



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 02:57 am BST

PDB ID : 5Z4P
Title : Crystal structure of tubulin-stathmin-TTL-Compound TCA complex
Authors : Zhang, H.; Luo, C.
Deposited on : 2018-01-12
Resolution : 2.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
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) : 2.11

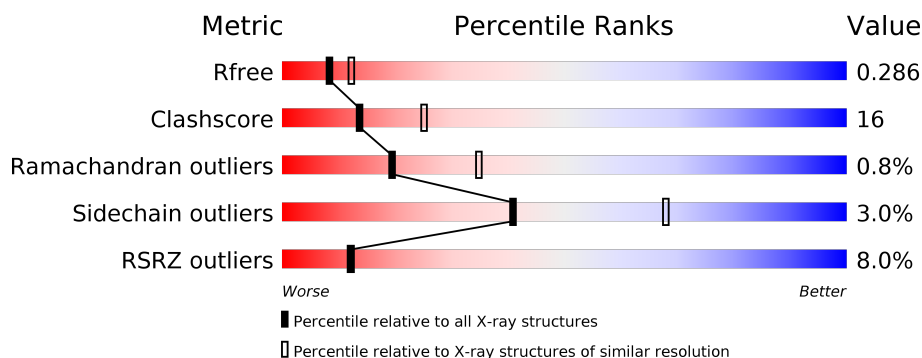
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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 on 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	440	<div> <div>3%</div> <div> <div></div> <div>72%</div> <div>27%</div> <div></div> </div> </div>
1	C	440	<div> <div>%</div> <div> <div></div> <div>76%</div> <div>23%</div> <div></div> </div> </div>
2	B	431	<div> <div>6%</div> <div> <div></div> <div>68%</div> <div>29%</div> <div></div> </div> </div>
2	D	431	<div> <div>9%</div> <div> <div></div> <div>61%</div> <div>33%</div> <div></div> </div> </div>
3	E	185	<div> <div>4%</div> <div> <div></div> <div>45%</div> <div>18%</div> <div></div> <div>35%</div> </div> </div>
4	F	378	<div> <div>22%</div> <div> <div></div> <div>48%</div> <div>35%</div> <div></div> <div>16%</div> </div> </div>

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	ACP	F	401	-	-	X	X
7	GOL	C	501	-	-	-	X
7	GOL	C	505	-	-	X	-
7	GOL	C	506	-	-	-	X

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 17477 atoms, of which 0 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	2	0
			3433	2175	582	653	23			
1	C	440	Total	C	N	O	S	0	3	0
			3451	2184	586	658	23			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	424	Total	C	N	O	S	0	2	0
			3347	2104	568	648	27			
2	D	421	Total	C	N	O	S	0	0	0
			3309	2080	562	640	27			

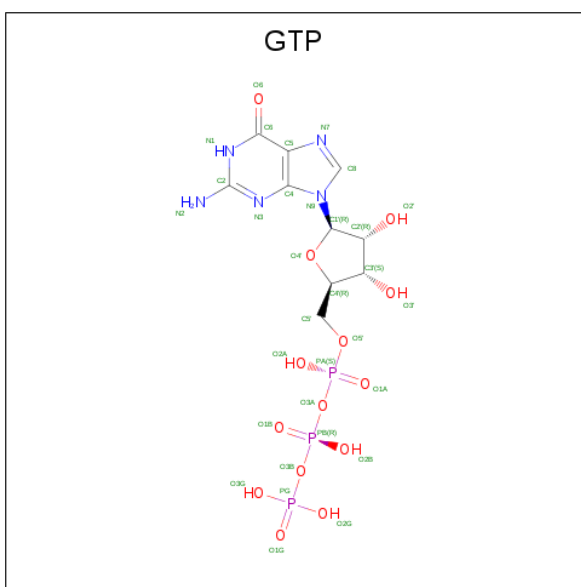
- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	121	Total	C	N	O	S	0	2	0
			1011	624	183	199	5			

- Molecule 4 is a protein called Tubulin tyrosine ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	317	Total	C	N	O	S	0	0	0
			2596	1677	434	471	14			

- Molecule 5 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).



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

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

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

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total	C	O	0	0
			6	3	3		
7	C	1	Total	C	O	0	0
			6	3	3		
7	C	1	Total	C	O	0	0
			6	3	3		
7	C	1	Total	C	O	0	0
			6	3	3		
7	C	1	Total	C	O	0	0
			6	3	3		
7	D	1	Total	C	O	0	0
			6	3	3		
7	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 8 is CALCIUM ION (three-letter code: CA) (formula: Ca).

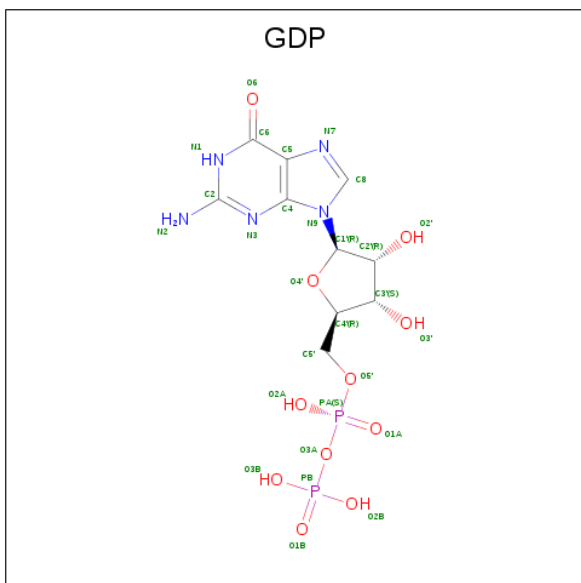
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	1	Total	Ca	0	0
			1	1		

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

- Molecule 9 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $\text{C}_{10}\text{H}_{15}\text{N}_5\text{O}_{11}\text{P}_2$).



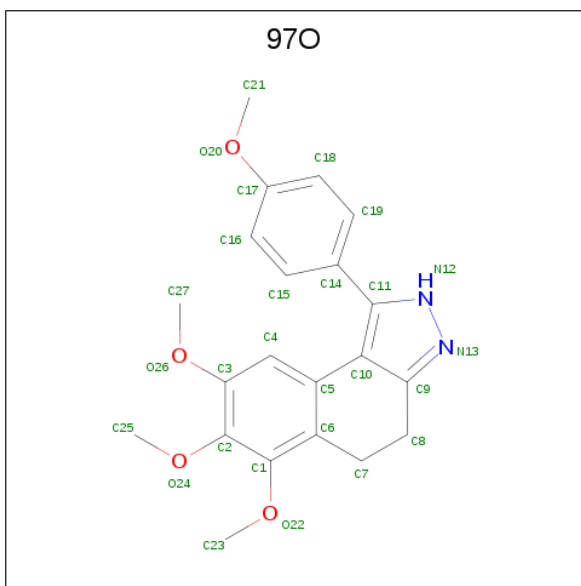
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	B	1	Total 28	C 10	N 5	O 11	P 2	0	0
9	D	1	Total 28	C 10	N 5	O 11	P 2	0	0

- Molecule 10 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $\text{C}_6\text{H}_{13}\text{NO}_4\text{S}$).



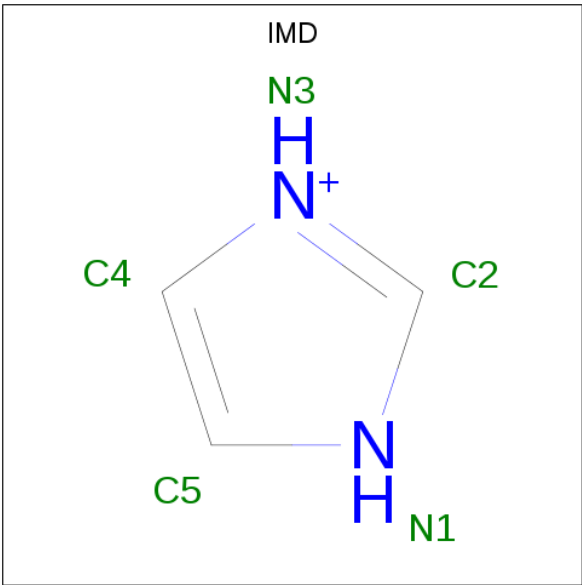
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 11 is 6,7,8-trimethoxy-1-(4-methoxyphenyl)-4,5-dihydro-2 {H}-benzo[e]indazole (three-letter code: 97O) (formula: $C_{21}H_{22}N_2O_4$).



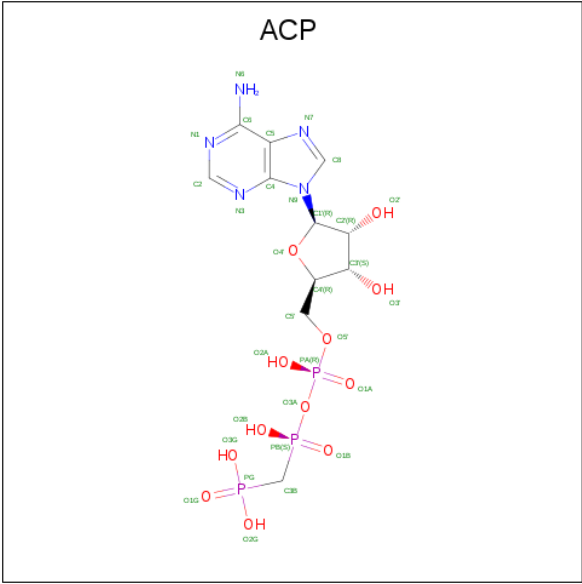
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	B	1	Total	C	N	O	0	0
			27	21	2	4		

- Molecule 12 is IMIDAZOLE (three-letter code: IMD) (formula: $C_3H_5N_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	C	1	Total	C	N	0	0
			5	3	2		
12	C	1	Total	C	N	0	0
			5	3	2		
12	C	1	Total	C	N	0	0
			5	3	2		

- Molecule 13 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (three-letter code: ACP) (formula: C₁₁H₁₈N₅O₁₂P₃).



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

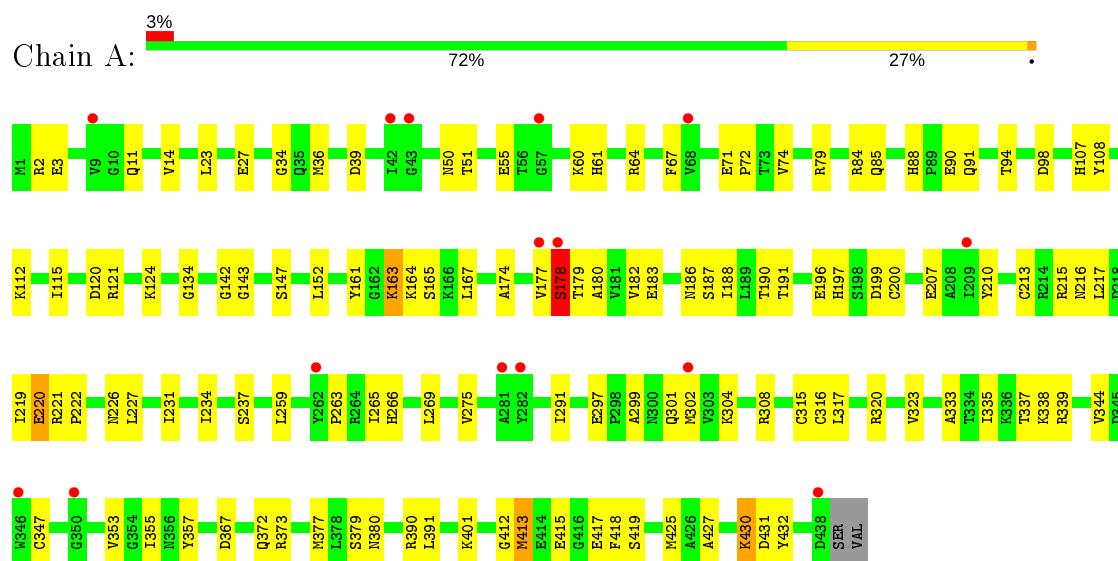
- Molecule 14 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	11	Total	O	0	0
			11	11		
14	B	13	Total	O	0	0
			13	13		
14	C	17	Total	O	0	0
			17	17		
14	D	4	Total	O	0	0
			4	4		
14	F	7	Total	O	0	0
			7	7		

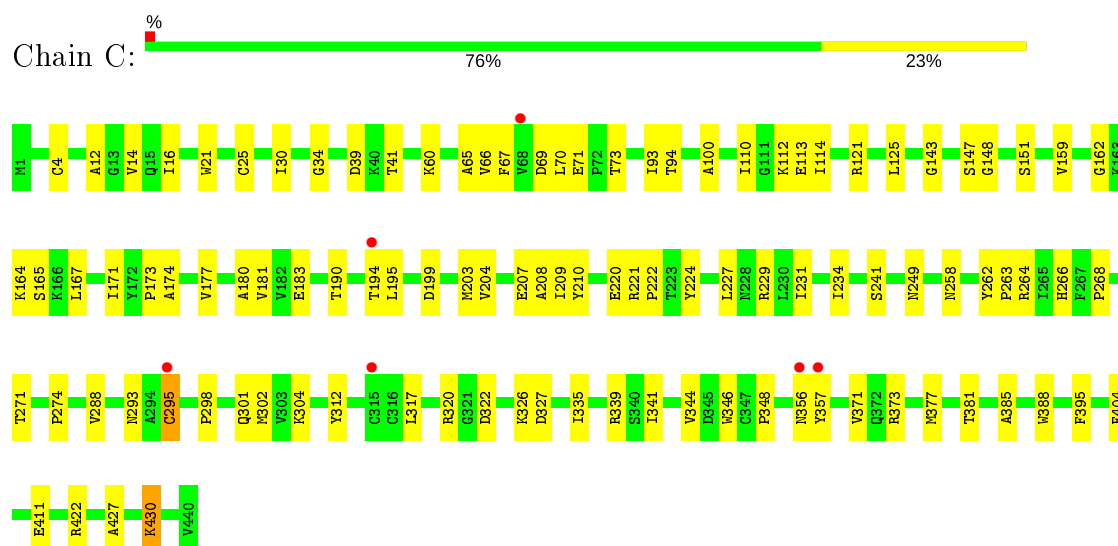
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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

