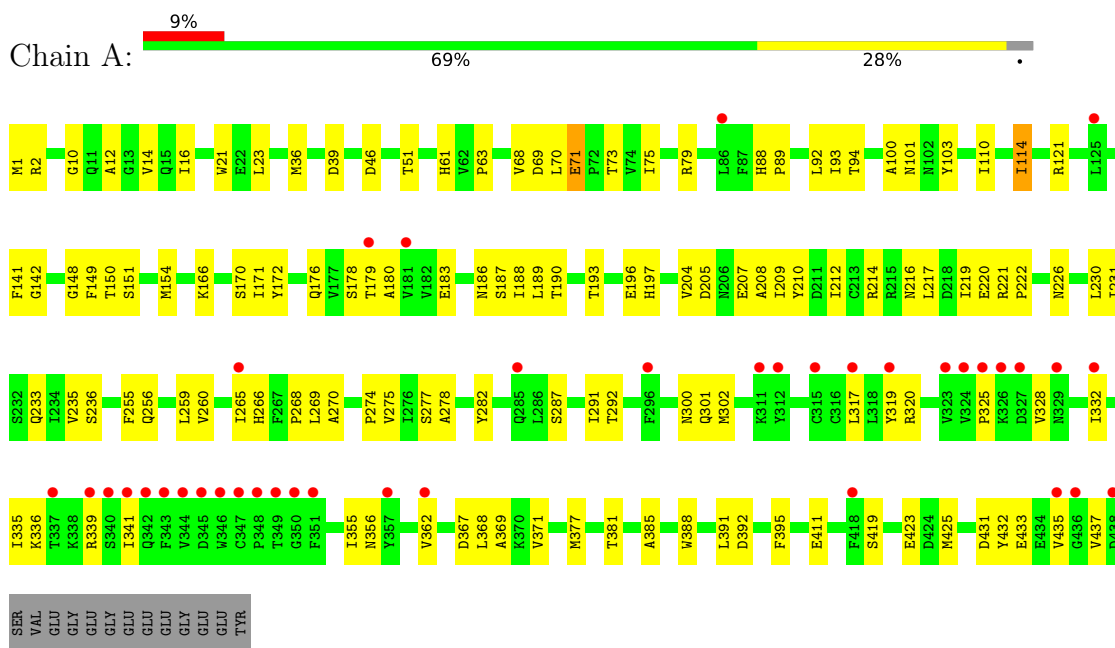
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	16	Total	O	0	0
			16	16		
12	B	26	Total	O	0	0
			26	26		
12	C	44	Total	O	0	0
			44	44		
12	D	3	Total	O	0	0
			3	3		
12	E	3	Total	O	0	0
			3	3		

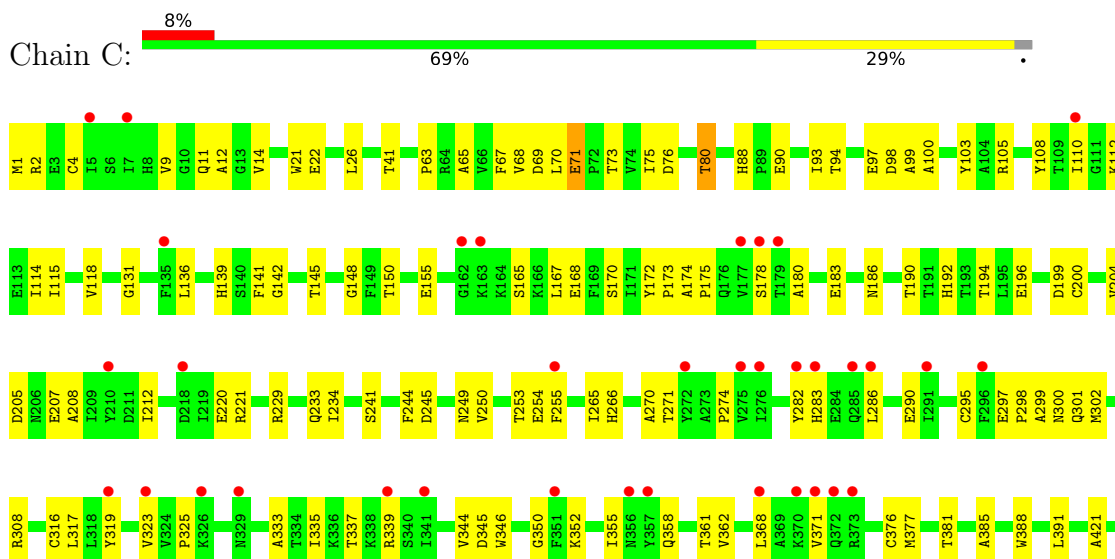
3 Residue-property plots [i](#)

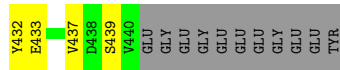
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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

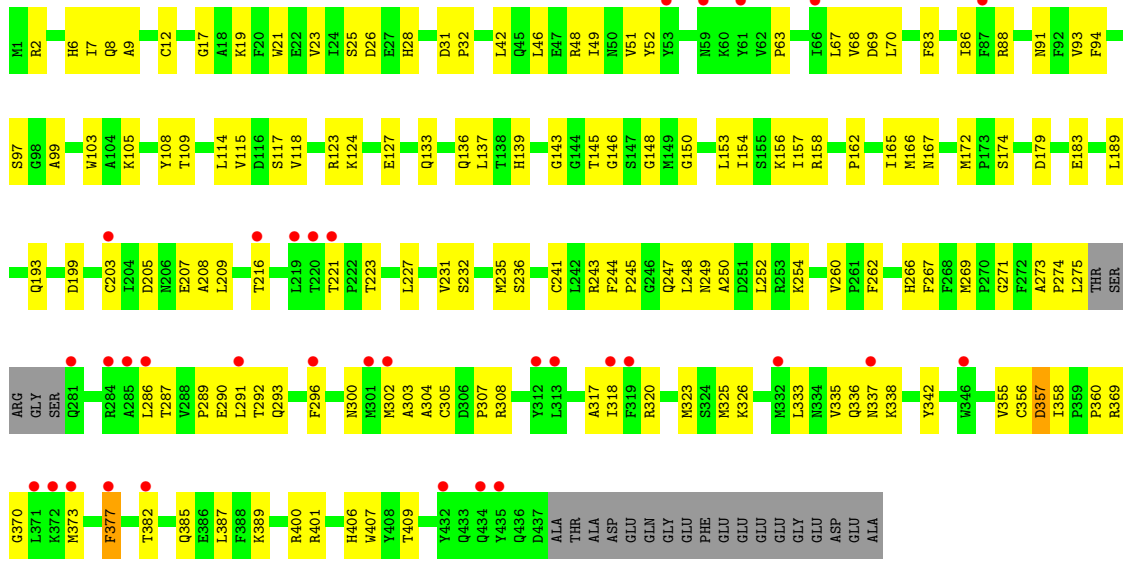


- Molecule 1: Tubulin alpha-1B chain

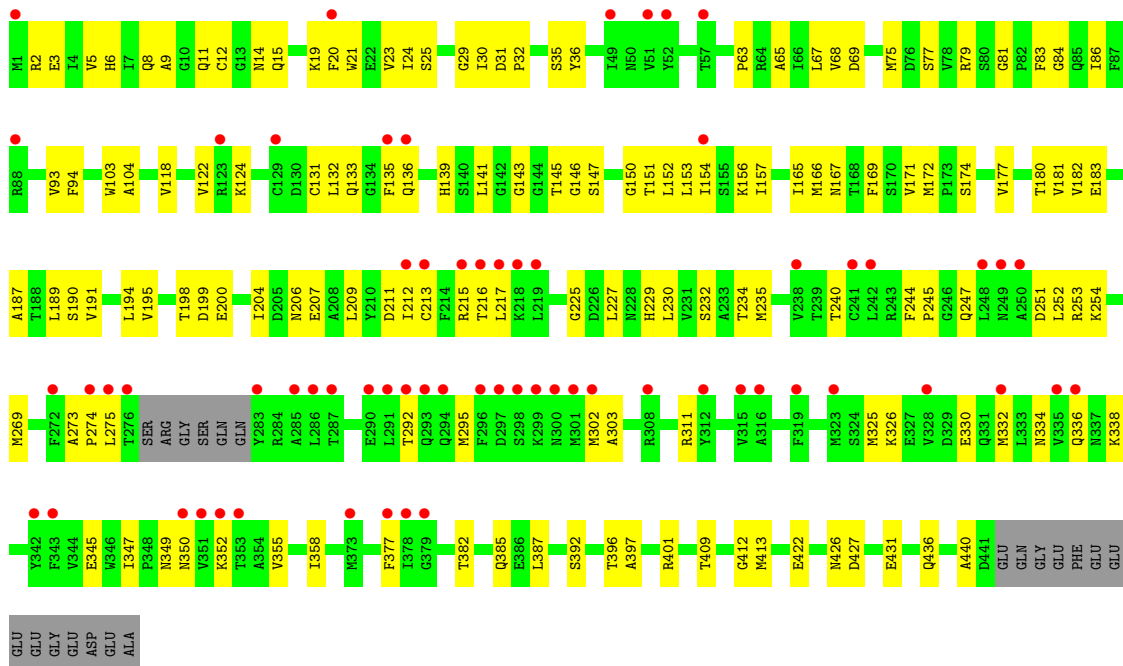




• Molecule 2: Tubulin beta-2B chain



• Molecule 2: Tubulin beta-2B chain



• Molecule 3: Stathmin-4

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	105.61Å 159.43Å 179.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	63.62 – 2.90 119.20 – 2.90	Depositor EDS
% Data completeness (in resolution range)	97.3 (63.62-2.90) 97.4 (119.20-2.90)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.27 (at 2.91Å)	Xtrriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.222 , 0.274 0.225 , 0.276	Depositor DCC
R_{free} test set	3303 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	81.0	Xtrriage
Anisotropy	0.589	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 38.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	17728	wwPDB-VP
Average B, all atoms (Å ²)	102.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.70% 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, CA, ACP, W0Y, GDP, MG

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	0.24	0/3502	0.40	0/4754
1	C	0.25	0/3521	0.41	0/4780
2	B	0.25	0/3397	0.40	0/4598
2	D	0.24	0/3429	0.40	0/4645
3	E	0.23	0/1016	0.34	0/1348
4	F	0.23	0/2929	0.38	0/3957
All	All	0.24	0/17794	0.39	0/24082

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	93	0
1	C	3443	0	3352	101	0
2	B	3324	0	3197	122	0
2	D	3354	0	3229	112	0
3	E	1008	0	1024	18	0
4	F	2863	0	2824	89	0
5	A	32	0	12	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	32	0	12	2	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	3	0
8	D	28	0	12	2	0
9	B	12	0	12	3	0
10	B	14	10	0	2	0
10	C	14	10	0	0	0
11	F	31	0	14	4	0
12	A	16	0	0	4	0
12	B	26	0	0	1	0
12	C	44	0	0	4	0
12	D	3	0	0	0	0
12	E	3	0	0	0	0
All	All	17708	20	17034	511	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

