



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:38 AM UTC

PDB ID : 8ZB8 / pdb_00008zb8
Title : Crystal structure of T2R-TTL-DPP21 complex
Authors : Wu, C.Y.; Chen, J.J.
Deposited on : 2024-04-26
Resolution : 2.94 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:

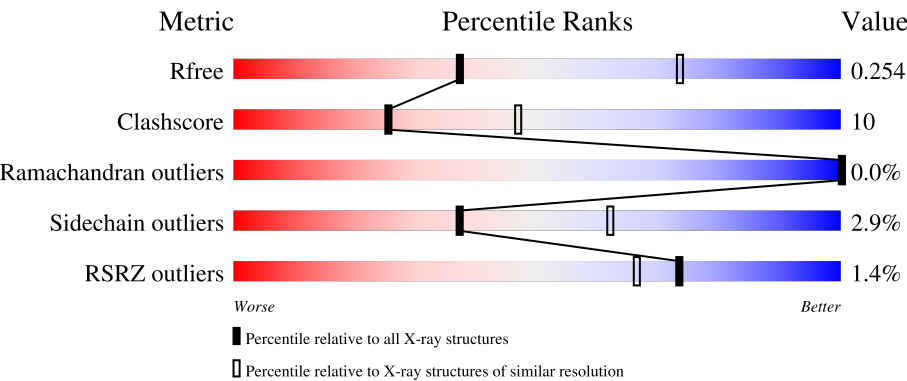
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.94 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	1159 (2.96-2.92)
Clashscore	190562	1184 (2.96-2.92)
Ramachandran outliers	187476	1131 (2.96-2.92)
Sidechain outliers	187428	1131 (2.96-2.92)
RSRZ outliers	180081	1159 (2.96-2.92)

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	450	% 76% 20% • •
1	C	450	% 81% 16% • •
2	B	445	73% 22% • •
2	D	445	% 67% 27% • 5%
3	E	143	2% 75% 8% • 15%

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Mol	Chain	Length	Quality of chain
4	F	384	4% 67% 20% • 13%

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 17485 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 Detyrosinated tubulin alpha-1B chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	437	Total	C	N	O	S	0	0	0
			3416	2163	581	650	22			
1	C	440	Total	C	N	O	S	0	0	0
			3437	2175	584	656	22			

- Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	427	Total	C	N	O	S	0	0	0
			3361	2110	576	649	26			
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	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

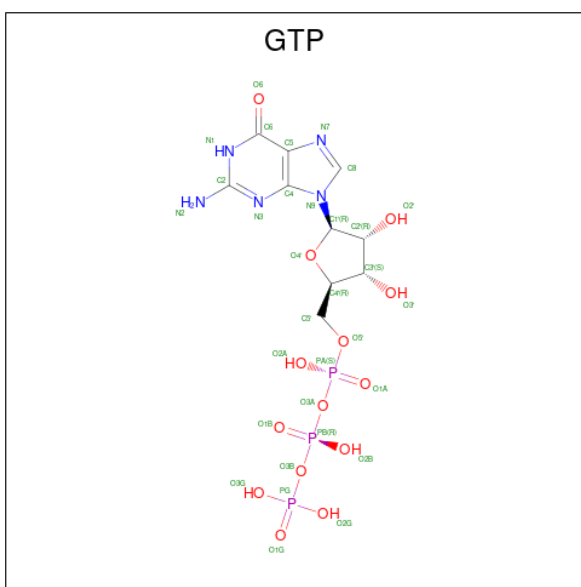
- Molecule 4 is a protein called Tubulin tyrosine ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	334	Total	C	N	O	S	0	0	0
			2744	1761	470	499	14			

