



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 02:01 PM UTC

PDB ID : 6QQN / pdb_00006qqn
Title : Tubulin-TH588 complex
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Deposited on : 2019-02-18
Resolution : 2.30 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

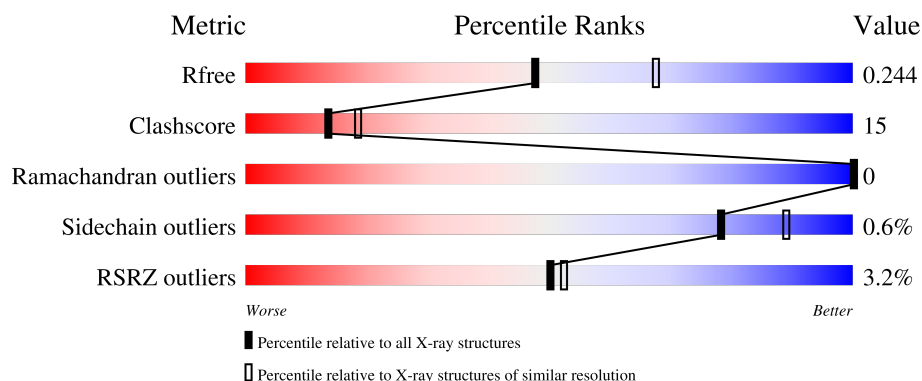
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	0% 74% 23% •
1	C	451	0% 75% 23% •
2	B	445	3% 65% 30% 5%
2	D	445	2% 68% 26% • 5%

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Mol	Chain	Length	Quality of chain
3	E	143	
4	F	384	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	2GE	B	504	-	-	X	-

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 17568 atoms, of which 18 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	436	Total	C	N	O	S	0	0	0
			3409	2159	580	648	22			
1	C	440	Total	C	N	O	S	0	1	0
			3444	2180	585	657	22			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	423	Total	C	N	O	S	0	1	0
			3344	2102	572	643	27			
2	D	421	Total	C	N	O	S	0	2	0
			3326	2089	567	642	28			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	121	Total	C	N	O	S	0	0	0
			1000	617	181	197	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	3	MET	-	initiating methionine	UNP P63043
E	4	ALA	-	expression tag	UNP P63043

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	314	Total	C	N	O	S	0	0	0
			2573	1659	437	464	13			

There are 6 discrepancies between the modelled and reference sequences:

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

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



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

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

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

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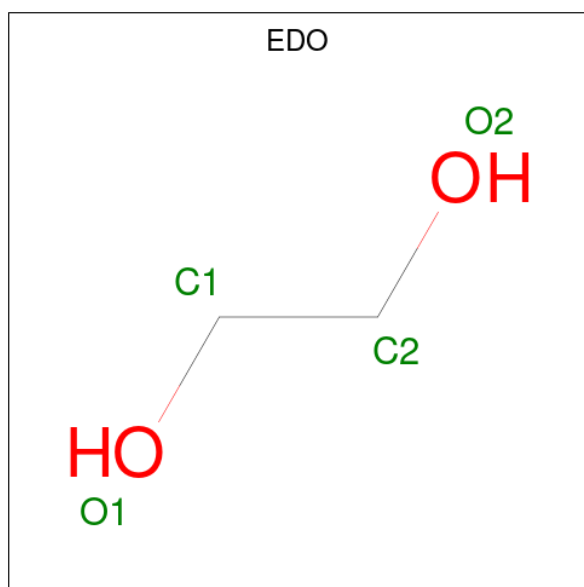
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	F	1	Total	Mg	0	0
			1	1		

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

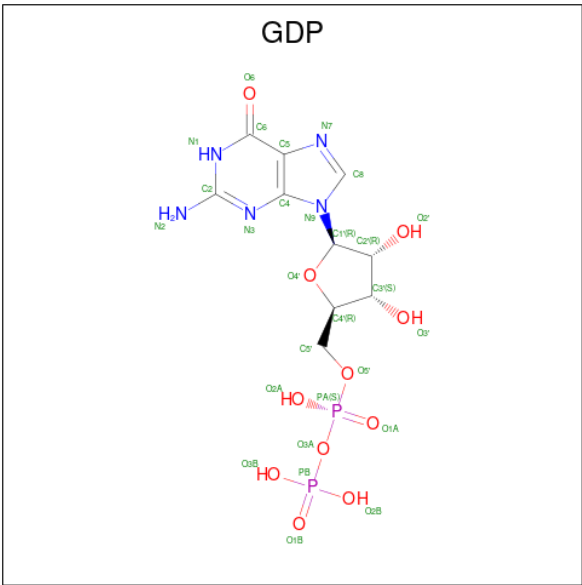
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Ca	0	0
			1	1		
7	B	2	Total	Ca	0	0
			2	2		
7	C	1	Total	Ca	0	0
			1	1		

- Molecule 8 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



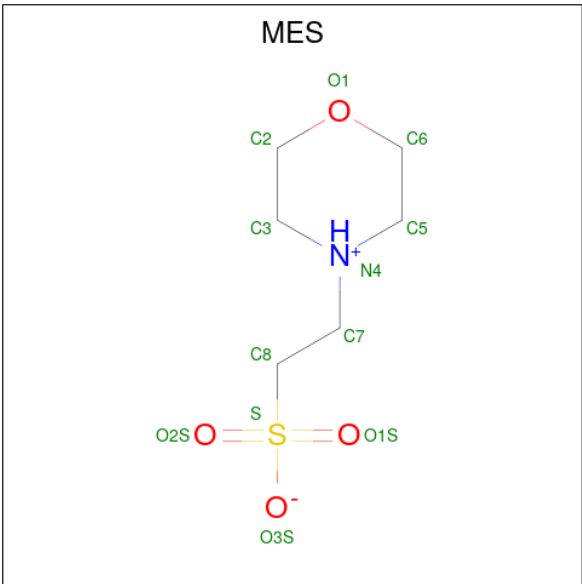
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	H	O	0	0
			10	2	6	2		

- Molecule 9 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



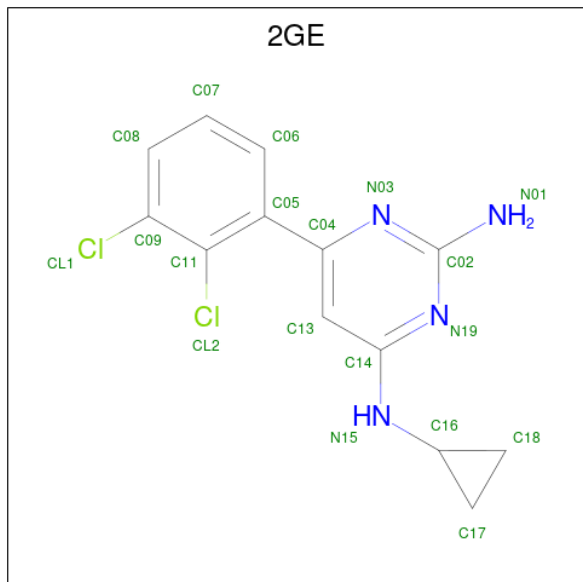
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	B	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
9	D	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- Molecule 10 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: C₆H₁₃NO₄S).



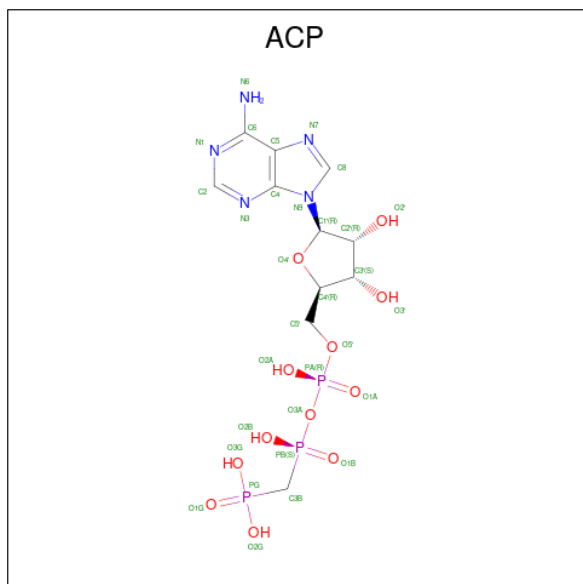
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 11 is N 4 -cyclopropyl-6-(2,3-dichlorophenyl)pyrimidine-2,4-diamine (CCD ID: 2GE) (formula: $C_{13}H_{12}Cl_2N_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	B	1	Total	C	Cl	H	N	0	0
			31	13	2	12	4		

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



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

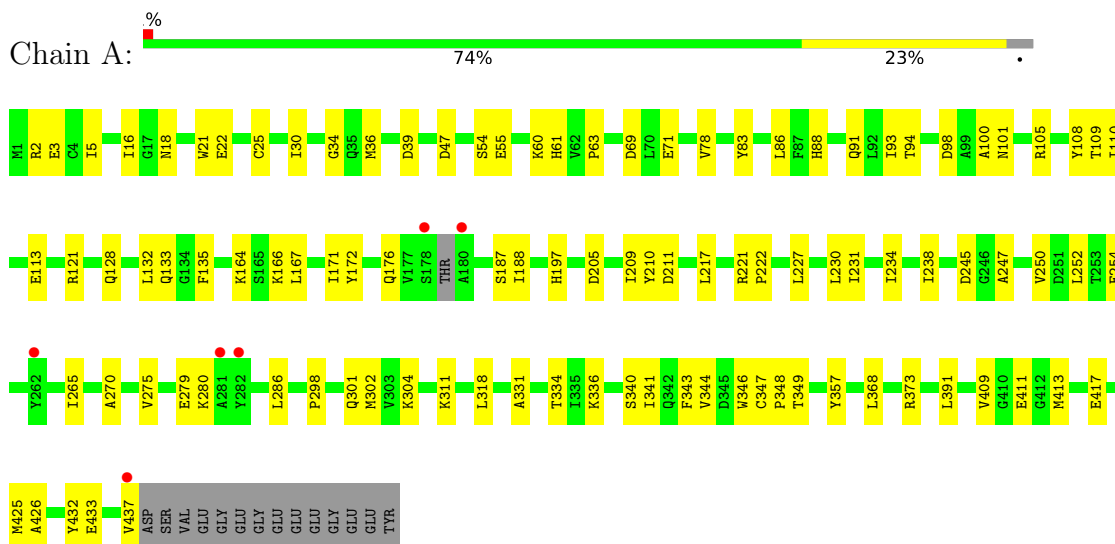
- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	50	Total 50	O 50	0	0
13	B	41	Total 41	O 41	0	0
13	C	117	Total 117	O 117	0	0
13	D	27	Total 27	O 27	0	0
13	E	11	Total 11	O 11	0	0
13	F	13	Total 13	O 13	0	0

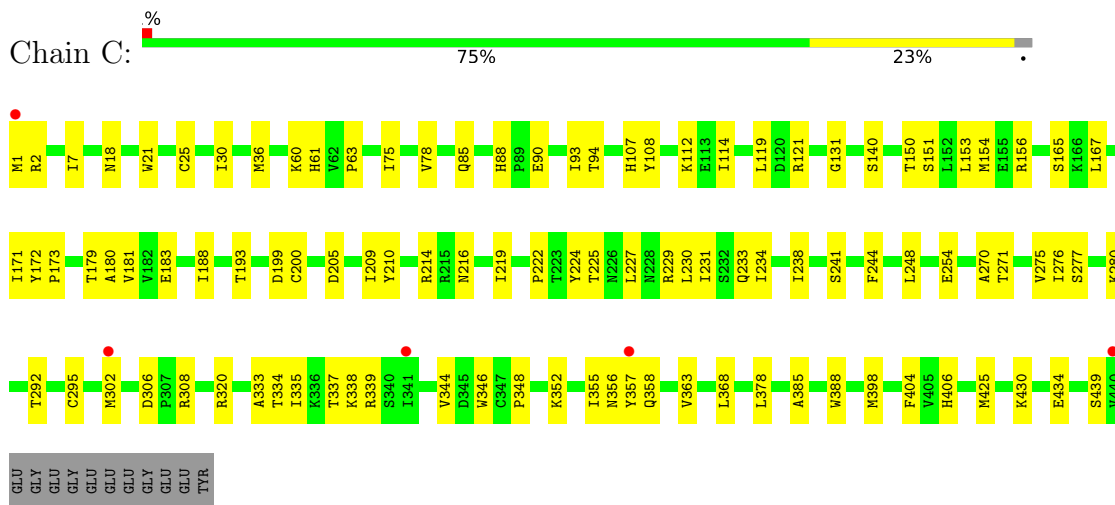
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Tubulin alpha-1B chain