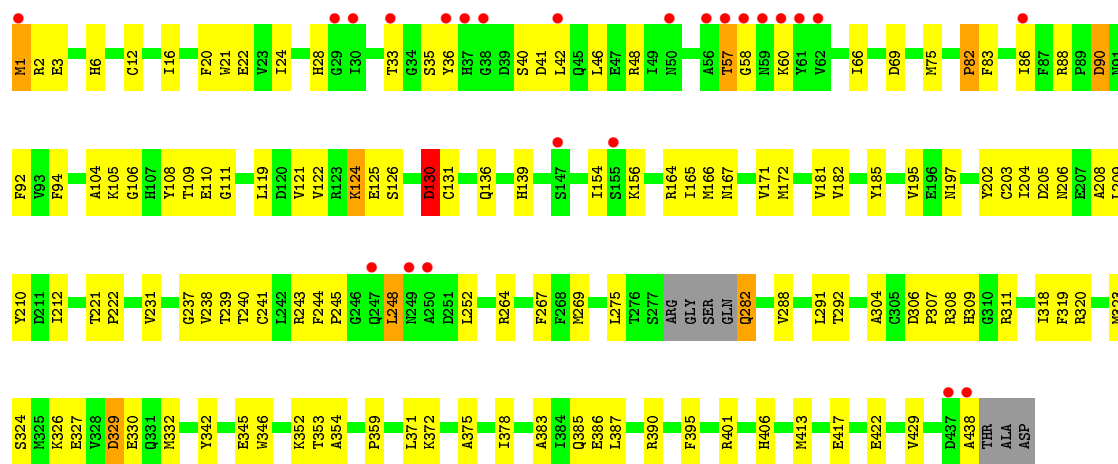


• Molecule 1: Tubulin alpha-1B chain

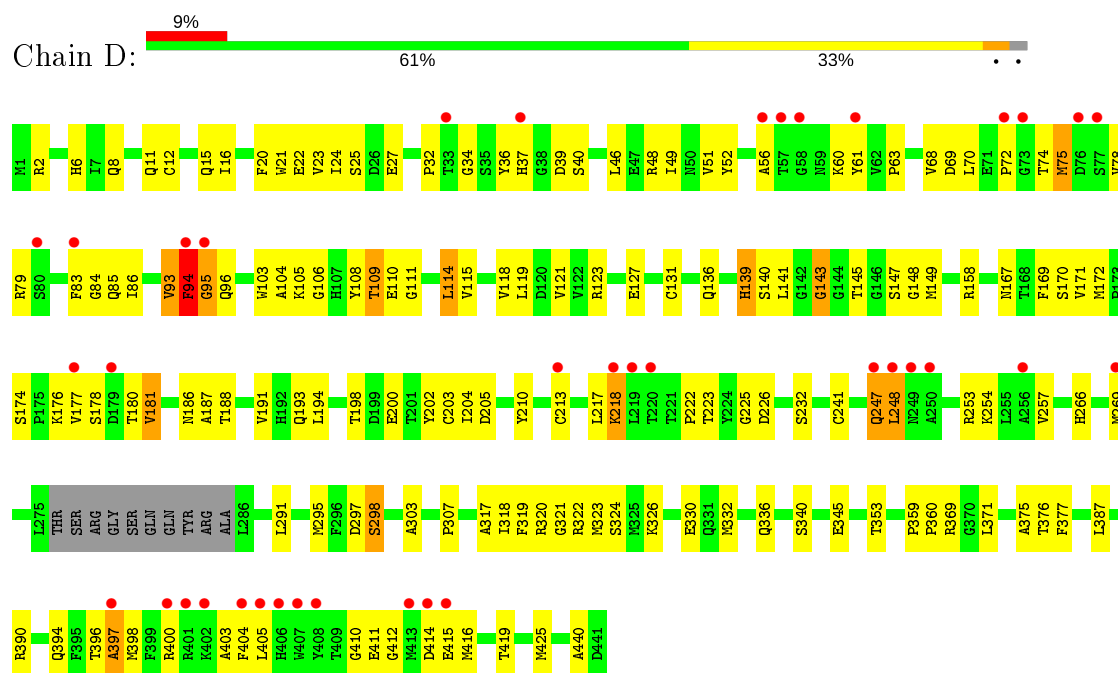


• Molecule 2: Tubulin beta-2B chain

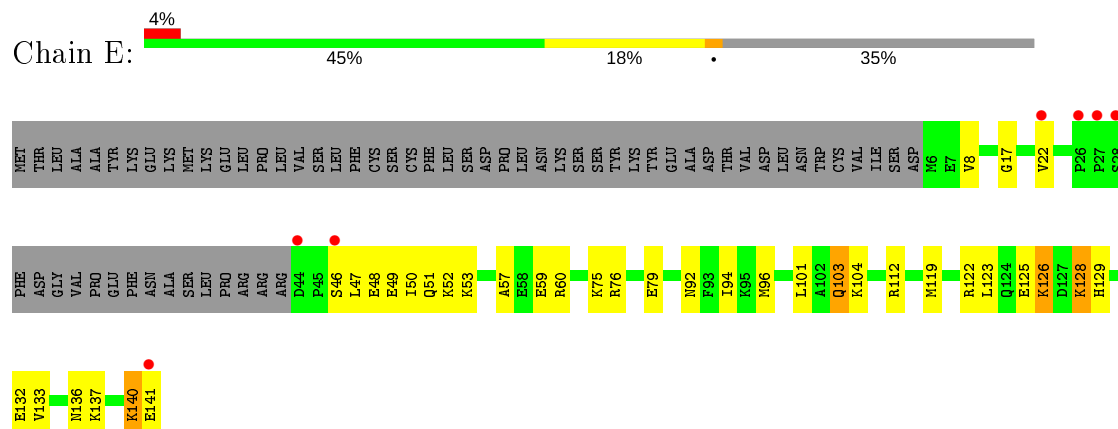




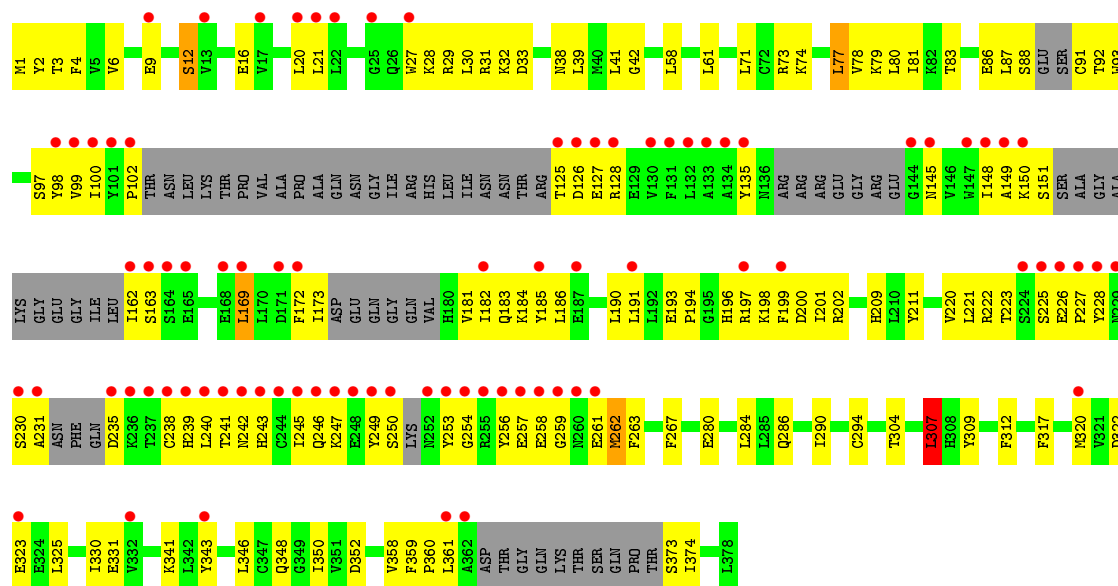
- Molecule 2: Tubulin beta-2B chain



- 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	103.83Å 154.84Å 181.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.64 – 2.50 49.64 – 2.49	Depositor EDS
% Data completeness (in resolution range)	99.7 (49.64-2.50) 99.7 (49.64-2.49)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.05 (at 2.48Å)	Xtriage
Refinement program	PHENIX (1.13 _2998: ???)	Depositor
R, R_{free}	0.222 , 0.286 0.222 , 0.286	Depositor DCC
R_{free} test set	813 reflections (0.80%)	wwPDB-VP
Wilson B-factor (Å ²)	61.3	Xtriage
Anisotropy	0.171	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 43.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	17477	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.57% 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: GDP, GOL, MG, IMD, CA, GTP, ACP, MES, 97O

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	0.46	0/3517	0.58	0/4774
1	C	0.54	1/3538 (0.0%)	0.64	1/4804 (0.0%)
2	B	0.50	0/3424	0.66	2/4638 (0.0%)
2	D	0.46	1/3382 (0.0%)	0.63	1/4581 (0.0%)
3	E	0.49	0/1025	0.62	0/1360
4	F	0.42	0/2652	0.62	2/3579 (0.1%)
All	All	0.48	2/17538 (0.0%)	0.63	6/23736 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	D	0	3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	295	CYS	CB-SG	-9.18	1.66	1.82
2	D	203	CYS	CB-SG	-5.32	1.73	1.81

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	130	ASP	CB-CG-OD1	8.52	125.97	118.30
2	B	130	ASP	CB-CG-OD2	-6.62	112.34	118.30
4	F	307	LEU	CA-CB-CG	6.52	130.29	115.30
2	D	248	LEU	CA-CB-CG	6.37	129.95	115.30
1	C	171	ILE	C-N-CA	5.83	136.28	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
4	F	169	LEU	CB-CG-CD2	-5.00	102.50	111.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	247	GLN	Peptide
2	D	93	VAL	Peptide
2	D	95	GLY	Peptide

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	3433	0	3352	93	0
1	C	3451	0	3368	82	0
2	B	3347	0	3220	105	0
2	D	3309	0	3189	121	0
3	E	1011	0	1032	38	0
4	F	2596	0	2570	125	0
5	A	32	0	12	2	0
5	C	32	0	12	1	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
7	A	18	0	24	1	0
7	B	6	0	8	0	0
7	C	30	0	40	8	0
7	D	12	0	16	0	0
8	A	1	0	0	0	0
8	B	1	0	0	0	0
8	C	1	0	0	0	0
9	B	28	0	12	1	0
9	D	28	0	12	1	0
10	B	12	0	12	0	0
11	B	27	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	C	15	0	15	5	0
13	F	31	0	12	13	0
14	A	11	0	0	2	0
14	B	13	0	0	2	0
14	C	17	0	0	1	0
14	D	4	0	0	0	0
14	F	7	0	0	1	0
All	All	17477	0	16906	545	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 16.