There are 39 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	?	-	ALA	deletion	UNP A0A8V0Z8P0
F	?	-	GLU	deletion	UNP A0A8V0Z8P0
F	?	-	MET	deletion	UNP A0A8V0Z8P0
F	?	-	GLN	deletion	UNP A0A8V0Z8P0
F	?	-	GLN	deletion	UNP A0A8V0Z8P0
F	?	-	GLN	deletion	UNP A0A8V0Z8P0
F	?	-	LEU	deletion	UNP A0A8V0Z8P0
F	?	-	LEU	deletion	UNP A0A8V0Z8P0
F	?	-	GLU	deletion	UNP A0A8V0Z8P0
F	?	-	GLY	deletion	UNP A0A8V0Z8P0
F	?	-	ASP	deletion	UNP A0A8V0Z8P0
F	?	-	GLN	deletion	UNP A0A8V0Z8P0
F	?	-	THR	deletion	UNP A0A8V0Z8P0
F	?	-	LEU	deletion	UNP A0A8V0Z8P0
F	?	-	VAL	deletion	UNP A0A8V0Z8P0
F	?	-	LEU	deletion	UNP A0A8V0Z8P0
F	?	-	ALA	deletion	UNP A0A8V0Z8P0
F	?	-	SER	deletion	UNP A0A8V0Z8P0
F	?	-	SER	deletion	UNP A0A8V0Z8P0
F	?	-	THR	deletion	UNP A0A8V0Z8P0
F	?	-	HIS	deletion	UNP A0A8V0Z8P0
F	?	-	PRO	deletion	UNP A0A8V0Z8P0
F	?	-	GLU	deletion	UNP A0A8V0Z8P0
F	?	-	SER	deletion	UNP A0A8V0Z8P0
F	?	-	VAL	deletion	UNP A0A8V0Z8P0
F	?	-	ASP	deletion	UNP A0A8V0Z8P0
F	?	-	SER	deletion	UNP A0A8V0Z8P0
F	?	-	ASP	deletion	UNP A0A8V0Z8P0
F	?	-	LYS	deletion	UNP A0A8V0Z8P0
F	?	-	ASN	deletion	UNP A0A8V0Z8P0
F	?	-	HIS	deletion	UNP A0A8V0Z8P0
F	?	-	GLY	deletion	UNP A0A8V0Z8P0
F	?	-	PHE	deletion	UNP A0A8V0Z8P0
F	379	HIS	-	expression tag	UNP A0A8V0Z8P0
F	380	HIS	-	expression tag	UNP A0A8V0Z8P0
F	381	HIS	-	expression tag	UNP A0A8V0Z8P0
F	382	HIS	-	expression tag	UNP A0A8V0Z8P0
F	383	HIS	-	expression tag	UNP A0A8V0Z8P0
F	384	HIS	-	expression tag	UNP A0A8V0Z8P0

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



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

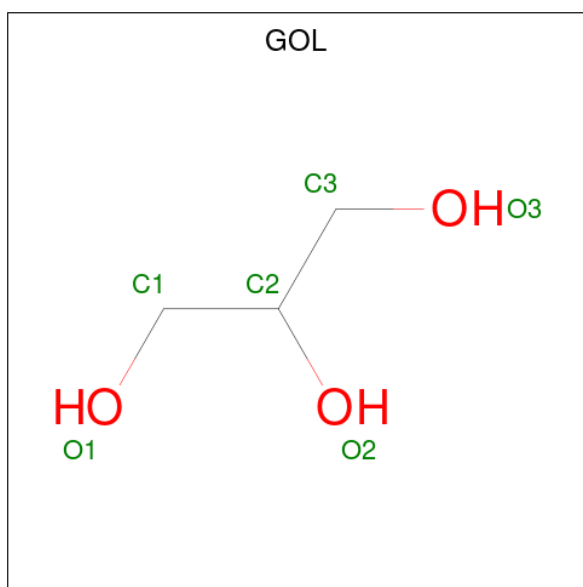
- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

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

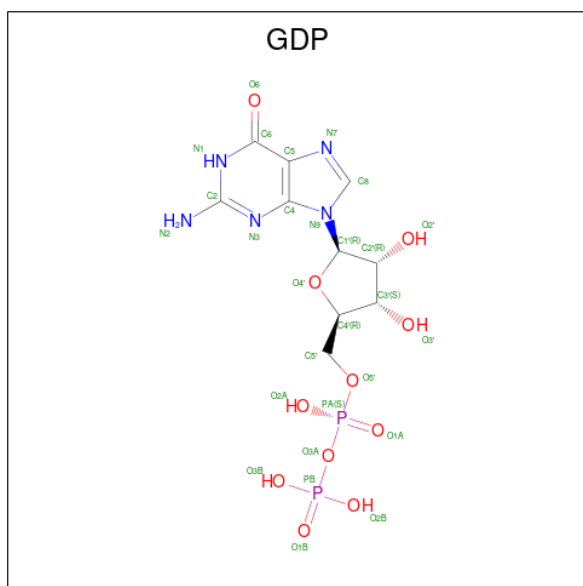
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total Ca 1 1	1	0
7	C	1	Total Ca 1 1	1	0