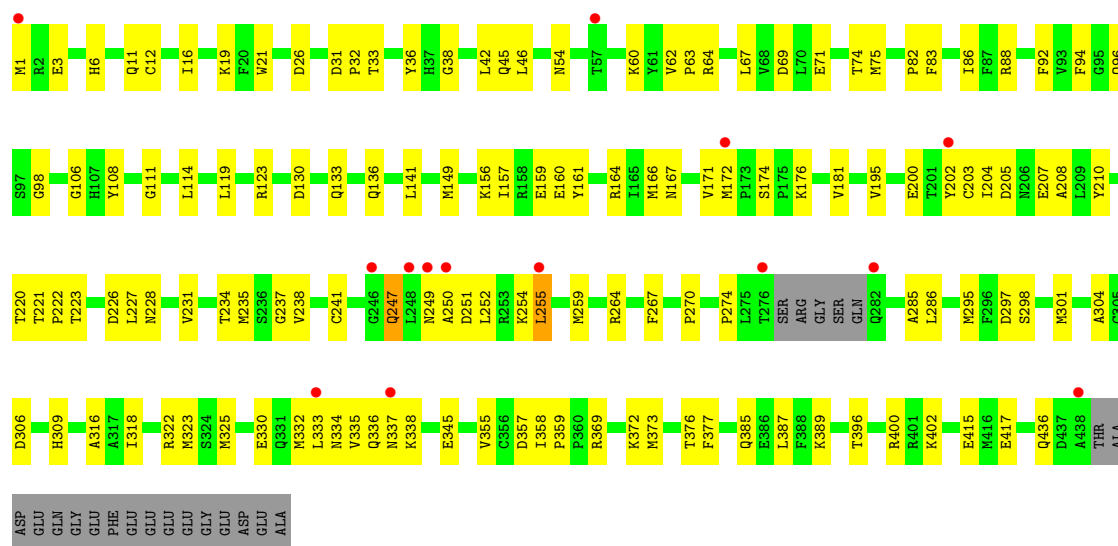


- Molecule 1: Tubulin alpha-1B chain

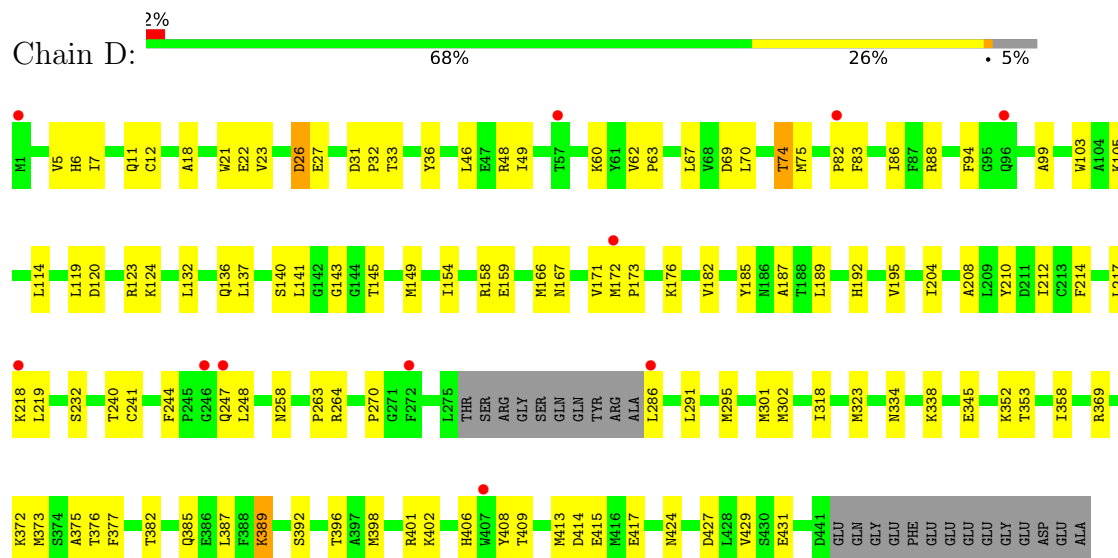


- Molecule 2: Tubulin beta-2B chain

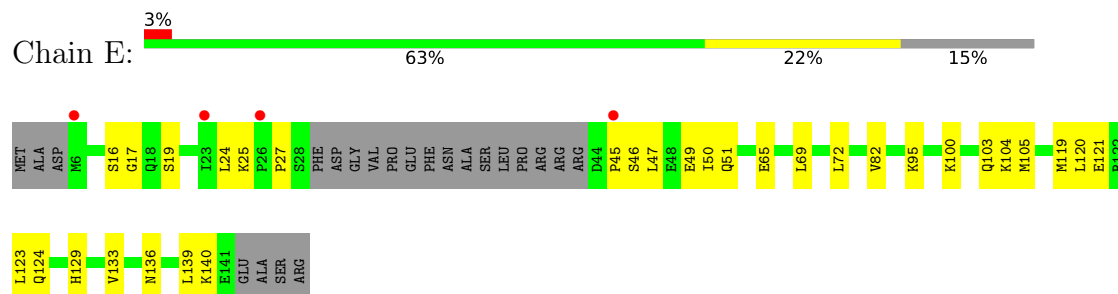




• Molecule 2: Tubulin beta-2B chain



• Molecule 3: Stathmin-4



• Molecule 4: Tubulin-Tyrosine Ligase



M1	ASN	V181	I283	PRO
Y2	GLY	I182	L284	T372
T3	ILE	Q183	L378	L378
F4	ARG	K184	I287	H379
V5	HIS	Y185	L291	H380
Y14	LEU	L186	R292	HIS
V17	ILE	E187	M296	HIS
ASN	ASN	K188	E299	HIS
THR	THR	P189	P300	HIS
L21	ARG	L190		
L21	THR	L191		
Q26	THR	L192		
K32	D126	H196	K305	
R36	E127	D200	H306	
F37	E129	V205	S311	
N38	V130	L206	F312	
L39	L132	H209	Q313	
M40	A133	Y216	L314	
R44	A134	R217	F319	
L58	Y135	E218	M320	
L61	G141	G219	V321	
R73	GLU	V220	D322	
S76	G144	L221	E323	
L77	N145	R222	V327	
V78	V146	A231	I330	
K82	V147	ASN	E331	
S88	I148	PHE	A335	
E89	K150	GLN	Q340	
C91	S151	ASP	K341	
P95	ALA	LYS	L342	
E96	GLY	T237	Y343	
S97	ALA	L240	A344	
Y98	LYS	N242	E345	
V99	GLY	H243	Q348	
I100	GLU	CYS	G349	
Y101	ILE	ILE	I350	
P102	LEU	GLN	V353	
THR	I162	LYS	F359	
ASN	S163	TYR	P360	
LEU	A166	SER	L361	
LYS	L169	LYS	A362	
THR	F172	ASN	ASP	
PRO	I173	TYR	THR	
VAL	ASP	GLY	GLY	
ALA	GLU	ARG	GLN	
ALA	GLN	Y256	LYS	
GLN	V179	M262	THR	
	H180	F263	SER	
		E280	GLN	

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 156.19Å 179.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.48 – 2.30 47.48 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.9 (47.48-2.30) 99.9 (47.48-2.30)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.33 (at 2.29Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.196 , 0.244 0.197 , 0.244	Depositor DCC
R_{free} test set	6477 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	56.9	Xtriage
Anisotropy	0.164	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 48.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	17568	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.38% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ACP, CA, GDP, MG, MES, EDO, 2GE, GTP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.11	0/3486	0.30	0/4730
1	C	0.13	0/3522	0.31	0/4782
2	B	0.12	0/3418	0.32	0/4628
2	D	0.10	0/3399	0.28	0/4603
3	E	0.11	0/1008	0.24	0/1337
4	F	0.09	0/2630	0.28	0/3551
All	All	0.11	0/17463	0.30	0/23631