All (511) 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:270:ALA:HB3	1:C:302:MET:HG3	1.53	0.90
5:A:501:GTP:O1G	12:A:601:HOH:O	1.90	0.89
2:B:325:MET:HG3	2:B:355:VAL:HG21	1.58	0.86
4:F:10:ASN:HB2	4:F:44:ARG:HH22	1.40	0.85
2:B:23:VAL:HG21	2:B:232:SER:HB3	1.57	0.85
1:A:209:ILE:HG23	1:A:230:LEU:HD23	1.58	0.85
1:A:178:SER:OG	1:A:183:GLU:OE1	1.96	0.84
4:F:102:PRO:HG2	4:F:105:LEU:HD13	1.59	0.84
2:D:136:GLN:HA	2:D:167:ASN:O	1.79	0.82
4:F:205:VAL:HG21	4:F:291:ILE:HD13	1.62	0.81
2:B:216:THR:HG21	2:B:275:LEU:HD12	1.62	0.80
1:C:93:ILE:HG22	1:C:114:ILE:HD11	1.64	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:197:ARG:NH1	4:F:257:GLU:OE2	2.14	0.79
1:C:69:ASP:OD2	12:C:601:HOH:O	2.02	0.77
4:F:214:TYR:HB3	4:F:375:PHE:HB3	1.67	0.77
4:F:236:LYS:HB3	4:F:240:LEU:HD13	1.68	0.76
2:D:347:ILE:HG22	2:D:350:ASN:HB3	1.65	0.75
1:A:172:TYR:HB3	1:A:205:ASP:HA	1.66	0.75
2:D:83:PHE:O	2:D:86:ILE:HG22	1.86	0.75
2:D:311:ARG:NH1	2:D:436:GLN:O	2.20	0.74
1:A:21:TRP:CZ3	1:A:63:PRO:HB3	2.23	0.74
1:C:271:THR:HG21	1:C:295:CYS:O	1.86	0.74
2:B:357:ASP:N	2:B:357:ASP:OD1	2.18	0.74
2:B:136:GLN:HA	2:B:167:ASN:O	1.89	0.73
2:B:199:ASP:OD1	9:B:504:MES:H62	1.90	0.72
2:B:83:PHE:O	2:B:86:ILE:HG22	1.90	0.71
4:F:280:GLU:OE1	4:F:284:LEU:HD23	1.92	0.70
2:B:244:PHE:HB3	2:B:245:PRO:HD2	1.74	0.70
4:F:102:PRO:HG2	4:F:105:LEU:CD1	2.20	0.70
2:B:21:TRP:CZ3	2:B:63:PRO:HB3	2.27	0.69
2:D:225:GLY:O	2:D:229[A]:HIS:ND1	2.24	0.69
1:C:350:GLY:O	12:C:602:HOH:O	2.10	0.68
1:A:70:LEU:HD13	1:A:110:ILE:HG21	1.76	0.68
1:C:180:ALA:O	1:C:183:GLU:HG3	1.94	0.67
1:C:21:TRP:CZ3	1:C:63:PRO:HB3	2.30	0.67
4:F:241:THR:HG1	11:F:401:ACP:HO3'	1.39	0.66
2:B:115:VAL:HG11	2:B:156:LYS:HE3	1.77	0.66
2:D:177:VAL:HG21	2:D:206:ASN:HB3	1.76	0.66
4:F:217:ARG:NH2	4:F:374:ILE:HA	2.10	0.66
4:F:146:VAL:HG22	4:F:164:SER:HB3	1.77	0.66
4:F:147:TRP:HB2	4:F:169:LEU:HD11	1.78	0.66
1:A:141:PHE:HB3	1:A:187:SER:OG	1.96	0.66
4:F:132:LEU:HD21	4:F:170:LEU:HD11	1.76	0.66
2:B:114:LEU:HD12	2:B:117:SER:OG	1.97	0.65
2:B:154:ILE:HG23	2:B:166:MET:HG2	1.78	0.65
4:F:205:VAL:CG2	4:F:291:ILE:HD13	2.26	0.65
1:A:69:ASP:OD1	12:A:602:HOH:O	2.15	0.65
2:B:42:LEU:HB2	2:B:358:ILE:HD11	1.78	0.65
2:B:48:ARG:HB2	2:B:243:ARG:O	1.97	0.65
4:F:128:ARG:NH2	4:F:174:ASP:OD1	2.30	0.65
2:B:360:PRO:C	2:B:369:ARG:HA	2.16	0.65
1:A:335:ILE:HG23	1:A:339:ARG:HG3	1.79	0.65
1:A:71:GLU:OE2	1:A:73:THR:OG1	2.10	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:328:VAL:O	1:A:332:ILE:HG13	1.97	0.64
1:C:71:GLU:HG2	1:C:98:ASP:HB3	1.79	0.64
2:B:2:ARG:HB3	2:B:133:GLN:CG	2.28	0.64
2:B:12:CYS:HB2	8:B:501:GDP:C8	2.32	0.64
2:D:2:ARG:HB3	2:D:133:GLN:HG2	1.79	0.64
2:B:145:THR:HB	8:B:501:GDP:O2B	1.98	0.63
2:D:21:TRP:CE3	2:D:24:ILE:HD11	2.33	0.63
2:D:397:ALA:O	2:D:401:ARG:NH1	2.31	0.63
2:B:305:CYS:O	2:B:307:PRO:HD3	1.98	0.63
2:B:287:THR:HB	2:B:289:PRO:HD2	1.80	0.62
1:C:335:ILE:HG23	1:C:339:ARG:HG3	1.80	0.62
1:A:278:ALA:HA	1:A:369:ALA:HB2	1.81	0.62
1:A:166:LYS:HE2	1:A:197:HIS:O	1.99	0.62
1:C:172:TYR:HB3	1:C:205:ASP:HA	1.81	0.62
4:F:219:GLY:HA3	4:F:264:PHE:CZ	2.34	0.62
2:B:46:LEU:HA	2:B:49:ILE:HB	1.80	0.62
2:D:21:TRP:CZ3	2:D:63:PRO:HB3	2.34	0.62
1:A:88:HIS:HB2	1:A:89:PRO:HD2	1.82	0.62
1:C:142:GLY:HA3	1:C:183:GLU:OE1	2.00	0.62
2:B:2:ARG:HE	2:B:133:GLN:HG2	1.65	0.62
1:A:220:GLU:HB3	2:B:326:LYS:HD2	1.82	0.61
1:C:220:GLU:HB3	2:D:326:LYS:HD2	1.81	0.61
4:F:226:GLU:HG3	4:F:237:THR:HG22	1.81	0.61
2:D:145:THR:HB	8:D:501:GDP:O2B	2.00	0.61
2:B:114:LEU:O	2:B:118:VAL:HG23	2.01	0.61
1:C:165:SER:HA	1:C:199:ASP:OD2	2.00	0.61
2:D:334:ASN:HD21	2:D:338:LYS:HE3	1.66	0.61
2:D:69:ASP:O	2:D:94:PHE:HA	2.01	0.61
2:D:143:GLY:O	2:D:147:SER:OG	2.18	0.60
4:F:246:GLN:O	4:F:250:SER:HB3	2.01	0.60
1:A:176:GLN:NE2	4:F:56:PRO:HB3	2.16	0.60
4:F:17:VAL:O	4:F:21:LEU:HG	2.01	0.60
4:F:63:ASN:HA	4:F:312:PHE:O	2.01	0.60
1:A:142:GLY:HA3	1:A:183:GLU:OE2	2.02	0.60
2:D:325:MET:HE2	2:D:355:VAL:HG21	1.84	0.60
1:C:234:ILE:HD12	1:C:234:ILE:H	1.66	0.60
1:C:196:GLU:HG2	12:C:613:HOH:O	2.00	0.60
1:C:186:ASN:O	1:C:190:THR:HG22	2.01	0.60
4:F:287:ILE:HG23	4:F:319:PHE:CZ	2.37	0.60
2:D:171:VAL:HA	2:D:204:ILE:O	2.02	0.59
1:A:336:LYS:HD2	1:A:341:ILE:HD12	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:114:ILE:O	1:C:118:VAL:HG23	2.01	0.59
2:D:2:ARG:O	2:D:133:GLN:NE2	2.31	0.59
1:A:187:SER:CB	1:A:391:LEU:HD21	2.32	0.59
1:A:231:ILE:O	1:A:235:VAL:HG23	2.02	0.59
2:D:181:VAL:HG13	2:D:182:VAL:HG13	1.83	0.59
1:C:250:VAL:HB	1:C:255:PHE:CE2	2.37	0.59
2:B:26:ASP:OD2	2:B:369:ARG:HD3	2.03	0.59
1:C:229:ARG:HG3	12:C:605:HOH:O	2.02	0.59
2:B:271:GLY:O	2:B:377:PHE:N	2.25	0.59
4:F:81:ILE:HA	4:F:87:LEU:HD12	1.84	0.58
2:B:70:LEU:HD12	2:B:99:ALA:HB2	1.85	0.58
2:B:2:ARG:HB3	2:B:133:GLN:HG2	1.85	0.58
2:D:212:ILE:O	2:D:216:THR:HB	2.04	0.58
4:F:201:ILE:HG12	4:F:221:LEU:HG	1.84	0.58
2:D:2:ARG:HB3	2:D:133:GLN:CG	2.34	0.58
2:D:180:THR:O	2:D:183:GLU:HG3	2.04	0.58
1:C:174:ALA:HB2	1:C:207:GLU:H	1.68	0.58
1:C:333:ALA:O	1:C:337:THR:HG23	2.04	0.58
1:A:188:ILE:HD12	1:A:395:PHE:HB2	1.86	0.58
1:C:1:MET:HE3	1:C:131:GLY:HA3	1.84	0.58
1:C:233:GLN:HG3	1:C:368:LEU:CD1	2.34	0.58
4:F:3:THR:HG22	4:F:28:LYS:HB3	1.86	0.58
1:A:216:ASN:HD22	1:A:275:VAL:HB	1.67	0.57
4:F:159:GLY:C	4:F:160:ILE:HD12	2.25	0.57
2:D:174:SER:OG	2:D:207:GLU:OE1	2.13	0.57
4:F:3:THR:HA	4:F:28:LYS:O	2.04	0.57
1:C:172:TYR:CE1	1:C:391:LEU:HD22	2.40	0.57
4:F:74:LYS:NZ	4:F:331:GLU:OE1	2.33	0.57
1:A:325:PRO:HB3	3:E:20:PHE:CE1	2.39	0.57
1:C:71:GLU:OE1	1:C:73:THR:OG1	2.15	0.57
1:C:139:HIS:CD2	1:C:150:THR:HG21	2.39	0.57
1:C:192:HIS:CG	1:C:421:ALA:HA	2.40	0.57
1:A:36:MET:HB3	1:A:61:HIS:CE1	2.39	0.57
1:C:21:TRP:CH2	1:C:63:PRO:HB3	2.39	0.57
3:E:128:LYS:O	3:E:128:LYS:HD3	2.05	0.57
1:C:100:ALA:HA	2:D:254:LYS:HG3	1.87	0.57
1:C:221:ARG:HG3	2:D:325:MET:HG2	1.85	0.57
1:A:10:GLY:O	1:A:14:VAL:HG23	2.05	0.57
4:F:2:TYR:CE1	4:F:359:PHE:HB3	2.39	0.57
2:B:42:LEU:H	2:B:42:LEU:HD12	1.70	0.57
2:D:154:ILE:HG23	2:D:166:MET:HG2	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:69:ASP:O	2:B:94:PHE:HA	2.05	0.56
2:B:325:MET:HE2	2:B:355:VAL:HG11	1.87	0.56
2:B:273:ALA:HB2	2:B:300:ASN:HD22	1.70	0.56
2:B:289:PRO:O	2:B:293:GLN:HG3	2.05	0.56
1:C:298:PRO:HG2	1:C:308:ARG:NH2	2.20	0.56
2:D:19:LYS:O	2:D:23:VAL:HG23	2.04	0.56
1:A:176:GLN:HE21	4:F:56:PRO:HB3	1.70	0.56
1:A:186:ASN:O	1:A:190:THR:HG22	2.06	0.56
4:F:10:ASN:CB	4:F:44:ARG:HH22	2.12	0.56
4:F:149:ALA:O	4:F:160:ILE:HG23	2.06	0.56
2:B:385:GLN:O	2:B:389:LYS:HG3	2.04	0.56
1:C:103:TYR:CD2	1:C:148:GLY:HA2	2.41	0.55
2:B:209:LEU:HD21	2:B:302:MET:HG2	1.87	0.55
2:D:153:LEU:O	2:D:157:ILE:HG13	2.06	0.55
5:A:501:GTP:O1B	12:A:601:HOH:O	2.18	0.55
3:E:137:LYS:HE2	3:E:141:GLU:OE2	2.06	0.55
2:D:295:MET:HE2	2:D:377:PHE:HB2	1.89	0.55
3:E:85:LYS:NZ	3:E:89:GLU:OE2	2.28	0.55
1:A:188:ILE:HD12	1:A:395:PHE:CD2	2.42	0.55
2:B:338:LYS:HZ2	4:F:1:MET:HB3	1.72	0.55
2:D:147:SER:HB2	2:D:190:SER:OG	2.06	0.55
4:F:14:TYR:HB3	4:F:41:LEU:HD13	1.86	0.55
1:A:23:LEU:HD23	1:A:236:SER:HB2	1.88	0.55
1:C:70:LEU:HB2	1:C:98:ASP:HA	1.88	0.55
1:A:21:TRP:CE3	1:A:63:PRO:HB3	2.41	0.54
1:A:70:LEU:HD13	1:A:110:ILE:CG2	2.37	0.54
2:B:205:ASP:OD1	2:B:207:GLU:N	2.39	0.54
2:B:286:LEU:HD23	2:B:291:LEU:CD2	2.37	0.54
2:D:209:LEU:HD22	2:D:230:LEU:HB2	1.88	0.54
2:B:124:LYS:HD3	2:B:124:LYS:C	2.27	0.54
1:A:431:ASP:O	1:A:435:VAL:HG23	2.08	0.54
2:B:382:THR:O	2:B:385:GLN:HG2	2.06	0.54
1:C:76:ASP:O	1:C:80:THR:HG22	2.07	0.54
1:C:271:THR:HG23	1:C:300:ASN:O	2.08	0.54
2:D:345:GLU:HG3	2:D:440:ALA:HB2	1.90	0.54
4:F:2:TYR:CZ	4:F:359:PHE:HB3	2.43	0.54
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.25	0.54