- Molecule 8 is GLYCEROL (CCD ID: GOL) (formula: $\text{C}_3\text{H}_8\text{O}_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			6	3	3		

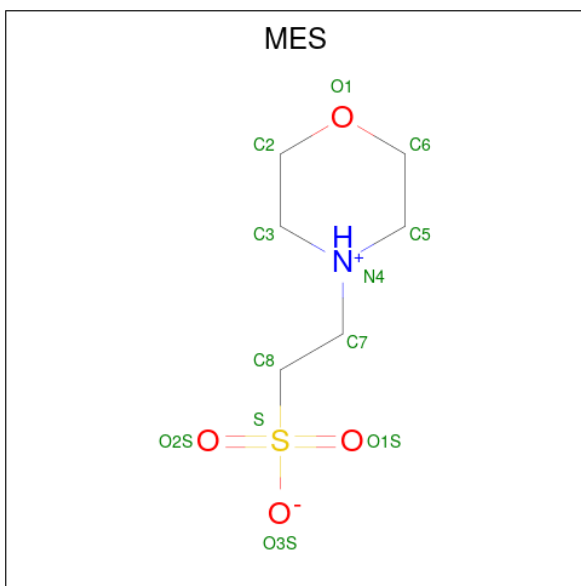
- Molecule 9 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



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

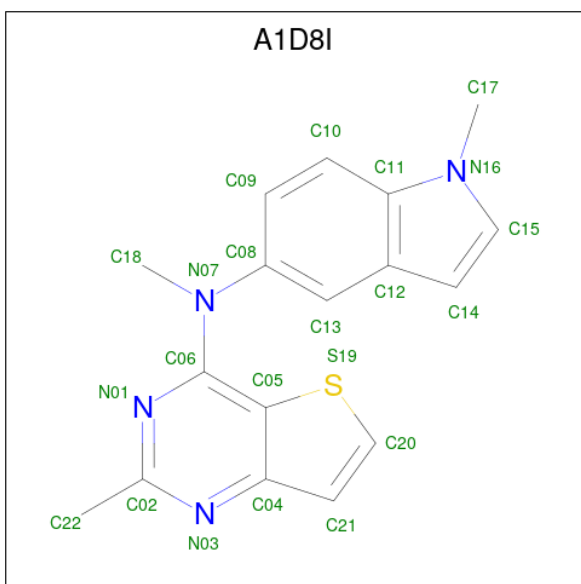
- Molecule 10 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES)

(formula: 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},2-dimethyl- {N}-(1-methylindol-5-yl)thieno[3,2-d]pyrimidin-4-amine (CCD ID: A1D8I) (formula: C₁₇H₁₆N₄S) (labeled as "Ligand of Interest" by depositor).



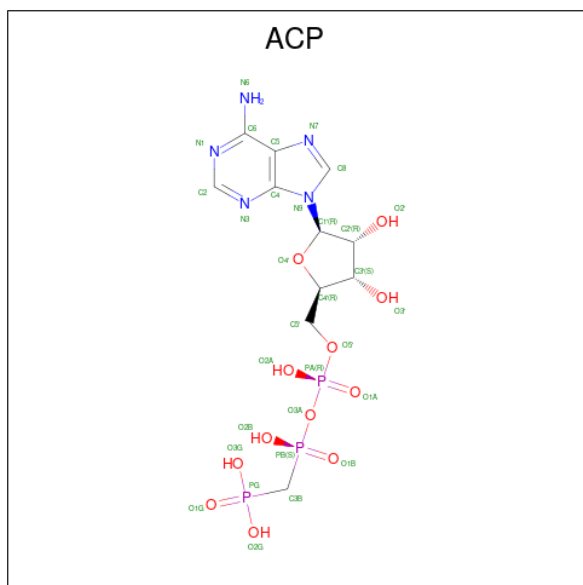
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	B	1	Total	C	N	S	0	0
			22	17	4	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	D	1	Total	C	N	S	0	0
			22	17	4	1		