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	3409	0	3322	96	0
1	C	3444	0	3356	87	0
2	B	3344	0	3227	126	0
2	D	3326	0	3205	100	0
3	E	1000	0	1018	29	0
4	F	2573	0	2550	95	0
5	A	32	0	12	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	32	0	12	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
6	F	1	0	0	0	0
7	A	1	0	0	0	0
7	B	2	0	0	0	0
7	C	1	0	0	0	0
8	A	4	6	6	0	0
9	B	28	0	12	1	0
9	D	28	0	12	3	0
10	B	12	0	12	0	0
11	B	19	12	12	7	0
12	F	31	0	14	3	0
13	A	50	0	0	5	0
13	B	41	0	0	0	0
13	C	117	0	0	1	0
13	D	27	0	0	1	0
13	E	11	0	0	1	0
13	F	13	0	0	1	0
All	All	17550	18	16770	498	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 (498) 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)
4:F:173:ILE:HD12	4:F:180:HIS:HB2	1.32	1.07
1:C:270:ALA:HB3	1:C:302:MET:HE2	1.42	1.02
2:B:62:VAL:HG11	2:B:88:ARG:HG3	1.41	1.00
4:F:292:ARG:HB3	4:F:296:MET:HE3	1.43	0.96
2:B:176:LYS:HE2	2:B:207:GLU:HG3	1.54	0.90
2:D:62:VAL:HG11	2:D:88:ARG:HG3	1.53	0.90
2:D:406:HIS:HA	2:D:409:THR:HG22	1.54	0.89
4:F:102:PRO:HB3	4:F:173:ILE:HG12	1.54	0.88
2:D:75:MET:HE2	2:D:94:PHE:HD2	1.39	0.87
2:B:301:MET:HE2	2:B:301:MET:HA	1.56	0.86
4:F:127:GLU:HB3	4:F:130:VAL:HG22	1.56	0.86
4:F:296:MET:HE2	4:F:380:HIS:HB3	1.58	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:217:LEU:HD21	1:A:368:LEU:HD23	1.61	0.82
2:B:181:VAL:HG23	1:C:348:PRO:HG2	1.62	0.82
4:F:100:ILE:HG23	4:F:128:ARG:HB2	1.63	0.80
1:A:18:ASN:HD21	1:A:78:VAL:HG22	1.44	0.80
4:F:146:VAL:HG13	4:F:185:TYR:HB3	1.64	0.79
4:F:78:VAL:HG21	4:F:181:VAL:HG21	1.64	0.78
2:B:249:ASN:HB3	2:B:255:LEU:HB3	1.65	0.78
4:F:292:ARG:HH11	4:F:296:MET:HE1	1.49	0.77
1:A:209:ILE:HG22	1:A:227:LEU:HD22	1.67	0.77
2:B:396:THR:HG22	2:B:400:ARG:HD2	1.66	0.77
4:F:280:GLU:HA	4:F:284:LEU:HB2	1.67	0.77
2:B:202:TYR:CE2	2:B:270:PRO:HB3	2.20	0.76
1:C:276:ILE:HG13	1:C:280:LYS:HE2	1.65	0.76
1:A:30:ILE:HG12	1:A:36:MET:HE2	1.67	0.76
1:A:36:MET:HE3	1:A:61:HIS:CD2	2.20	0.75
4:F:150:LYS:HD3	4:F:151:SER:H	1.49	0.75
2:B:306:ASP:HB3	2:B:309:HIS:ND1	2.01	0.75
2:B:325:MET:HE3	2:B:355:VAL:HG11	1.69	0.75
3:E:120:LEU:O	3:E:124:GLN:HG2	1.86	0.74
1:A:280:LYS:HG3	13:A:601:HOH:O	1.88	0.73
1:A:36:MET:HG2	1:A:61:HIS:CE1	2.24	0.73
1:A:110:ILE:O	1:A:113:GLU:HG2	1.89	0.72
1:C:234:ILE:HG21	1:C:302:MET:SD	2.29	0.72
2:D:136:GLN:HA	2:D:167:ASN:O	1.90	0.72
4:F:217:ARG:NH2	4:F:345:GLU:OE2	2.23	0.72
2:D:301:MET:HA	2:D:301:MET:HE2	1.72	0.72
2:D:270:PRO:HG2	2:D:302:MET:HB2	1.72	0.71
1:A:221:ARG:HH11	2:B:325:MET:HB3	1.55	0.71
2:D:75:MET:HE2	2:D:94:PHE:CD2	2.25	0.71
2:B:176:LYS:CE	2:B:207:GLU:HG3	2.20	0.71
1:A:30:ILE:CG1	1:A:36:MET:HE2	2.21	0.70
4:F:127:GLU:HB3	4:F:130:VAL:CG2	2.20	0.70
2:D:240:THR:HB	2:D:318:ILE:HD13	1.71	0.70
4:F:14:TYR:HA	4:F:17:VAL:HG22	1.74	0.70
4:F:292:ARG:NH1	4:F:296:MET:HE1	2.07	0.70
1:A:209:ILE:HD11	1:A:302:MET:CE	2.22	0.70
1:A:270:ALA:HB3	1:A:302:MET:HG2	1.72	0.69
1:C:238:ILE:CD1	1:C:378:LEU:HD21	2.23	0.69
2:D:83:PHE:O	2:D:86:ILE:HG22	1.93	0.68
2:B:316:ALA:HB1	11:B:504:2GE:H3	1.75	0.68
2:D:323:MET:HE2	2:D:373:MET:HG2	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:159:GLU:HB3	3:E:123:LEU:HD13	1.76	0.68
2:B:119:LEU:HD11	2:B:156:LYS:HB3	1.74	0.68
2:B:172:MET:HG3	2:B:387:LEU:HD11	1.76	0.68
2:B:400:ARG:HH12	1:C:439:SER:HB3	1.58	0.68
1:A:109:THR:OG1	1:A:411:GLU:HG3	1.94	0.67
3:E:24:LEU:O	3:E:25:LYS:HG3	1.95	0.67
4:F:200:ASP:HB3	4:F:222:ARG:HB2	1.76	0.67
2:B:202:TYR:HB2	11:B:504:2GE:CL1	2.32	0.66
1:A:100:ALA:HA	2:B:254:LYS:HG2	1.76	0.66
1:C:234:ILE:HD13	1:C:302:MET:SD	2.35	0.66
1:C:167:LEU:HD22	1:C:200:CYS:HB3	1.77	0.66
2:D:23:VAL:HG21	2:D:232:SER:OG	1.95	0.66
4:F:95:PRO:HG2	4:F:183:GLN:OE1	1.95	0.66
2:D:21:TRP:CZ3	2:D:63:PRO:HB3	2.31	0.66
2:B:247:GLN:HA	2:B:250:ALA:HB2	1.78	0.66
1:A:3:GLU:O	1:A:133:GLN:HG2	1.97	0.65
4:F:5:VAL:CG2	4:F:32:LYS:HA	2.27	0.65
1:A:209:ILE:HD11	1:A:302:MET:HE1	1.79	0.65
1:A:336:LYS:HG3	3:E:24:LEU:HD23	1.79	0.65
3:E:129:HIS:O	3:E:133:VAL:HG23	1.97	0.65
2:B:338:LYS:HZ1	4:F:1:MET:HB3	1.62	0.65
2:B:400:ARG:HH12	1:C:439:SER:CB	2.10	0.64
2:D:48:ARG:NH2	2:D:241[B]:CYS:O	2.30	0.64
2:D:214:PHE:O	2:D:218:LYS:HA	1.97	0.64
4:F:73:ARG:HB2	4:F:76:SER:OG	1.97	0.64
4:F:292:ARG:HD3	4:F:378:LEU:HB3	1.78	0.64
1:A:221:ARG:NH1	2:B:325:MET:HB3	2.12	0.64
1:A:234:ILE:HD13	1:A:302:MET:SD	2.37	0.64
2:D:286:LEU:HD11	2:D:372:LYS:HE2	1.77	0.64
2:B:71:GLU:HG3	2:B:98:GLY:HA2	1.80	0.64
2:D:241[B]:CYS:SG	2:D:318:ILE:HD12	2.38	0.64
2:B:202:TYR:CZ	2:B:270:PRO:HB3	2.33	0.63
2:D:33:THR:HG22	2:D:60:LYS:NZ	2.13	0.63
2:D:318:ILE:CG2	2:D:376:THR:HB	2.27	0.63
1:C:334:THR:CG2	1:C:338:LYS:HE2	2.27	0.63
2:B:202:TYR:CZ	2:B:238:VAL:HG11	2.33	0.63
2:D:154:ILE:HG23	2:D:166:MET:HG2	1.81	0.63
1:C:30:ILE:CG1	1:C:36:MET:HE2	2.29	0.63
4:F:101:TYR:CE2	4:F:126:ASP:HB2	2.34	0.63
1:A:279:GLU:HB2	13:A:601:HOH:O	1.99	0.62
2:B:83:PHE:O	2:B:86:ILE:HG22	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:157:ILE:HG21	2:B:166:MET:HE1	1.81	0.62
1:C:320:ARG:HA	1:C:356:ASN:O	1.99	0.62
1:A:18:ASN:ND2	1:A:78:VAL:HG22	2.13	0.61
4:F:192:LEU:HD13	4:F:262:MET:HE1	1.82	0.61
2:B:195:VAL:HG13	2:B:264[A]:ARG:HG2	1.81	0.60
1:A:413:MET:HE3	1:A:417:GLU:HB3	1.83	0.60
4:F:287:ILE:HD13	4:F:327:VAL:HG11	1.83	0.60
2:B:36:TYR:CD1	2:B:46:LEU:HD21	2.35	0.60
1:A:270:ALA:HB3	1:A:302:MET:CG	2.31	0.60
2:D:291:LEU:HD22	2:D:375:ALA:CB	2.32	0.60
4:F:200:ASP:O	4:F:221:LEU:HA	2.01	0.60
4:F:200:ASP:HB2	4:F:241:THR:OG1	2.01	0.60
2:B:26:ASP:OD2	2:B:369:ARG:HD3	2.02	0.60
1:A:340:SER:O	1:A:341:ILE:HD13	2.02	0.59
2:B:114:LEU:HD23	2:B:149:MET:HE1	1.84	0.59
2:D:48:ARG:NH2	2:D:241[A]:CYS:O	2.36	0.59
2:B:259:MET:HG3	11:B:504:2GE:N01	2.17	0.59
2:D:240:THR:HB	2:D:318:ILE:CD1	2.32	0.59
2:B:334:ASN:O	2:B:338:LYS:HG2	2.03	0.58
1:C:248:LEU:HD23	1:C:357:TYR:CE2	2.38	0.58
2:D:295:MET:CG	2:D:377:PHE:HB2	2.32	0.58
2:B:42:LEU:HD22	2:B:358:ILE:HD11	1.85	0.58
1:A:302:MET:HE3	1:A:302:MET:HA	1.85	0.58
2:B:338:LYS:NZ	4:F:1:MET:HB3	2.18	0.58
4:F:100:ILE:CD1	4:F:128:ARG:HA	2.32	0.58
4:F:287:ILE:HD12	4:F:319:PHE:CD2	2.38	0.58
2:B:333:LEU:HD22	4:F:36:ARG:HH22	1.67	0.58
1:C:277:SER:OG	1:C:280:LYS:HD3	2.03	0.58
2:D:143:GLY:HA3	9:D:501:GDP:O3A	2.03	0.58
4:F:169:LEU:HD13	4:F:182:ILE:CD1	2.33	0.58
2:D:21:TRP:CE3	2:D:63:PRO:HB3	2.38	0.57
2:D:124:LYS:C	2:D:124:LYS:HD3	2.29	0.57
1:A:166:LYS:HE2	1:A:197:HIS:O	2.04	0.57
2:D:392:SER:O	2:D:396:THR:HG23	2.04	0.57
4:F:150:LYS:CD	4:F:151:SER:H	2.17	0.57
1:C:216:ASN:O	1:C:280:LYS:NZ	2.37	0.57
1:A:343:PHE:CD1	1:A:349:THR:HG23	2.39	0.57
2:B:167:ASN:ND2	2:B:252:LEU:HD22	2.19	0.57
2:B:172:MET:HE2	2:B:387:LEU:HD21	1.87	0.57
1:C:107:HIS:CE1	3:E:105:MET:HE1	2.40	0.57
2:B:181:VAL:HG23	1:C:348:PRO:CG	2.34	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:CYS:SG	1:A:86:LEU:HD11	2.45	0.56
1:A:69:ASP:O	1:A:94:THR:HA	2.05	0.56
2:B:295:MET:HG2	2:B:377:PHE:HB2	1.87	0.56
1:A:98:ASP:HB2	5:A:501:GTP:O1G	2.04	0.56
1:A:211:ASP:OD2	1:A:304:LYS:NZ	2.28	0.56
2:B:285:ALA:CB	2:B:372:LYS:HD3	2.35	0.56
3:E:136:ASN:OD1	3:E:140:LYS:HE2	2.05	0.56
4:F:186:LEU:HD21	4:F:322:ASP:HB3	1.88	0.56
2:D:217:LEU:HB2	2:D:219:LEU:HD13	1.88	0.56
4:F:101:TYR:CD2	4:F:126:ASP:HB2	2.41	0.56
2:B:259:MET:HG3	11:B:504:2GE:H5	1.69	0.56
4:F:146:VAL:CG1	4:F:187:GLU:HG2	2.36	0.56
1:A:21:TRP:CZ3	1:A:63:PRO:HB3	2.41	0.55
2:B:223:THR:HG23	2:B:226:ASP:H	1.72	0.55
2:D:248:LEU:HD23	2:D:353:THR:O	2.05	0.55
2:D:345:GLU:OE1	2:D:345:GLU:N	2.21	0.55
4:F:320:MET:HB2	4:F:330:ILE:HD11	1.88	0.55
4:F:82:LYS:NZ	4:F:127:GLU:OE1	2.37	0.55
4:F:169:LEU:HD13	4:F:182:ILE:HD12	1.88	0.55
1:A:245:ASP:HB3	3:E:16:SER:OG	2.07	0.55
2:B:325:MET:HE3	2:B:355:VAL:CG1	2.35	0.55
1:A:22:GLU:HG3	1:A:83:TYR:CE1	2.41	0.55
4:F:17:VAL:O	4:F:21:LEU:HG	2.06	0.55
2:B:295:MET:CG	2:B:377:PHE:HB2	2.37	0.55
4:F:263:PHE:CE2	4:F:341:LYS:HD3	2.42	0.55
4:F:102:PRO:HD3	4:F:173:ILE:HD11	1.88	0.55
1:A:209:ILE:CD1	1:A:302:MET:HE1	2.35	0.55
2:D:172:MET:HG3	2:D:387:LEU:HD11	1.88	0.55
2:B:69:ASP:O	2:B:94:PHE:HA	2.07	0.54
2:B:176:LYS:HE2	2:B:207:GLU:CG	2.32	0.54
1:C:181[A]:VAL:HG21	1:C:404:PHE:CZ	2.42	0.54
1:C:210:TYR:CZ	1:C:222:PRO:HD2	2.42	0.54
2:D:18:ALA:O	2:D:22:GLU:HG3	2.07	0.54
1:A:30:ILE:CD1	1:A:36:MET:HE2	2.38	0.54
1:C:276:ILE:HD11	1:C:280:LYS:C	2.32	0.54
4:F:37:PHE:CZ	4:F:40:MET:HE3	2.42	0.54
4:F:131:PHE:HD2	4:F:132:LEU:HD12	1.72	0.54
4:F:320:MET:HE1	12:F:701:ACP:C4	2.38	0.54
4:F:340:GLN:HA	4:F:343:TYR:HD2	1.72	0.54
1:C:271:THR:HG21	1:C:295:CYS:O	2.08	0.54
1:A:108:TYR:CE2	1:A:413:MET:HG3	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:286:LEU:CD1	2:D:372:LYS:HE2	2.37	0.54
1:C:93:ILE:HD11	1:C:121:ARG:HG3	1.89	0.54
2:D:413:MET:HE3	2:D:417:GLU:OE2	2.08	0.54
1:C:234:ILE:O	1:C:238:ILE:HG12	2.08	0.53
2:D:171:VAL:HA	2:D:204:ILE:O	2.08	0.53
2:D:173:PRO:HG3	2:D:187:ALA:HB2	1.91	0.53
2:D:406:HIS:HA	2:D:409:THR:CG2	2.32	0.53
1:C:21:TRP:CZ3	1:C:63:PRO:HB3	2.44	0.53
4:F:150:LYS:HD3	4:F:151:SER:N	2.22	0.53
2:B:67:LEU:N	2:B:67:LEU:HD12	2.24	0.53
4:F:14:TYR:HD1	4:F:17:VAL:HG21	1.72	0.53
4:F:44:ARG:HH11	4:F:335:ALA:HB1	1.73	0.53
2:B:141:LEU:HD12	2:B:172:MET:SD	2.48	0.53
2:B:402:LYS:HE2	2:B:415:GLU:OE1	2.09	0.53
1:C:173:PRO:HB3	1:C:183:GLU:OE1	2.09	0.53
1:C:229:ARG:NE	1:C:363:VAL:HG21	2.24	0.53
4:F:340:GLN:OE1	4:F:340:GLN:N	2.33	0.53
2:B:12:CYS:HB2	9:B:501:GDP:C8	2.44	0.53
1:A:209:ILE:HG22	1:A:227:LEU:CD2	2.36	0.53
2:D:141:LEU:HD12	2:D:172:MET:SD	2.48	0.53
4:F:242:ASN:ND2	12:F:701:ACP:H3B2	2.23	0.53
2:D:248:LEU:HD23	2:D:353:THR:C	2.34	0.53
4:F:296:MET:CE	4:F:380:HIS:HB3	2.36	0.53
1:A:34:GLY:O	1:A:61:HIS:N	2.33	0.53
2:B:62:VAL:CG1	2:B:88:ARG:HG3	2.27	0.53
1:C:140:SER:HA	1:C:171:ILE:HB	1.91	0.52
2:B:106:GLY:O	2:B:111:GLY:HA3	2.09	0.52
2:D:145:THR:HB	9:D:501:GDP:O2B	2.10	0.52
3:E:45:PRO:HA	3:E:49:GLU:OE1	2.09	0.52
2:B:332:MET:O	2:B:336:GLN:HG2	2.09	0.52
1:A:93:ILE:HD11	1:A:121:ARG:HG3	1.91	0.52
1:A:357:TYR:CZ	3:E:17:GLY:HA2	2.44	0.52
2:B:318:ILE:N	2:B:318:ILE:HD12	2.24	0.52
1:C:172:TYR:HB3	1:C:205:ASP:HA	1.92	0.52
2:D:103:TRP:CE3	2:D:189:LEU:HD13	2.45	0.52
2:B:33:THR:O	2:B:60:LYS:HE3	2.10	0.52
2:B:82:PRO:O	2:B:83:PHE:HB2	2.10	0.52
4:F:88:SER:C	4:F:90:SER:H	2.18	0.52
4:F:100:ILE:HD13	4:F:128:ARG:HA	1.91	0.52
2:B:67:LEU:HD22	2:B:92:PHE:CE2	2.44	0.52
2:B:251:ASP:O	2:B:255:LEU:HG	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:SER:HB3	1:A:391:LEU:HD21	1.91	0.51
1:C:244:PHE:CZ	1:C:358:GLN:HG2	2.45	0.51
4:F:97:SER:OG	4:F:183:GLN:HB3	2.10	0.51
1:A:132:LEU:O	1:A:164:LYS:HE3	2.10	0.51
2:B:119:LEU:HD11	2:B:156:LYS:CB	2.40	0.51
2:B:208:ALA:HB2	2:B:304:ALA:H	1.74	0.51
2:D:192:HIS:O	2:D:195:VAL:HG12	2.10	0.51
1:A:30:ILE:HD11	1:A:36:MET:HE2	1.93	0.51
2:B:252:LEU:HA	2:B:255:LEU:HD11	1.91	0.51
2:D:176:LYS:HD3	2:D:210:TYR:CD2	2.46	0.51
2:D:240:THR:CG2	2:D:318:ILE:HD11	2.41	0.51
1:A:286:LEU:O	1:A:373:ARG:NH1	2.42	0.51
2:B:205:ASP:OD2	2:B:304:ALA:HB3	2.10	0.51
2:B:357:ASP:O	2:B:359:PRO:HD3	2.11	0.51
2:D:295:MET:HG2	2:D:377:PHE:HB2	1.92	0.51
4:F:148:ILE:HD12	4:F:162:ILE:HG12	1.92	0.51
1:A:88:HIS:O	1:A:91:GLN:HG2	2.09	0.51
2:B:274:PRO:HB3	2:B:286:LEU:HD11	1.92	0.51
2:D:82:PRO:O	2:D:83:PHE:HB2	2.11	0.51
1:A:101:ASN:OD1	2:B:254:LYS:HE2	2.11	0.51
2:B:71:GLU:HG3	2:B:98:GLY:CA	2.41	0.51
2:B:136:GLN:HA	2:B:167:ASN:O	2.11	0.51
2:D:158:ARG:HG3	3:E:119:MET:HE2	1.92	0.50
1:C:238:ILE:HD12	1:C:378:LEU:HD21	1.93	0.50
1:C:292:THR:HG22	1:C:335:ILE:CD1	2.42	0.50
2:D:31:ASP:HB2	2:D:32:PRO:HD2	1.93	0.50
4:F:2:TYR:CE1	4:F:359:PHE:HB3	2.47	0.50
1:C:406:HIS:CD2	2:D:263:PRO:HD3	2.47	0.50
2:D:6:HIS:CD2	2:D:21:TRP:HE1	2.30	0.50
1:C:229:ARG:CD	1:C:363:VAL:HG21	2.42	0.50
1:C:406:HIS:CG	2:D:263:PRO:HD3	2.47	0.50
4:F:314:LEU:HD22	4:F:350:ILE:HD11	1.93	0.50
1:A:71:GLU:HG2	1:A:98:ASP:HB3	1.93	0.49
2:D:385:GLN:HB2	2:D:429:VAL:HG13	1.93	0.49
1:A:188:ILE:HG13	1:A:425:MET:HG3	1.93	0.49
1:A:346:TRP:H	1:A:346:TRP:CD1	2.30	0.49
1:A:34:GLY:HA2	1:A:86:LEU:CD2	2.43	0.49
1:A:55:GLU:HA	1:A:60:LYS:O	2.12	0.49
2:B:19:LYS:NZ	2:B:19:LYS:HB3	2.27	0.49
1:C:385:ALA:HA	1:C:388:TRP:CD1	2.46	0.49
2:D:31:ASP:HB2	2:D:32:PRO:CD	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:318:LEU:HD13	13:A:605:HOH:O	2.12	0.49
2:B:274:PRO:HB3	2:B:286:LEU:CD1	2.43	0.49
2:D:33:THR:HG22	2:D:60:LYS:HZ1	1.77	0.49
2:D:120:ASP:OD1	2:D:123:ARG:NH1	2.45	0.49
1:A:280:LYS:N	13:A:601:HOH:O	2.45	0.49
1:C:238:ILE:HD11	1:C:378:LEU:HD21	1.93	0.49
1:C:93:ILE:HG22	1:C:114:ILE:HD11	1.94	0.49
3:E:65:GLU:HG3	3:E:69:LEU:HD23	1.95	0.49
1:A:311:LYS:HE3	1:A:344:VAL:HG12	1.95	0.49
2:B:208:ALA:HB2	2:B:304:ALA:N	2.28	0.49
2:B:123:ARG:NH1	2:B:160:GLU:OE2	2.45	0.49
4:F:131:PHE:CD2	4:F:132:LEU:HD12	2.48	0.49
1:A:2:ARG:HB2	1:A:133:GLN:NE2	2.28	0.49
2:B:75:MET:HE3	2:B:92:PHE:CD2	2.48	0.49
1:A:265:ILE:HG23	1:A:432:TYR:CE1	2.47	0.48
1:C:334:THR:HG23	1:C:338:LYS:HE2	1.95	0.48
2:D:67:LEU:N	2:D:67:LEU:HD12	2.28	0.48
2:D:99:ALA:O	2:D:105:LYS:HD2	2.13	0.48
2:B:38:GLY:HA3	2:B:45:GLN:OE1	2.12	0.48
2:B:54:ASN:OD1	2:B:64:ARG:NH2	2.44	0.48
2:D:382:THR:O	2:D:385:GLN:HG2	2.12	0.48
3:E:139:LEU:HD23	3:E:139:LEU:C	2.38	0.48
1:C:180:ALA:O	1:C:183:GLU:HG3	2.14	0.48
4:F:216:TYR:CZ	4:F:218:GLU:HB2	2.48	0.48
2:B:174:SER:CB	2:B:207:GLU:HB2	2.43	0.48
1:C:1:MET:HE3	1:C:131:GLY:HA3	1.94	0.48
2:B:16:ILE:HD11	2:B:228:ASN:OD1	2.14	0.48
1:A:30:ILE:HD11	1:A:36:MET:CE	2.43	0.48
2:D:414:ASP:OD1	2:D:415:GLU:N	2.46	0.48
3:E:65:GLU:HG3	3:E:69:LEU:CD2	2.43	0.48
4:F:131:PHE:CE1	4:F:182:ILE:HD13	2.48	0.48
2:D:36:TYR:CD1	2:D:46:LEU:HD21	2.49	0.48
1:C:181[A]:VAL:O	1:C:398:MET:HE1	2.14	0.48
2:B:11:GLN:HA	2:B:74:THR:HG21	1.95	0.47
2:B:387:LEU:C	2:B:387:LEU:HD23	2.39	0.47
1:A:54:SER:O	1:A:61:HIS:HA	2.14	0.47
2:B:204:ILE:HD13	2:B:231:VAL:HG13	1.95	0.47
4:F:146:VAL:HG12	4:F:187:GLU:HG2	1.96	0.47
2:B:96:GLN:HB3	1:C:1:MET:HE2	1.96	0.47
2:B:3:GLU:OE2	2:B:130:ASP:N	2.46	0.47
2:D:12:CYS:HB2	9:D:501:GDP:C8	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:191:LEU:HD12	4:F:196:HIS:CE1	2.50	0.47
1:A:409:VAL:HA	1:A:413:MET:O	2.14	0.47
1:C:188:ILE:HG13	1:C:425:MET:HG3	1.96	0.47
1:A:210:TYR:OH	1:A:221:ARG:HD2	2.15	0.47
2:B:1:MET:HB3	2:B:3:GLU:OE2	2.15	0.47
1:C:209:ILE:HG23	1:C:230:LEU:HD23	1.96	0.47
4:F:132:LEU:HD12	4:F:132:LEU:N	2.29	0.47
1:C:151:SER:HB3	1:C:193:THR:HG21	1.96	0.47
2:D:185:TYR:OH	2:D:398:MET:O	2.33	0.47
1:C:30:ILE:HG12	1:C:36:MET:HE2	1.96	0.47
1:C:344:VAL:HG21	1:C:346:TRP:CE2	2.50	0.46
1:C:119:LEU:HD11	1:C:156:ARG:HB3	1.95	0.46
2:D:12:CYS:HB3	2:D:140:SER:HB3	1.97	0.46
2:D:291:LEU:HD22	2:D:375:ALA:HB2	1.96	0.46
1:A:210:TYR:CD1	1:A:222:PRO:HG2	2.50	0.46
1:A:247:ALA:HB3	3:E:19:SER:OG	2.15	0.46
1:C:88:HIS:HE1	1:C:90:GLU:HG3	1.80	0.46
4:F:101:TYR:HD1	4:F:179:VAL:HG22	1.79	0.46
2:D:195:VAL:HG11	2:D:424:ASN:OD1	2.15	0.46
2:D:387:LEU:HD23	2:D:387:LEU:C	2.40	0.46
4:F:292:ARG:HH11	4:F:296:MET:CE	2.24	0.46
2:B:161:TYR:HB3	2:B:164:ARG:HG3	1.96	0.46
2:B:202:TYR:HE2	2:B:234:THR:CG2	2.29	0.46
1:C:7:ILE:HG21	1:C:153:LEU:HD21	1.97	0.46
4:F:26:GLN:NE2	4:F:361:LEU:HD22	2.30	0.46
4:F:61:LEU:HD11	4:F:312:PHE:HD2	1.81	0.46
4:F:283:ILE:HG23	4:F:327:VAL:CG2	2.46	0.46
2:B:210:TYR:CE1	2:B:222:PRO:HD2	2.51	0.46
2:D:26:ASP:CG	2:D:369:ARG:HE	2.24	0.46
4:F:146:VAL:HG12	4:F:187:GLU:CD	2.41	0.46
4:F:296:MET:HE2	4:F:380:HIS:CB	2.38	0.46
1:A:227:LEU:O	1:A:231:ILE:HG13	2.15	0.46
2:B:255:LEU:HD13	11:B:504:2GE:N03	2.30	0.46
2:B:301:MET:HE1	2:B:377:PHE:CD2	2.51	0.46
1:C:275:VAL:HG13	1:C:368:LEU:HD21	1.97	0.46
1:C:88:HIS:CE1	1:C:90:GLU:HG3	2.51	0.45
1:A:270:ALA:O	1:A:302:MET:HG2	2.17	0.45
2:B:119:LEU:HD11	2:B:156:LYS:HG2	1.99	0.45
1:C:36:MET:HE3	1:C:61:HIS:CD2	2.51	0.45
1:A:349:THR:HB	3:E:25:LYS:HB2	1.99	0.45
2:B:323:MET:HB3	2:B:373:MET:HE1	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:333:ALA:O	1:C:337:THR:HG23	2.16	0.45
2:D:291:LEU:HD22	2:D:375:ALA:HB3	1.99	0.45
1:A:433:GLU:O	1:A:437:VAL:HG23	2.16	0.45
2:B:396:THR:O	2:B:400:ARG:HG3	2.17	0.45
1:C:179:THR:HG21	2:D:247:GLN:HE21	1.81	0.45
2:B:75:MET:HE3	2:B:92:PHE:HD2	1.82	0.45
2:B:345:GLU:OE1	2:B:345:GLU:N	2.39	0.45
2:D:12:CYS:CB	2:D:140:SER:HB3	2.47	0.45
4:F:287:ILE:HG23	4:F:319:PHE:CE2	2.51	0.45
1:A:298:PRO:HA	1:A:301:GLN:CD	2.41	0.45
2:B:241:CYS:SG	11:B:504:2GE:N15	2.81	0.45
2:D:69:ASP:O	2:D:94:PHE:HA	2.16	0.45
2:D:248:LEU:HD21	2:D:352:LYS:HB3	1.99	0.45
4:F:132:LEU:HD12	4:F:132:LEU:H	1.80	0.45
1:A:347:CYS:C	3:E:27:PRO:HB3	2.41	0.45
2:B:309:HIS:O	2:B:436:GLN:NE2	2.50	0.45
1:C:165:SER:HA	1:C:199:ASP:OD2	2.17	0.45
1:A:105:ARG:HA	1:A:411:GLU:HG2	1.99	0.45
2:B:96:GLN:CB	1:C:1:MET:HE2	2.47	0.45
2:B:159:GLU:HB2	3:E:72:LEU:HD13	1.98	0.45
1:C:254:GLU:HG2	1:C:352:LYS:HE2	1.99	0.45
2:D:427:ASP:O	2:D:431:GLU:HG3	2.17	0.45
4:F:146:VAL:HG12	4:F:187:GLU:CG	2.47	0.45
2:D:114:LEU:HD21	2:D:149:MET:SD	2.57	0.44
2:D:264:ARG:HH12	2:D:424:ASN:HD21	1.65	0.44
4:F:283:ILE:HG23	4:F:327:VAL:HG21	1.99	0.44
2:B:255:LEU:HB2	11:B:504:2GE:N01	2.32	0.44
1:C:60:LYS:HE2	1:C:85:GLN:O	2.18	0.44
4:F:100:ILE:HG12	4:F:128:ARG:HA	1.99	0.44
4:F:189:PRO:HA	4:F:322:ASP:HA	1.98	0.44
1:A:167:LEU:HD13	1:A:252:LEU:HD22	2.00	0.44
2:B:330:GLU:O	2:B:334:ASN:HB2	2.18	0.44
1:C:227:LEU:O	1:C:231:ILE:HG13	2.17	0.44
4:F:206:LEU:HD23	4:F:353:VAL:CG2	2.48	0.44
1:C:2:ARG:HA	1:C:2:ARG:NE	2.32	0.44
4:F:216:TYR:CE2	4:F:218:GLU:HB2	2.53	0.44
4:F:283:ILE:O	4:F:287:ILE:HG12	2.17	0.44
2:B:203:CYS:SG	2:B:267:PHE:HB3	2.58	0.44
1:A:331:ALA:O	1:A:334:THR:HG22	2.18	0.44
2:D:33:THR:HG22	2:D:60:LYS:HZ2	1.81	0.44
3:E:47:LEU:O	3:E:51:GLN:HG2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:231:VAL:O	2:B:235:MET:HG3	2.18	0.43
4:F:220:VAL:HG12	4:F:263:PHE:CD1	2.53	0.43
1:A:36:MET:HG3	1:A:39:ASP:HB2	2.00	0.43
1:A:217:LEU:HD21	1:A:368:LEU:CD2	2.41	0.43
2:D:247:GLN:O	2:D:247:GLN:HG2	2.18	0.43
4:F:146:VAL:HG12	4:F:187:GLU:OE2	2.19	0.43
2:B:171:VAL:HA	2:B:204:ILE:O	2.17	0.43
1:C:75:ILE:HD12	1:C:94:THR:HG22	2.00	0.43
1:C:335:ILE:O	1:C:339:ARG:HB3	2.18	0.43
1:A:36:MET:HG3	1:A:36:MET:O	2.18	0.43
2:B:108:TYR:OH	2:B:417:GLU:OE2	2.36	0.43
2:B:167:ASN:OD1	2:B:200:GLU:HB2	2.18	0.43
1:A:128:GLN:O	1:A:128:GLN:HG3	2.18	0.43
1:A:209:ILE:HG23	1:A:230:LEU:HD23	2.00	0.43
2:D:46:LEU:HA	2:D:49:ILE:HB	2.00	0.43
2:B:174:SER:HB2	2:B:207:GLU:HB2	2.01	0.43
2:D:23:VAL:O	2:D:27:GLU:HG3	2.19	0.43
4:F:3:THR:O	4:F:38:ASN:HB2	2.17	0.43
1:A:426:ALA:HA	13:A:628:HOH:O	2.19	0.43
2:B:31:ASP:HB2	2:B:32:PRO:HD2	2.01	0.43
2:B:332:MET:O	2:B:335:VAL:HG12	2.19	0.43
2:B:345:GLU:HG3	13:F:811:HOH:O	2.18	0.43
1:C:209:ILE:HG22	1:C:227:LEU:HD22	2.01	0.43
1:C:225:THR:OG1	13:C:601:HOH:O	2.21	0.43
2:D:417:GLU:OE1	3:E:129:HIS:NE2	2.48	0.43
4:F:132:LEU:HA	4:F:135:TYR:HB3	2.01	0.43
1:A:270:ALA:CB	1:A:302:MET:HG2	2.45	0.43
1:A:275:VAL:HG13	1:A:368:LEU:HD21	2.01	0.43
1:C:1:MET:O	1:C:2:ARG:HB2	2.18	0.43
1:A:16:ILE:HD13	1:A:171:ILE:HD11	2.01	0.43
2:B:385:GLN:OE1	2:B:389:LYS:HE3	2.19	0.43
1:C:21:TRP:CE3	1:C:63:PRO:HB3	2.54	0.43
2:D:318:ILE:HG22	2:D:376:THR:HB	1.98	0.43
2:D:431:GLU:OE1	13:D:601:HOH:O	2.21	0.43
4:F:205:VAL:HG21	4:F:291:ILE:HD13	2.01	0.43
2:D:119:LEU:O	2:D:123:ARG:HG3	2.19	0.42
4:F:340:GLN:HA	4:F:343:TYR:CD2	2.54	0.42
4:F:102:PRO:HB3	4:F:173:ILE:CG1	2.38	0.42
4:F:305:LYS:HE2	4:F:306:HIS:NE2	2.33	0.42
1:A:234:ILE:O	1:A:238:ILE:HG13	2.20	0.42
2:B:42:LEU:H	2:B:42:LEU:HD12	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:181:VAL:HG23	1:C:348:PRO:CD	2.49	0.42
2:D:11:GLN:HA	2:D:74:THR:HG21	2.00	0.42
2:B:337:ASN:ND2	4:F:58:LEU:HD21	2.34	0.42
4:F:320:MET:HE1	12:F:701:ACP:N3	2.34	0.42
1:A:348:PRO:HB3	3:E:27:PRO:HD3	2.01	0.42
2:B:297:ASP:OD1	2:B:298:SER:N	2.53	0.42
4:F:188:LYS:HB2	4:F:323:GLU:CD	2.45	0.42
2:B:1:MET:HB3	2:B:3:GLU:CD	2.45	0.42
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.37	0.42
1:C:334:THR:HG22	1:C:338:LYS:HE2	2.02	0.42
2:D:70:LEU:H	2:D:145:THR:HG21	1.84	0.42
1:A:172:TYR:HB3	1:A:205:ASP:HA	2.02	0.42
1:A:187:SER:CB	1:A:391:LEU:HD21	2.49	0.42
1:A:357:TYR:CE2	3:E:17:GLY:HA2	2.54	0.42
2:B:21:TRP:CZ3	2:B:63:PRO:HB3	2.55	0.42
1:C:224:TYR:HE2	2:D:247:GLN:OE1	2.02	0.42
1:C:280:LYS:HE2	1:C:280:LYS:HB2	1.80	0.42
2:D:385:GLN:O	2:D:389:LYS:HB2	2.20	0.42
4:F:299:GLU:HB3	4:F:300:PRO:HD3	2.02	0.42
1:A:16:ILE:CD1	1:A:171:ILE:HD11	2.49	0.42
2:B:220:THR:O	2:B:221:THR:HB	2.20	0.42
1:C:108:TYR:O	1:C:112:LYS:HG2	2.20	0.42
1:C:306:ASP:OD1	1:C:308:ARG:HG2	2.19	0.42
1:A:34:GLY:O	1:A:60:LYS:HA	2.20	0.41
1:C:25:CYS:HB3	1:C:30:ILE:O	2.20	0.41
2:D:218:LYS:HA	2:D:218:LYS:HD2	1.80	0.41
1:A:250:VAL:HG22	1:A:254:GLU:OE1	2.20	0.41
2:B:195:VAL:CG1	2:B:264[A]:ARG:HG2	2.47	0.41
3:E:46:SER:O	3:E:50:ILE:HG13	2.20	0.41
4:F:220:VAL:HG12	4:F:263:PHE:CE1	2.55	0.41
1:A:210:TYR:CE1	1:A:222:PRO:HG2	2.55	0.41
2:D:398:MET:HA	2:D:401:ARG:HE	1.85	0.41
2:B:237:GLY:HA3	2:B:376:THR:OG1	2.21	0.41
2:D:244:PHE:CE1	2:D:358:ILE:HD12	2.56	0.41
3:E:65:GLU:O	3:E:69:LEU:HD23	2.21	0.41
4:F:209:HIS:HA	4:F:311:SER:O	2.20	0.41
2:B:227:LEU:O	2:B:231:VAL:HG23	2.20	0.41
1:C:180:ALA:HA	2:D:258:ASN:OD1	2.21	0.41
1:C:233:GLN:HG3	1:C:368:LEU:CD1	2.50	0.41
3:E:100:LYS:HE3	3:E:100:LYS:HB2	1.85	0.41
1:C:181[B]:VAL:O	1:C:398:MET:HE1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:214:ARG:HG2	1:C:219:ILE:O	2.21	0.41
1:C:248:LEU:HD23	1:C:357:TYR:HE2	1.84	0.41
4:F:150:LYS:CG	4:F:151:SER:H	2.34	0.41
1:A:36:MET:CG	1:A:39:ASP:HB2	2.51	0.41
1:A:47:ASP:OD1	1:A:47:ASP:N	2.54	0.41
2:B:108:TYR:CG	3:E:82:VAL:HG11	2.56	0.41
2:B:181:VAL:CG2	1:C:348:PRO:HD2	2.50	0.41
1:C:385:ALA:HA	1:C:388:TRP:HD1	1.86	0.41
2:D:7:ILE:O	2:D:137:LEU:HA	2.21	0.41
2:D:33:THR:HG22	2:D:33:THR:O	2.20	0.41
2:D:208:ALA:O	2:D:212:ILE:HG13	2.20	0.41
1:C:270:ALA:CB	1:C:302:MET:HE2	2.30	0.41
2:D:5:VAL:HG23	2:D:132:LEU:CD1	2.51	0.41
2:D:334:ASN:OD1	2:D:338:LYS:HE3	2.20	0.41
3:E:121:GLU:HA	3:E:124:GLN:HG2	2.02	0.41
2:B:133:GLN:OE1	2:B:252:LEU:N	2.51	0.40
2:B:234:THR:O	2:B:238:VAL:HG13	2.21	0.40
2:B:285:ALA:HB2	2:B:372:LYS:HD3	2.02	0.40
1:C:248:LEU:HB3	1:C:355:ILE:HB	2.02	0.40
1:A:5:ILE:O	1:A:135:PHE:HA	2.21	0.40
1:A:34:GLY:HA2	1:A:86:LEU:HD23	2.02	0.40
1:A:209:ILE:CG2	1:A:227:LEU:HD22	2.42	0.40
1:A:234:ILE:HD13	1:A:302:MET:CE	2.51	0.40
2:D:114:LEU:HD23	2:D:114:LEU:H	1.86	0.40
2:D:389:LYS:HD3	2:D:429:VAL:HG11	2.02	0.40
4:F:163:SER:HB2	4:F:169:LEU:CD2	2.51	0.40
2:B:119:LEU:HD11	2:B:156:LYS:CG	2.51	0.40
2:D:182:VAL:HG22	2:D:408:TYR:OH	2.22	0.40
1:C:150:THR:O	1:C:154:MET:HG2	2.22	0.40
3:E:95:LYS:HD2	13:E:205:HOH:O	2.20	0.40
3:E:103:GLN:HG3	3:E:104:LYS:N	2.36	0.40
2:B:31:ASP:HB2	2:B:32:PRO:CD	2.51	0.40
1:C:18:ASN:OD1	1:C:78:VAL:HG22	2.22	0.40
1:C:75:ILE:HB	1:C:94:THR:CG2	2.51	0.40
1:C:430:LYS:NZ	1:C:434:GLU:OE2	2.45	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	432/451 (96%)	423 (98%)	9 (2%)	0	100	100
1	C	439/451 (97%)	426 (97%)	13 (3%)	0	100	100
2	B	420/445 (94%)	407 (97%)	13 (3%)	0	100	100
2	D	419/445 (94%)	404 (96%)	15 (4%)	0	100	100
3	E	117/143 (82%)	116 (99%)	1 (1%)	0	100	100
4	F	298/384 (78%)	284 (95%)	14 (5%)	0	100	100
All	All	2125/2319 (92%)	2060 (97%)	65 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	367/379 (97%)	366 (100%)	1 (0%)	86	93
1	C	372/379 (98%)	371 (100%)	1 (0%)	86	93
2	B	367/383 (96%)	364 (99%)	3 (1%)	73	86
2	D	366/383 (96%)	362 (99%)	4 (1%)	65	81
3	E	109/127 (86%)	109 (100%)	0	100	100
4	F	283/342 (83%)	281 (99%)	2 (1%)	76	87
All	All	1864/1993 (94%)	1853 (99%)	11 (1%)	78	89