1:C:178:SER:OG	2:D:352:LYS:NZ	2.40	0.54
1:C:344:VAL:HG21	1:C:346:TRP:CE2	2.43	0.54
2:B:360:PRO:O	2:B:369:ARG:HA	2.07	0.54
2:B:333:LEU:O	2:B:337:ASN:ND2	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:136:LEU:HD23	1:C:167:LEU:HB2	1.90	0.53
1:A:233:GLN:HG3	1:A:368:LEU:HD12	1.89	0.53
2:B:179:ASP:N	2:B:183:GLU:OE2	2.41	0.53
1:A:233:GLN:HG3	1:A:368:LEU:CD1	2.39	0.53
1:A:209:ILE:CG2	1:A:230:LEU:HD23	2.35	0.53
1:C:108:TYR:O	1:C:112:LYS:HG2	2.09	0.53
1:A:214:ARG:HG2	1:A:219:ILE:O	2.09	0.53
1:C:174:ALA:HB2	1:C:207:GLU:N	2.23	0.53
1:C:175:PRO:HB3	2:D:349:ASN:ND2	2.22	0.53
2:D:124:LYS:C	2:D:124:LYS:HD3	2.29	0.53
2:D:194:LEU:O	2:D:198:THR:OG1	2.26	0.53
2:B:223:THR:O	2:B:227:LEU:HD13	2.08	0.53
2:B:236:SER:O	2:B:243:ARG:NH2	2.39	0.53
2:D:11:GLN:O	2:D:15:GLN:HG2	2.08	0.53
2:D:152:LEU:O	2:D:156:LYS:HG2	2.08	0.53
1:A:75:ILE:HD12	1:A:94:THR:HG22	1.89	0.53
2:D:392:SER:O	2:D:396:THR:HG22	2.08	0.53
1:A:100:ALA:HA	2:B:254:LYS:HG3	1.91	0.52
1:A:103:TYR:CD1	1:A:148:GLY:HA2	2.43	0.52
1:A:433:GLU:HG3	1:A:437:VAL:HG21	1.92	0.52
2:B:286:LEU:HD12	2:B:290:GLU:OE1	2.08	0.52
1:C:174:ALA:HB1	1:C:207:GLU:HB2	1.90	0.52
4:F:225:SER:O	4:F:252:ASN:HB2	2.09	0.52
1:A:79:ARG:HG2	1:A:92:LEU:HD12	1.91	0.52
2:B:292:THR:HG22	2:B:335:VAL:HG21	1.92	0.52
3:E:135:LYS:O	3:E:139:LEU:HG	2.10	0.52
4:F:341:LYS:HG2	4:F:341:LYS:O	2.09	0.52
1:A:180:ALA:HB3	1:A:183:GLU:HG3	1.92	0.52
1:C:22:GLU:O	1:C:26:LEU:HG	2.09	0.52
4:F:220:VAL:HG12	4:F:263:PHE:CE2	2.44	0.52
1:C:385:ALA:HA	1:C:388:TRP:CD1	2.45	0.52
2:D:77:SER:O	2:D:81:GLY:N	2.42	0.52
2:B:338:LYS:NZ	4:F:1:MET:HB3	2.25	0.52
2:D:9:ALA:HA	2:D:68:VAL:O	2.10	0.52
2:D:103:TRP:CE3	2:D:189:LEU:HD13	2.45	0.52
4:F:147:TRP:HB2	4:F:169:LEU:CD1	2.39	0.52
2:B:221:THR:HG21	1:C:325:PRO:HB2	1.92	0.52
2:B:244:PHE:CD2	2:B:358:ILE:HD12	2.45	0.52
2:B:269:MET:HG2	2:B:303:ALA:HB2	1.92	0.52
2:D:172:MET:HG3	2:D:387:LEU:HD11	1.92	0.52
2:D:165:ILE:HG21	2:D:252:LEU:HB3	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:240:THR:HG23	2:D:244:PHE:CD2	2.45	0.51
1:C:11:GLN:HE22	2:D:247:GLN:NE2	2.08	0.51
1:C:14:VAL:HG13	1:C:67:PHE:HD2	1.75	0.51
2:D:269:MET:HG3	2:D:303:ALA:HB3	1.90	0.51
1:C:4[A]:CYS:SG	1:C:136:LEU:HG	2.51	0.51
3:E:9:ILE:HD11	3:E:21:GLU:OE1	2.11	0.51
2:B:103:TRP:CE3	2:B:189:LEU:HD13	2.45	0.51
2:B:244:PHE:CE2	2:B:358:ILE:HD12	2.44	0.51
4:F:220:VAL:HG12	4:F:263:PHE:CD2	2.45	0.51
1:A:187:SER:HB2	1:A:391:LEU:HD21	1.91	0.51
1:A:188:ILE:HD12	1:A:395:PHE:CB	2.40	0.51
2:D:187:ALA:O	2:D:191:VAL:HG23	2.10	0.51
2:B:2:ARG:NE	2:B:133:GLN:HG2	2.26	0.51
4:F:226:GLU:HG3	4:F:237:THR:CG2	2.41	0.51
2:B:9:ALA:HA	2:B:68:VAL:O	2.10	0.51
1:C:297:GLU:HG3	1:C:299:ALA:H	1.76	0.51
3:E:60:ARG:O	3:E:64:GLN:HG3	2.10	0.51
1:A:141:PHE:CE1	1:A:170:SER:HB3	2.46	0.50
1:A:274:PRO:HG2	1:A:371:VAL:HG11	1.92	0.50
2:B:269:MET:HG2	2:B:303:ALA:CB	2.41	0.50
1:C:200:CYS:HA	1:C:266:HIS:HB2	1.92	0.50
1:C:316:CYS:O	1:C:377:MET:HG3	2.11	0.50
2:B:174:SER:CB	2:B:207:GLU:HB2	2.40	0.50
1:C:254:GLU:HG2	1:C:352:LYS:HE2	1.92	0.50
1:A:210:TYR:CE1	1:A:222:PRO:HD2	2.47	0.50
2:D:31:ASP:OD1	2:D:35:SER:N	2.44	0.50
2:D:332:MET:O	2:D:336:GLN:HG3	2.11	0.50
1:A:142:GLY:HA3	1:A:183:GLU:HG2	1.93	0.50
2:B:317:ALA:C	2:B:318:ILE:HD12	2.31	0.50
3:E:11:LEU:HD12	3:E:20:PHE:HB3	1.92	0.50
4:F:225:SER:OG	4:F:250:SER:OG	2.22	0.50
1:A:176:GLN:CG	4:F:56:PRO:HB3	2.41	0.50
4:F:216:TYR:CZ	4:F:218:GLU:HB2	2.47	0.50
1:C:271:THR:CG2	1:C:295:CYS:HA	2.42	0.50
4:F:349:GLY:O	4:F:353:VAL:HG22	2.11	0.50
1:A:208:ALA:O	1:A:212:ILE:HG13	2.12	0.50
2:B:19:LYS:O	2:B:23:VAL:HG23	2.12	0.50
1:C:21:TRP:CZ2	1:C:65:ALA:HB2	2.46	0.50
4:F:53:GLY:N	4:F:60:GLN:OE1	2.33	0.50
2:D:212:ILE:HG21	2:D:275:LEU:HD13	1.94	0.49
4:F:287:ILE:HG23	4:F:319:PHE:CE2	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:265:ILE:HG23	1:A:432:TYR:CZ	2.48	0.49
2:B:296:PHE:CD1	2:B:377:PHE:HE1	2.30	0.49
2:D:6:HIS:CD2	2:D:21:TRP:HE1	2.30	0.49
4:F:286:GLN:O	4:F:290:ILE:HG13	2.13	0.49
4:F:267:PHE:CE2	4:F:279:LEU:HD13	2.47	0.49
1:A:151:SER:HB2	1:A:193:THR:OG1	2.12	0.49
2:B:208:ALA:HB2	2:B:304:ALA:HB2	1.94	0.49
2:D:21:TRP:CE3	2:D:63:PRO:HB3	2.48	0.49
2:D:32:PRO:HA	2:D:83:PHE:CD2	2.47	0.49
2:D:325:MET:CE	2:D:355:VAL:HG21	2.42	0.49
1:A:256:GLN:HG2	1:A:260:VAL:HB	1.93	0.49
2:D:12:CYS:HB2	8:D:501:GDP:C8	2.48	0.49
1:C:9:VAL:HG12	1:C:145:THR:HG22	1.95	0.49
2:D:104:ALA:HB2	2:D:413:MET:SD	2.52	0.49
1:A:101:ASN:ND2	1:A:180:ALA:HB2	2.28	0.49
2:B:48:ARG:NH2	2:B:250:ALA:O	2.46	0.49
1:C:204:VAL:HG13	1:C:302:MET:HE3	1.94	0.49
3:E:77:GLU:O	3:E:81:GLU:HG3	2.12	0.49
1:A:226:ASN:ND2	1:A:367:ASP:OD2	2.43	0.49
2:D:146:GLY:O	2:D:150:GLY:HA3	2.12	0.49
2:D:334:ASN:ND2	2:D:338:LYS:HE3	2.28	0.49
2:B:286:LEU:HD23	2:B:291:LEU:HD23	1.94	0.48
1:C:271:THR:HG21	1:C:295:CYS:HA	1.95	0.48
2:D:213:CYS:SG	2:D:227:LEU:HD23	2.52	0.48
2:D:409:THR:O	3:E:140:LYS:NZ	2.31	0.48
4:F:350:ILE:O	4:F:354:ALA:HB3	2.13	0.48
1:A:103:TYR:CD2	1:A:189:LEU:HD13	2.47	0.48
1:C:172:TYR:HE1	1:C:391:LEU:HD22	1.78	0.48
2:D:5:VAL:HB	2:D:135:PHE:CD2	2.49	0.48
2:B:241:CYS:HB3	2:B:249:ASN:O	2.14	0.48
1:C:99:ALA:HB3	5:C:501:GTP:O2G	2.13	0.48
1:C:234:ILE:HG12	1:C:302:MET:SD	2.53	0.48
2:B:88:ARG:HD3	2:B:91:ASN:OD1	2.13	0.48
1:C:433:GLU:O	1:C:437:VAL:HG23	2.13	0.48
2:B:172:MET:HG3	2:B:387:LEU:HD11	1.95	0.48
2:B:174:SER:OG	2:B:207:GLU:HB2	2.14	0.48
1:A:2:ARG:O	1:A:51:THR:HG22	2.13	0.48
2:B:93:VAL:HG12	2:B:114:LEU:HD11	1.96	0.48
1:C:317:LEU:HB3	1:C:319:TYR:CE2	2.49	0.48
3:E:22:VAL:HG13	3:E:22:VAL:O	2.14	0.48
4:F:103:THR:HG23	4:F:128:ARG:NH2	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:241:SER:HA	1:C:249:ASN:OD1	2.14	0.47
2:D:244:PHE:CE1	2:D:358:ILE:HD12	2.49	0.47
4:F:296:MET:SD	4:F:380:HIS:HB2	2.54	0.47
1:A:142:GLY:CA	1:A:183:GLU:HG2	2.44	0.47
1:A:320:ARG:HA	1:A:356:ASN:O	2.14	0.47
1:C:99:ALA:O	1:C:105:ARG:HD3	2.14	0.47
1:A:385:ALA:HB2	1:A:432:TYR:CG	2.49	0.47
1:C:141:PHE:HB2	1:C:173:PRO:HD3	1.95	0.47
2:D:5:VAL:HB	2:D:135:PHE:HD2	1.79	0.47
2:D:147:SER:O	2:D:151:THR:HG23	2.14	0.47
4:F:267:PHE:CE2	4:F:271:LEU:HD11	2.49	0.47
1:A:266:HIS:O	1:A:268:PRO:HD3	2.13	0.47
2:B:193:GLN:HB3	12:B:603:HOH:O	2.13	0.47
2:B:320:ARG:HA	2:B:356:CYS:O	2.14	0.47
1:C:70:LEU:CB	1:C:98:ASP:HA	2.44	0.47
4:F:171:ASP:O	4:F:175:GLU:HG3	2.15	0.47
2:D:67:LEU:N	2:D:67:LEU:HD12	2.29	0.47
1:A:142:GLY:HA3	1:A:183:GLU:CG	2.45	0.47
1:A:217:LEU:HA	1:A:277:SER:HB2	1.95	0.47
1:C:14:VAL:HG13	1:C:67:PHE:CD2	2.49	0.47
1:C:168:GLU:OE2	1:C:194:THR:HG21	2.14	0.47
2:D:412:GLY:C	3:E:133:VAL:HG13	2.35	0.47
2:B:308:ARG:HA	2:B:342:TYR:CE1	2.49	0.47
2:B:369:ARG:HG3	2:B:370:GLY:N	2.30	0.47
4:F:89:GLU:O	4:F:89:GLU:HG2	2.15	0.47
4:F:126:ASP:OD2	4:F:128:ARG:HG3	2.15	0.47
1:C:97:GLU:HB2	2:D:131:CYS:SG	2.54	0.47
4:F:79:LYS:O	4:F:83:THR:OG1	2.23	0.47
1:C:75:ILE:HD12	1:C:94:THR:HG22	1.97	0.46
2:D:251:ASP:OD1	2:D:253:ARG:N	2.48	0.46
2:B:2:ARG:O	2:B:51:VAL:HG22	2.15	0.46
1:C:174:ALA:CB	1:C:207:GLU:HB2	2.44	0.46
1:C:208:ALA:O	1:C:212:ILE:HG13	2.15	0.46
4:F:3:THR:O	4:F:38:ASN:HB2	2.15	0.46
2:D:427:ASP:O	2:D:431:GLU:HG3	2.14	0.46
4:F:24:THR:O	4:F:26:GLN:HG3	2.16	0.46
2:D:167:ASN:HA	2:D:200:GLU:O	2.16	0.46
4:F:87:LEU:O	4:F:88:SER:OG	2.23	0.46
2:B:93:VAL:CG1	2:B:114:LEU:HD11	2.46	0.46
1:A:188:ILE:HD12	1:A:395:PHE:CG	2.51	0.46
1:A:207:GLU:OE2	4:F:54:HIS:ND1	2.42	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:165:ILE:HG21	2:B:252:LEU:HB3	1.97	0.46
1:C:361:THR:HG22	1:C:362:VAL:H	1.81	0.46
2:D:29:GLY:O	2:D:36:TYR:HA	2.16	0.46
2:D:273:ALA:HB1	2:D:274:PRO:HA	1.98	0.46
1:A:69:ASP:O	1:A:94:THR:HA	2.15	0.46
1:A:93:ILE:HD11	1:A:121:ARG:HG3	1.98	0.46