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

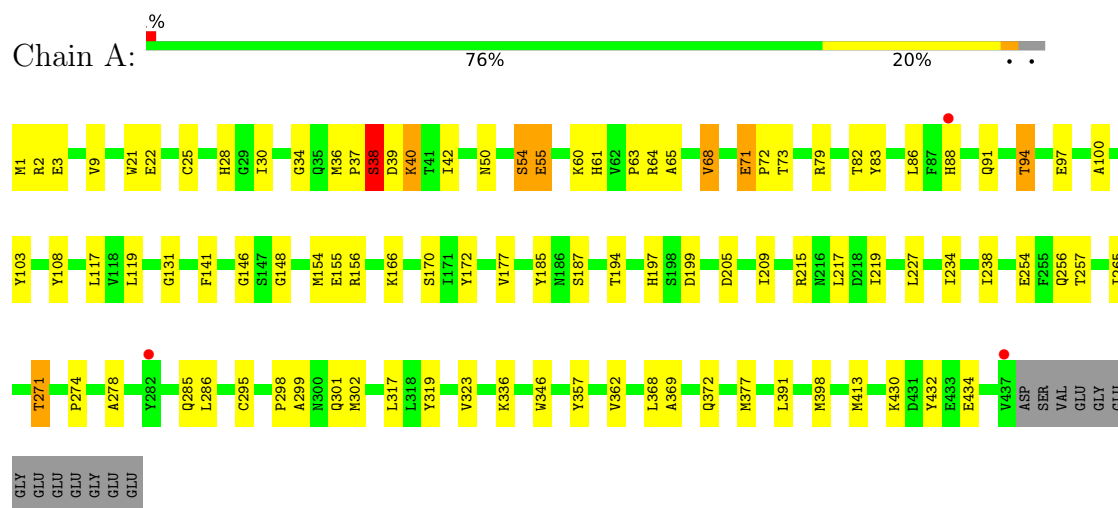


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
12	F	1	Total	C	N	O	P	0	0
			31	11	5	12	3		

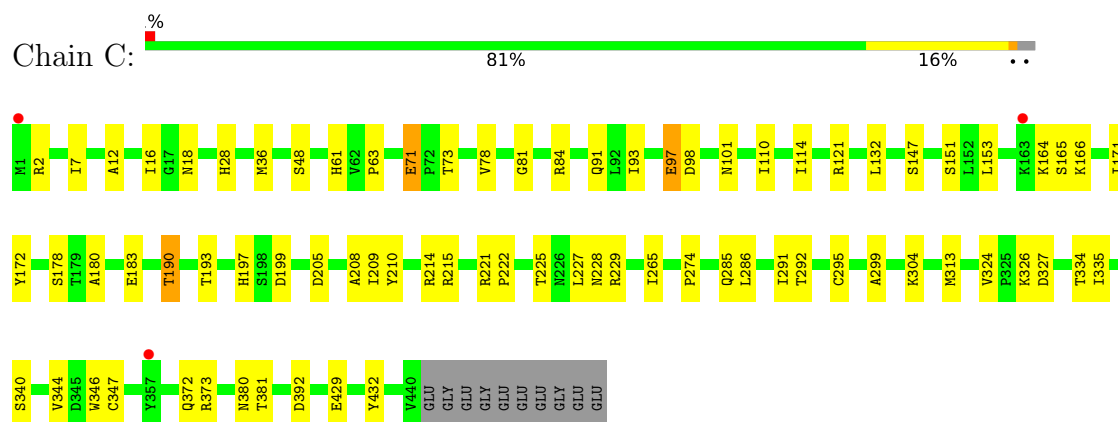
3 Residue-property plots [i](#)

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.