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	176	GLN
2	B	247	GLN
2	B	255	LEU
2	B	322	ARG
1	C	241	SER
2	D	26	ASP
2	D	74	THR
2	D	389	LYS
2	D	402	LYS
4	F	331	GLU
4	F	348	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	300	ASN
1	A	372	GLN
2	B	8	GLN
2	B	14	ASN
2	B	136	GLN
2	B	247	GLN
2	B	258	ASN
2	B	282	GLN
2	B	436	GLN
1	C	15	GLN
1	C	101	ASN
1	C	300	ASN
3	E	18	GLN
3	E	103	GLN
3	E	115	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 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
9	GDP	B	501	6	29,30,30	1.17	4 (13%)	45,47,47	1.75	7 (15%)
5	GTP	C	501	6	33,34,34	1.00	3 (9%)	50,54,54	1.54	10 (20%)
8	EDO	A	504	-	3,3,3	0.43	0	2,2,2	0.37	0
12	ACP	F	701	6	31,33,33	1.36	5 (16%)	47,52,52	1.99	9 (19%)
9	GDP	D	501	6	29,30,30	1.17	3 (10%)	45,47,47	1.71	6 (13%)
10	MES	B	503	-	12,12,12	2.26	1 (8%)	15,16,16	1.79	2 (13%)
5	GTP	A	501	6	33,34,34	0.98	3 (9%)	50,54,54	1.53	10 (20%)
11	2GE	B	504	-	21,21,21	1.31	2 (9%)	28,30,30	2.16	9 (32%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	GDP	B	501	6	-	3/16/32/32	0/3/3/3
5	GTP	C	501	6	-	9/22/38/38	0/3/3/3
8	EDO	A	504	-	-	0/1/1/1	-
12	ACP	F	701	6	-	5/19/38/38	0/3/3/3
9	GDP	D	501	6	-	4/16/32/32	0/3/3/3
10	MES	B	503	-	-	0/6/14/14	0/1/1/1
5	GTP	A	501	6	-	9/22/38/38	0/3/3/3
11	2GE	B	504	-	-	4/8/10/10	0/3/3/3