1:A:188:ILE:HD11	1:A:392:ASP:HA	1.97	0.46
2:B:235:MET:HB3	2:B:235:MET:HE2	1.76	0.46
2:D:169:PHE:CE2	2:D:235:MET:HG2	2.50	0.46
4:F:316:GLY:N	4:F:336:PRO:HG3	2.30	0.46
1:A:1:MET:HB2	1:A:46:ASP:HB2	1.98	0.46
2:B:21:TRP:CH2	2:B:63:PRO:HB3	2.50	0.46
4:F:214:TYR:HB3	4:F:375:PHE:CB	2.42	0.46
2:D:234:THR:OG1	2:D:302:MET:HG3	2.16	0.46
2:D:326:LYS:O	2:D:330:GLU:HG3	2.15	0.46
4:F:196:HIS:O	4:F:227:PRO:HA	2.16	0.46
4:F:220:VAL:HG11	4:F:339:ALA:HB2	1.98	0.46
4:F:318:ASP:OD2	11:F:401:ACP:O2G	2.34	0.46
2:B:103:TRP:CD1	2:B:148:GLY:HA2	2.52	0.45
2:D:23:VAL:HG21	2:D:232:SER:HB2	1.97	0.45
1:C:1:MET:HG3	1:C:2:ARG:H	1.80	0.45
1:C:1:MET:HG3	1:C:2:ARG:N	2.32	0.45
1:A:187:SER:HB3	1:A:391:LEU:HD21	1.97	0.45
2:B:318:ILE:HD12	2:B:318:ILE:N	2.32	0.45
2:D:292:THR:O	2:D:295:MET:HG2	2.17	0.45
4:F:299:GLU:HB3	4:F:300:PRO:HD3	1.98	0.45
11:F:401:ACP:O3G	11:F:401:ACP:O1B	2.34	0.45
2:D:6:HIS:HD2	2:D:65:ALA:HB1	1.80	0.45
2:D:295:MET:HE2	2:D:295:MET:HB2	1.81	0.45
4:F:220:VAL:HG11	4:F:339:ALA:CB	2.46	0.45
2:B:67:LEU:N	2:B:67:LEU:HD12	2.32	0.45
2:B:105:LYS:HA	2:B:109:THR:OG1	2.17	0.45
2:B:114:LEU:O	2:B:114:LEU:HG	2.16	0.45
1:C:270:ALA:HB3	1:C:302:MET:CG	2.35	0.45
1:C:344:VAL:HG21	1:C:346:TRP:CZ2	2.52	0.45
2:D:387:LEU:HD23	2:D:387:LEU:C	2.37	0.45
1:A:317:LEU:HD23	1:A:377:MET:HG3	1.99	0.45
4:F:10:ASN:HB2	4:F:44:ARG:NH2	2.21	0.45
2:D:3:GLU:O	2:D:132:LEU:HD12	2.17	0.45
3:E:92:ASN:O	3:E:96:MET:HG2	2.17	0.45
1:A:336:LYS:NZ	1:A:341:ILE:HB	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:8:GLN:OE1	2:B:17:GLY:HA3	2.17	0.45
1:C:361:THR:HG22	1:C:362:VAL:N	2.32	0.45
2:B:21:TRP:O	2:B:25:SER:OG	2.22	0.45
2:B:23:VAL:CG2	2:B:232:SER:HB3	2.39	0.45
1:C:274:PRO:HG2	1:C:371:VAL:HG11	1.98	0.45
2:D:169:PHE:CD2	2:D:235:MET:HG2	2.52	0.45
4:F:287:ILE:O	4:F:291:ILE:HG13	2.17	0.45
2:D:75:MET:SD	2:D:94:PHE:HB3	2.57	0.44
1:A:287:SER:O	1:A:291:ILE:HG23	2.17	0.44
1:A:362:VAL:HG22	12:A:608:HOH:O	2.17	0.44
2:B:231:VAL:O	2:B:235:MET:HG3	2.17	0.44
1:A:16:ILE:CD1	1:A:171:ILE:HD11	2.48	0.44
2:B:174:SER:HB2	2:B:207:GLU:HB2	1.98	0.44
1:C:323:VAL:HG12	1:C:355:ILE:HD13	1.99	0.44
2:B:292:THR:CG2	2:B:335:VAL:HG21	2.48	0.44
1:C:88:HIS:HE1	1:C:90:GLU:HG3	1.81	0.44
1:C:205:ASP:HB3	1:C:302:MET:O	2.17	0.44
2:D:69:ASP:HA	2:D:145:THR:HG21	1.99	0.44
2:D:141:LEU:HA	2:D:147:SER:HB3	1.98	0.44
2:D:412:GLY:HA3	3:E:133:VAL:HG13	1.98	0.44
2:D:347:ILE:CG2	2:D:350:ASN:HB3	2.44	0.44
2:D:382:THR:O	2:D:385:GLN:HG2	2.17	0.44
2:B:7:ILE:O	2:B:137:LEU:HA	2.18	0.44
2:B:123:ARG:O	2:B:127:GLU:HG3	2.17	0.44
4:F:330:ILE:HG21	11:F:401:ACP:H5'2	2.00	0.44
1:A:179:THR:HG21	2:B:248:LEU:CB	2.48	0.44
1:C:234:ILE:HD12	1:C:234:ILE:N	2.31	0.44
4:F:222:ARG:HA	4:F:260:ASN:O	2.18	0.44
1:A:1:MET:CB	1:A:46:ASP:HB2	2.49	0.43
2:B:154:ILE:CG2	2:B:166:MET:HG2	2.48	0.43
2:D:68:VAL:HA	2:D:93:VAL:O	2.18	0.43
4:F:205:VAL:HG21	4:F:291:ILE:HG21	1.99	0.43
1:A:196:GLU:OE1	1:A:196:GLU:HA	2.18	0.43
2:D:118:VAL:O	2:D:122:VAL:HG23	2.19	0.43
2:D:275:LEU:HD23	2:D:275:LEU:HA	1.84	0.43
2:B:26:ASP:OD1	2:B:369:ARG:NH1	2.52	0.43
2:B:336:GLN:OE1	4:F:36:ARG:NH2	2.52	0.43
1:C:194:THR:O	1:C:194:THR:HG22	2.18	0.43
2:D:25:SER:HB3	2:D:30:ILE:HB	2.00	0.43
1:A:255:PHE:O	1:A:259:LEU:HB2	2.19	0.43
2:D:240:THR:HG23	2:D:244:PHE:HD2	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:ILE:HG12	1:A:114:ILE:O	2.18	0.43
2:B:143:GLY:HA3	8:B:501:GDP:O3A	2.19	0.43
2:B:209:LEU:CD2	2:B:302:MET:HG2	2.48	0.43
1:C:286:LEU:HD23	1:C:290:GLU:OE1	2.18	0.43
2:D:204:ILE:HG22	2:D:209:LEU:HD11	2.01	0.43
2:B:31:ASP:HB2	2:B:32:PRO:HD2	2.01	0.43
1:C:250:VAL:HG11	1:C:352:LYS:HE3	1.99	0.43
1:C:319:TYR:HB2	1:C:355:ILE:HG12	2.01	0.43
2:D:211:ASP:O	2:D:215:ARG:HB2	2.19	0.43
1:A:12:ALA:HB2	5:A:501:GTP:C8	2.54	0.42
2:B:97:SER:HA	1:C:2:ARG:NH1	2.35	0.42
1:A:176:GLN:HG3	4:F:56:PRO:CG	2.48	0.42
2:D:191:VAL:O	2:D:195:VAL:HG23	2.18	0.42
4:F:163:SER:OG	4:F:168:GLU:OE1	2.25	0.42
2:B:260:VAL:HG12	2:B:262:PHE:O	2.19	0.42
1:C:141:PHE:CE1	1:C:170:SER:HB3	2.55	0.42
1:C:155:GLU:HB3	3:E:101:LEU:HD22	2.02	0.42
2:D:154:ILE:HG23	2:D:166:MET:CG	2.47	0.42
2:B:158:ARG:HG3	9:B:504:MES:H32	2.02	0.42
2:B:323:MET:HB3	2:B:373:MET:HE2	2.01	0.42
10:B:505:W0Y:O	1:C:253:THR:HG22	2.20	0.42
4:F:135:TYR:CZ	4:F:166:ALA:HB2	2.55	0.42
4:F:197:ARG:HB2	4:F:224:SER:O	2.19	0.42
2:B:274:PRO:HB3	2:B:286:LEU:HD22	2.00	0.42
1:C:282:TYR:O	1:C:283:HIS:HB2	2.19	0.42
2:B:360:PRO:O	2:B:369:ARG:HD2	2.19	0.42
2:D:2:ARG:HB2	2:D:133:GLN:NE2	2.34	0.42
2:B:407:TRP:HB3	10:B:505:W0Y:O2	2.20	0.42
2:D:345:GLU:H	2:D:345:GLU:HG2	1.69	0.42
4:F:17:VAL:HG13	4:F:351:VAL:HG22	2.01	0.42
2:B:108:TYR:CG	3:E:82:VAL:HG11	2.55	0.42
2:B:153:LEU:O	2:B:157:ILE:HG13	2.20	0.42
2:B:406:HIS:HA	2:B:409:THR:OG1	2.20	0.42
2:D:21:TRP:HA	2:D:24:ILE:HG12	2.02	0.42
2:D:212:ILE:CG2	2:D:275:LEU:HD13	2.50	0.42
3:E:100:LYS:O	3:E:103:GLN:HB3	2.19	0.42
2:B:287:THR:CB	2:B:289:PRO:HD2	2.49	0.42
4:F:199:PHE:CE2	4:F:221:LEU:HD23	2.54	0.42
1:A:291:ILE:HG13	1:A:292:THR:N	2.34	0.41
2:B:28:HIS:NE2	2:B:243:ARG:HD2	2.35	0.41
2:B:199:ASP:O	2:B:266:HIS:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:97:GLU:O	1:C:110:ILE:HG21	2.19	0.41
2:D:141:LEU:HD12	2:D:172:MET:SD	2.60	0.41
4:F:204:TRP:CZ2	4:F:338:CYS:HA	2.54	0.41
1:A:68:VAL:HG11	1:A:149:PHE:CE2	2.56	0.41
2:D:20:PHE:CE1	2:D:24:ILE:HG21	2.55	0.41
2:D:79:ARG:O	2:D:84:GLY:HA3	2.21	0.41
4:F:58:LEU:HD23	4:F:58:LEU:HA	1.90	0.41
1:A:36:MET:SD	1:A:39:ASP:HB2	2.61	0.41
1:A:150:THR:O	1:A:154:MET:HG2	2.20	0.41
1:A:204:VAL:HG13	1:A:209:ILE:HD11	2.02	0.41
1:A:269:LEU:HD11	1:A:301:GLN:HB3	2.02	0.41
1:C:112:LYS:O	1:C:115:ILE:HG22	2.20	0.41
1:C:265:ILE:HG23	1:C:432:TYR:CZ	2.55	0.41
1:C:271:THR:O	1:C:376:CYS:HA	2.19	0.41
4:F:275:LEU:N	4:F:275:LEU:HD22	2.35	0.41
1:A:319:TYR:HB2	1:A:355:ILE:HG12	2.02	0.41
2:B:69:ASP:OD1	2:B:70:LEU:N	2.53	0.41
4:F:217:ARG:HH22	4:F:374:ILE:HG22	1.85	0.41
2:B:162:PRO:O	9:B:504:MES:H72	2.20	0.41
1:C:12:ALA:HB2	5:C:501:GTP:C8	2.55	0.41
1:C:345:ASP:OD2	1:C:439:SER:N	2.42	0.41
2:D:165:ILE:HA	2:D:199:ASP:OD2	2.20	0.41
1:A:385:ALA:HA	1:A:388:TRP:HD1	1.86	0.41
1:A:411:GLU:O	3:E:61:ARG:HD3	2.21	0.41
2:B:51:VAL:HG12	2:B:52:TYR:CD2	2.55	0.41
1:C:244:PHE:CE1	1:C:358:GLN:HG2	2.55	0.41
2:B:325:MET:CG	2:B:355:VAL:HG21	2.39	0.41
4:F:217:ARG:NH1	4:F:345:GLU:OE2	2.54	0.41
1:A:270:ALA:HB3	1:A:302:MET:CG	2.51	0.41
1:A:419:SER:O	1:A:423:GLU:HG3	2.21	0.41
2:B:400:ARG:HG3	2:B:401:ARG:HG2	2.02	0.41
2:D:213:CYS:HA	2:D:217:LEU:HB2	2.03	0.41
2:D:422:GLU:HG2	2:D:426:ASN:ND2	2.36	0.41
2:B:31:ASP:HB2	2:B:32:PRO:CD	2.51	0.41
2:B:42:LEU:HD12	2:B:42:LEU:N	2.35	0.41
2:B:203:CYS:SG	2:B:267:PHE:HB3	2.61	0.41
2:D:8:GLN:NE2	2:D:14:ASN:HA	2.36	0.41
2:D:154:ILE:HG23	2:D:166:MET:SD	2.60	0.41
1:A:388:TRP:CE3	1:A:425:MET:HE1	2.56	0.40
2:B:146:GLY:O	2:B:150:GLY:HA3	2.21	0.40
1:C:68:VAL:HG21	1:C:118:VAL:HG13	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:19:ARG:C	4:F:19:ARG:HD2	2.42	0.40
2:B:68:VAL:HG21	2:B:118:VAL:HG11	2.03	0.40
2:D:21:TRP:CZ2	2:D:65:ALA:HB2	2.56	0.40
4:F:131:PHE:CD2	4:F:132:LEU:HD23	2.57	0.40
4:F:240:LEU:HD12	4:F:240:LEU:N	2.37	0.40
1:C:208:ALA:HB1	1:C:301:GLN:O	2.22	0.40
2:D:24:ILE:HG13	2:D:25:SER:N	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	436/451 (97%)	418 (96%)	17 (4%)	1 (0%)	47	78
1	C	439/451 (97%)	418 (95%)	21 (5%)	0	100	100
2	B	416/445 (94%)	397 (95%)	19 (5%)	0	100	100
2	D	422/445 (95%)	399 (94%)	22 (5%)	1 (0%)	47	78
3	E	118/143 (82%)	118 (100%)	0	0	100	100
4	F	342/384 (89%)	318 (93%)	24 (7%)	0	100	100
All	All	2173/2319 (94%)	2068 (95%)	103 (5%)	2 (0%)	51	82