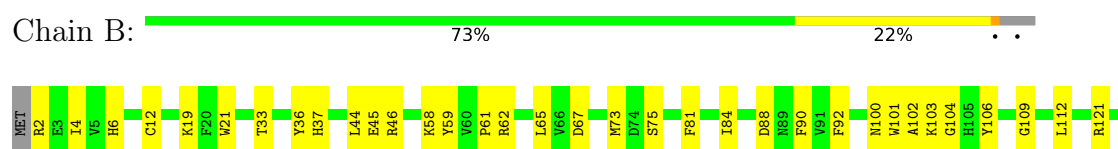
- Molecule 1: Detyrosinated tubulin alpha-1B chain



- Molecule 1: Detyrosinated tubulin alpha-1B chain

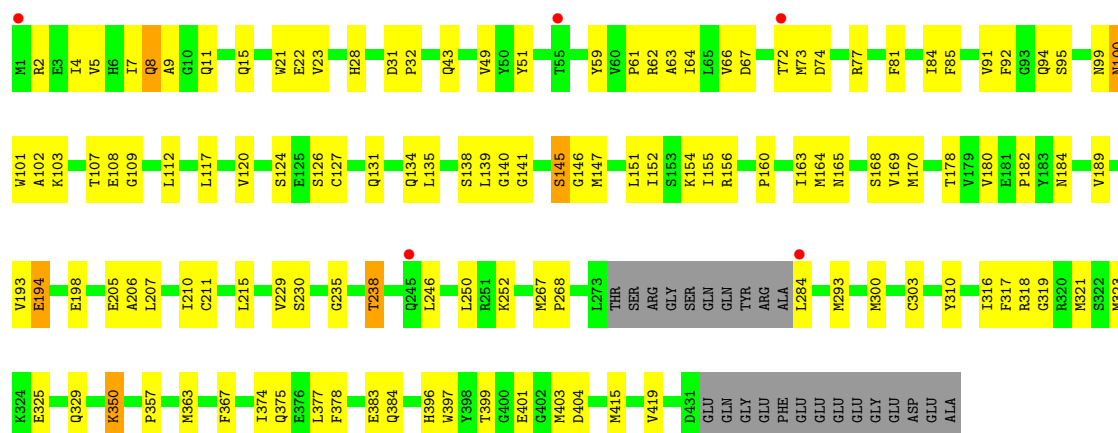


- Molecule 2: Tubulin beta chain

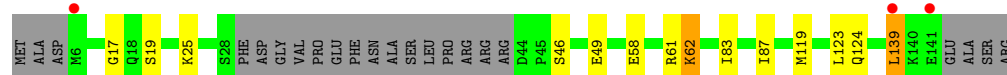
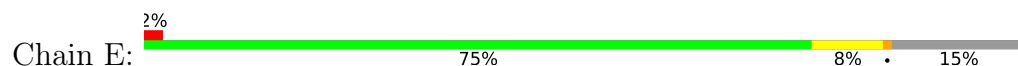