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	503	MES	C8-S	-7.54	1.67	1.77
12	F	701	ACP	PB-O3A	3.33	1.62	1.58
11	B	504	2GE	C02-N01	3.22	1.40	1.33
9	D	501	GDP	C5-C4	3.07	1.47	1.38
9	B	501	GDP	C5-C4	3.01	1.47	1.38
12	F	701	ACP	PG-O2G	2.92	1.61	1.55
12	F	701	ACP	PG-O3G	2.84	1.61	1.55
9	B	501	GDP	C6-N1	-2.40	1.34	1.38
12	F	701	ACP	PA-O3A	2.39	1.62	1.59
5	A	501	GTP	PA-O3A	2.33	1.62	1.59
9	D	501	GDP	C6-N1	-2.26	1.34	1.38
5	C	501	GTP	PB-O3A	2.22	1.61	1.59
11	B	504	2GE	C07-C06	2.16	1.42	1.38
9	D	501	GDP	C5-N7	-2.15	1.34	1.39
5	A	501	GTP	PB-O3A	2.08	1.61	1.59
5	C	501	GTP	PB-O3B	2.08	1.61	1.59
5	C	501	GTP	C2-N3	2.07	1.38	1.33
9	B	501	GDP	PA-O3A	2.06	1.61	1.59
12	F	701	ACP	PB-O2B	2.06	1.61	1.56
9	B	501	GDP	C5-N7	-2.05	1.35	1.39
5	A	501	GTP	C2-N3	2.02	1.38	1.33