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	114	ILE
2	D	245	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	369/379 (97%)	364 (99%)	5 (1%)	67	89
1	C	372/379 (98%)	367 (99%)	5 (1%)	69	90
2	B	364/383 (95%)	360 (99%)	4 (1%)	73	92
2	D	368/383 (96%)	367 (100%)	1 (0%)	92	98
3	E	109/127 (86%)	109 (100%)	0	100	100
4	F	313/342 (92%)	312 (100%)	1 (0%)	92	98
All	All	1895/1993 (95%)	1879 (99%)	16 (1%)	81	94

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

Mol	Chain	Res	Type
1	A	71	GLU
1	A	221	ARG
1	A	282	TYR
1	A	300	ASN
1	A	381	THR
2	B	139	HIS
2	B	247	GLN
2	B	357	ASP
2	B	377	PHE
1	C	41	THR
1	C	71	GLU
1	C	80	THR
1	C	245	ASP
1	C	381	THR
2	D	139	HIS
4	F	73	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	GLN

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Mol	Chain	Res	Type
1	A	88	HIS
1	A	300	ASN
2	B	15	GLN
2	B	133	GLN
2	B	247	GLN
2	B	282	GLN
2	B	294	GLN
2	B	300	ASN
1	C	11	GLN
1	C	85	GLN
1	C	133	GLN
1	C	372	GLN
2	D	6	HIS
2	D	294	GLN
4	F	180	HIS
4	F	183	GLN
4	F	229	ASN
4	F	269	GLN
4	F	333	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 17 ligands modelled in this entry, 9 are monoatomic - leaving 8 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	B	501	6	24,30,30	0.94	1 (4%)	30,47,47	1.19	3 (10%)
10	W0Y	C	504	-	14,14,14	0.45	0	20,20,20	0.75	0
8	GDP	D	501	6	24,30,30	0.93	1 (4%)	30,47,47	1.25	4 (13%)
11	ACP	F	401	6	27,33,33	1.38	5 (18%)	32,52,52	1.48	4 (12%)
10	W0Y	B	505	-	14,14,14	0.47	0	20,20,20	0.89	0
9	MES	B	504	-	12,12,12	2.27	1 (8%)	14,16,16	1.93	6 (42%)
5	GTP	A	501	6	26,34,34	1.11	2 (7%)	32,54,54	1.51	6 (18%)
5	GTP	C	501	6	26,34,34	1.14	2 (7%)	32,54,54	1.52	7 (21%)

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	B	501	6	-	2/12/32/32	0/3/3/3
10	W0Y	C	504	-	-	2/12/12/12	0/1/1/1
8	GDP	D	501	6	-	2/12/32/32	0/3/3/3
11	ACP	F	401	6	-	9/15/38/38	0/3/3/3
10	W0Y	B	505	-	-	3/12/12/12	0/1/1/1
9	MES	B	504	-	-	4/6/14/14	0/1/1/1
5	GTP	A	501	6	-	8/18/38/38	0/3/3/3
5	GTP	C	501	6	-	8/18/38/38	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	504	MES	C8-S	-7.59	1.66	1.77
5	C	501	GTP	C5-C6	-4.08	1.39	1.47
5	A	501	GTP	C5-C6	-3.86	1.39	1.47
11	F	401	ACP	PG-O2G	2.92	1.61	1.54
11	F	401	ACP	PG-O3G	2.89	1.61	1.54
11	F	401	ACP	PB-O3A	2.73	1.61	1.58
11	F	401	ACP	C5-C4	2.55	1.47	1.40
8	D	501	GDP	C6-N1	-2.39	1.34	1.37
8	B	501	GDP	C6-N1	-2.35	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	501	GTP	C2-N3	2.23	1.38	1.33
11	F	401	ACP	PB-O2B	2.18	1.61	1.56
5	A	501	GTP	C2-N3	2.15	1.38	1.33

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	F	401	ACP	PB-O3A-PA	-4.29	118.97	132.56
9	B	504	MES	C5-N4-C3	3.84	117.47	108.83
8	D	501	GDP	PA-O3A-PB	-3.59	120.52	132.83
11	F	401	ACP	C3'-C2'-C1'	3.52	106.28	100.98
5	A	501	GTP	PA-O3A-PB	-3.39	121.20	132.83
8	B	501	GDP	PA-O3A-PB	-3.27	121.60	132.83
5	C	501	GTP	PA-O3A-PB	-3.27	121.62	132.83
5	C	501	GTP	C5-C6-N1	3.14	119.50	113.95
5	A	501	GTP	C5-C6-N1	3.14	119.49	113.95
5	A	501	GTP	C8-N7-C5	3.10	108.89	102.99
11	F	401	ACP	N3-C2-N1	-3.09	123.85	128.68
5	C	501	GTP	PB-O3B-PG	-3.00	122.53	132.83
5	C	501	GTP	C8-N7-C5	3.00	108.70	102.99
5	A	501	GTP	PB-O3B-PG	-2.94	122.74	132.83
5	C	501	GTP	C2-N1-C6	-2.86	119.83	125.10
5	A	501	GTP	C2-N1-C6	-2.85	119.85	125.10
9	B	504	MES	C6-C5-N4	-2.75	105.93	110.10
11	F	401	ACP	C4-C5-N7	-2.58	106.71	109.40
9	B	504	MES	C7-N4-C5	2.55	117.75	111.23
8	D	501	GDP	C3'-C2'-C1'	2.52	104.78	100.98
8	B	501	GDP	C8-N7-C5	2.46	107.68	102.99
5	C	501	GTP	C3'-C2'-C1'	2.39	104.57	100.98
5	A	501	GTP	C3'-C2'-C1'	2.38	104.56	100.98
8	B	501	GDP	C5-C6-N1	2.35	118.10	113.95
8	D	501	GDP	C8-N7-C5	2.34	107.45	102.99
9	B	504	MES	O3S-S-C8	2.33	109.54	105.77
5	C	501	GTP	O6-C6-C5	-2.24	119.99	124.37
9	B	504	MES	O2S-S-C8	2.24	109.62	106.92
8	D	501	GDP	C5-C6-N1	2.22	117.88	113.95
9	B	504	MES	O1S-S-C8	2.12	109.47	106.92

There are no chirality outliers.

All (38) torsion outliers are listed below:

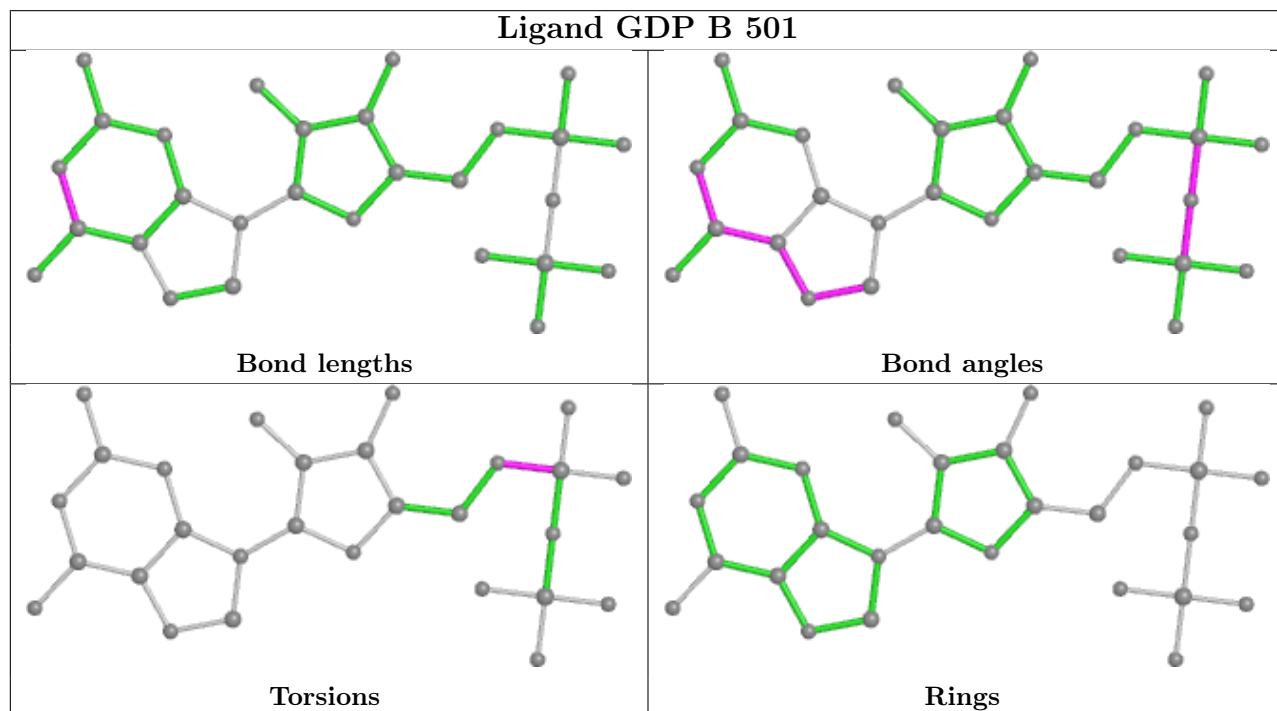
Mol	Chain	Res	Type	Atoms
5	A	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	PB-O3B-PG-O2G
5	C	501	GTP	C5'-O5'-PA-O1A
8	B	501	GDP	C5'-O5'-PA-O3A
8	B	501	GDP	C5'-O5'-PA-O2A
8	D	501	GDP	C5'-O5'-PA-O3A
9	B	504	MES	C8-C7-N4-C5
9	B	504	MES	C7-C8-S-O2S
9	B	504	MES	C7-C8-S-O3S
10	B	505	W0Y	C2-C1-N-C
10	B	505	W0Y	O-C1-N-C
10	C	504	W0Y	C2-C1-N-C
10	C	504	W0Y	O-C1-N-C
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-O3A
11	F	401	ACP	C5'-O5'-PA-O1A
11	F	401	ACP	C5'-O5'-PA-O2A
5	A	501	GTP	C3'-C4'-C5'-O5'
5	A	501	GTP	O4'-C4'-C5'-O5'
5	A	501	GTP	PB-O3B-PG-O2G
5	A	501	GTP	C5'-O5'-PA-O3A
5	C	501	GTP	C5'-O5'-PA-O3A
11	F	401	ACP	C5'-O5'-PA-O3A
5	A	501	GTP	C5'-O5'-PA-O2A
5	C	501	GTP	C5'-O5'-PA-O2A
8	D	501	GDP	C5'-O5'-PA-O2A
9	B	504	MES	C7-C8-S-O1S
5	C	501	GTP	C3'-C4'-C5'-O5'
5	A	501	GTP	PB-O3A-PA-O2A
5	C	501	GTP	PB-O3A-PA-O2A
5	C	501	GTP	C4'-C5'-O5'-PA
11	F	401	ACP	PB-O3A-PA-O1A
5	A	501	GTP	C4'-C5'-O5'-PA
5	C	501	GTP	O4'-C4'-C5'-O5'
11	F	401	ACP	PB-O3A-PA-O2A
10	B	505	W0Y	C4-C5-S-O2