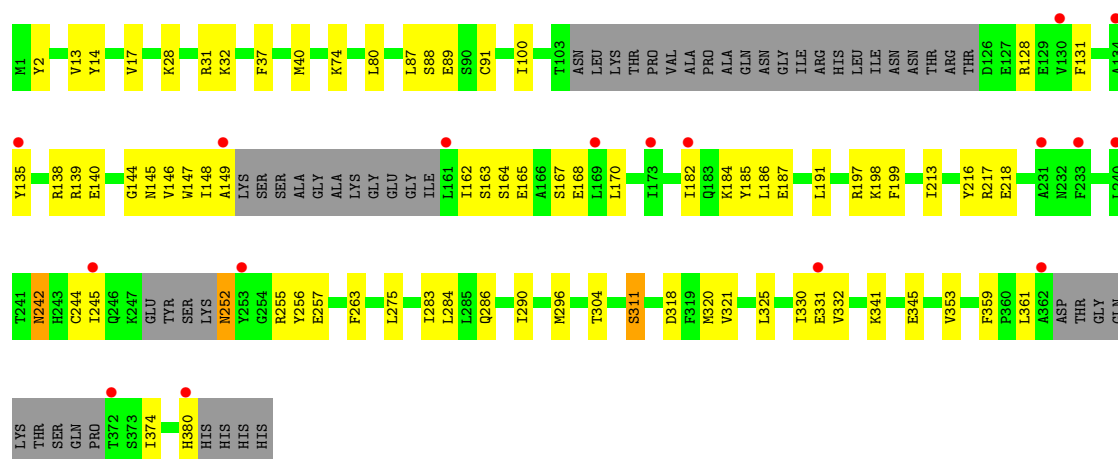
• Molecule 2: Tubulin beta chain



• Molecule 3: Stathmin-4



• Molecule 4: Tubulin tyrosine ligase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	105.60Å 158.20Å 180.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	52.28 – 2.94 52.28 – 2.94	Depositor EDS
% Data completeness (in resolution range)	99.9 (52.28-2.94) 99.9 (52.28-2.94)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.43 (at 2.96Å)	Xtriage
Refinement program	PHENIX (1.19_4092: ???)	Depositor
R, R_{free}	0.198 , 0.259 0.196 , 0.254	Depositor DCC
R_{free} test set	2000 reflections (3.07%)	wwPDB-VP
Wilson B-factor (Å ²)	65.6	Xtriage
Anisotropy	0.212	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 43.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	17485	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.46% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ACP, GDP, CA, GOL, GTP, A1D8I, MES, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.51	0/3494	0.72	1/4743 (0.0%)
1	C	0.53	1/3515 (0.0%)	0.72	4/4772 (0.1%)
2	B	0.50	0/3436	0.67	1/4654 (0.0%)
2	D	0.45	0/3382	0.64	1/4581 (0.0%)
3	E	0.50	0/1008	0.64	0/1337
4	F	0.42	0/2806	0.58	0/3791
All	All	0.48	1/17641 (0.0%)	0.67	7/23878 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	340	SER	N-CA	-6.19	1.38	1.46

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	38	SER	N-CA-C	10.08	122.35	111.36
2	D	95	SER	N-CA-C	7.61	119.21	111.07
2	B	301	ALA	N-CA-C	-6.85	97.73	108.90
1	C	171	ILE	CA-C-N	6.53	133.34	120.94
1	C	171	ILE	C-N-CA	6.53	133.34	120.94
1	C	97	GLU	CA-C-N	-5.28	111.45	121.54
1	C	97	GLU	C-N-CA	-5.28	111.45	121.54

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	3416	0	3330	64	0
1	C	3437	0	3348	41	0
2	B	3361	0	3238	77	0
2	D	3309	0	3189	91	0
3	E	1000	0	1018	9	0
4	F	2744	0	2709	57	0
5	A	32	0	12	1	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
7	A	1	0	0	0	0
7	C	1	0	0	0	0
8	A	6	0	8	0	0
9	B	28	0	12	1	0
9	D	28	0	12	5	0
10	B	12	0	12	1	0
11	B	22	0	0	1	0
11	D	22	0	0	0	0
12	F	31	0	14	1	0
All	All	17485	0	16914	331	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 10.