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	F	701	ACP	PB-O3A-PA	-6.05	112.64	132.37
9	B	501	GDP	C5-C4-N3	-5.98	118.88	128.39
9	D	501	GDP	C5-C4-N3	-5.84	119.10	128.39
11	B	504	2GE	C11-C09-CL1	-5.63	115.34	120.51
12	F	701	ACP	C5-C4-N3	-5.60	119.00	126.72
9	B	501	GDP	C2-N3-C4	5.05	121.00	112.30
11	B	504	2GE	C05-C11-CL2	4.98	123.99	119.67
10	B	503	MES	C5-N4-C3	4.93	119.45	108.84
9	D	501	GDP	C2-N3-C4	4.87	120.69	112.30
12	F	701	ACP	N3-C4-N9	4.71	135.18	127.17
5	A	501	GTP	C5-C4-N3	-4.65	120.99	128.39
5	C	501	GTP	C5-C4-N3	-4.46	121.28	128.39
5	C	501	GTP	C2-N3-C4	4.39	119.86	112.30
9	D	501	GDP	N9-C4-N3	4.38	134.72	125.95
5	A	501	GTP	C2-N3-C4	4.37	119.82	112.30
9	B	501	GDP	N9-C4-N3	4.33	134.61	125.95
12	F	701	ACP	N3-C2-N1	-4.01	122.51	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	F	701	ACP	C5-N7-C8	3.71	109.28	103.45
11	B	504	2GE	N15-C14-N19	3.64	122.29	117.03
12	F	701	ACP	C2-N3-C4	3.56	120.52	111.83
9	B	501	GDP	C6-C5-N7	3.52	136.69	130.29
9	D	501	GDP	C6-C5-N7	3.24	136.19	130.29
11	B	504	2GE	C04-N03-C02	3.10	118.19	116.35
5	C	501	GTP	N9-C8-N7	-2.97	107.89	113.40
5	C	501	GTP	N9-C4-N3	2.89	131.74	125.95
12	F	701	ACP	C4-C5-N7	-2.85	107.33	110.58
11	B	504	2GE	N01-C02-N19	2.84	121.48	117.22
5	A	501	GTP	N9-C4-N3	2.81	131.58	125.95
9	B	501	GDP	C4-C5-N7	-2.79	106.25	110.67
5	A	501	GTP	C2-N1-C6	-2.76	120.11	125.11
11	B	504	2GE	C04-C05-C11	2.74	125.10	121.01
12	F	701	ACP	N9-C8-N7	-2.71	110.09	113.94
5	A	501	GTP	N9-C8-N7	-2.70	108.39	113.40
5	C	501	GTP	C2-N1-C6	-2.60	120.40	125.11
5	C	501	GTP	C8-N7-C5	2.58	108.86	104.26
5	A	501	GTP	C8-N7-C5	2.54	108.79	104.26
11	B	504	2GE	C09-C11-CL2	-2.52	116.82	120.02
11	B	504	2GE	N01-C02-N03	-2.48	113.51	117.22
9	D	501	GDP	C4-C5-N7	-2.46	106.78	110.67
10	B	503	MES	O1S-S-C8	2.45	110.42	106.73
5	C	501	GTP	O6-C6-C5	-2.42	120.14	126.53
5	A	501	GTP	C5-C6-N1	2.36	119.27	113.25
5	C	501	GTP	O2A-PA-O3A	2.32	113.54	107.27
5	C	501	GTP	C5-C6-N1	2.32	119.16	113.25
5	A	501	GTP	O3G-PG-O3B	2.32	112.41	104.64
12	F	701	ACP	PA-O5'-C5'	-2.30	108.15	121.35
9	D	501	GDP	O6-C6-C5	-2.30	120.46	126.53
5	A	501	GTP	O6-C6-C5	-2.18	120.77	126.53
9	B	501	GDP	O6-C6-C5	-2.16	120.83	126.53
5	A	501	GTP	O2A-PA-O3A	2.12	113.00	107.27
11	B	504	2GE	C08-C09-CL1	2.07	122.50	118.42
5	C	501	GTP	O3G-PG-O3B	2.05	111.51	104.64
9	B	501	GDP	C8-N7-C5	2.04	107.89	104.26

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	501	GTP	PB-O3B-PG-O3G

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Mol	Chain	Res	Type	Atoms
5	A	501	GTP	C5'-O5'-PA-O3A
5	A	501	GTP	C5'-O5'-PA-O1A
5	A	501	GTP	C5'-O5'-PA-O2A
5	C	501	GTP	PB-O3B-PG-O2G
5	C	501	GTP	PB-O3B-PG-O3G
5	C	501	GTP	C5'-O5'-PA-O3A
5	C	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O2A
9	B	501	GDP	C5'-O5'-PA-O3A
9	B	501	GDP	C5'-O5'-PA-O1A
9	B	501	GDP	C5'-O5'-PA-O2A
9	D	501	GDP	C5'-O5'-PA-O3A
9	D	501	GDP	C5'-O5'-PA-O1A
9	D	501	GDP	C5'-O5'-PA-O2A
11	B	504	2GE	C13-C14-N15-C16
11	B	504	2GE	N19-C14-N15-C16
12	F	701	ACP	C5'-O5'-PA-O2A
5	A	501	GTP	PB-O3B-PG-O2G
12	F	701	ACP	PB-C3B-PG-O2G
12	F	701	ACP	PG-C3B-PB-O2B
12	F	701	ACP	C5'-O5'-PA-O1A
12	F	701	ACP	C5'-O5'-PA-O3A
5	A	501	GTP	PB-O3A-PA-O2A
5	A	501	GTP	C4'-C5'-O5'-PA
5	C	501	GTP	PB-O3A-PA-O2A
5	A	501	GTP	PB-O3B-PG-O1G
5	C	501	GTP	PB-O3B-PG-O1G
9	D	501	GDP	PA-O3A-PB-O2B
5	C	501	GTP	PB-O3A-PA-O1A
11	B	504	2GE	C13-C04-C05-C11
5	C	501	GTP	C4'-C5'-O5'-PA
11	B	504	2GE	N03-C04-C05-C11
5	A	501	GTP	PB-O3A-PA-O1A

There are no ring outliers.

5 monomers are involved in 15 short contacts:

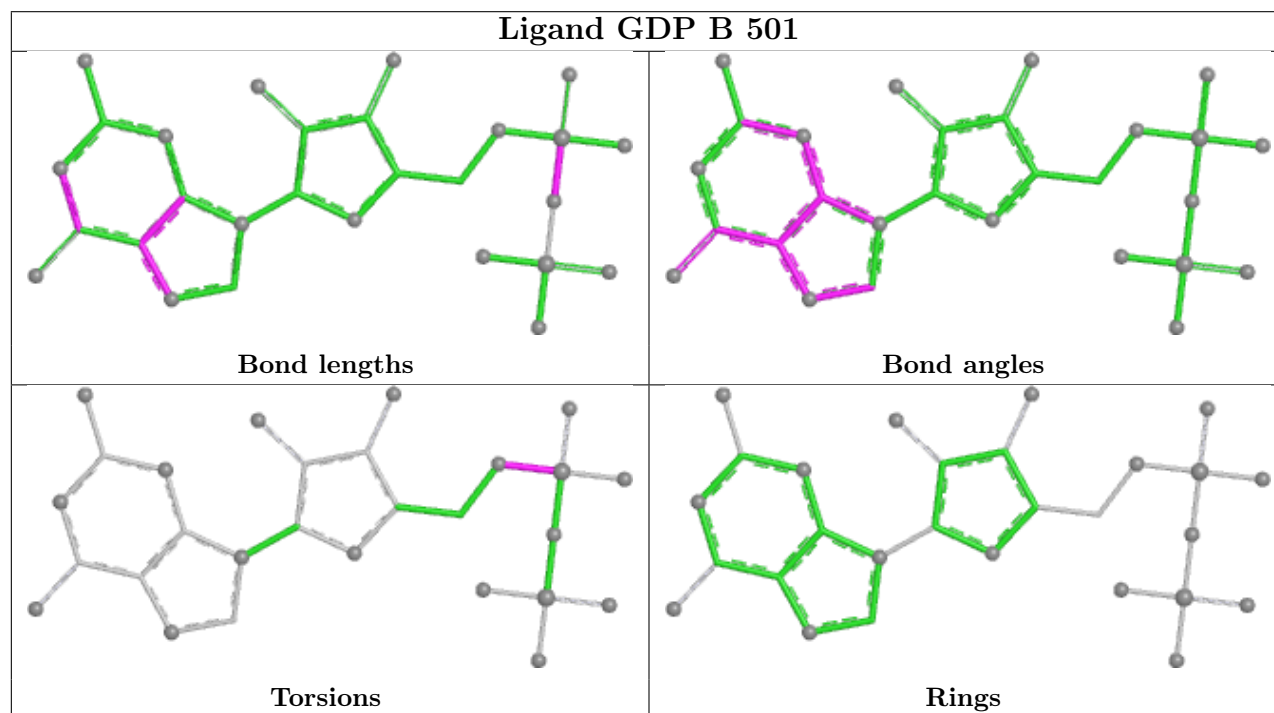
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	B	501	GDP	1	0
12	F	701	ACP	3	0
9	D	501	GDP	3	0
5	A	501	GTP	1	0

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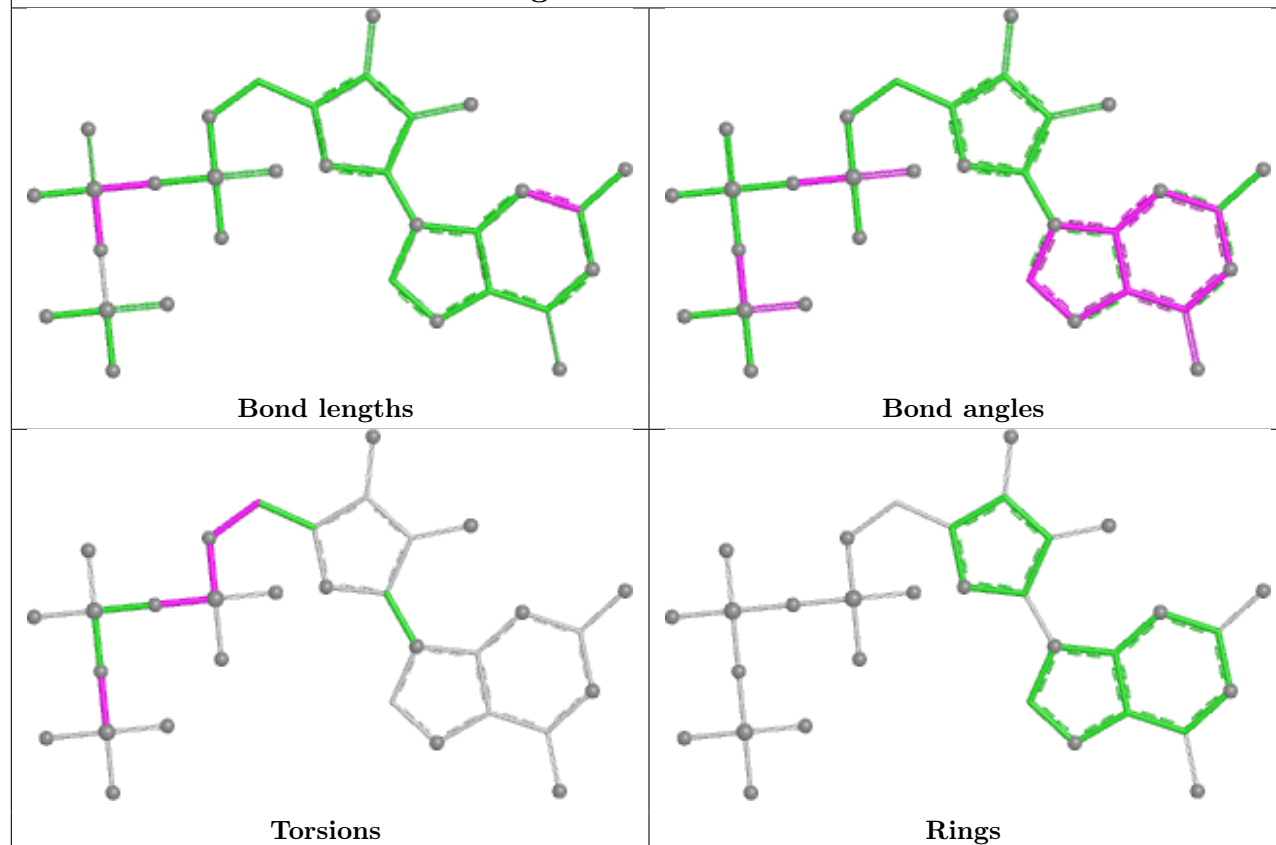
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	B	504	2GE	7	0

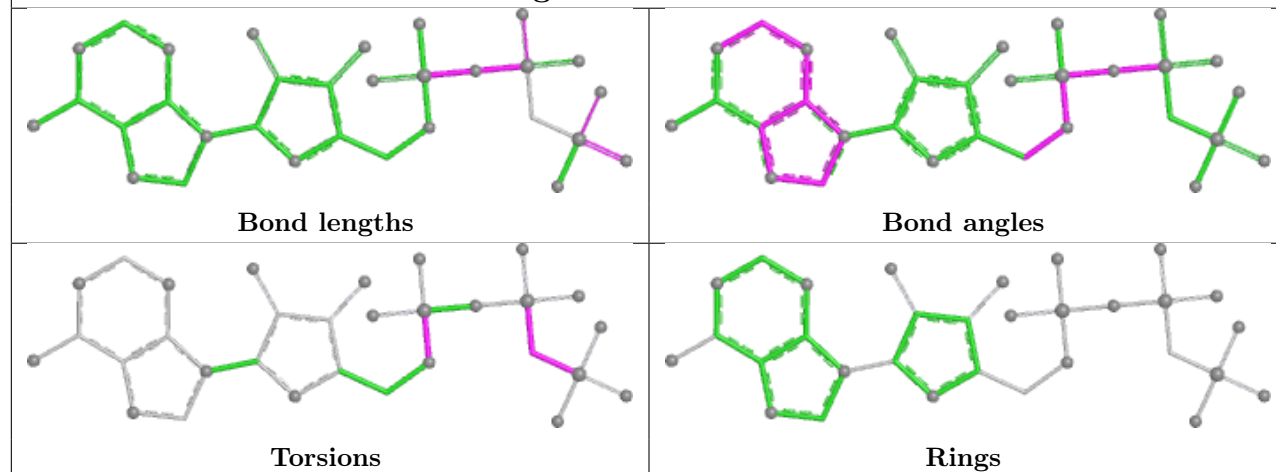
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