All (545) 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)
13:F:401:ACP:C3'	13:F:401:ACP:O3'	1.80	1.30
4:F:241:THR:N	13:F:401:ACP:O3'	1.73	1.21
3:E:103:GLN:OE1	3:E:104:LYS:CE	1.95	1.14
4:F:148:ILE:HA	4:F:162:ILE:HD12	1.30	1.09
4:F:241:THR:HG22	13:F:401:ACP:HO3'	1.24	1.01
2:D:103:TRP:HD1	2:D:147:SER:HG	1.12	0.97
12:C:510:IMD:H5	3:E:112:ARG:HE	1.33	0.94
4:F:29:ARG:HH21	4:F:31:ARG:HH22	1.21	0.89
4:F:99:VAL:O	4:F:128:ARG:NH2	2.06	0.89
3:E:103:GLN:OE1	3:E:104:LYS:NZ	2.05	0.88
3:E:103:GLN:OE1	3:E:104:LYS:HE2	1.72	0.87
4:F:241:THR:HG22	13:F:401:ACP:O3'	1.75	0.87
2:B:172:MET:HG3	2:B:387:LEU:HD11	1.56	0.86
4:F:148:ILE:HA	4:F:162:ILE:CD1	2.06	0.86
13:F:401:ACP:C2'	13:F:401:ACP:O3'	2.22	0.86
2:B:205:ASP:OD2	2:B:390:ARG:NH2	2.07	0.86
4:F:241:THR:CG2	13:F:401:ACP:O3'	2.24	0.86
4:F:31:ARG:HH21	4:F:32:LYS:HG3	1.38	0.86
2:B:2:ARG:NH1	2:B:131:CYS:SG	2.49	0.85
11:B:506:97O:N12	14:B:601:HOH:O	2.10	0.84
2:D:396:THR:O	2:D:400:ARG:NH1	2.10	0.83
4:F:320:MET:HG3	4:F:330:ILE:HD11	1.61	0.83
2:D:21:TRP:O	2:D:25:SER:OG	1.99	0.81
2:D:75:MET:N	2:D:75:MET:SD	2.53	0.81
4:F:201:ILE:HG12	4:F:221:LEU:HD13	1.63	0.80
2:D:158:ARG:HG2	3:E:123:LEU:HD11	1.64	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:396:THR:C	2:D:400:ARG:HH12	1.85	0.79
2:D:193:GLN:OE1	3:E:126:LYS:NZ	2.18	0.77
2:B:240:THR:HG21	2:B:320:ARG:HD2	1.67	0.76
2:B:33:THR:O	2:B:60:LYS:NZ	2.19	0.76
2:B:318:ILE:HG22	2:B:354:ALA:HB3	1.68	0.75
4:F:126:ASP:OD1	4:F:128:ARG:NH2	2.18	0.75
1:A:71:GLU:HG2	1:A:72:PRO:HD2	1.69	0.74
4:F:196:HIS:HE1	4:F:228:TYR:HB3	1.52	0.73
4:F:148:ILE:CD1	4:F:162:ILE:HD13	2.17	0.73
1:C:249:ASN:OD1	1:C:356[A]:ASN:ND2	2.21	0.73
2:D:72:PRO:HA	2:D:75:MET:HE2	1.71	0.73
4:F:348:GLN:NE2	4:F:352:ASP:OD1	2.22	0.72
1:A:71:GLU:HB2	1:A:98:ASP:HB3	1.72	0.72
3:E:103:GLN:OE1	3:E:104:LYS:HE3	1.90	0.72
3:E:140:LYS:HD2	3:E:140:LYS:O	1.88	0.72
1:A:79:ARG:HH22	1:A:94:THR:HG23	1.55	0.71
2:D:321:GLY:HA2	2:D:359:PRO:HG3	1.73	0.70
1:A:297:GLU:OE2	1:A:339:ARG:NH2	2.25	0.70
4:F:201:ILE:HG13	4:F:221:LEU:HD11	1.74	0.70
4:F:201:ILE:CG1	4:F:221:LEU:HD13	2.21	0.70
2:B:237:GLY:O	2:B:318:ILE:HD11	1.92	0.69
4:F:148:ILE:HD13	4:F:162:ILE:HD13	1.75	0.69
4:F:29:ARG:NH2	4:F:31:ARG:HH22	1.88	0.69
4:F:1:MET:SD	4:F:28:LYS:NZ	2.59	0.69
4:F:102:PRO:HB3	4:F:173:ILE:HG23	1.73	0.69
2:D:332:MET:HG3	2:D:353:THR:HG21	1.75	0.69
4:F:125:THR:N	4:F:127:GLU:OE1	2.26	0.69
4:F:196:HIS:ND1	4:F:196:HIS:O	2.26	0.69
2:B:119:LEU:HA	2:B:122:VAL:HG22	1.75	0.68
4:F:241:THR:H	13:F:401:ACP:HO3'	1.36	0.68
2:B:1:MET:SD	2:B:130:ASP:HB3	2.34	0.68
4:F:97:SER:HA	4:F:183:GLN:CG	2.24	0.67
2:D:12:CYS:SG	2:D:171:VAL:HG21	2.34	0.67
1:A:427:ALA:O	1:A:430:LYS:HG3	1.94	0.67
4:F:201:ILE:HG13	4:F:221:LEU:CD1	2.23	0.67
4:F:235:ASP:O	4:F:239:HIS:NE2	2.28	0.67
1:C:288:VAL:HG13	7:C:506:GOL:H2	1.77	0.67
1:A:335:ILE:HG23	1:A:339:ARG:HD2	1.76	0.67
4:F:31:ARG:HE	4:F:32:LYS:H	1.43	0.67
2:D:253:ARG:O	2:D:257:VAL:HG23	1.94	0.67
1:A:11:GLN:HG3	1:A:74:VAL:HG21	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:226:GLU:OE2	4:F:246:GLN:NE2	2.29	0.66
2:D:180:THR:HG22	2:D:181:VAL:H	1.60	0.66
2:D:213:CYS:HA	2:D:217:LEU:HB2	1.78	0.66
4:F:149:ALA:HA	4:F:182:ILE:HD13	1.78	0.65
4:F:149:ALA:HA	4:F:182:ILE:CD1	2.26	0.65
2:D:48:ARG:O	2:D:51:VAL:HG12	1.97	0.65
4:F:61:LEU:HD21	4:F:312:PHE:CE1	2.31	0.65
4:F:73:ARG:HD2	4:F:74:LYS:N	2.12	0.65
1:A:304:LYS:NZ	14:A:601:HOH:O	2.28	0.64
2:B:324:SER:HB3	2:B:327:GLU:HB2	1.78	0.64
4:F:196:HIS:CE1	4:F:228:TYR:HB3	2.32	0.64
2:D:6:HIS:HD2	2:D:136:GLN:HE21	1.42	0.64
4:F:201:ILE:CG1	4:F:221:LEU:CD1	2.76	0.64
4:F:185:TYR:OH	4:F:198:LYS:NZ	2.31	0.64
2:B:282:GLN:OE1	2:B:371:LEU:HD22	1.97	0.63
2:D:56:ALA:HB3	2:D:60:LYS:HB2	1.81	0.63
2:D:319:PHE:HB3	2:D:323:MET:HE1	1.80	0.63
1:C:204:VAL:HA	1:C:302:MET:HE3	1.81	0.63
1:A:304:LYS:HB2	1:A:304:LYS:HZ3	1.63	0.63
2:B:136:GLN:HA	2:B:167:ASN:O	1.98	0.62
2:B:241:CYS:HB2	11:B:506:97O:O22	1.98	0.62
2:D:23:VAL:HG21	2:D:232:SER:HB2	1.80	0.62
1:A:220:GLU:CD	1:A:220:GLU:H	2.02	0.62
4:F:241:THR:CA	13:F:401:ACP:O3'	2.47	0.62
2:D:140:SER:HA	2:D:171:VAL:CG2	2.30	0.62
1:A:79:ARG:NH2	1:A:94:THR:HG23	2.15	0.62
1:C:204:VAL:HG22	1:C:302:MET:CE	2.30	0.62
1:C:221:ARG:NH1	7:C:505:GOL:O3	2.30	0.62
2:B:106:GLY:O	2:B:111:GLY:HA3	2.00	0.61
1:C:4:CYS:SG	12:C:511:IMD:H5	2.39	0.61
4:F:92:THR:O	4:F:92:THR:OG1	2.19	0.61
1:C:167:LEU:HD13	12:C:511:IMD:H2	1.82	0.61
1:C:71:GLU:OE2	1:C:73:THR:HB	2.01	0.61
4:F:97:SER:HA	4:F:183:GLN:HG2	1.82	0.61
4:F:148:ILE:O	4:F:182:ILE:HD12	2.01	0.60
4:F:29:ARG:HH21	4:F:31:ARG:NH2	1.97	0.60
2:D:194:LEU:O	2:D:198:THR:HG22	2.01	0.60
4:F:163:SER:HB3	4:F:169:LEU:HD11	1.83	0.60
4:F:286:GLN:O	4:F:290:ILE:HG12	2.02	0.60
2:D:176:LYS:HD2	2:D:210:TYR:CD2	2.37	0.60
2:D:269:MET:HG3	2:D:303:ALA:HB3	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:72:PRO:HA	2:D:75:MET:CE	2.31	0.60
2:B:181:VAL:HG12	1:C:258:ASN:OD1	2.02	0.60
2:B:212:ILE:HG23	2:B:275:LEU:HD13	1.83	0.60
2:D:414:ASP:OD2	2:D:415:GLU:N	2.34	0.60
4:F:61:LEU:HD21	4:F:312:PHE:HE1	1.67	0.60
1:A:167:LEU:HG	1:A:200:CYS:HB3	1.84	0.59
2:B:385:GLN:HG3	2:B:429:VAL:HG13	1.85	0.59
1:C:209:ILE:HD11	1:C:302:MET:HG2	1.84	0.59
4:F:31:ARG:NE	4:F:32:LYS:H	1.99	0.59
1:A:187:SER:HB3	1:A:391:LEU:HD21	1.83	0.59
1:A:88:HIS:O	1:A:91:GLN:HG2	2.03	0.59
1:A:107:HIS:ND1	1:A:152:LEU:HB2	2.18	0.59
1:A:178:SER:OG	1:A:179:THR:N	2.34	0.59
1:A:188:ILE:HG23	1:A:425:MET:HG3	1.84	0.59
2:B:306:ASP:HB3	2:B:309:HIS:CD2	2.38	0.59
3:E:137:LYS:O	3:E:140:LYS:HE3	2.03	0.59
2:D:2:ARG:NH1	2:D:131:CYS:SG	2.71	0.59
2:D:83:PHE:O	2:D:86:ILE:HG22	2.03	0.58
1:C:220:GLU:HG2	2:D:326:LYS:HD3	1.84	0.58
1:C:271:THR:HG21	1:C:295:CYS:O	2.02	0.58
2:D:12:CYS:HB2	9:D:501:GDP:C8	2.39	0.58
4:F:148:ILE:O	4:F:182:ILE:CD1	2.50	0.58
2:B:165:ILE:HG21	2:B:252:LEU:HB3	1.86	0.58
2:B:57:THR:OG1	2:B:58:GLY:N	2.36	0.58
2:D:318:ILE:HG23	2:D:376:THR:HB	1.85	0.58
2:D:140:SER:HA	2:D:171:VAL:HG23	1.85	0.58
1:A:196:GLU:HG3	1:A:197:HIS:CD2	2.38	0.58
2:D:115:VAL:O	2:D:119:LEU:HG	2.04	0.58
2:D:6:HIS:CE1	2:D:21:TRP:HE1	2.21	0.58
2:D:69:ASP:OD2	2:D:74:THR:HG21	2.04	0.58
2:D:172:MET:HG3	2:D:387:LEU:HD11	1.85	0.58
2:D:79:ARG:HA	2:D:84:GLY:HA3	1.86	0.57
4:F:280:GLU:HA	4:F:284:LEU:HB2	1.86	0.57
2:B:208:ALA:HB2	2:B:304:ALA:HB2	1.86	0.57
2:B:40:SER:OG	2:B:41:ASP:N	2.37	0.57
7:C:505:GOL:O1	2:D:247:GLN:NE2	2.38	0.57
2:D:109:THR:OG1	2:D:110:GLU:N	2.37	0.57
2:B:181:VAL:HG23	1:C:348:PRO:CG	2.35	0.57
4:F:12:SER:OG	14:F:501:HOH:O	2.13	0.57
1:A:217:LEU:HB3	1:A:219:ILE:HD12	1.85	0.57
2:B:36:TYR:CZ	2:B:46:LEU:HD11	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:210:TYR:CE1	2:B:222:PRO:HD2	2.40	0.57
2:B:36:TYR:CD1	2:B:46:LEU:HD21	2.39	0.57
1:A:220:GLU:HG2	1:A:221:ARG:H	1.70	0.57
4:F:243:HIS:HB3	4:F:247:LYS:HD2	1.86	0.57
1:C:249:ASN:OD1	1:C:356[B]:ASN:ND2	2.38	0.57
1:A:88:HIS:CE1	1:A:90:GLU:HG3	2.40	0.57
2:B:203:CYS:SG	2:B:267:PHE:HB3	2.45	0.57
1:C:34:GLY:HA3	1:C:60:LYS:HG3	1.86	0.56
4:F:9:GLU:OE2	4:F:29:ARG:NH2	2.34	0.56
1:C:112:LYS:NZ	1:C:113:GLU:OE2	2.38	0.56
1:C:221:ARG:HH11	7:C:505:GOL:HO3	1.52	0.56
1:C:14:VAL:HG13	1:C:67:PHE:HD2	1.71	0.56
2:D:223:THR:HG22	2:D:225:GLY:H	1.70	0.56
2:B:291:LEU:HD13	2:B:375:ALA:HB2	1.88	0.56
2:D:191:VAL:HG21	2:D:425:MET:SD	2.46	0.56
1:A:179:THR:HG22	14:B:601:HOH:O	2.06	0.55
3:E:103:GLN:CD	3:E:104:LYS:CE	2.73	0.55
1:C:288:VAL:HG12	1:C:373:ARG:HD3	1.88	0.55
2:D:104:ALA:HB1	2:D:411:GLU:HB2	1.88	0.55
2:B:48:ARG:NH2	2:B:245:PRO:HA	2.22	0.55
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.25	0.55
2:D:123:ARG:O	2:D:127:GLU:HG2	2.07	0.55
1:A:90:GLU:O	1:A:121:ARG:HD2	2.07	0.55
2:B:269:MET:HE1	2:B:307:PRO:HG3	1.89	0.55
2:D:171:VAL:HA	2:D:204:ILE:O	2.07	0.55
2:D:298:SER:HB2	2:D:307:PRO:HD2	1.88	0.55
1:C:220:GLU:CG	2:D:326:LYS:HD3	2.37	0.55
4:F:100:ILE:HG13	4:F:128:ARG:NE	2.21	0.55
1:A:163:LYS:CD	1:A:163:LYS:H	2.20	0.55
2:B:48:ARG:CZ	2:B:245:PRO:HA	2.37	0.55
1:A:220:GLU:HB2	2:B:326:LYS:HD3	1.89	0.55
2:B:3:GLU:CD	2:B:3:GLU:N	2.60	0.55
2:D:397:ALA:C	2:D:400:ARG:HH22	2.10	0.55
1:A:207:GLU:OE1	1:A:304:LYS:NZ	2.28	0.54
1:A:210:TYR:CE2	1:A:222:PRO:HD2	2.42	0.54
2:D:106:GLY:O	2:D:111:GLY:HA3	2.07	0.54
2:D:108:TYR:CD1	3:E:133:VAL:HG11	2.42	0.54
2:D:96:GLN:H	2:D:96:GLN:CD	2.11	0.54
2:D:218:LYS:O	2:D:218:LYS:HG3	2.07	0.54
3:E:52:LYS:HD3	3:E:52:LYS:C	2.28	0.54
4:F:77:LEU:O	4:F:81:ILE:HD12	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:221:THR:HG21	1:C:326:LYS:HA	1.89	0.54
2:B:282:GLN:CD	2:B:371:LEU:HD22	2.28	0.54
3:E:140:LYS:O	3:E:141:GLU:HB2	2.07	0.54
3:E:92:ASN:O	3:E:96:MET:HG3	2.08	0.54
1:A:174:ALA:O	1:A:178:SER:HB3	2.07	0.54
1:A:2:ARG:O	1:A:51:THR:HG23	2.08	0.54
4:F:182:ILE:HG23	4:F:182:ILE:O	2.08	0.54
2:D:188:THR:HA	2:D:191:VAL:HG22	1.90	0.53
2:B:326:LYS:NZ	2:B:330:GLU:OE2	2.35	0.53
1:C:344:VAL:HG21	1:C:346:TRP:CE2	2.43	0.53
2:D:105:LYS:O	2:D:111:GLY:N	2.41	0.53
2:B:124:LYS:O	2:B:124:LYS:HD3	2.09	0.53
2:B:282:GLN:O	2:B:282:GLN:HG3	2.08	0.53
2:B:156:LYS:NZ	3:E:79:GLU:OE1	2.41	0.53
4:F:241:THR:N	13:F:401:ACP:HO3'	1.93	0.53
4:F:3:THR:HB	4:F:30:LEU:HD11	1.89	0.53
4:F:163:SER:HB3	4:F:169:LEU:CD1	2.38	0.53
4:F:220:VAL:HG23	4:F:263:PHE:CE1	2.44	0.53
4:F:71:LEU:HD11	4:F:294:CYS:HB3	1.91	0.53
1:C:274:PRO:HG2	1:C:371:VAL:HG11	1.89	0.53
2:B:172:MET:HE2	2:B:387:LEU:HD21	1.90	0.53
1:C:317:LEU:HD23	1:C:377:MET:HB2	1.90	0.53
3:E:57:ALA:HA	3:E:60:ARG:NH1	2.24	0.53
1:C:322:ASP:OD2	1:C:373:ARG:NH2	2.39	0.53
1:A:120:ASP:OD2	1:A:124:LYS:NZ	2.38	0.52
1:A:227:LEU:O	1:A:231:ILE:HG13	2.09	0.52
2:B:69:ASP:O	2:B:94:PHE:HA	2.08	0.52
2:D:405:LEU:H	2:D:405:LEU:HD22	1.74	0.52
1:A:412:GLY:O	3:E:60:ARG:NH1	2.43	0.52
2:B:66:ILE:HD13	2:B:122:VAL:HG12	1.90	0.52
1:A:207:GLU:HG2	1:A:304:LYS:HZ2	1.73	0.52
1:A:415:GLU:O	1:A:418:PHE:HB2	2.09	0.52
2:B:288:VAL:O	2:B:292:THR:HG23	2.09	0.52
3:E:103:GLN:CD	3:E:104:LYS:HE3	2.29	0.52
4:F:262:MET:HG2	4:F:267:PHE:HB2	1.91	0.52
2:D:141:LEU:HD12	2:D:172:MET:HE3	1.92	0.52
4:F:197:ARG:HB3	4:F:225:SER:HA	1.92	0.52
4:F:230:SER:OG	4:F:231:ALA:N	2.43	0.52
1:A:143:GLY:HA3	5:A:501:GTP:O3A	2.10	0.52
2:D:141:LEU:HD21	2:D:170:SER:HB3	1.90	0.52
2:D:326:LYS:O	2:D:330:GLU:HG3	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:129:HIS:O	3:E:133:VAL:HG12	2.10	0.52
3:E:47:LEU:O	3:E:50:ILE:HG12	2.09	0.52
2:B:202:TYR:HE2	2:B:378:ILE:HD13	1.75	0.51
1:C:147:SER:HB2	1:C:190:THR:HB	1.92	0.51
1:A:275:VAL:N	7:A:503:GOL:O1	2.39	0.51
4:F:190:LEU:HD12	4:F:191:LEU:H	1.76	0.51
4:F:323:GLU:C	4:F:325:LEU:H	2.14	0.51
2:D:143:GLY:O	2:D:186:ASN:ND2	2.43	0.51
1:A:108:TYR:OH	1:A:417:GLU:OE1	2.22	0.51
1:A:269:LEU:HD11	1:A:301:GLN:HB3	1.92	0.51
2:B:125:GLU:OE1	2:B:125:GLU:HA	2.11	0.51
1:C:335:ILE:O	1:C:339:ARG:HB2	2.10	0.51
4:F:74:LYS:HA	4:F:77:LEU:HB3	1.93	0.51
1:A:337:THR:OG1	1:A:338:LYS:N	2.41	0.51
2:D:198:THR:HG23	2:D:266:HIS:CD2	2.46	0.51
1:A:60:LYS:NZ	1:A:85:GLN:O	2.32	0.51
3:E:47:LEU:O	3:E:51:GLN:HG2	2.10	0.51
1:C:93:ILE:HG22	1:C:114:ILE:HD11	1.93	0.51
1:A:401:LYS:HG3	2:B:346:TRP:CE3	2.46	0.50
2:B:324:SER:CB	2:B:327:GLU:HB2	2.42	0.50
1:C:100:ALA:HA	2:D:254:LYS:HG3	1.94	0.50
2:D:139:HIS:O	2:D:171:VAL:HG22	2.11	0.50
4:F:102:PRO:HA	4:F:173:ILE:HG12	1.93	0.50
1:C:173:PRO:HB3	1:C:183:GLU:OE2	2.12	0.50
4:F:86:GLU:O	4:F:87:LEU:HD23	2.12	0.50
1:A:179:THR:HA	2:B:352:LYS:NZ	2.27	0.50
2:D:34:GLY:HA3	2:D:86:ILE:HD11	1.93	0.50
1:C:12:ALA:O	1:C:16:ILE:HG12	2.11	0.50
1:A:39:ASP:OD2	1:A:61:HIS:NE2	2.38	0.50
1:A:265:ILE:HG23	1:A:432:TYR:CZ	2.47	0.50
2:B:237:GLY:O	2:B:240:THR:HG23	2.12	0.50
1:A:304:LYS:HB2	1:A:304:LYS:NZ	2.27	0.49
1:A:291:ILE:HD13	1:A:373:ARG:HG3	1.92	0.49
2:D:70:LEU:HG	2:D:145:THR:HG23	1.93	0.49
1:C:151:SER:HA	1:C:194:THR:HG22	1.93	0.49
1:C:174:ALA:HB2	1:C:207:GLU:N	2.27	0.49
4:F:33:ASP:OD2	4:F:33:ASP:N	2.43	0.49
4:F:93:TRP:CD2	4:F:290:ILE:HD12	2.47	0.49
2:B:401:ARG:HE	7:C:501:GOL:H2	1.77	0.49
1:C:224:TYR:CD2	7:C:505:GOL:H12	2.47	0.49
2:D:75:MET:O	2:D:79:ARG:HG3	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:151:SER:HB2	4:F:181:VAL:H	1.76	0.49
1:C:293:ASN:HA	1:C:335:ILE:HD11	1.93	0.49
1:A:3:GLU:HG2	1:A:64:ARG:CZ	2.43	0.49