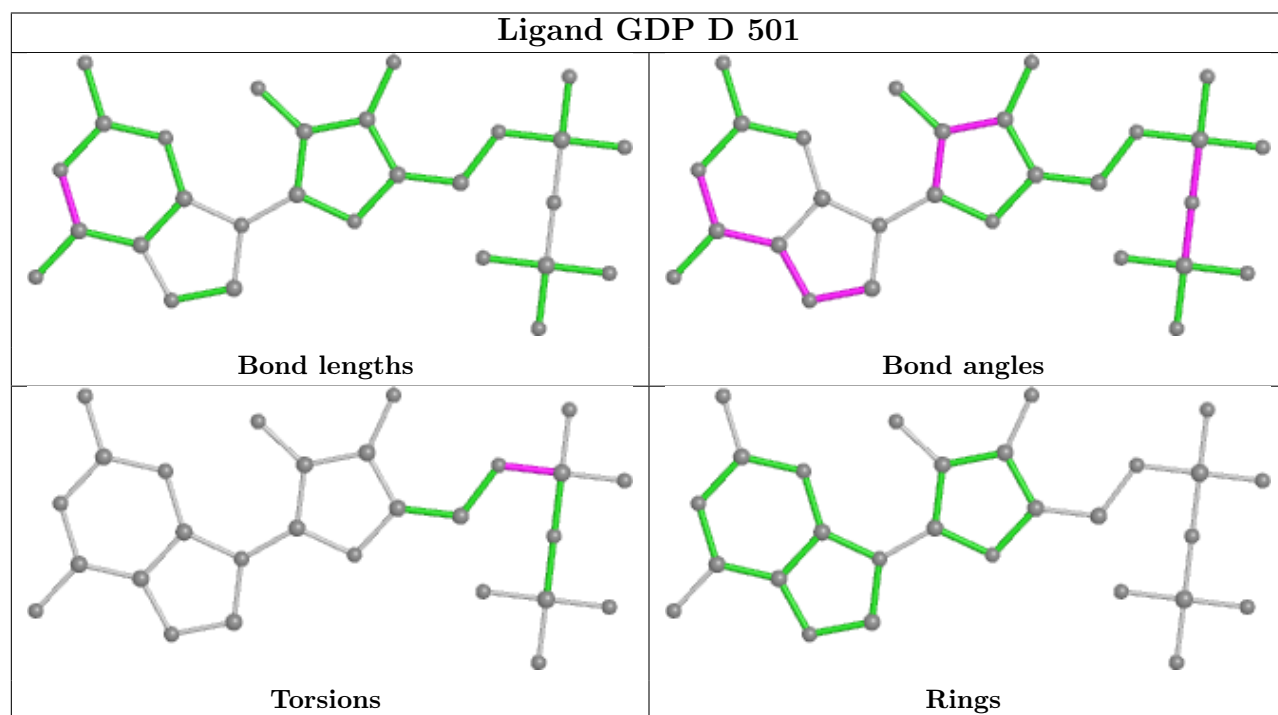
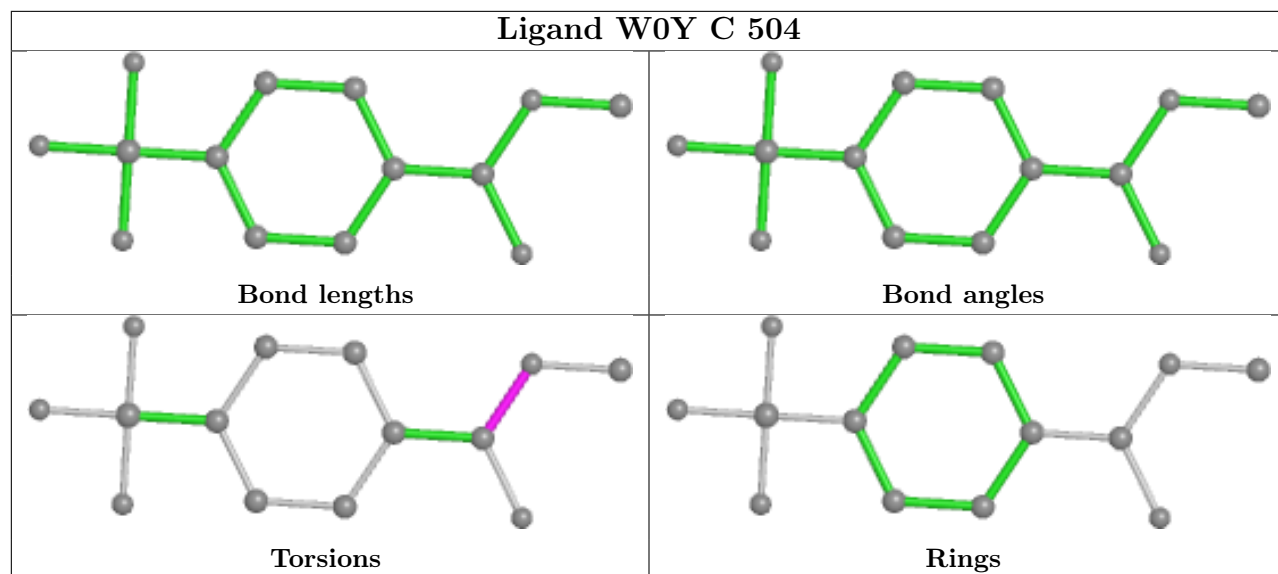
There are no ring outliers.

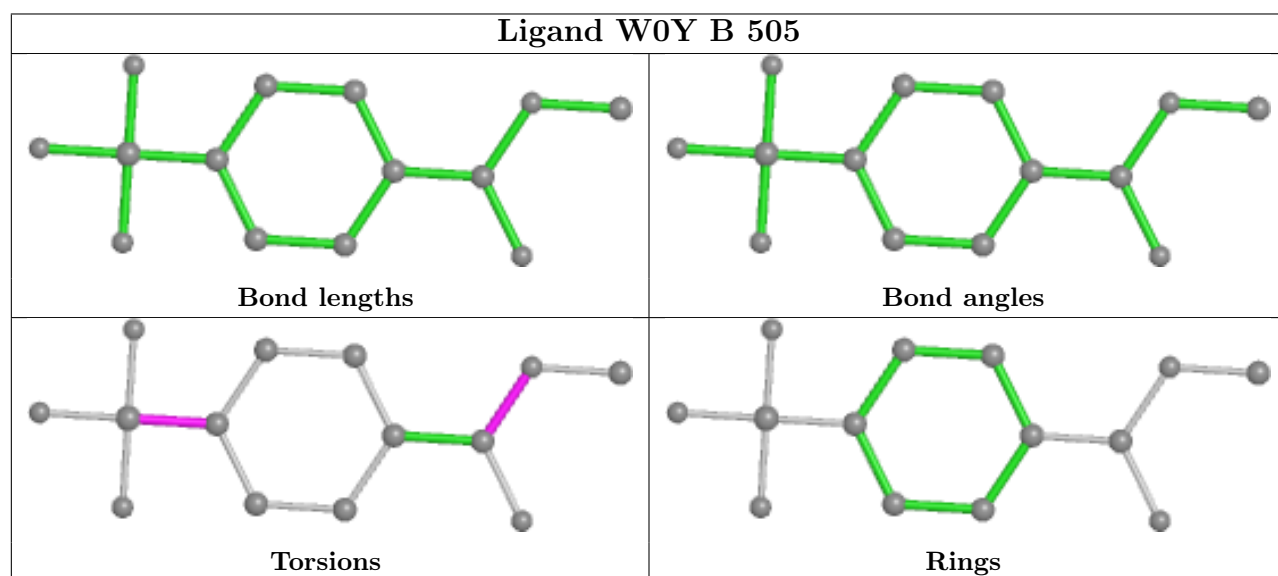
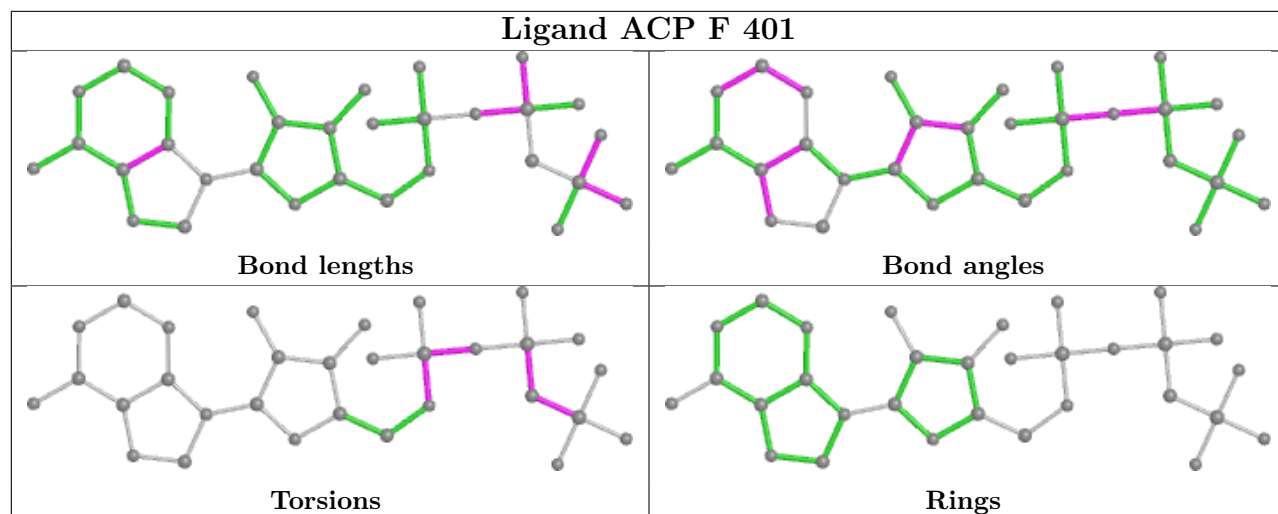
7 monomers are involved in 19 short contacts:

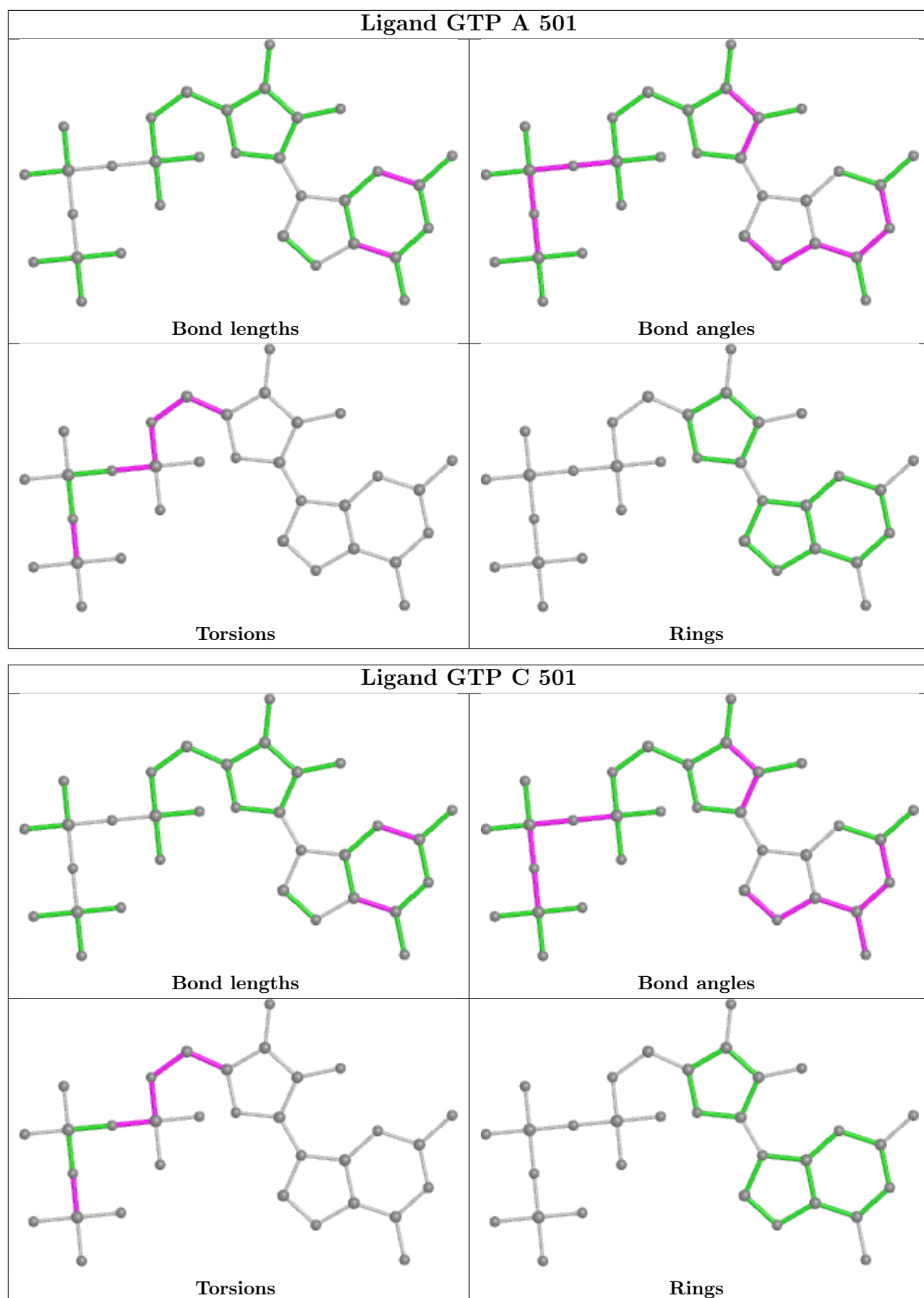
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	501	GDP	3	0
8	D	501	GDP	2	0
11	F	401	ACP	4	0
10	B	505	W0Y	2	0
9	B	504	MES	3	0
5	A	501	GTP	3	0
5	C	501	GTP	2	0

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.