All (331) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:ARG:HH22	1:A:94:THR:HG22	1.31	0.94
4:F:87:LEU:O	4:F:88:SER:HB3	1.68	0.91
2:D:101:TRP:HD1	2:D:145:SER:HG	1.26	0.84
4:F:263:PHE:HZ	4:F:341:LYS:HD3	1.42	0.83
2:D:11:GLN:HB3	9:D:501:GDP:O1A	1.76	0.83
2:B:2:ARG:HH11	2:B:131:GLN:HB3	1.42	0.82
4:F:341:LYS:H	4:F:341:LYS:HD2	1.41	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:238:THR:HG21	2:D:318:ARG:HD2	1.61	0.81
4:F:197:ARG:NH2	4:F:257:GLU:OE2	2.13	0.80
2:D:317:PHE:HB3	2:D:321:MET:HE1	1.62	0.79
2:D:267:MET:HE1	2:D:303:CYS:HB2	1.66	0.77
1:A:295:CYS:HB3	1:A:377:MET:HE2	1.66	0.77
2:D:206:ALA:O	2:D:210:ILE:HG13	1.82	0.77
4:F:31:ARG:HE	4:F:31:ARG:HA	1.49	0.77
2:D:151:LEU:O	2:D:155:ILE:HG13	1.84	0.77
2:D:11:GLN:N	9:D:501:GDP:O2B	2.18	0.75
2:B:238:THR:HG21	2:B:318:ARG:HD3	1.67	0.75
2:B:106:TYR:OH	2:B:407:GLU:OE2	2.04	0.74
2:B:228:LEU:HB3	2:B:300:MET:HE1	1.69	0.74
4:F:263:PHE:CZ	4:F:341:LYS:HD3	2.23	0.73
2:D:99:ASN:HD22	2:D:178:THR:HG21	1.52	0.72
2:D:375:GLN:HB2	2:D:419:VAL:HG13	1.71	0.72
4:F:252:ASN:N	4:F:252:ASN:HD22	1.87	0.72
4:F:100:ILE:HD12	4:F:128:ARG:HG3	1.72	0.71
2:B:321:MET:HE2	2:B:363:MET:HE2	1.72	0.71
2:B:73:MET:HE2	2:B:92:PHE:HB3	1.73	0.71
1:A:79:ARG:HH22	1:A:94:THR:CG2	2.03	0.71
1:A:1:MET:HE2	1:A:50:ASN:HB3	1.73	0.70
1:A:28:HIS:O	1:A:36:MET:HE3	1.91	0.70
2:D:235:GLY:O	2:D:238:THR:HG23	1.92	0.69
2:B:81:PHE:O	2:B:84:ILE:HG22	1.93	0.69
4:F:331:GLU:HG2	4:F:332:VAL:N	2.07	0.69
2:D:73:MET:HG3	2:D:92:PHE:HD2	1.58	0.68
2:B:33:THR:HG22	2:B:58:LYS:NZ	2.07	0.68
1:C:221:ARG:HD2	2:D:323:MET:SD	2.34	0.68
2:D:102:ALA:HB2	2:D:403:MET:HE3	1.76	0.67
4:F:213:ILE:HD11	4:F:296:MET:HE2	1.74	0.67
1:C:285:GLN:OE1	1:C:372:GLN:NE2	2.28	0.67
2:D:396:HIS:HA	2:D:399:THR:HG22	1.76	0.67
2:D:141:GLY:O	2:D:184:ASN:ND2	2.29	0.66
1:A:39:ASP:OD2	1:A:55:GLU:OE2	2.12	0.66
2:B:112:LEU:HD23	2:B:147:MET:HE1	1.78	0.65
4:F:138:ARG:HB3	4:F:145:ASN:OD1	1.97	0.65
3:E:58:GLU:OE1	3:E:61:ARG:NH2	2.27	0.64
1:A:166:LYS:HE2	1:A:197:HIS:O	1.98	0.64
2:D:11:GLN:HB2	9:D:501:GDP:O2B	1.98	0.64
4:F:139:ARG:NH1	4:F:140:GLU:OE2	2.31	0.63
4:F:341:LYS:HD2	4:F:341:LYS:N	2.13	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:128:ARG:HH21	4:F:170:LEU:HB3	1.63	0.63
2:B:317:PHE:CE1	2:B:330:MET:HE3	2.34	0.63
2:D:321:MET:HB3	2:D:363:MET:HE1	1.81	0.63
2:B:392:LYS:HE3	2:B:405:GLU:OE2	1.99	0.62
2:B:2:ARG:NH1	2:B:131:GLN:HB3	2.15	0.62
1:C:12:ALA:O	1:C:16:ILE:HG13	1.99	0.61
1:A:34:GLY:O	1:A:61:HIS:N	2.32	0.61
2:B:197:ASP:OD2	10:B:503:MES:H52	2.00	0.61
2:D:134:GLN:HA	2:D:165:ASN:O	2.00	0.61