2:B:83:PHE:HB3	2:B:86:ILE:HD13	1.94	0.49
1:C:181:VAL:HG21	1:C:404:PHE:CZ	2.48	0.49
2:D:75:MET:HA	2:D:78:VAL:HG22	1.95	0.49
1:C:227:LEU:O	1:C:231:ILE:HG13	2.13	0.49
3:E:104:LYS:HE2	3:E:104:LYS:HA	1.94	0.49
2:B:292:THR:HG22	2:B:319:PHE:CZ	2.47	0.48
1:C:66:VAL:HG23	1:C:125:LEU:HD11	1.95	0.48
2:B:154:ILE:HG23	2:B:166:MET:HG2	1.95	0.48
2:D:136:GLN:HA	2:D:167:ASN:O	2.13	0.48
2:D:291:LEU:HG	2:D:375:ALA:HB2	1.94	0.48
2:D:70:LEU:HA	2:D:95:GLY:O	2.13	0.48
2:B:240:THR:HG21	2:B:320:ARG:CD	2.42	0.48
4:F:241:THR:H	13:F:401:ACP:C3'	2.23	0.48
1:A:390:ARG:NH2	14:A:603:HOH:O	2.46	0.48
4:F:16:GLU:O	4:F:20:LEU:HD12	2.13	0.48
4:F:190:LEU:HB2	4:F:322:ASP:O	2.14	0.48
2:D:295:MET:CG	2:D:377:PHE:HB2	2.43	0.48
3:E:46:SER:OG	3:E:49:GLU:HG3	2.13	0.48
2:D:410:GLY:O	3:E:137:LYS:HG3	2.14	0.48
4:F:148:ILE:HD12	4:F:162:ILE:HD13	1.95	0.48
13:F:401:ACP:C2'	13:F:401:ACP:HO3'	2.22	0.48
13:F:401:ACP:O2'	13:F:401:ACP:O3'	2.29	0.48
4:F:87:LEU:O	4:F:91:CYS:HB3	2.14	0.48
12:C:510:IMD:H5	3:E:112:ARG:NE	2.15	0.47
1:C:411:GLU:HA	3:E:112:ARG:HD2	1.95	0.47
2:B:320:ARG:HB3	2:B:359:PRO:HA	1.97	0.47
1:A:142:GLY:HA3	1:A:183:GLU:OE1	2.15	0.47
2:B:292:THR:HG22	2:B:319:PHE:CE2	2.49	0.47
2:D:6:HIS:CE1	2:D:8:GLN:HG2	2.49	0.47
2:D:20:PHE:CE1	2:D:24:ILE:HG21	2.50	0.47
2:D:332:MET:O	2:D:336:GLN:HG3	2.15	0.47
2:B:352:LYS:HG3	2:B:353:THR:N	2.29	0.47
2:B:90:ASP:OD1	2:B:90:ASP:N	2.46	0.47
4:F:186:LEU:HA	4:F:186:LEU:HD13	1.62	0.47
2:B:36:TYR:CE2	2:B:46:LEU:HD11	2.50	0.47
2:D:223:THR:HB	2:D:226:ASP:H	1.78	0.47
4:F:220:VAL:HG23	4:F:263:PHE:CD1	2.50	0.47
4:F:320:MET:CG	4:F:330:ILE:HD11	2.38	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:58:LEU:HA	4:F:58:LEU:HD23	1.60	0.47
2:D:6:HIS:CD2	2:D:136:GLN:HE21	2.28	0.47
2:D:167:ASN:HD21	2:D:202:TYR:HE1	1.63	0.47
2:B:238:VAL:HG13	2:B:378:ILE:HD11	1.97	0.47
1:A:179:THR:HG23	2:B:352:LYS:NZ	2.30	0.47
2:D:345:GLU:CD	2:D:345:GLU:H	2.16	0.47
2:D:109:THR:CG2	2:D:411:GLU:HB3	2.45	0.46
4:F:12:SER:HB2	4:F:343:TYR:OH	2.15	0.46
1:A:161:TYR:HA	1:A:163:LYS:NZ	2.30	0.46
2:B:181:VAL:HG23	1:C:348:PRO:HG2	1.96	0.46
1:C:210:TYR:CE1	1:C:222:PRO:HD2	2.50	0.46
1:A:187:SER:O	1:A:191:THR:HG23	2.16	0.46
1:C:164:LYS:HB2	1:C:164:LYS:HE2	1.76	0.46
4:F:245:ILE:O	4:F:249:TYR:HB2	2.16	0.46
2:B:282:GLN:OE1	2:B:371:LEU:CD2	2.63	0.46
1:A:36:MET:HB3	1:A:61:HIS:CE1	2.51	0.46
2:B:88:ARG:NH1	2:B:125:GLU:OE2	2.48	0.46
2:D:136:GLN:HG2	2:D:169:PHE:HE1	1.81	0.46
2:D:403:ALA:HB1	2:D:404:PHE:CD2	2.50	0.46
2:D:22:GLU:HG2	2:D:83:PHE:HD2	1.80	0.46
1:A:215:ARG:NH2	1:A:299:ALA:HB1	2.31	0.46
2:D:210:TYR:CD1	2:D:222:PRO:HG2	2.51	0.46
1:A:220:GLU:CD	1:A:220:GLU:N	2.69	0.46
1:C:234:ILE:HG21	1:C:302:MET:SD	2.56	0.46
2:D:319:PHE:HB3	2:D:323:MET:CE	2.46	0.46
2:D:319:PHE:CB	2:D:323:MET:HE1	2.46	0.46
2:D:345:GLU:HG2	2:D:440:ALA:HB2	1.98	0.46
2:D:34:GLY:HA3	2:D:86:ILE:CD1	2.46	0.46
2:D:412:GLY:HA3	3:E:133:VAL:O	2.16	0.46
2:B:40:SER:OG	2:B:42:LEU:N	2.47	0.45
2:D:63:PRO:HD3	2:D:86:ILE:HG13	1.96	0.45
1:A:34:GLY:O	1:A:61:HIS:N	2.45	0.45
4:F:79:LYS:O	4:F:83:THR:HG23	2.15	0.45
1:C:288:VAL:HG21	1:C:327:ASP:HB3	1.99	0.45
1:A:142:GLY:O	1:A:186:ASN:ND2	2.35	0.45
1:A:98:ASP:HB2	5:A:501:GTP:O2G	2.16	0.45
2:B:1:MET:HE3	2:B:130:ASP:HB3	1.98	0.45
2:B:171:VAL:HA	2:B:204:ILE:O	2.16	0.45
2:D:174:SER:O	2:D:178:SER:HB2	2.17	0.45
3:E:103:GLN:NE2	3:E:104:LYS:HE3	2.31	0.45
1:A:71:GLU:HG2	1:A:72:PRO:CD	2.44	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:172:MET:CE	2:B:387:LEU:HD21	2.46	0.45
2:B:291:LEU:HD23	2:B:291:LEU:HA	1.66	0.45
1:A:213:CYS:O	1:A:217:LEU:HB2	2.17	0.45
1:A:259:LEU:O	1:A:380:ASN:ND2	2.40	0.45
1:A:88:HIS:HE1	1:A:90:GLU:HG3	1.80	0.45
1:C:427:ALA:HA	1:C:430:LYS:HG3	1.97	0.45
2:D:37:HIS:O	2:D:37:HIS:CG	2.69	0.45
4:F:259:GLY:O	4:F:261:GLU:HG3	2.15	0.45
1:A:265:ILE:HD11	1:A:431:ASP:HB3	1.99	0.45
2:D:398:MET:HB3	2:D:403:ALA:HB3	1.99	0.44
4:F:6:VAL:HG22	4:F:41:LEU:HD12	1.99	0.44
1:A:14:VAL:HG13	1:A:67:PHE:CD2	2.53	0.44
1:A:263:PRO:O	1:A:266:HIS:ND1	2.33	0.44
1:C:207:GLU:OE1	1:C:304:LYS:NZ	2.42	0.44
1:C:385:ALA:HA	1:C:388:TRP:CD1	2.52	0.44
2:B:108:TYR:OH	2:B:417:GLU:OE2	2.32	0.44
1:C:312:TYR:CE1	1:C:341:ILE:HG23	2.52	0.44
2:D:36:TYR:HB2	2:D:61:TYR:HE2	1.83	0.44
1:C:69:ASP:O	1:C:94:THR:HA	2.17	0.44
3:E:119:MET:HA	3:E:122:ARG:HH21	1.82	0.44
4:F:100:ILE:HG13	4:F:128:ARG:CZ	2.48	0.44
4:F:150:LYS:HB3	4:F:150:LYS:HE2	1.69	0.44
1:A:430:LYS:HE3	1:A:431:ASP:OD1	2.17	0.44
1:C:71:GLU:OE2	1:C:73:THR:CB	2.65	0.44
4:F:221:LEU:HD12	4:F:221:LEU:HA	1.70	0.44
2:B:154:ILE:HG22	2:B:197:ASN:HB3	1.99	0.44
4:F:149:ALA:HB3	4:F:162:ILE:N	2.33	0.44
1:C:93:ILE:HD11	1:C:121:ARG:HG3	1.99	0.44
4:F:221:LEU:HB3	4:F:262:MET:HB3	1.99	0.44
1:C:147:SER:OG	1:C:148:GLY:N	2.51	0.44
1:C:209:ILE:HG22	1:C:227:LEU:HD22	1.99	0.44
4:F:31:ARG:HG3	4:F:33:ASP:OD2	2.18	0.44
4:F:373:SER:OG	4:F:374:ILE:N	2.51	0.44
1:A:163:LYS:HE2	1:A:164:LYS:HE2	1.99	0.44
1:A:372:GLN:OE1	1:A:372:GLN:HA	2.18	0.44
2:B:22:GLU:HB2	2:B:83:PHE:CD1	2.53	0.44
2:D:68:VAL:HA	2:D:93:VAL:O	2.18	0.44
2:D:94:PHE:C	2:D:94:PHE:CD1	2.91	0.44
4:F:228:TYR:HB2	4:F:238:CYS:SG	2.58	0.44
1:A:226:ASN:ND2	1:A:367:ASP:OD2	2.51	0.43
1:A:79:ARG:HH12	1:A:94:THR:HG21	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:165:SER:HA	1:C:199:ASP:OD2	2.18	0.43
1:C:204:VAL:HG11	1:C:231:ILE:HD13	1.99	0.43
4:F:3:THR:O	4:F:38:ASN:HB2	2.18	0.43
4:F:4:PHE:O	4:F:29:ARG:HA	2.18	0.43
1:A:108:TYR:CE2	1:A:413:MET:HG3	2.53	0.43
1:A:147:SER:HB2	1:A:190:THR:HB	2.00	0.43
2:B:1:MET:CE	2:B:130:ASP:HB3	2.48	0.43
4:F:200:ASP:HB2	4:F:241:THR:HG23	1.99	0.43
4:F:246:GLN:HA	4:F:250:SER:HB3	1.99	0.43
4:F:98:TYR:H	4:F:183:GLN:NE2	2.16	0.43
2:B:332:MET:HG3	2:B:353:THR:HG21	1.99	0.43
1:C:71:GLU:HG2	1:C:73:THR:H	1.83	0.43
2:D:187:ALA:O	2:D:191:VAL:HG13	2.19	0.43
2:D:210:TYR:CE1	2:D:222:PRO:HG2	2.54	0.43
4:F:331:GLU:OE2	13:F:401:ACP:H3B1	2.18	0.43
2:B:3:GLU:CD	2:B:3:GLU:H	2.22	0.43
2:D:114:LEU:HD11	2:D:149:MET:SD	2.58	0.43
4:F:39:LEU:HD13	4:F:61:LEU:CD2	2.49	0.43
2:D:178:SER:OG	2:D:180:THR:O	2.36	0.43
2:D:360:PRO:HG2	2:D:371:LEU:HD12	2.01	0.43
3:E:132:GLU:O	3:E:136:ASN:HB2	2.18	0.43
4:F:346:LEU:O	4:F:350:ILE:HG13	2.19	0.43
2:B:345:GLU:H	2:B:345:GLU:HG3	1.61	0.43
2:B:406:HIS:CG	1:C:263:PRO:HD3	2.54	0.43
1:C:344:VAL:HG21	1:C:346:TRP:CZ2	2.54	0.43
2:D:36:TYR:CD1	2:D:46:LEU:HD21	2.54	0.43
2:D:109:THR:HG21	2:D:411:GLU:HB3	2.00	0.43
2:D:114:LEU:O	2:D:118:VAL:HG23	2.19	0.43
4:F:257:GLU:HB3	4:F:258:GLU:H	1.67	0.43
1:A:50:ASN:O	1:A:64:ARG:NH1	2.51	0.43
2:B:104:ALA:HB2	2:B:413:MET:SD	2.59	0.43
1:C:143:GLY:HA3	5:C:503:GTP:O3A	2.19	0.43
1:A:180:ALA:HB1	1:A:182:VAL:HG22	2.01	0.42
2:B:248:LEU:HD23	2:B:248:LEU:HA	1.74	0.42
1:C:177:VAL:HG12	7:C:505:GOL:H32	2.00	0.42
2:D:297:ASP:OD1	2:D:298:SER:N	2.52	0.42
4:F:194:PRO:O	4:F:197:ARG:NH1	2.52	0.42
1:A:221:ARG:HD2	2:B:329:ASP:OD2	2.19	0.42
2:D:75:MET:HE2	2:D:94:PHE:CZ	2.54	0.42
4:F:102:PRO:HG3	4:F:172:PHE:CE2	2.53	0.42
4:F:202:ARG:HA	4:F:317:PHE:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:307:LEU:HD12	4:F:309:TYR:O	2.20	0.42
2:B:12:CYS:HB2	9:B:501:GDP:C8	2.53	0.42
4:F:2:TYR:CZ	4:F:359:PHE:HB3	2.53	0.42
2:D:167:ASN:ND2	2:D:200:GLU:HB2	2.35	0.42
4:F:21:LEU:HD22	4:F:27:TRP:CD2	2.55	0.42
1:A:165:SER:HA	1:A:199:ASP:OD2	2.20	0.42
1:A:134:GLY:HA3	1:A:165:SER:O	2.18	0.42
1:A:27:GLU:CD	1:A:320:ARG:HH22	2.23	0.42
1:C:395:PHE:CD1	1:C:422:ARG:HD3	2.54	0.42
2:D:52:TYR:OH	2:D:136:GLN:OE1	2.29	0.42
3:E:125:GLU:OE1	3:E:128:LYS:HE2	2.20	0.42
1:A:377:MET:HE2	1:A:379:SER:HB3	2.02	0.42
2:B:66:ILE:HG12	2:B:121:VAL:HG12	2.01	0.42
1:C:66:VAL:HG23	1:C:125:LEU:CD1	2.49	0.42
1:A:112:LYS:HA	1:A:115:ILE:HG22	2.02	0.42
1:A:333:ALA:O	1:A:337:THR:HG23	2.20	0.42
2:B:20:PHE:CZ	2:B:24:ILE:HD13	2.54	0.42
2:B:311:ARG:HH22	2:B:345:GLU:HG3	1.84	0.42
1:C:262:TYR:CZ	7:C:501:GOL:H12	2.54	0.42
2:D:48:ARG:NH2	2:D:241:CYS:O	2.53	0.42
2:B:82:PRO:HB2	2:B:83:PHE:H	1.65	0.42
2:B:75:MET:HE3	2:B:92:PHE:CD2	2.55	0.42
1:C:298:PRO:HA	1:C:301:GLN:NE2	2.35	0.42
2:D:205:ASP:CG	2:D:390:ARG:HH22	2.24	0.42
4:F:191:LEU:HD11	4:F:196:HIS:HA	2.00	0.42
4:F:360:PRO:C	4:F:361:LEU:HD12	2.40	0.42
1:A:216:ASN:HB3	1:A:275:VAL:O	2.19	0.42
2:B:124:LYS:HA	2:B:124:LYS:HE2	2.02	0.42
2:B:205:ASP:OD1	2:B:206:ASN:N	2.52	0.42
1:C:162:GLY:HA2	3:E:94:ILE:HD11	2.01	0.42
1:C:203:MET:O	1:C:302:MET:CE	2.68	0.42
2:D:320:ARG:HD3	2:D:360:PRO:HD3	2.02	0.42
4:F:98:TYR:H	4:F:183:GLN:CD	2.23	0.42
4:F:193:GLU:HB3	4:F:194:PRO:HA	2.02	0.42
4:F:31:ARG:NH2	4:F:32:LYS:HG3	2.20	0.42
4:F:209:HIS:CE1	4:F:358:VAL:HG22	2.54	0.42
2:B:3:GLU:N	2:B:3:GLU:OE2	2.53	0.41
2:B:36:TYR:CE1	2:B:46:LEU:HD21	2.54	0.41
2:D:12:CYS:O	2:D:16:ILE:HG12	2.20	0.41
3:E:101:LEU:HD23	3:E:101:LEU:HA	1.71	0.41
3:E:8:VAL:HG22	3:E:22:VAL:HG12	2.00	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:135:TYR:O	4:F:145:ASN:ND2	2.53	0.41
4:F:197:ARG:HD3	4:F:256:TYR:HB2	2.01	0.41
1:A:14:VAL:HG13	1:A:67:PHE:HD2	1.84	0.41
1:C:180:ALA:O	1:C:183:GLU:HG3	2.20	0.41
1:C:264:ARG:HG3	14:C:614:HOH:O	2.20	0.41
2:D:93:VAL:HG21	2:D:121:VAL:HG11	2.01	0.41
2:B:182:VAL:O	2:B:185:TYR:HB2	2.20	0.41
3:E:50:ILE:HA	3:E:53:LYS:HE3	2.02	0.41
4:F:304:THR:HB	4:F:307:LEU:HD11	2.01	0.41
1:C:427:ALA:O	1:C:430:LYS:HG3	2.20	0.41
2:D:317:ALA:O	2:D:353:THR:HA	2.21	0.41
2:B:16:ILE:HD13	2:B:231:VAL:HG11	2.02	0.41
1:C:159:VAL:HA	3:E:94:ILE:HG23	2.03	0.41
1:C:21:TRP:CZ2	1:C:65:ALA:HB2	2.55	0.41
2:D:46:LEU:HA	2:D:49:ILE:HB	2.03	0.41
1:A:357:TYR:CZ	3:E:17:GLY:HA2	2.56	0.41
4:F:31:ARG:HE	4:F:32:LYS:N	2.15	0.41
2:B:1:MET:HG2	2:B:3:GLU:OE2	2.21	0.41
1:C:208:ALA:HB2	1:C:304:LYS:HG3	2.02	0.41
4:F:263:PHE:CZ	4:F:341:LYS:HG3	2.56	0.41
2:B:383:ALA:O	2:B:386:GLU:HG3	2.21	0.41
2:B:395:PHE:CE1	2:B:422:GLU:HB2	2.55	0.41
1:C:25:CYS:HB3	1:C:30:ILE:O	2.20	0.41
1:C:266:HIS:O	1:C:268:PRO:HD3	2.20	0.41
2:D:23:VAL:O	2:D:27:GLU:HG3	2.21	0.41
2:D:416:MET:O	2:D:419:THR:N	2.53	0.41
1:A:308:ARG:HB2	1:A:308:ARG:HE	1.70	0.41
1:A:317:LEU:HD12	1:A:353:VAL:HG22	2.02	0.41
2:B:195:VAL:CG1	2:B:264:ARG:HG2	2.51	0.41
2:D:318:ILE:CG2	2:D:376:THR:HB	2.49	0.41
2:D:390:ARG:O	2:D:394:GLN:HG2	2.19	0.41
4:F:222:ARG:HA	4:F:222:ARG:HD3	1.83	0.41
1:A:85:GLN:HG3	1:A:85:GLN:H	1.72	0.41
1:C:195:LEU:HD12	1:C:266:HIS:CE1	2.56	0.41
1:C:67:PHE:CD1	1:C:67:PHE:N	2.88	0.41
1:A:179:THR:HB	1:A:180:ALA:H	1.72	0.41
1:A:23:LEU:HD12	1:A:23:LEU:HA	1.68	0.41
2:B:308:ARG:HD2	2:B:342:TYR:CE2	2.55	0.41
2:B:346:TRP:HE1	2:B:438:ALA:HB3	1.85	0.41
1:C:14:VAL:HG13	1:C:67:PHE:CD2	2.54	0.41
2:D:103:TRP:NE1	2:D:148:GLY:HA2	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:32:PRO:HB3	2:D:85:GLN:NE2	2.35	0.41
2:D:405:LEU:N	2:D:405:LEU:HD22	2.36	0.41
1:A:234:ILE:HG12	1:A:302[B]:MET:SD	2.60	0.41
1:C:204:VAL:HG22	1:C:302:MET:HE3	2.03	0.41
2:B:109:THR:OG1	2:B:110:GLU:N	2.54	0.40
2:B:48:ARG:NH1	2:B:244:PHE:O	2.54	0.40
1:A:55:GLU:HG2	1:A:61:HIS:CD2	2.56	0.40
2:B:105:LYS:HA	2:B:109:THR:OG1	2.21	0.40
2:D:63:PRO:CD	2:D:86:ILE:HG13	2.51	0.40
4:F:151:SER:OG	4:F:151:SER:O	2.36	0.40
2:B:28:HIS:CE1	2:B:243:ARG:HB3	2.56	0.40
1:C:70:LEU:HD13	1:C:110:ILE:CG2	2.51	0.40
4:F:61:LEU:HD21	4:F:312:PHE:CD1	2.57	0.40
1:A:344:VAL:CG2	1:A:347:CYS:HB2	2.52	0.40
2:B:205:ASP:O	2:B:209:LEU:HG	2.21	0.40
2:B:239:THR:O	2:B:243:ARG:HG3	2.22	0.40
1:C:39:ASP:OD2	1:C:41:THR:OG1	2.40	0.40
2:D:34:GLY:CA	2:D:86:ILE:CD1	2.99	0.40
3:E:76:ARG:HA	3:E:76:ARG:HD3	1.91	0.40
4:F:150:LYS:NZ	4:F:240:LEU:HD13	2.36	0.40
4:F:97:SER:CA	4:F:183:GLN:HG2	2.50	0.40
4:F:190:LEU:HD12	4:F:191:LEU:N	2.37	0.40
4:F:199:PHE:HA	4:F:223:THR:HA	2.04	0.40
4:F:77:LEU:O	4:F:80:LEU:N	2.53	0.40
1:A:323:VAL:HG12	1:A:355:ILE:HD13	2.02	0.40
1:C:167:LEU:CD1	12:C:511:IMD:H2	2.48	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	438/440 (100%)	412 (94%)	24 (6%)	2 (0%)	29	48
1	C	441/440 (100%)	428 (97%)	13 (3%)	0	100	100
2	B	422/431 (98%)	395 (94%)	25 (6%)	2 (0%)	29	48
2	D	417/431 (97%)	387 (93%)	23 (6%)	7 (2%)	9	16
3	E	119/185 (64%)	112 (94%)	7 (6%)	0	100	100
4	F	299/378 (79%)	246 (82%)	47 (16%)	6 (2%)	7	12
All	All	2136/2305 (93%)	1980 (93%)	139 (6%)	17 (1%)	19	35