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	360:PRO	C	369:ARG	N	3.41

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%)	0.48	39 (8%) 9 7	68, 91, 135, 206	0
1	C	440/451 (97%)	0.54	35 (7%) 12 9	57, 77, 112, 157	0
2	B	422/445 (94%)	0.62	33 (7%) 13 10	64, 91, 141, 178	4 (0%)
2	D	425/445 (95%)	0.72	65 (15%) 2 1	70, 104, 142, 204	5 (1%)
3	E	122/143 (85%)	0.50	12 (9%) 7 5	85, 105, 159, 212	0
4	F	350/384 (91%)	0.34	29 (8%) 11 8	92, 130, 199, 221	0
All	All	2197/2319 (94%)	0.54	213 (9%) 7 6	57, 97, 161, 221	9 (0%)

All (213) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	E	6	MET	9.3
2	D	216	THR	8.7
3	E	27	PRO	8.4
2	D	275	LEU	7.7
4	F	142	ARG	7.6
2	D	294	GLN	7.4
1	A	349	THR	6.5
4	F	143	GLU	6.2
1	A	340	SER	5.7
2	D	218	LYS	5.6
2	D	276	THR	5.4
2	D	299	LYS	5.4
3	E	25	LYS	5.3
1	A	346	TRP	5.1
4	F	98	TYR	5.0
4	F	141	GLY	5.0
2	D	215	ARG	5.0
2	D	217	LEU	4.9
4	F	131	PHE	4.8

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Mol	Chain	Res	Type	RSRZ
3	E	26	PRO	4.7
3	E	24	LEU	4.7
2	D	296	PHE	4.6
1	A	341	ILE	4.5
1	C	368	LEU	4.5
4	F	100	ILE	4.5
1	C	372	GLN	4.5
1	C	285	GLN	4.4
4	F	240	LEU	4.4
1	C	339	ARG	4.3
2	D	248	LEU	4.3
1	C	323	VAL	4.2
1	A	312	TYR	4.2
4	F	89	GLU	4.0
4	F	138	ARG	4.0
2	D	353	THR	4.0
1	C	371	VAL	4.0
1	A	350	GLY	4.0
1	C	286	LEU	3.9
2	D	290	GLU	3.9
2	D	293	GLN	3.9
2	D	297	ASP	3.8
1	C	296	PHE	3.8
2	B	284	ARG	3.8
3	E	7	GLU	3.7
3	E	22	VAL	3.7
2	D	286	LEU	3.7
4	F	137	ARG	3.7
1	C	135	PHE	3.6
1	A	339	ARG	3.6
2	B	286	LEU	3.6
2	B	377	PHE	3.6
2	B	219	LEU	3.6
1	A	438	ASP	3.6
2	B	332	MET	3.6
1	C	178	SER	3.5
2	B	372	LYS	3.5
2	D	212	ILE	3.5
2	D	1	MET	3.5
2	D	323	MET	3.4
1	C	276	ILE	3.4
2	D	301	MET	3.4

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Mol	Chain	Res	Type	RSRZ
1	C	291	ILE	3.4
1	A	325	PRO	3.4
2	D	57	THR	3.4
1	A	435	VAL	3.4
2	B	319	PHE	3.4
2	D	312	TYR	3.4
2	D	319	PHE	3.3
2	D	308	ARG	3.3
2	D	287	THR	3.3
1	A	342	GLN	3.3
2	D	219	LEU	3.3
1	A	436	GLY	3.2
2	B	337	ASN	3.2
1	C	179	THR	3.2
1	A	326	LYS	3.1
2	D	250	ALA	3.1
2	D	300	ASN	3.1
4	F	99	VAL	3.1
4	F	182	ILE	3.1
2	D	379	GLY	3.1
2	B	371	LEU	3.1
2	B	285	ALA	3.0
2	B	203	CYS	3.0
2	D	377	PHE	3.0
2	D	335	VAL	3.0
2	D	351	VAL	3.0
2	B	221	THR	3.0
4	F	134	ALA	3.0
1	C	177	VAL	3.0
4	F	328	TRP	2.9
1	A	344	VAL	2.9
1	A	345	ASP	2.9
1	A	351	PHE	2.9
2	D	135	PHE	2.9
4	F	90	SER	2.9
4	F	140	GLU	2.9
1	C	210	TYR	2.9
1	C	341	ILE	2.8
2	B	435	TYR	2.8
2	B	216	THR	2.8
2	D	274	PRO	2.8
2	D	291	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
2	D	328	VAL	2.8
1	A	323	VAL	2.8
4	F	169	LEU	2.8
2	D	283	TYR	2.8
2	B	281	GLN	2.7
2	D	336	GLN	2.7
4	F	97	SER	2.7
2	D	241	CYS	2.7
3	E	116	LEU	2.7
1	C	357	TYR	2.7
2	B	61	TYR	2.7
2	D	350	ASN	2.7
3	E	23	ILE	2.7
1	A	348	PRO	2.7
2	D	292	THR	2.7
3	E	139	LEU	2.7
4	F	162	ILE	2.6
1	A	315	CYS	2.6
2	D	378	ILE	2.6
2	B	301	MET	2.6
1	A	86	LEU	2.6
1	C	275	VAL	2.6
1	A	418	PHE	2.6
2	B	296	PHE	2.6
1	C	370	LYS	2.6
1	C	163	LYS	2.6
4	F	36	ARG	2.6
2	D	49	ILE	2.6
2	D	20	PHE	2.6
2	D	352	LYS	2.5
2	D	213	CYS	2.5
1	A	311	LYS	2.5
2	B	346	TRP	2.5
2	B	53	TYR	2.5
2	D	316	ALA	2.5
1	A	317	LEU	2.5
2	D	332	MET	2.5
2	D	343	PHE	2.5
2	D	298	SER	2.5
1	A	337	THR	2.5
2	B	220	THR	2.5
2	B	291	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	181	VAL	2.4
2	B	432	TYR	2.4
4	F	136	ASN	2.4
2	D	249	ASN	2.4
4	F	294	CYS	2.4
1	A	332	ILE	2.4
1	A	296	PHE	2.3
2	D	272	PHE	2.3
1	C	272	TYR	2.3
1	C	282	TYR	2.3
1	C	319	TYR	2.3
1	C	162	GLY	2.3
2	B	87	PHE	2.3
1	A	285	GLN	2.3
1	A	327	ASP	2.3
1	C	373	ARG	2.3
4	F	96	GLU	2.3
2	D	373	MET	2.3
1	C	329	ASN	2.3
2	B	313	LEU	2.3
2	D	123	ARG	2.3
2	D	302	MET	2.3
2	D	51	VAL	2.2
2	D	129	CYS	2.2
1	A	343	PHE	2.2
1	A	324	VAL	2.2
2	D	242	LEU	2.2
2	D	238	VAL	2.2
1	A	329	ASN	2.2
2	D	154	ILE	2.2
1	A	357	TYR	2.2
2	D	88	ARG	2.2
3	E	84	GLN	2.2
4	F	234	GLN	2.2
2	D	285	ALA	2.2
4	F	94	PHE	2.2
2	B	302	MET	2.2
2	D	52	TYR	2.2
2	D	342	TYR	2.2
1	C	7	ILE	2.2
2	B	312	TYR	2.2
1	C	218	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	347	CYS	2.2
1	A	319	TYR	2.2
2	B	373	MET	2.1
1	A	362	VAL	2.1
2	D	136	GLN	2.1
4	F	173	ILE	2.1
2	B	59	ASN	2.1
3	E	50	ILE	2.1
2	D	315	VAL	2.1
1	C	255	PHE	2.1
1	C	283	HIS	2.1
1	C	351	PHE	2.1
4	F	329	LEU	2.0
1	C	5	ILE	2.0
1	A	265	ILE	2.0
2	B	66	ILE	2.0
1	A	179	THR	2.0
1	C	110	ILE	2.0
1	C	356	ASN	2.0
2	B	434	GLN	2.0
4	F	31	ARG	2.0
4	F	161	LEU	2.0
1	C	326	LYS	2.0
2	B	318	ILE	2.0
2	B	382	THR	2.0
1	A	125	LEU	2.0

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

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

6.3 Carbohydrates [\(i\)](#)

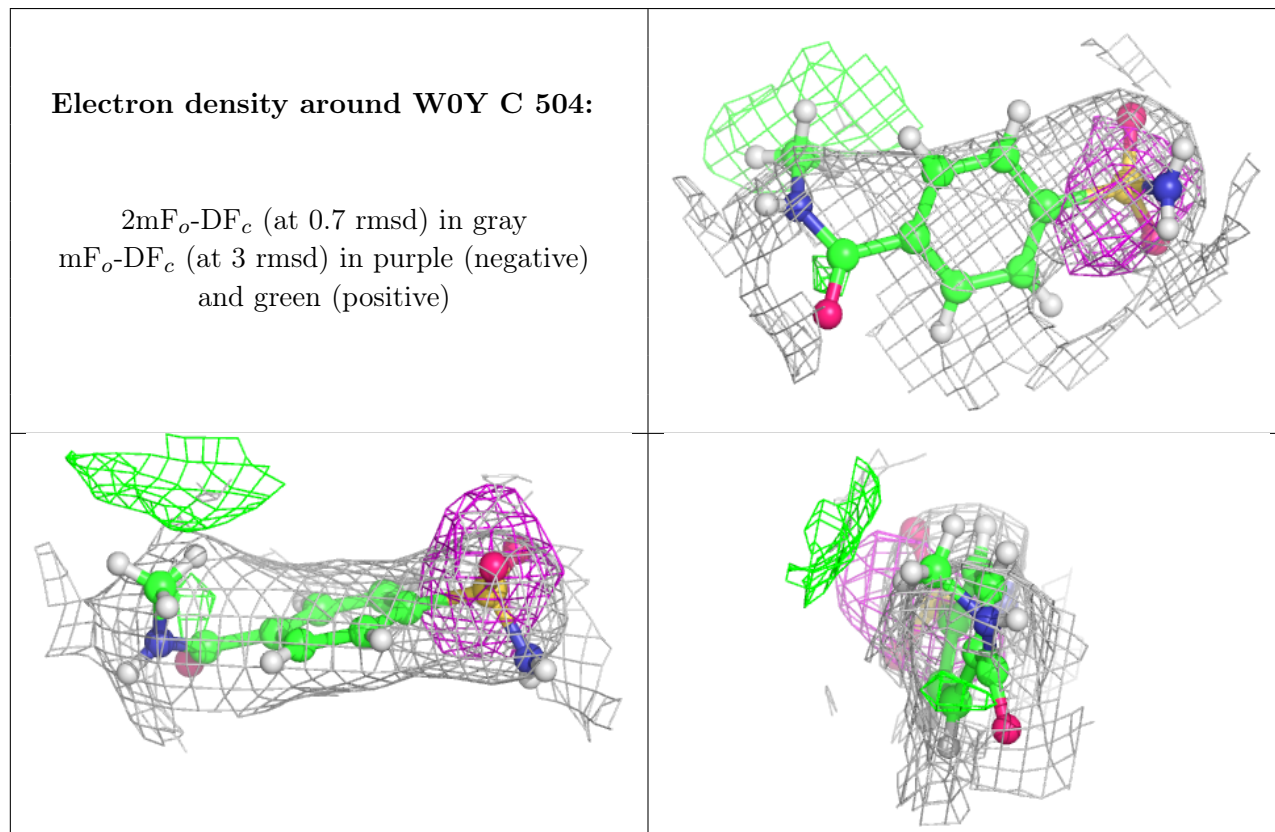
There are no monosaccharides in this entry.