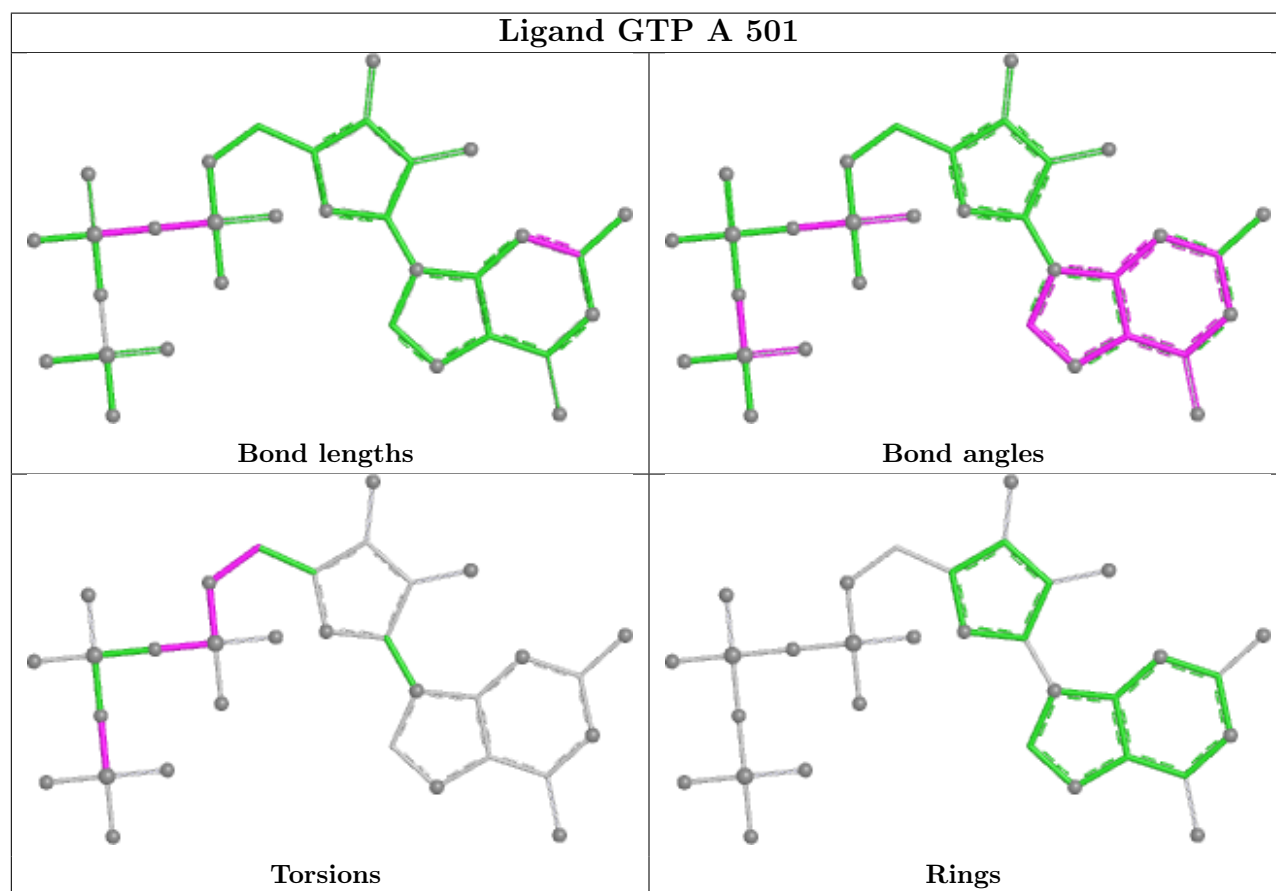
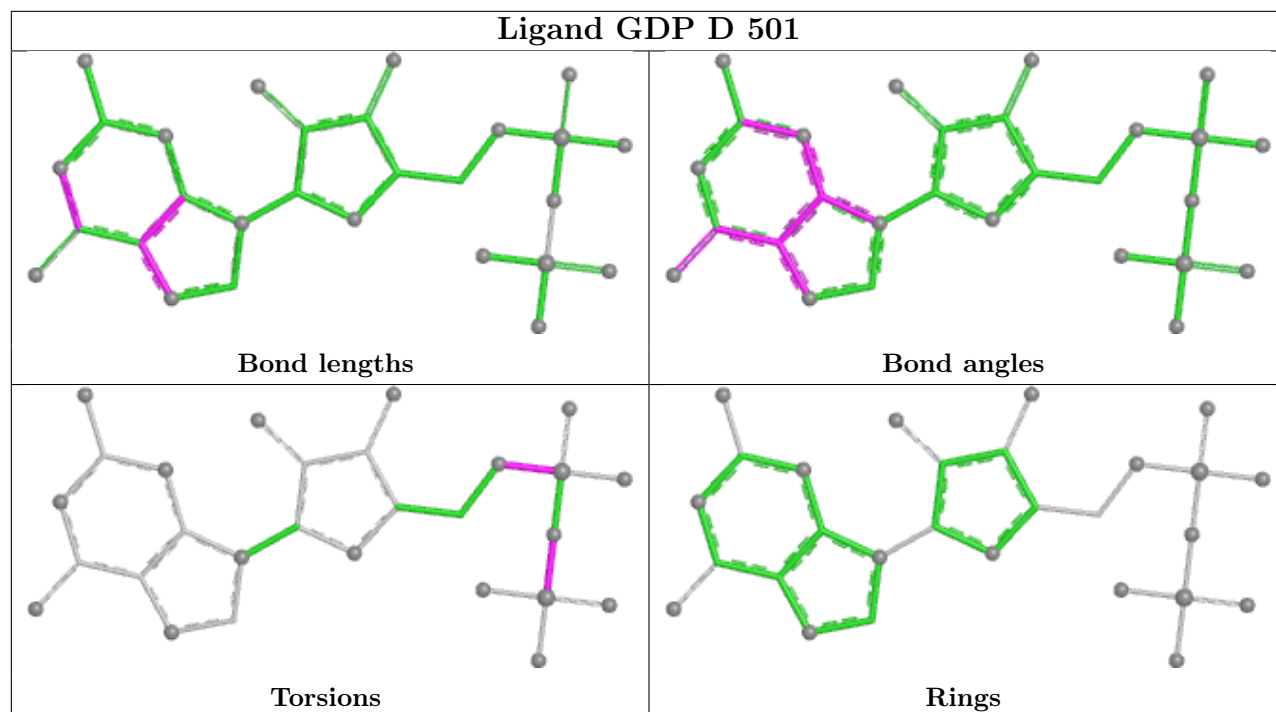


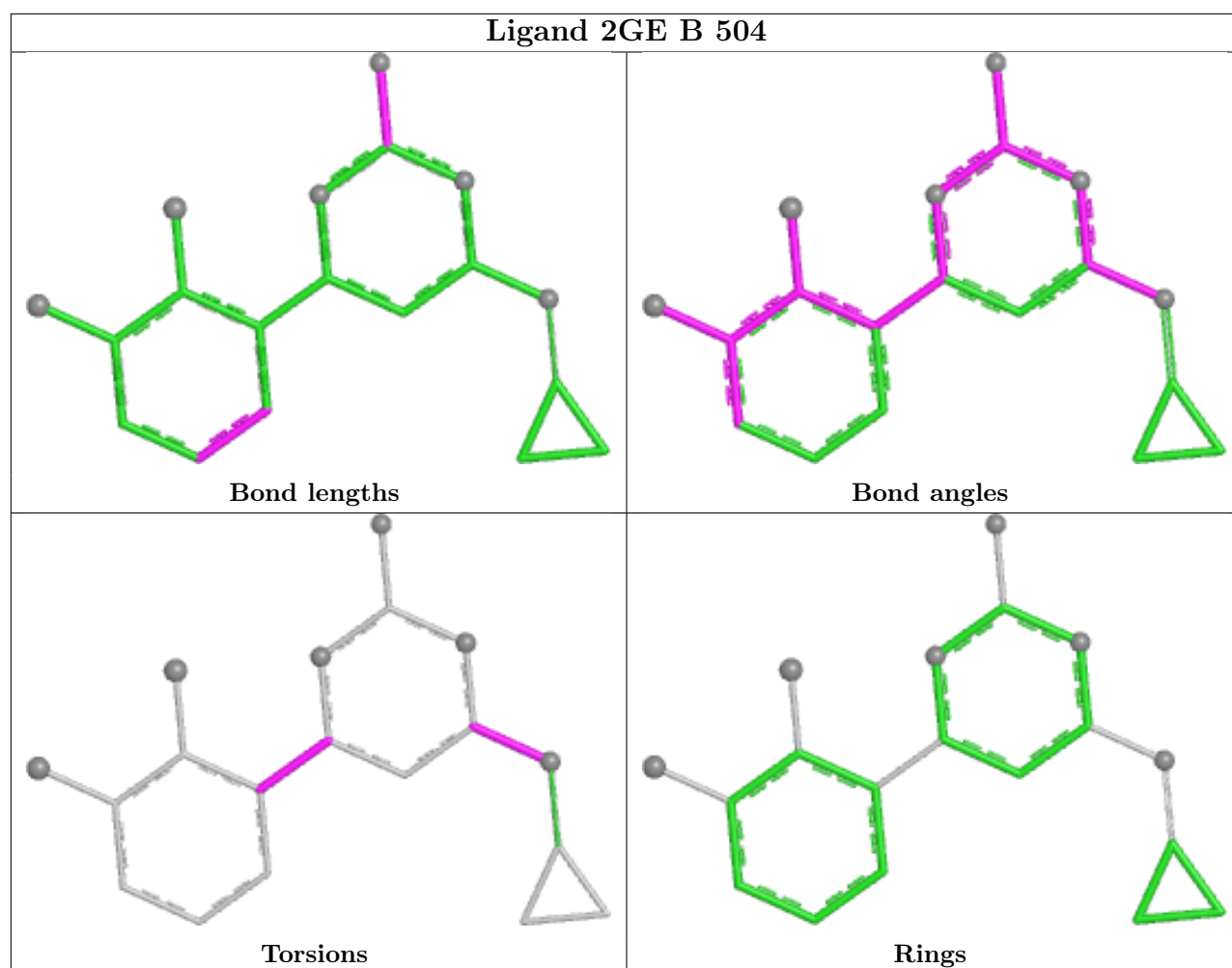
Ligand GTP C 501



Ligand ACP F 701







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	436/451 (96%)	0.01	6 (1%)	73	75	44, 64, 101, 142	0
1	C	440/451 (97%)	-0.19	5 (1%)	78	79	24, 52, 79, 100	1 (0%)
2	B	423/445 (95%)	0.15	14 (3%)	49	51	24, 62, 104, 124	1 (0%)
2	D	421/445 (94%)	0.26	11 (2%)	57	59	30, 75, 106, 126	2 (0%)
3	E	121/143 (84%)	0.39	4 (3%)	49	51	54, 81, 119, 124	0
4	F	314/384 (81%)	0.63	30 (9%)	13	15	57, 91, 145, 164	0
All	All	2155/2319 (92%)	0.16	70 (3%)	50	52	24, 67, 117, 164	4 (0%)

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	248	LEU	6.2
2	D	286	LEU	4.9
2	B	249	ASN	4.9
2	D	172	MET	4.1
2	B	202	TYR	4.0
2	B	276	THR	3.8
4	F	102	PRO	3.7
4	F	231	ALA	3.6
2	D	1	MET	3.6
1	A	282	TYR	3.5
4	F	144	GLY	3.5
2	B	246	GLY	3.5
2	B	250	ALA	3.3
4	F	141	GLY	3.3
2	B	438	ALA	3.3
4	F	186	LEU	3.3
4	F	134	ALA	3.3
4	F	372	THR	3.3
1	C	302	MET	3.2

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Mol	Chain	Res	Type	RSRZ
4	F	173	ILE	3.2
1	C	440	VAL	3.2
1	A	437	VAL	3.1
4	F	362	ALA	3.0
1	A	281	ALA	3.0
4	F	184	LYS	3.0
4	F	91	CYS	3.0
2	B	57	THR	2.9
4	F	99	VAL	2.9
1	A	180	ALA	2.9
2	B	337	ASN	2.9
2	B	1	MET	2.8
2	D	246	GLY	2.8
4	F	240	LEU	2.8
2	D	407	TRP	2.7
4	F	237	THR	2.7
4	F	130	VAL	2.6
4	F	166	ALA	2.6
4	F	179	VAL	2.6
2	B	333	LEU	2.6
3	E	45	PRO	2.5
4	F	146	VAL	2.5
4	F	169	LEU	2.5
3	E	6	MET	2.5
2	B	255	LEU	2.5
1	C	357	TYR	2.4
3	E	23	ILE	2.4
1	C	1	MET	2.4
1	A	262	TYR	2.4
3	E	26	PRO	2.4
2	D	218	LYS	2.4
4	F	149	ALA	2.3
1	A	178	SER	2.3
4	F	132	LEU	2.3
2	D	82	PRO	2.3
4	F	44	ARG	2.3
2	D	247	GLN	2.3
2	D	57	THR	2.2
4	F	172	PHE	2.1
1	C	341	ILE	2.1
4	F	335	ALA	2.1
4	F	380	HIS	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	172	MET	2.1
2	D	96	GLN	2.1
4	F	243	HIS	2.1
4	F	379	HIS	2.1
4	F	100	ILE	2.1
4	F	182	ILE	2.1
4	F	330	ILE	2.1
2	D	272	PHE	2.0
2	B	282	GLN	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	CA	B	505	1/1	0.79	0.16	96,96,96,96	0
7	CA	B	506	1/1	0.79	0.12	124,124,124,124	0
6	MG	F	702	1/1	0.80	0.12	83,83,83,83	0
12	ACP	F	701	31/31	0.80	0.13	89,102,159,161	0
11	2GE	B	504	19/19	0.90	0.17	73,88,107,108	31
6	MG	D	502	1/1	0.92	0.09	71,71,71,71	0
9	GDP	D	501	28/28	0.92	0.10	64,68,78,86	0
10	MES	B	503	12/12	0.93	0.10	51,60,77,82	0
8	EDO	A	504	4/4	0.93	0.10	71,86,94,98	0
7	CA	A	503	1/1	0.93	0.07	89,89,89,89	0
7	CA	C	503	1/1	0.97	0.04	72,72,72,72	0
5	GTP	A	501	32/32	0.98	0.05	37,47,53,59	0
9	GDP	B	501	28/28	0.98	0.05	33,46,53,63	0
5	GTP	C	501	32/32	0.98	0.05	37,42,50,52	0