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	57	THR
2	B	82	PRO
2	D	177	VAL
4	F	254	GLY
1	A	177	VAL
2	D	143	GLY
4	F	242	ASN
2	D	94	PHE
2	D	109	THR
4	F	42	GLY
4	F	77	LEU
1	A	178	SER
2	D	11	GLN
2	D	397	ALA
4	F	227	PRO
2	D	181	VAL
4	F	78	VAL

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	371/371 (100%)	361 (97%)	10 (3%)	44	71

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	374/371 (101%)	369 (99%)	5 (1%)	69	87
2	B	368/372 (99%)	355 (96%)	13 (4%)	36	62
2	D	364/372 (98%)	350 (96%)	14 (4%)	33	58
3	E	111/168 (66%)	104 (94%)	7 (6%)	18	34
4	F	286/336 (85%)	279 (98%)	7 (2%)	49	74
All	All	1874/1990 (94%)	1818 (97%)	56 (3%)	41	68

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	84	ARG
1	A	163	LYS
1	A	178	SER
1	A	220	GLU
1	A	237	SER
1	A	315	CYS
1	A	316	CYS
1	A	413	MET
1	A	419	SER
1	A	430	LYS
2	B	1	MET
2	B	35	SER
2	B	90	ASP
2	B	124	LYS
2	B	126	SER
2	B	130	ASP
2	B	139	HIS
2	B	164	ARG
2	B	248	LEU
2	B	282	GLN
2	B	323	MET
2	B	329	ASP
2	B	372	LYS
1	C	229	ARG
1	C	241	SER
1	C	357	TYR
1	C	381	THR
1	C	430	LYS
2	D	15	GLN
2	D	39	ASP

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Mol	Chain	Res	Type
2	D	40	SER
2	D	75	MET
2	D	94	PHE
2	D	114	LEU
2	D	139	HIS
2	D	218	LYS
2	D	248	LEU
2	D	298	SER
2	D	322	ARG
2	D	324	SER
2	D	340	SER
2	D	369	ARG
3	E	48	GLU
3	E	59	GLU
3	E	75	LYS
3	E	103	GLN
3	E	126	LYS
3	E	128	LYS
3	E	140	LYS
4	F	12	SER
4	F	88	SER
4	F	184	LYS
4	F	211	TYR
4	F	253	TYR
4	F	262	MET
4	F	307	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	309	HIS
2	D	6	HIS
2	D	15	GLN
2	D	85	GLN
2	D	96	GLN
2	D	101	ASN
2	D	247	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 28 ligands modelled in this entry, 7 are monoatomic - leaving 21 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	$\# Z > 2$
7	GOL	A	504	-	5,5,5	1.41	2 (40%)	5,5,5	0.88	0
11	97O	B	506	-	28,30,30	6.27	19 (67%)	35,43,43	3.52	13 (37%)
7	GOL	D	503	-	5,5,5	0.98	0	5,5,5	0.97	0
5	GTP	C	503	6	26,34,34	0.97	1 (3%)	33,54,54	1.98	9 (27%)
13	ACP	F	401	-	27,33,33	4.73	12 (44%)	32,52,52	2.90	9 (28%)
7	GOL	C	505	-	5,5,5	0.87	0	5,5,5	0.98	0
12	IMD	C	510	-	3,5,5	0.30	0	4,5,5	0.84	0
9	GDP	D	501	6	24,30,30	1.28	2 (8%)	31,47,47	1.96	7 (22%)
7	GOL	C	501	-	5,5,5	0.60	0	5,5,5	1.33	1 (20%)
7	GOL	A	506	-	5,5,5	1.10	0	5,5,5	0.88	0
7	GOL	C	506	-	5,5,5	1.54	2 (40%)	5,5,5	0.72	0
12	IMD	C	509	-	3,5,5	0.44	0	4,5,5	0.34	0
9	GDP	B	501	6	24,30,30	1.17	2 (8%)	31,47,47	1.89	6 (19%)
12	IMD	C	511	-	3,5,5	0.45	0	4,5,5	0.18	0
10	MES	B	505	-	12,12,12	2.23	1 (8%)	14,16,16	1.99	4 (28%)
5	GTP	A	501	6	26,34,34	1.06	1 (3%)	33,54,54	1.86	9 (27%)
7	GOL	D	504	-	5,5,5	0.85	0	5,5,5	1.13	0
7	GOL	C	502	-	5,5,5	1.12	0	5,5,5	0.87	0
7	GOL	C	507	-	5,5,5	1.35	1 (20%)	5,5,5	0.76	0
7	GOL	B	503	-	5,5,5	1.19	1 (20%)	5,5,5	0.65	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	GOL	A	503	-	5,5,5	0.95	0	5,5,5	0.83	0

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
7	GOL	A	504	-	-	2/4/4/4	-
11	97O	B	506	-	-	4/12/21/21	0/4/4/4
7	GOL	D	503	-	-	2/4/4/4	-
5	GTP	C	503	6	-	8/18/38/38	0/3/3/3
13	ACP	F	401	-	-	4/15/38/38	0/3/3/3
7	GOL	C	505	-	-	2/4/4/4	-
12	IMD	C	509	-	-	-	0/1/1/1
7	GOL	C	501	-	-	2/4/4/4	-
7	GOL	A	506	-	-	0/4/4/4	-
7	GOL	C	506	-	-	2/4/4/4	-
9	GDP	D	501	6	-	3/12/32/32	0/3/3/3
9	GDP	B	501	6	-	4/12/32/32	0/3/3/3
7	GOL	C	502	-	-	4/4/4/4	-
10	MES	B	505	-	-	4/6/14/14	0/1/1/1
5	GTP	A	501	6	-	6/18/38/38	0/3/3/3
7	GOL	D	504	-	-	4/4/4/4	-
12	IMD	C	511	-	-	-	0/1/1/1
7	GOL	C	507	-	-	2/4/4/4	-
7	GOL	B	503	-	-	0/4/4/4	-
7	GOL	A	503	-	-	2/4/4/4	-
12	IMD	C	510	-	-	-	0/1/1/1