6.4 Ligands [\(i\)](#)

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

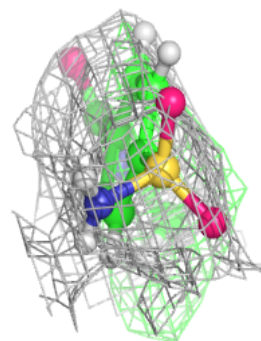
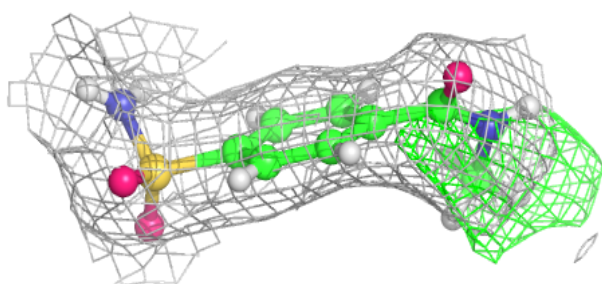
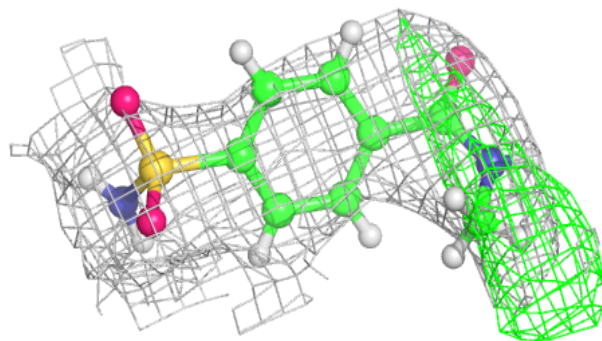
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
10	W0Y	C	504	14/14	0.69	0.28	93,112,131,137	24
7	CA	E	201	1/1	0.77	0.12	97,97,97,97	0
10	W0Y	B	505	14/14	0.79	0.28	79,88,98,102	24
9	MES	B	504	12/12	0.88	0.15	99,107,116,122	0
11	ACP	F	401	31/31	0.88	0.14	126,135,144,148	0
6	MG	D	502	1/1	0.92	0.21	88,88,88,88	0
7	CA	B	503	1/1	0.94	0.05	122,122,122,122	0
8	GDP	D	501	28/28	0.94	0.19	91,97,103,109	0
8	GDP	B	501	28/28	0.96	0.17	63,73,81,82	0
5	GTP	A	501	32/32	0.96	0.18	66,75,80,86	0
7	CA	C	503	1/1	0.97	0.15	101,101,101,101	0
5	GTP	C	501	32/32	0.97	0.20	60,68,74,76	0
7	CA	A	503	1/1	0.97	0.16	117,117,117,117	0
6	MG	B	502	1/1	0.97	0.13	75,75,75,75	0
6	MG	A	502	1/1	0.99	0.16	81,81,81,81	0
6	MG	F	402	1/1	0.99	0.09	125,125,125,125	0
6	MG	C	502	1/1	0.99	0.14	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.

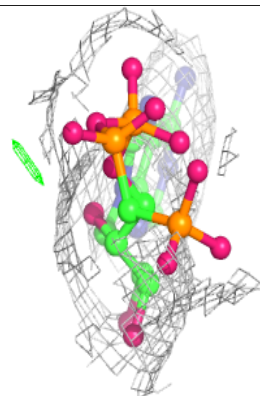
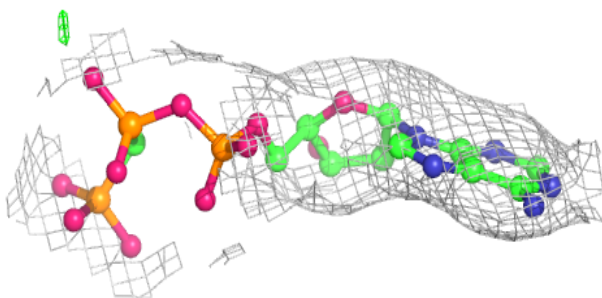
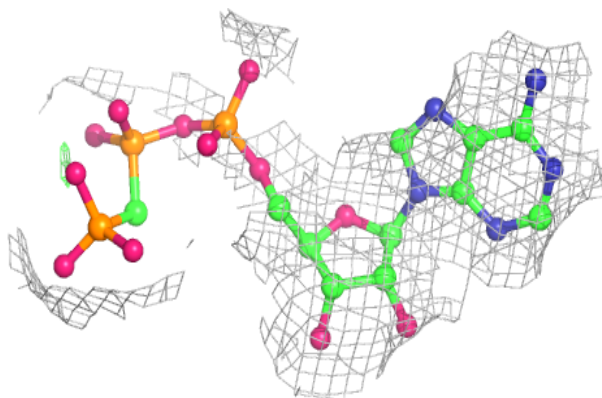


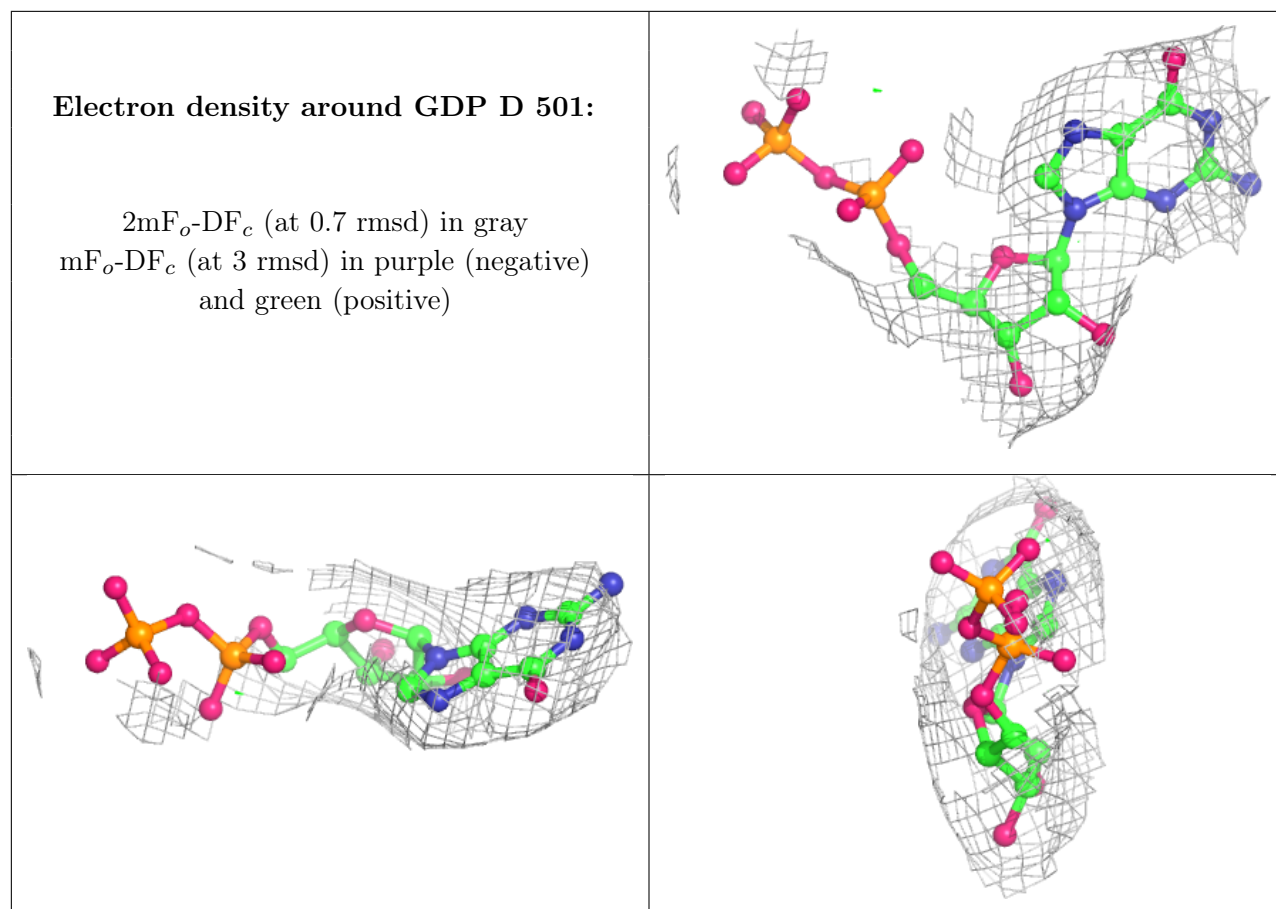
Electron density around W0Y B 505:

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

**Electron density around ACP F 401:**

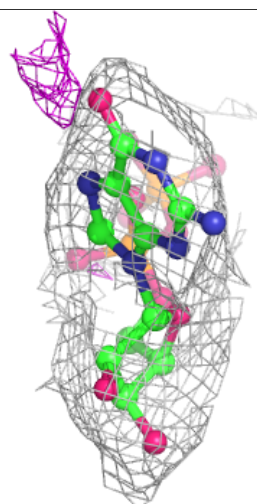
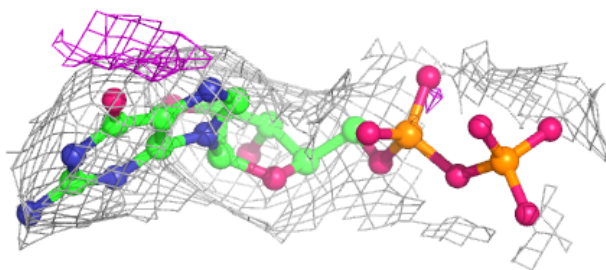
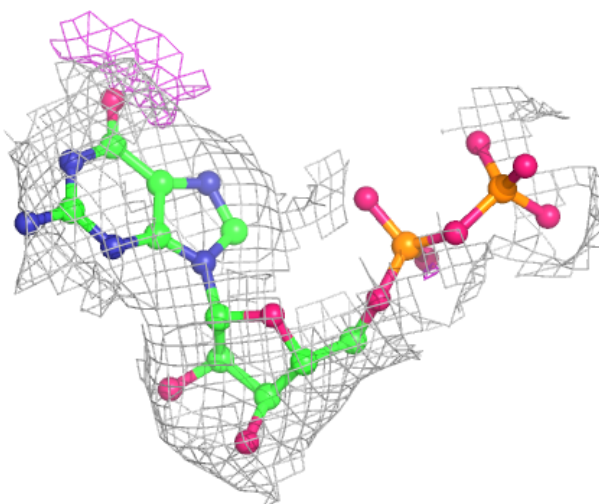
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





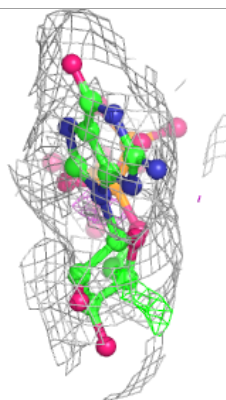
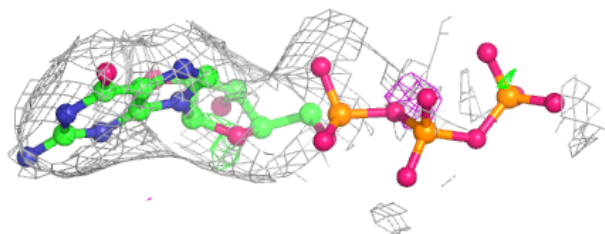
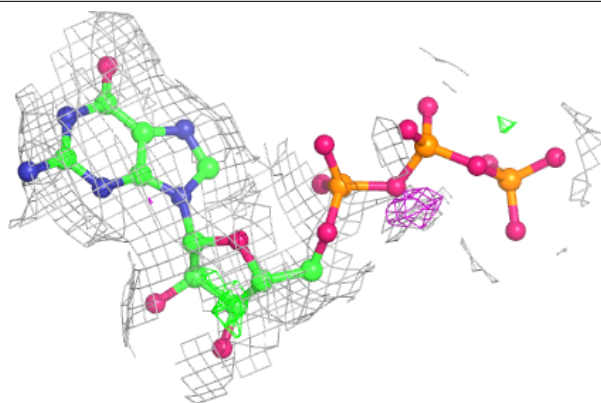
Electron density around GDP B 501:

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

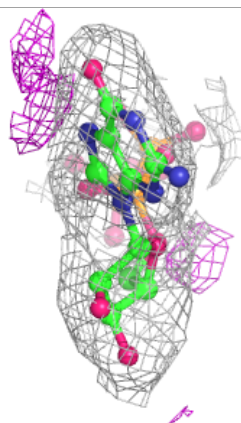
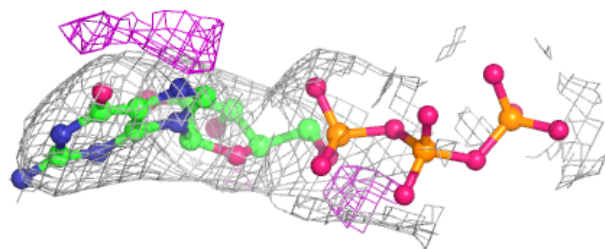
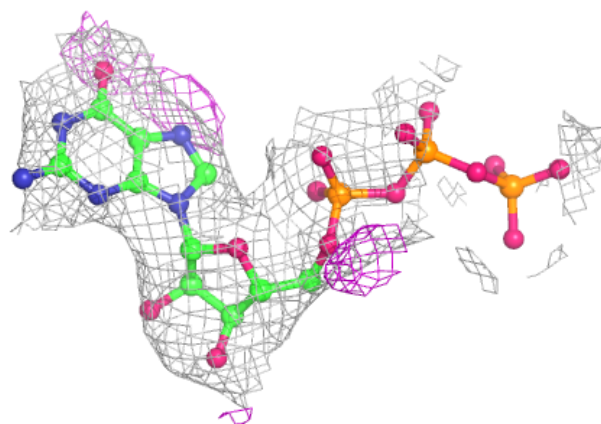


Electron density around GTP A 501:

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

**Electron density around GTP C 501:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.