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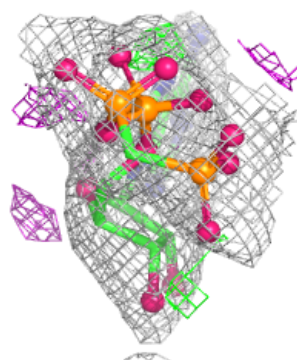
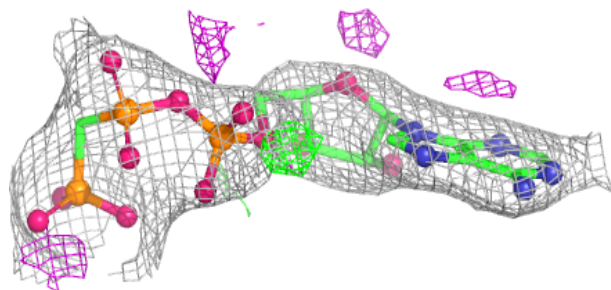
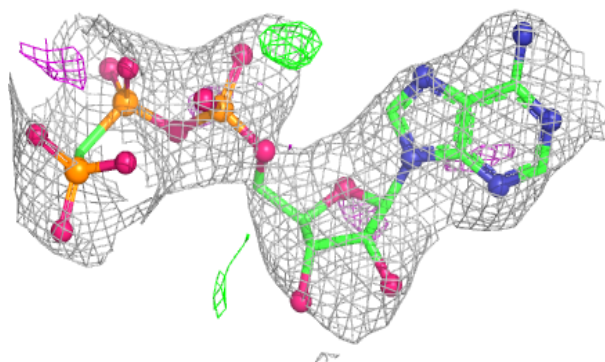
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	MG	A	502	1/1	0.99	0.03	46,46,46,46	0
6	MG	B	502	1/1	0.99	0.04	45,45,45,45	0
6	MG	C	502	1/1	0.99	0.02	46,46,46,46	0

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.

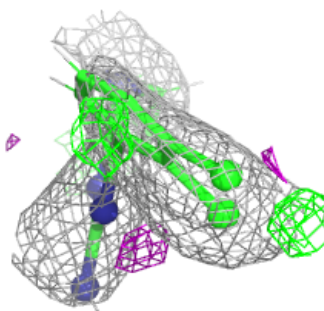
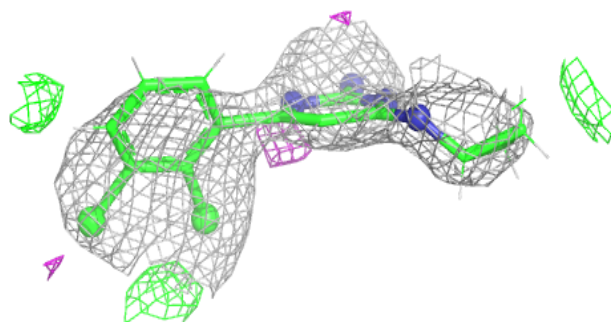
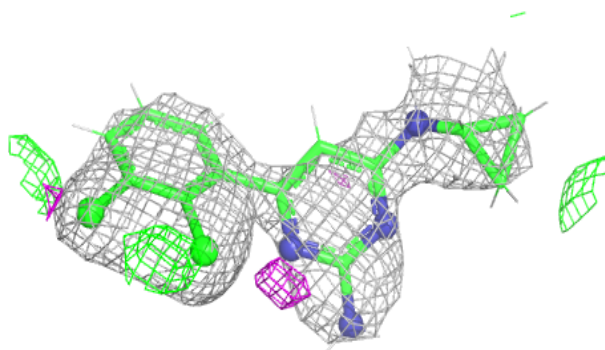
Electron density around ACP F 701:

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

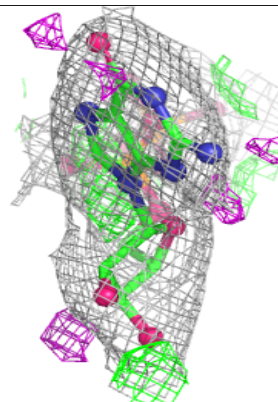
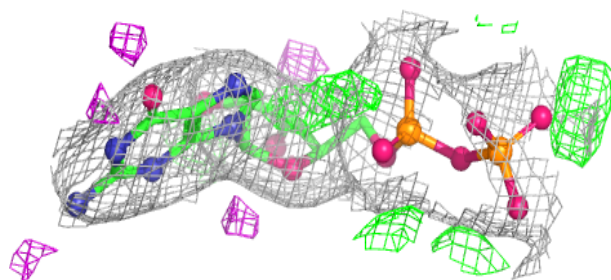
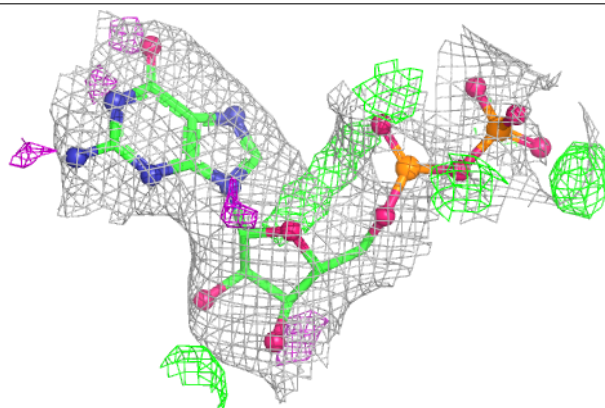


Electron density around 2GE B 504:

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

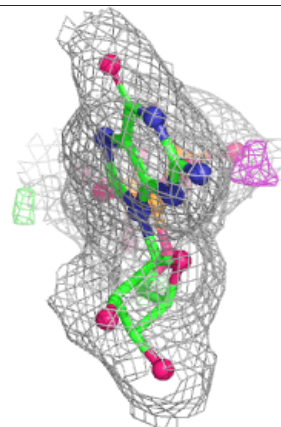
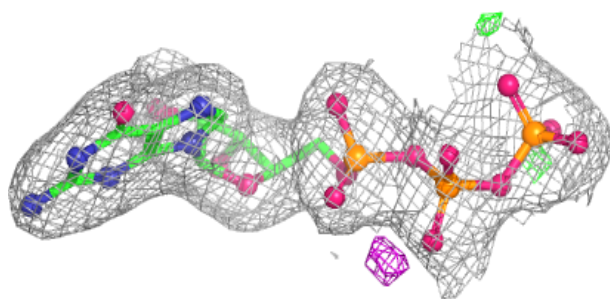
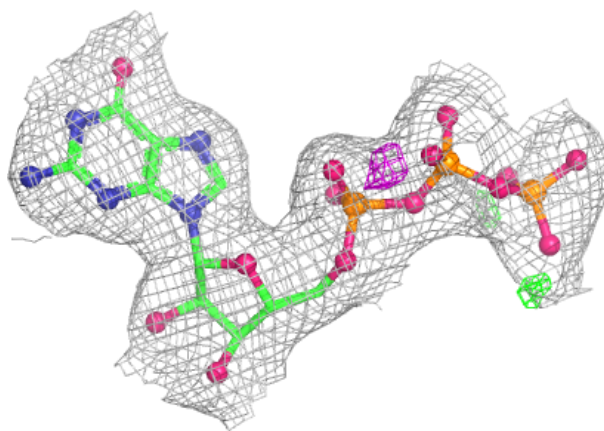
**Electron density around GDP D 501:**

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



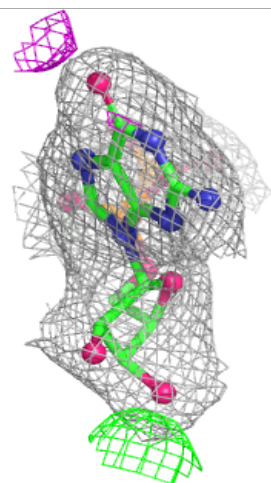
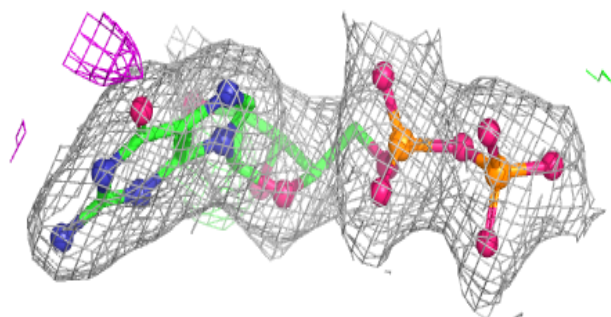
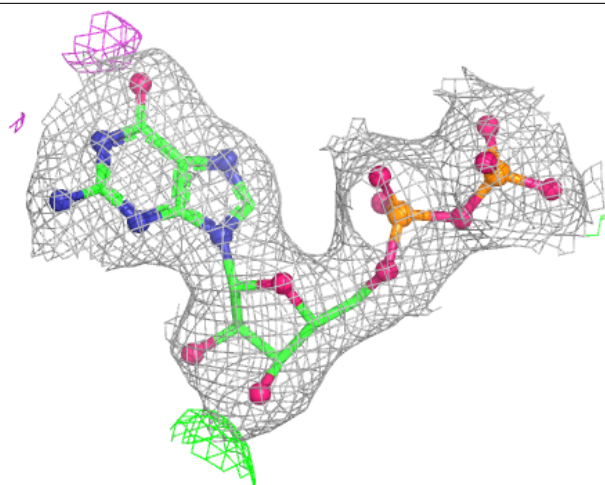
Electron density around GTP A 501:

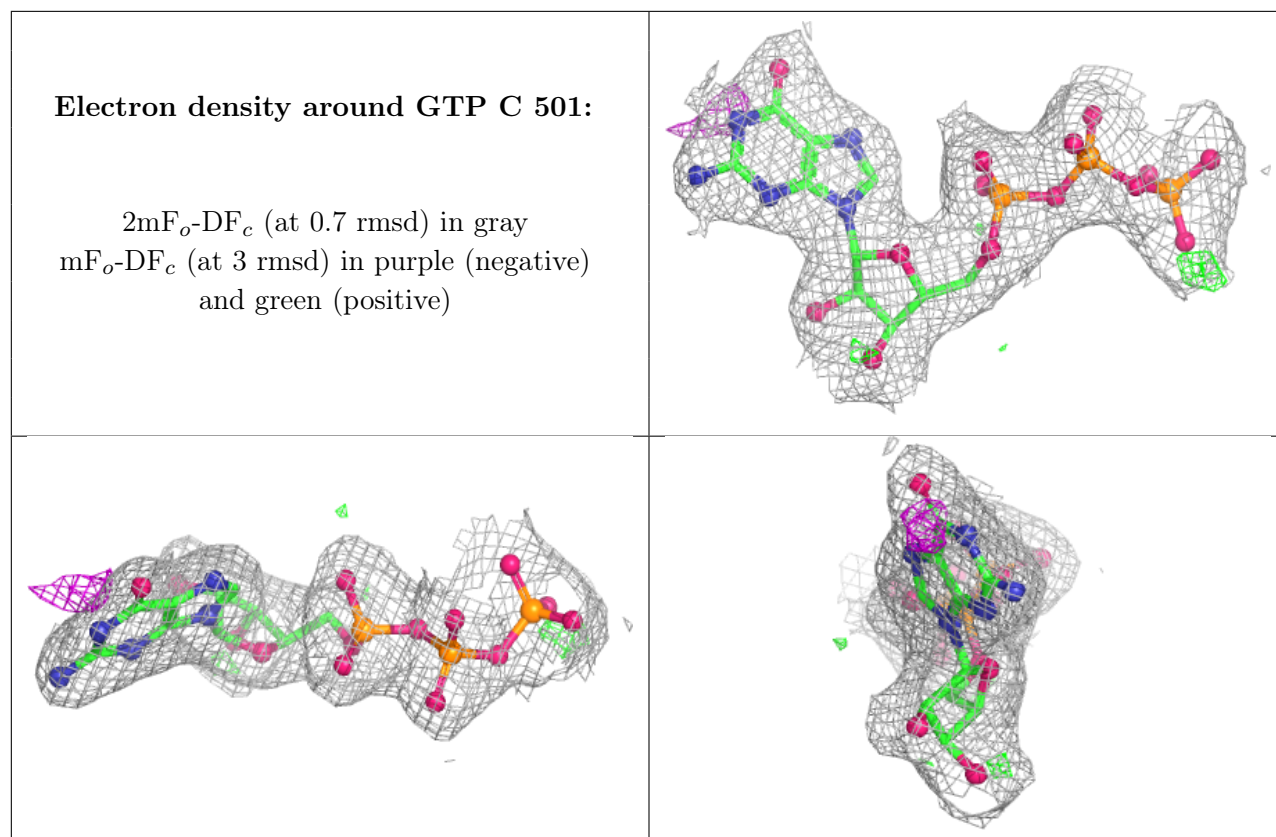
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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.