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	F	401	ACP	O3'-C3'	15.73	1.80	1.43
11	B	506	97O	C3-C2	-15.56	1.08	1.41
11	B	506	97O	C8-C9	13.66	1.72	1.50
13	F	401	ACP	C2'-C3'	-12.74	1.18	1.53
11	B	506	97O	C4-C3	-10.75	1.19	1.38
11	B	506	97O	C5-C6	9.68	1.57	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	B	506	97O	C1-C6	9.67	1.55	1.39
11	B	506	97O	C1-C2	-9.00	1.21	1.39
13	F	401	ACP	PB-O3A	8.74	1.68	1.58
11	B	506	97O	C7-C6	-7.62	1.39	1.51
10	B	505	MES	C8-S	-7.37	1.67	1.77
11	B	506	97O	C5-C10	-7.31	1.37	1.48
11	B	506	97O	C14-C11	7.28	1.57	1.49
13	F	401	ACP	O4'-C1'	6.73	1.50	1.41
11	B	506	97O	C4-C5	5.16	1.48	1.39
9	D	501	GDP	C6-C5	4.96	1.49	1.41
11	B	506	97O	O22-C1	4.22	1.46	1.38
9	B	501	GDP	C6-C5	3.96	1.48	1.41
11	B	506	97O	O26-C3	3.75	1.43	1.37
13	F	401	ACP	C6-N6	3.58	1.47	1.34
11	B	506	97O	C15-C16	3.49	1.45	1.38
5	A	501	GTP	C6-N1	3.29	1.38	1.33
13	F	401	ACP	C2'-C1'	-3.17	1.49	1.53
11	B	506	97O	O20-C17	3.00	1.43	1.37
13	F	401	ACP	C4-N3	-2.95	1.31	1.35
11	B	506	97O	O24-C2	2.95	1.43	1.38
5	C	503	GTP	C6-N1	2.75	1.37	1.33
11	B	506	97O	C7-C8	2.73	1.60	1.51
11	B	506	97O	C10-C11	2.70	1.45	1.41
11	B	506	97O	C18-C19	2.48	1.43	1.38
13	F	401	ACP	PB-O2B	-2.40	1.50	1.56
13	F	401	ACP	C5-N7	2.30	1.48	1.39
9	D	501	GDP	C5-C4	2.27	1.46	1.40
13	F	401	ACP	C3'-C4'	2.27	1.58	1.53
7	C	506	GOL	C3-C2	2.26	1.61	1.51
13	F	401	ACP	PA-O5'	2.24	1.68	1.59
7	A	504	GOL	C1-C2	2.20	1.60	1.51
7	C	506	GOL	C1-C2	2.19	1.60	1.51
13	F	401	ACP	O4'-C4'	2.16	1.49	1.45
7	A	504	GOL	C3-C2	2.15	1.60	1.51
11	B	506	97O	C18-C17	2.09	1.42	1.38
7	C	507	GOL	C3-C2	2.05	1.60	1.51
7	B	503	GOL	C3-C2	2.02	1.60	1.51
9	B	501	GDP	C2'-C1'	-2.01	1.50	1.53

All (58) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	B	506	97O	C5-C6-C1	-10.38	106.49	118.41
13	F	401	ACP	O3'-C3'-C4'	7.33	132.25	111.05
11	B	506	97O	C4-C3-C2	7.29	128.47	120.22
11	B	506	97O	O26-C3-C4	-6.98	112.11	124.12
11	B	506	97O	C4-C5-C10	6.96	135.33	123.35
13	F	401	ACP	C2'-C3'-C4'	6.91	116.07	102.64
11	B	506	97O	C4-C5-C6	-6.01	110.63	119.05
5	C	503	GTP	N3-C2-N1	-5.98	119.24	127.22
13	F	401	ACP	C3'-C2'-C1'	5.92	109.90	100.98
13	F	401	ACP	C5'-C4'-C3'	-5.90	93.08	115.18
13	F	401	ACP	O3'-C3'-C2'	-5.52	93.97	111.82
11	B	506	97O	C3-C2-C1	5.52	126.42	119.56
5	A	501	GTP	N3-C2-N1	-5.26	120.20	127.22
11	B	506	97O	C7-C6-C5	5.02	129.54	119.48
5	C	503	GTP	C2-N3-C4	4.95	121.02	115.36
13	F	401	ACP	O2'-C2'-C3'	4.93	127.78	111.82
9	D	501	GDP	C2-N3-C4	4.90	120.95	115.36
10	B	505	MES	C5-N4-C3	4.80	119.64	108.83
5	A	501	GTP	C2-N3-C4	4.71	120.73	115.36
9	B	501	GDP	C2-N3-C4	4.70	120.72	115.36
9	D	501	GDP	C6-C5-C4	-4.49	116.51	120.80
9	B	501	GDP	C6-C5-C4	-4.07	116.91	120.80
9	B	501	GDP	C6-N1-C2	4.00	122.29	115.93
13	F	401	ACP	N3-C2-N1	-3.96	122.49	128.68
9	D	501	GDP	C6-N1-C2	3.85	122.05	115.93
9	B	501	GDP	C5-C6-N1	-3.76	118.29	123.43
10	B	505	MES	O3S-S-C8	3.70	111.76	105.77
11	B	506	97O	C11-C10-C9	-3.66	98.58	104.23
9	D	501	GDP	C5-C6-N1	-3.61	118.49	123.43
11	B	506	97O	C27-O26-C3	-3.59	112.11	117.53
9	D	501	GDP	C4-C5-N7	-3.43	105.82	109.40
9	B	501	GDP	N3-C2-N1	-3.38	122.71	127.22
5	A	501	GTP	C5-C6-N1	-3.34	118.86	123.43
9	D	501	GDP	N3-C2-N1	-3.22	122.93	127.22
5	C	503	GTP	PA-O3A-PB	-2.95	122.69	132.83
11	B	506	97O	C7-C8-C9	-2.94	102.98	110.37
5	C	503	GTP	C6-N1-C2	2.89	120.52	115.93
9	B	501	GDP	C4-C5-N7	-2.89	106.39	109.40
5	A	501	GTP	N2-C2-N1	2.81	121.63	117.25
5	C	503	GTP	C5-C6-N1	-2.81	119.58	123.43
13	F	401	ACP	C4-C5-N7	-2.72	106.56	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	F	401	ACP	O4'-C4'-C3'	-2.70	99.77	105.11
11	B	506	97O	C8-C7-C6	-2.66	103.96	111.22
5	C	503	GTP	O4'-C1'-C2'	-2.59	103.14	106.93
5	A	501	GTP	C6-N1-C2	2.51	119.92	115.93
5	A	501	GTP	C4-C5-N7	-2.51	106.79	109.40
5	C	503	GTP	PB-O3B-PG	-2.50	124.24	132.83
11	B	506	97O	O24-C2-C3	-2.50	116.53	120.12
11	B	506	97O	O26-C3-C2	2.42	119.41	115.16
9	D	501	GDP	O2B-PB-O3A	2.36	112.56	104.64
5	A	501	GTP	PB-O3B-PG	-2.30	124.92	132.83
5	C	503	GTP	C4-C5-N7	-2.24	107.07	109.40
5	C	503	GTP	O3'-C3'-C4'	-2.22	104.62	111.05
5	A	501	GTP	O3G-PG-O3B	2.19	111.97	104.64
10	B	505	MES	C6-C5-N4	-2.10	106.93	110.10
5	A	501	GTP	PA-O3A-PB	-2.04	125.81	132.83
10	B	505	MES	C7-N4-C5	2.02	116.40	111.23
7	C	501	GOL	C3-C2-C1	-2.02	103.86	111.70

There are no chirality outliers.

All (55) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	F	401	ACP	C5'-O5'-PA-O2A
13	F	401	ACP	C5'-O5'-PA-O3A
9	D	501	GDP	C5'-O5'-PA-O1A
9	D	501	GDP	C5'-O5'-PA-O2A
7	C	507	GOL	O1-C1-C2-C3
7	A	503	GOL	O1-C1-C2-C3
9	B	501	GDP	C5'-O5'-PA-O1A
9	B	501	GDP	C5'-O5'-PA-O2A
5	C	503	GTP	PB-O3B-PG-O3G
5	C	503	GTP	C5'-O5'-PA-O1A
5	C	503	GTP	C5'-O5'-PA-O2A
7	C	506	GOL	C1-C2-C3-O3
7	C	506	GOL	O2-C2-C3-O3
7	C	502	GOL	O1-C1-C2-C3
10	B	505	MES	C8-C7-N4-C5
10	B	505	MES	C7-C8-S-O1S
5	A	501	GTP	PB-O3B-PG-O3G
5	A	501	GTP	C5'-O5'-PA-O1A
5	A	501	GTP	C5'-O5'-PA-O2A
7	D	504	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
11	B	506	97O	C2-C3-O26-C27
10	B	505	MES	C7-C8-S-O3S
7	C	505	GOL	O1-C1-C2-C3
7	C	501	GOL	O1-C1-C2-C3
7	A	504	GOL	C1-C2-C3-O3
7	C	502	GOL	C1-C2-C3-O3
7	D	504	GOL	C1-C2-C3-O3
7	C	505	GOL	O1-C1-C2-O2
7	C	507	GOL	O1-C1-C2-O2
7	A	504	GOL	O2-C2-C3-O3
7	C	502	GOL	O1-C1-C2-O2
7	D	504	GOL	O1-C1-C2-O2
7	D	504	GOL	O2-C2-C3-O3
11	B	506	97O	C4-C3-O26-C27
7	A	503	GOL	O1-C1-C2-O2
7	C	501	GOL	O1-C1-C2-O2
7	C	502	GOL	O2-C2-C3-O3
9	D	501	GDP	C5'-O5'-PA-O3A
7	D	503	GOL	O1-C1-C2-O2
13	F	401	ACP	C5'-O5'-PA-O1A
10	B	505	MES	C7-C8-S-O2S
11	B	506	97O	C10-C11-C14-C19
9	B	501	GDP	PB-O3A-PA-O1A
5	C	503	GTP	PG-O3B-PB-O1B
5	C	503	GTP	PB-O3B-PG-O1G
5	A	501	GTP	PB-O3B-PG-O1G
5	C	503	GTP	PB-O3B-PG-O2G
5	A	501	GTP	PB-O3B-PG-O2G
13	F	401	ACP	PB-O3A-PA-O2A
9	B	501	GDP	C5'-O5'-PA-O3A
5	C	503	GTP	C5'-O5'-PA-O3A
5	A	501	GTP	C5'-O5'-PA-O3A
11	B	506	97O	C10-C11-C14-C15
5	C	503	GTP	PG-O3B-PB-O2B
7	D	503	GOL	O1-C1-C2-C3

There are no ring outliers.

12 monomers are involved in 34 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	B	506	97O	2	0
5	C	503	GTP	1	0

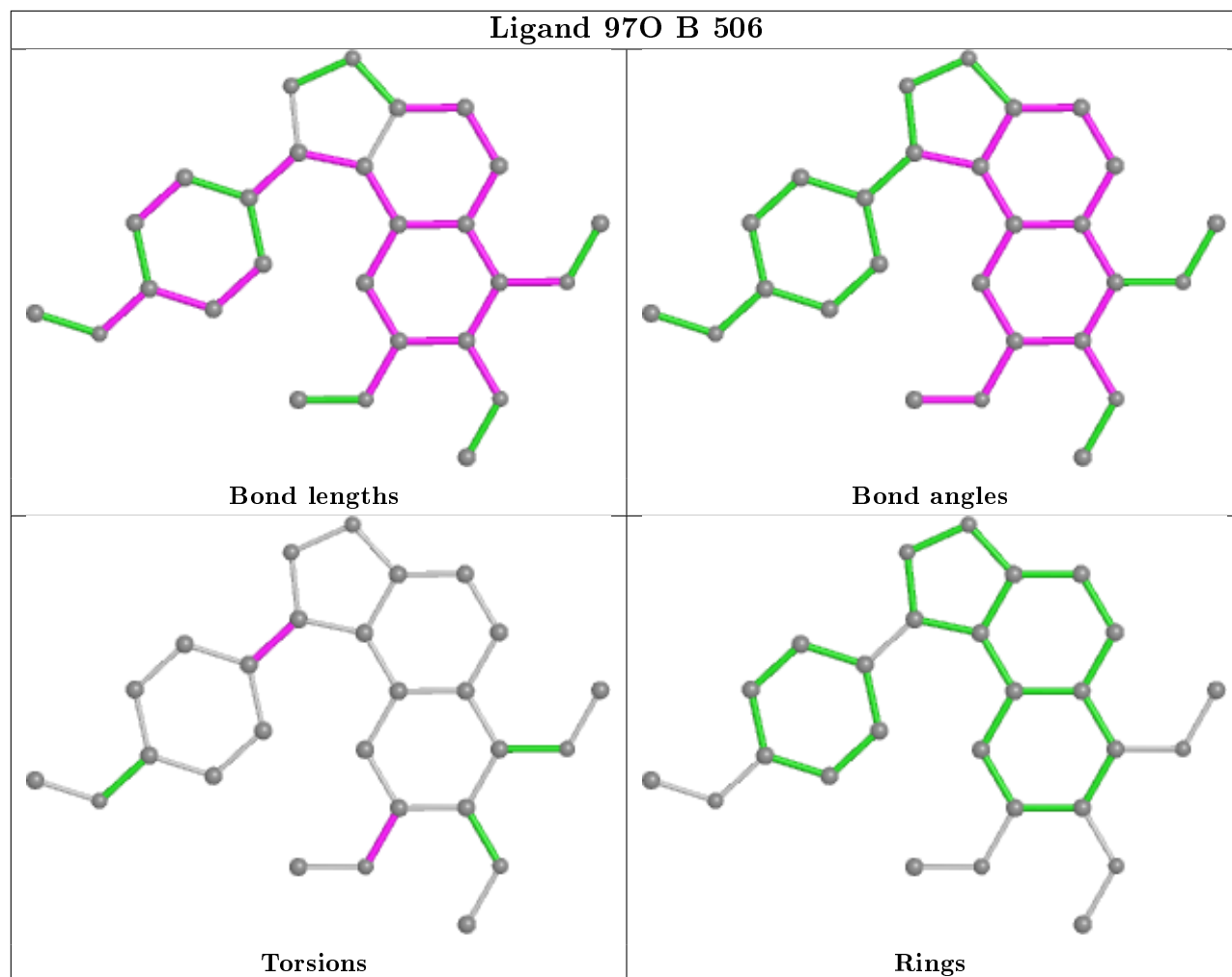
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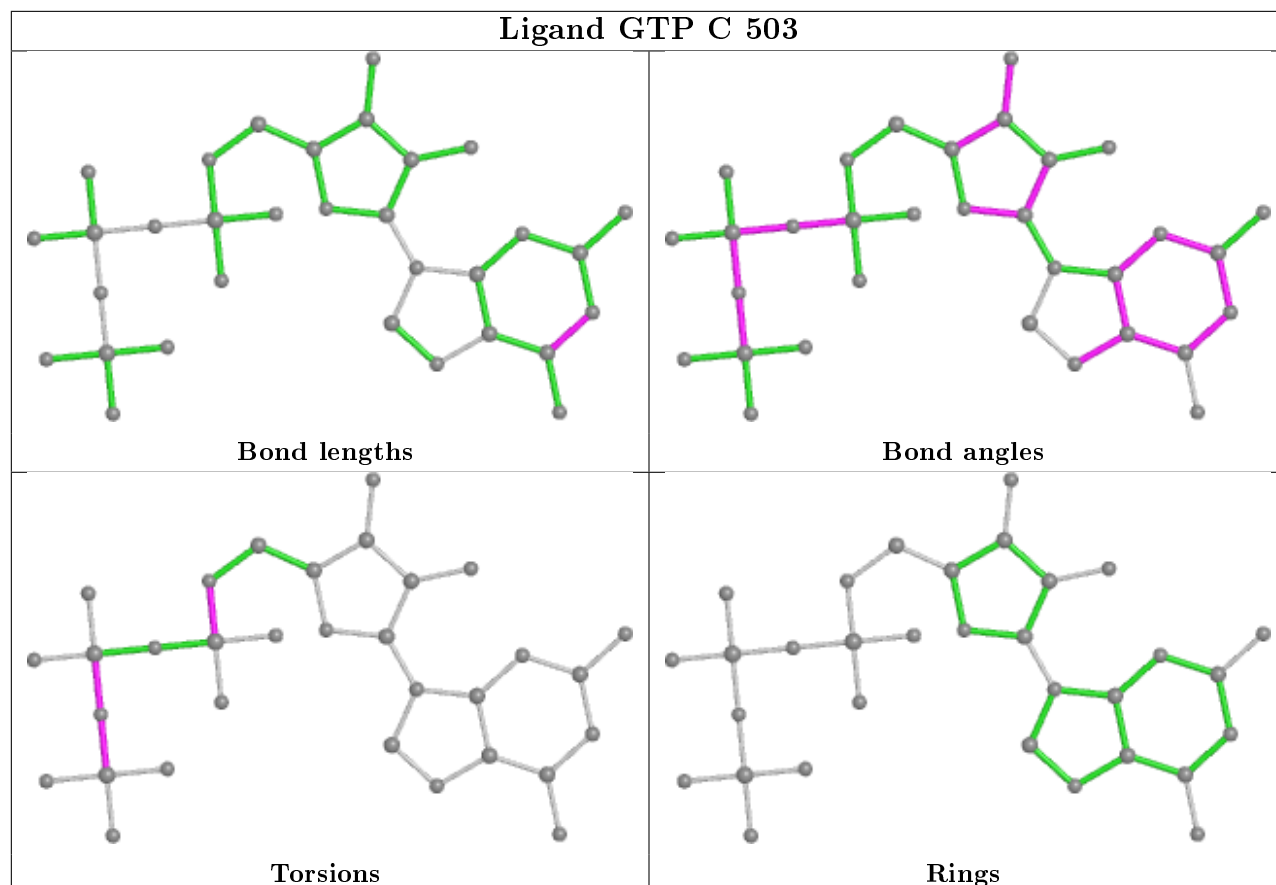
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	F	401	ACP	13	0
7	C	505	GOL	5	0
12	C	510	IMD	2	0
9	D	501	GDP	1	0
7	C	501	GOL	2	0
7	C	506	GOL	1	0
9	B	501	GDP	1	0
12	C	511	IMD	3	0
5	A	501	GTP	2	0
7	A	503	GOL	1	0

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.

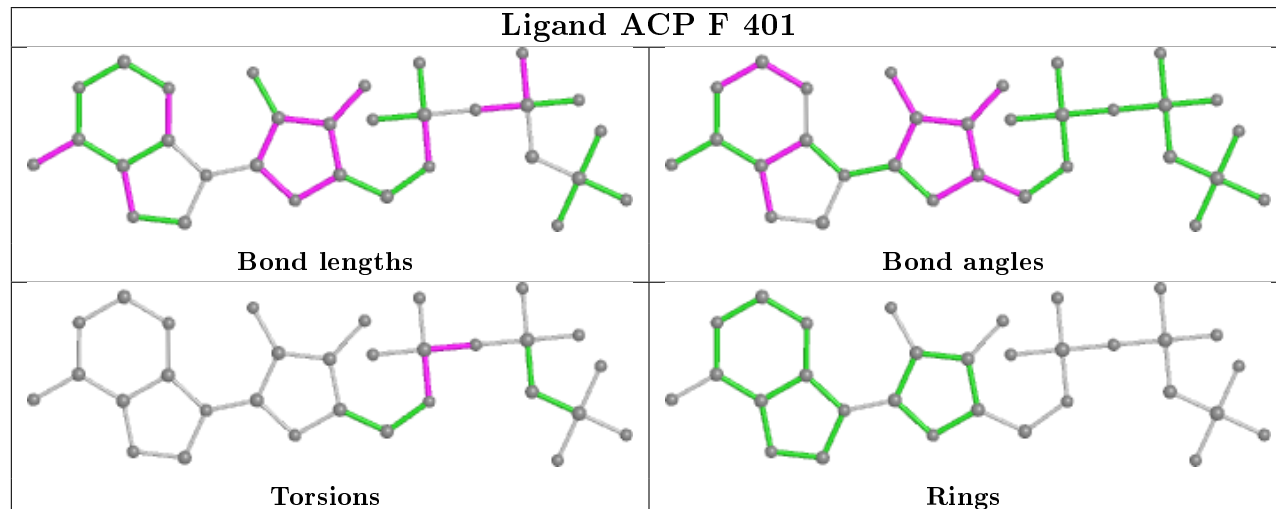
Ligand 97O B 506

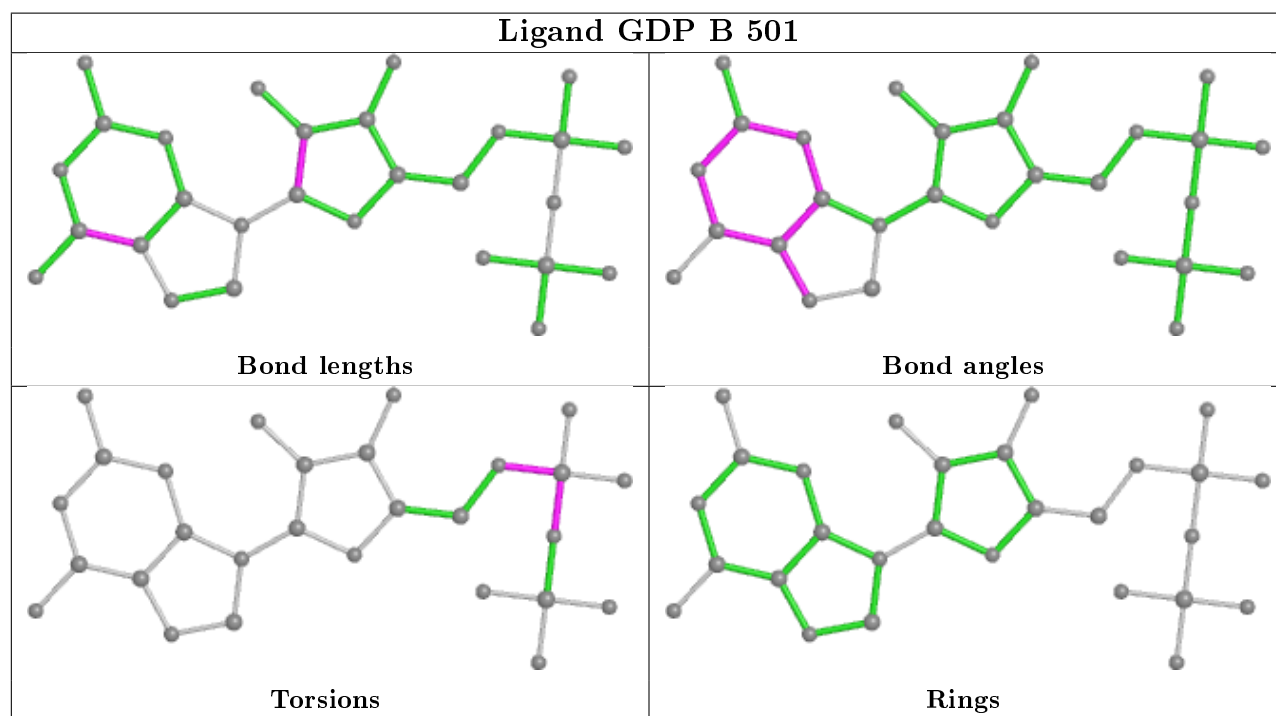
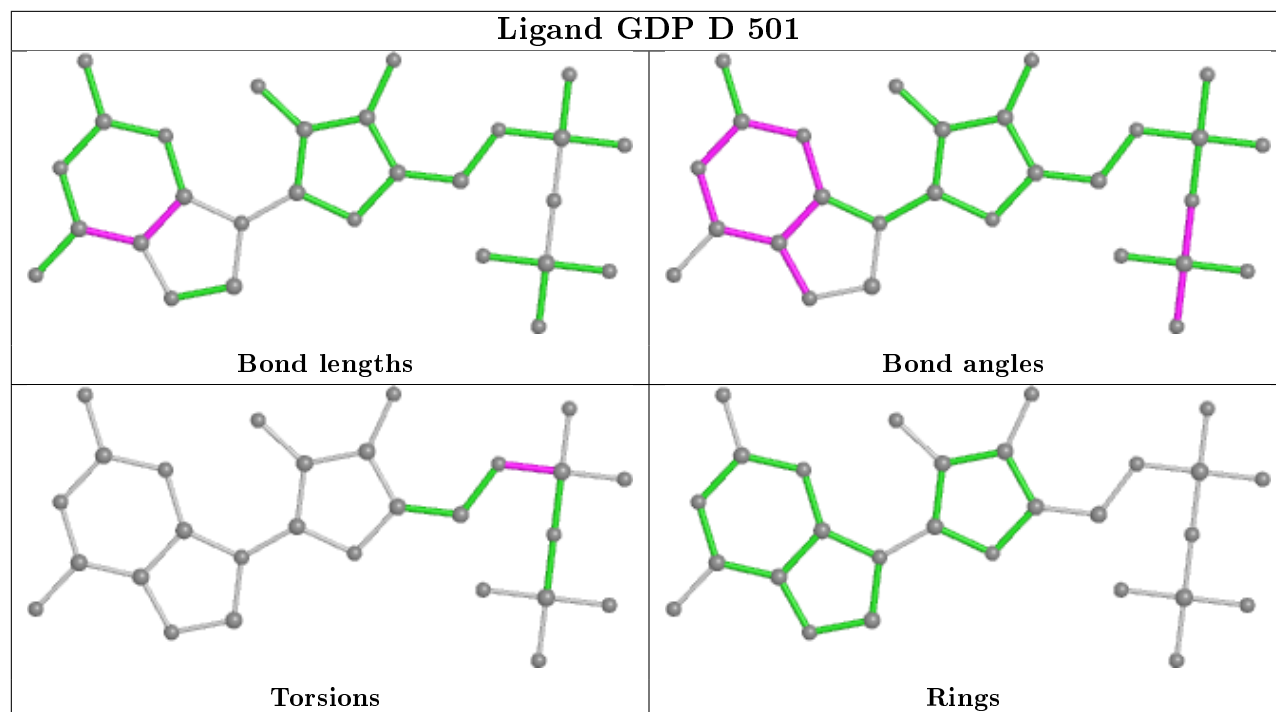


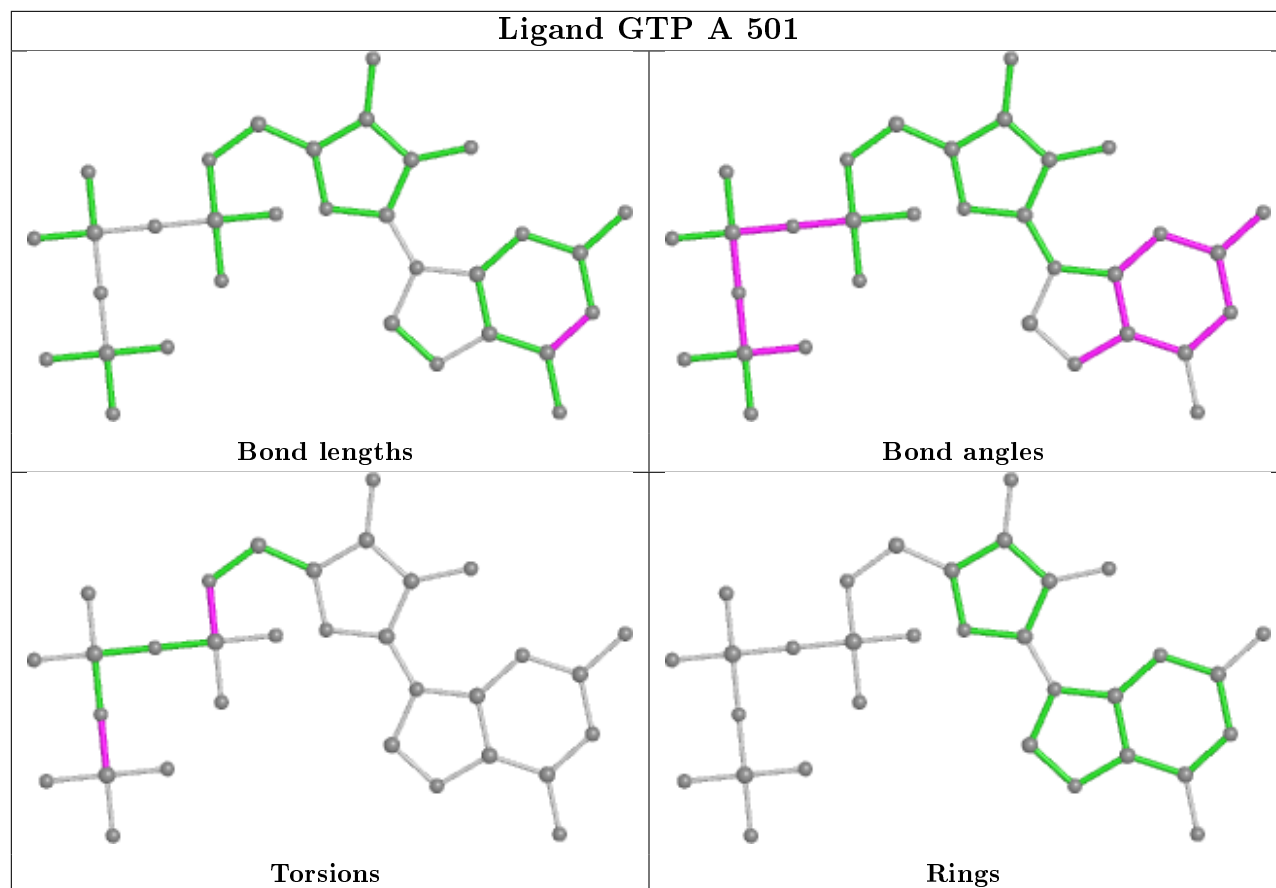
Ligand GTP C 503



Ligand ACP F 401







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	438/440 (99%)	0.36	15 (3%) 45 48	44, 63, 80, 146	0
1	C	440/440 (100%)	0.01	6 (1%) 75 77	37, 51, 71, 149	0
2	B	424/431 (98%)	0.31	24 (5%) 23 25	38, 58, 91, 135	0
2	D	421/431 (97%)	0.55	38 (9%) 9 9	46, 70, 102, 118	0
3	E	121/185 (65%)	0.39	7 (5%) 23 24	49, 71, 94, 148	0
4	F	317/378 (83%)	1.66	83 (26%) 0 0	52, 81, 247, 320	0
All	All	2161/2305 (93%)	0.51	173 (8%) 12 12	37, 64, 117, 320	0

All (173) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	244	CYS	24.9
4	F	249	TYR	18.6
4	F	240	LEU	14.1
4	F	235	ASP	10.9
4	F	250	SER	10.8
4	F	254	GLY	10.7
4	F	248	GLU	10.6
4	F	225	SER	9.6
4	F	239	HIS	9.4
4	F	231	ALA	9.1
4	F	245	ILE	8.7
4	F	256	TYR	8.6
4	F	252	ASN	8.2
4	F	238	CYS	8.0
4	F	133	ALA	7.7
4	F	255	ARG	7.3
4	F	259	GLY	7.0
2	D	249	ASN	7.0
4	F	149	ALA	6.6

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Mol	Chain	Res	Type	RSRZ
4	F	243	HIS	6.6
4	F	229	ASN	6.5
4	F	148	ILE	6.2
4	F	182	ILE	6.1
4	F	257	GLU	6.1
2	D	401	ARG	6.0
4	F	230	SER	5.9
4	F	224	SER	5.9
4	F	150	LYS	5.9
4	F	100	ILE	5.7
4	F	247	LYS	5.7
4	F	246	GLN	5.4
4	F	131	PHE	5.3
4	F	237	THR	5.2
4	F	98	TYR	5.2
2	B	57	THR	5.1
4	F	253	TYR	5.1
4	F	258	GLU	5.1
4	F	227	PRO	5.0
4	F	130	VAL	4.9
4	F	236	LYS	4.9
4	F	172	PHE	4.8
4	F	242	ASN	4.7
2	B	59	ASN	4.7
4	F	125	THR	4.5
3	E	27	PRO	4.4
4	F	228	TYR	4.4
2	D	219	LEU	4.4
4	F	101	TYR	4.4
4	F	171	ASP	4.3
4	F	126	ASP	4.3
2	D	397	ALA	4.2
4	F	102	PRO	4.1
2	B	247	GLN	4.0
4	F	134	ALA	4.0
1	A	68[A]	VAL	4.0
4	F	226	GLU	4.0
2	D	247	GLN	3.9
2	D	37	HIS	3.9
2	D	400	ARG	3.8
2	B	62	VAL	3.8
2	D	57	THR	3.8

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Mol	Chain	Res	Type	RSRZ
1	C	356[A]	ASN	3.8
2	B	249	ASN	3.8
4	F	197	ARG	3.7
2	D	406	HIS	3.7
2	D	179	ASP	3.7
4	F	162	ILE	3.7
3	E	26	PRO	3.6
4	F	22	LEU	3.6
4	F	99	VAL	3.6
2	D	405	LEU	3.5
1	C	315[A]	CYS	3.5
4	F	145	ASN	3.5
4	F	260	ASN	3.5
2	D	94	PHE	3.5
4	F	17	VAL	3.5
2	D	269	MET	3.3
2	D	402	LYS	3.3
4	F	135	TYR	3.3
2	B	37	HIS	3.2
2	B	56	ALA	3.2
1	A	262	TYR	3.2
4	F	27	TRP	3.2
2	B	60	LYS	3.2
2	B	61	TYR	3.1
4	F	323	GLU	3.1
3	E	46	SER	3.1
4	F	362	ALA	3.1
2	D	408	TYR	3.1
4	F	187	GLU	3.1
2	B	58	GLY	3.1
4	F	343	TYR	3.1
3	E	28	SER	3.1
2	B	86	ILE	3.0
4	F	199	PHE	3.0
4	F	21	LEU	3.0
4	F	241	THR	3.0
2	D	220	THR	3.0
4	F	144	GLY	3.0
2	D	218	LYS	3.0
2	D	415	GLU	2.9
4	F	20	LEU	2.9
2	D	177	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
4	F	25	GLY	2.9
2	D	76	ASP	2.9
2	B	438	ALA	2.9
2	D	77	SER	2.8
4	F	13	VAL	2.8
2	B	36	TYR	2.8
2	B	437	ASP	2.8
4	F	185	TYR	2.7
1	A	209	ILE	2.7
2	D	83	PHE	2.7
2	B	30	ILE	2.7
2	D	407	TRP	2.7
4	F	332	VAL	2.6
2	D	256	ALA	2.6
4	F	261	GLU	2.6
2	D	414	ASP	2.6
1	A	302[A]	MET	2.6
2	D	413	MET	2.6
4	F	132	LEU	2.6
1	A	346	TRP	2.6
4	F	147	TRP	2.5
4	F	165	GLU	2.5
1	C	357	TYR	2.5
4	F	128	ARG	2.5
4	F	168	GLU	2.5
4	F	320	MET	2.5
2	B	155	SER	2.4
2	B	33	THR	2.4
1	C	194	THR	2.4
2	D	248	LEU	2.4
2	B	29	GLY	2.4
2	D	56	ALA	2.4
1	A	178	SER	2.4
2	B	147	SER	2.4
4	F	191	LEU	2.4
2	D	58	GLY	2.4
1	A	42	ILE	2.4
1	C	68	VAL	2.3
2	B	42	LEU	2.3
4	F	163	SER	2.3
1	A	43	GLY	2.3
1	A	350	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	438	ASP	2.3
3	E	141	GLU	2.3
1	A	282	TYR	2.3
4	F	127	GLU	2.3
2	D	213	CYS	2.3
4	F	169	LEU	2.3
4	F	9	GLU	2.2
2	D	95	GLY	2.2
2	B	250	ALA	2.2
4	F	361	LEU	2.2
2	D	250	ALA	2.2
1	A	177	VAL	2.1
2	D	80	SER	2.1
1	C	295	CYS	2.1
1	A	9	VAL	2.1
3	E	22	VAL	2.1
1	A	281	ALA	2.1
2	D	404	PHE	2.1
2	D	61	TYR	2.1
2	D	73	GLY	2.1
2	D	72	PRO	2.1
4	F	164	SER	2.1
1	A	57	GLY	2.1
2	B	38	GLY	2.1
2	B	1	MET	2.0
3	E	44	ASP	2.0
2	D	33	THR	2.0
2	B	50[A]	ASN	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 carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

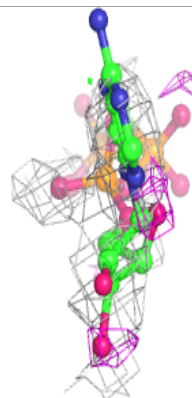
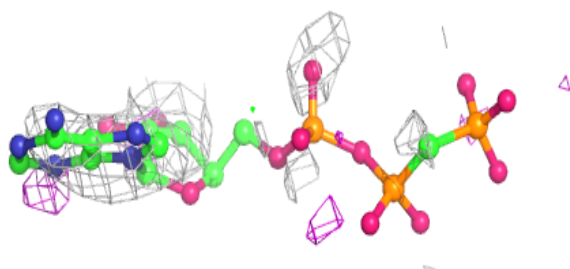
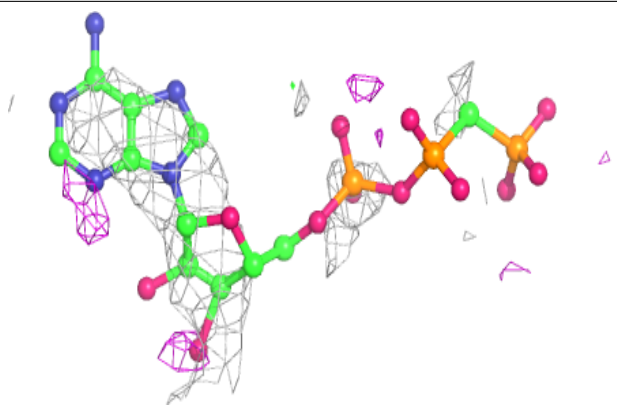
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
13	ACP	F	401	31/31	0.54	0.57	86,205,221,231	0
7	GOL	C	506	6/6	0.71	0.44	63,69,69,69	0
7	GOL	A	504	6/6	0.75	0.23	62,74,81,82	0
7	GOL	B	503	6/6	0.77	0.30	57,71,76,89	0
7	GOL	D	503	6/6	0.78	0.30	82,90,92,96	0
7	GOL	C	501	6/6	0.80	0.41	50,56,66,76	0
7	GOL	C	502	6/6	0.80	0.28	64,68,73,78	0
7	GOL	A	506	6/6	0.81	0.19	68,71,73,76	0
7	GOL	D	504	6/6	0.83	0.26	67,68,75,79	0
7	GOL	C	507	6/6	0.85	0.17	56,63,66,66	0
7	GOL	C	505	6/6	0.89	0.31	66,72,74,78	0
12	IMD	C	509	5/5	0.89	0.24	51,53,67,67	0
11	97O	B	506	27/27	0.89	0.18	58,73,78,80	0
12	IMD	C	510	5/5	0.90	0.18	61,65,71,74	0
12	IMD	C	511	5/5	0.91	0.21	65,69,75,76	0
7	GOL	A	503	6/6	0.92	0.24	67,72,75,79	0
9	GDP	D	501	28/28	0.95	0.14	66,71,81,92	0
6	MG	B	502	1/1	0.95	0.41	51,51,51,51	0
6	MG	D	502	1/1	0.95	0.14	76,76,76,76	0
6	MG	A	502	1/1	0.95	0.51	59,59,59,59	0
6	MG	C	504	1/1	0.96	0.25	50,50,50,50	0
5	GTP	C	503	32/32	0.97	0.17	35,44,50,57	0
10	MES	B	505	12/12	0.97	0.14	45,54,69,70	0
8	CA	B	504	1/1	0.97	0.09	97,97,97,97	0
8	CA	A	505	1/1	0.97	0.04	82,82,82,82	0
5	GTP	A	501	32/32	0.98	0.25	46,53,58,60	0
8	CA	C	508	1/1	0.98	0.06	85,85,85,85	0
9	GDP	B	501	28/28	0.98	0.21	38,47,50,58	0

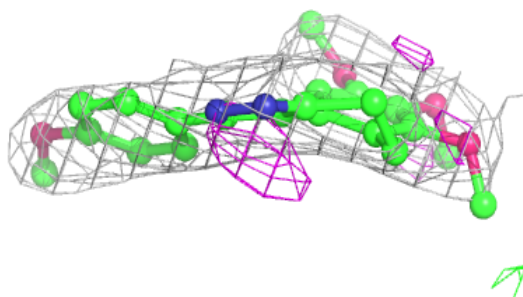
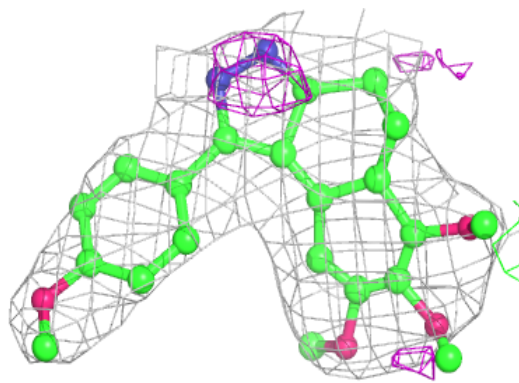
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

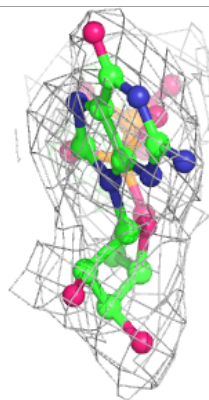
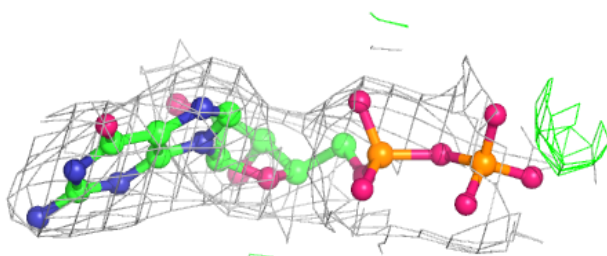
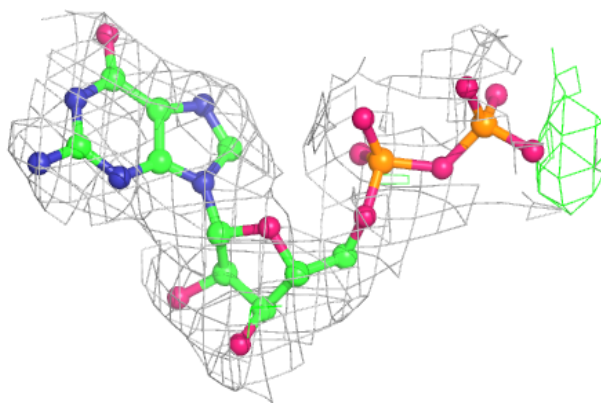
**Electron density around 97O B 506:**

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

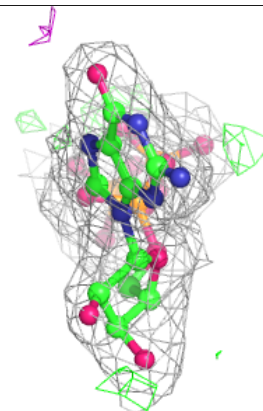
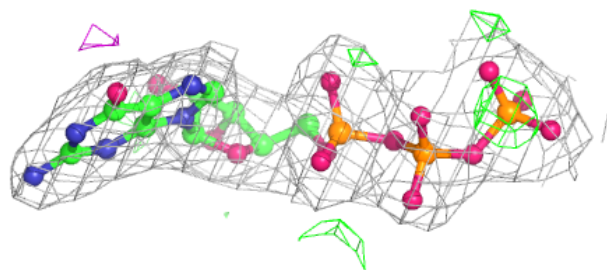
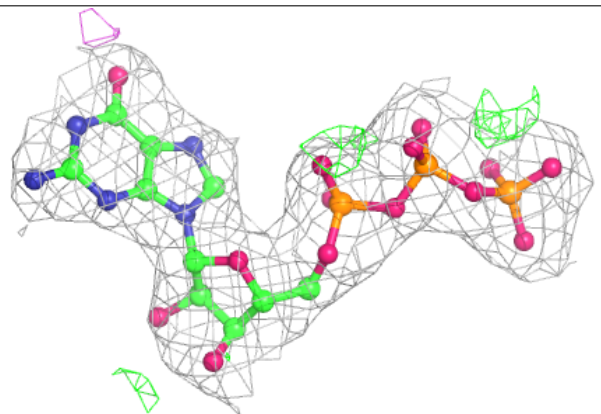


Electron density around GDP D 501:

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

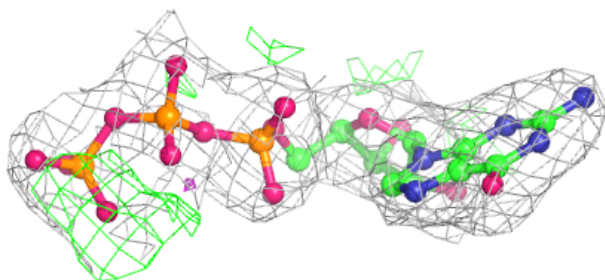
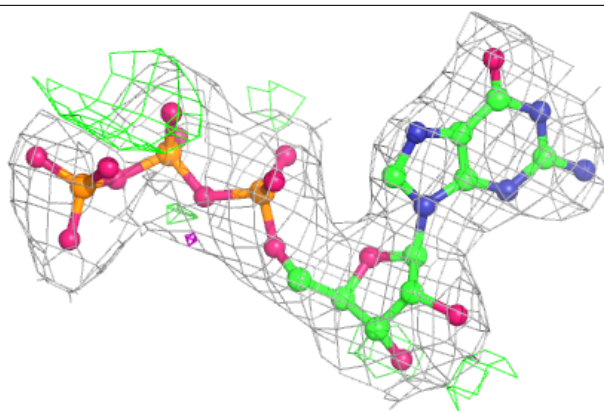
**Electron density around GTP C 503:**

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

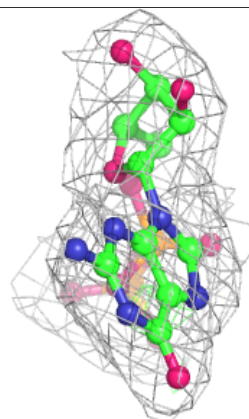
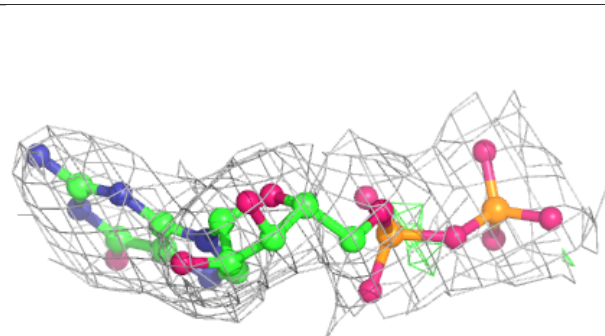
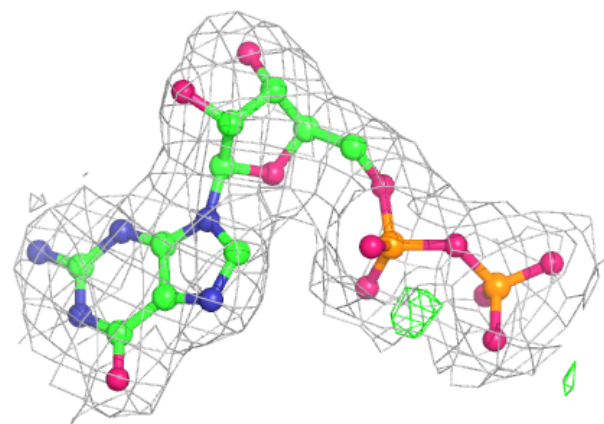


Electron density around GTP A 501:

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

**Electron density around GDP B 501:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.