2:B:140:GLY:O	2:B:184:ASN:ND2	2.30	0.61
2:B:2:ARG:HD2	2:B:131:GLN:HB3	1.82	0.60
2:B:343:GLU:H	2:B:343:GLU:CD	2.08	0.60
2:D:207:LEU:HD11	2:D:229:VAL:HG23	1.84	0.60
2:B:101:TRP:CE3	2:B:187:LEU:HD13	2.37	0.60
2:B:158:GLU:HG2	2:B:159:TYR:CE1	2.37	0.60
1:A:295:CYS:HB3	1:A:377:MET:CE	2.32	0.60
4:F:163:SER:OG	4:F:168:GLU:OE2	2.18	0.59
2:D:101:TRP:CD1	2:D:145:SER:HG	2.14	0.59
4:F:87:LEU:O	4:F:88:SER:CB	2.43	0.59
2:D:101:TRP:HD1	2:D:145:SER:OG	1.84	0.59
2:B:232:THR:OG1	2:B:300:MET:HE2	2.03	0.58
4:F:197:ARG:HH22	4:F:257:GLU:CD	2.10	0.58
1:C:178:SER:O	2:D:350:LYS:HE3	2.02	0.58
4:F:286:GLN:O	4:F:290:ILE:HG13	2.02	0.58
2:D:11:GLN:CB	9:D:501:GDP:O2B	2.52	0.58
4:F:146:VAL:HG23	4:F:187:GLU:OE2	2.04	0.58
1:A:265:ILE:HG23	1:A:432:TYR:CZ	2.39	0.57
2:B:21:TRP:CZ3	2:B:61:PRO:HB3	2.38	0.57
2:D:268:PRO:HG2	2:D:300:MET:HB2	1.86	0.57
2:D:32:PRO:HB3	2:D:81:PHE:HA	1.86	0.57
1:A:119:LEU:HD11	1:A:156:ARG:HB3	1.84	0.57
4:F:144:GLY:HA3	4:F:187:GLU:OE1	2.05	0.57
1:A:88:HIS:N	1:A:91:GLN:OE1	2.36	0.57
1:A:34:GLY:HA3	1:A:60:LYS:HG3	1.87	0.56
2:D:11:GLN:O	2:D:15:GLN:HG2	2.06	0.56
2:D:141:GLY:HA3	9:D:501:GDP:O3A	2.06	0.56
2:B:321:MET:HB3	2:B:363:MET:HE1	1.86	0.56
1:A:39:ASP:OD2	1:A:55:GLU:CD	2.48	0.56
4:F:296:MET:HE3	4:F:380:HIS:CG	2.41	0.56
1:A:185:TYR:CZ	1:A:398:MET:HE3	2.41	0.56
1:A:285:GLN:HG3	1:A:372:GLN:OE1	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:302:MET:N	1:A:302:MET:HE2	2.21	0.55
1:A:187:SER:HB3	1:A:391:LEU:HD21	1.87	0.55
2:D:94:GLN:N	2:D:94:GLN:OE1	2.40	0.55
4:F:31:ARG:HE	4:F:31:ARG:CA	2.18	0.54
2:B:134:GLN:HA	2:B:165:ASN:O	2.07	0.54
4:F:213:ILE:CD1	4:F:296:MET:HE2	2.38	0.54
2:D:63:ALA:O	2:D:64:ILE:HD13	2.07	0.54
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.25	0.54
4:F:31:ARG:NE	4:F:32:LYS:H	2.05	0.54
1:C:324:VAL:HG22	1:C:327:ASP:OD2	2.08	0.54
1:C:93:ILE:HG22	1:C:114:ILE:HD11	1.89	0.53
2:D:103:LYS:HG3	2:D:401:GLU:OE2	2.08	0.53
1:A:71:GLU:HG2	1:A:73:THR:H	1.73	0.53
1:A:1:MET:HE2	1:A:50:ASN:CB	2.38	0.53
1:C:392:ASP:OD2	1:C:429:GLU:OE2	2.26	0.53
1:A:21:TRP:CZ3	1:A:63:PRO:HB3	2.43	0.53
1:A:103:TYR:CD1	1:A:148:GLY:HA2	2.44	0.53
1:A:274:PRO:HB3	1:A:286:LEU:HD12	1.89	0.53
2:D:117:LEU:HD11	2:D:154:LYS:HB3	1.91	0.53
2:D:321:MET:HB3	2:D:363:MET:CE	2.40	0.52
2:B:106:TYR:CD2	2:B:403:MET:HE2	2.45	0.52
2:D:182:PRO:HG3	2:D:384:GLN:HB3	1.91	0.52
2:D:152:ILE:HG23	2:D:164:MET:HG2	1.92	0.52
2:B:267:MET:HG2	2:B:374:ILE:HD13	1.91	0.52
3:E:58:GLU:HG3	3:E:62:LYS:HD2	1.91	0.52
4:F:304:THR:HG21	4:F:311:SER:HB2	1.91	0.52
1:A:336:LYS:NZ	3:E:25:LYS:HE2	2.25	0.52
2:D:21:TRP:CZ3	2:D:61:PRO:HB3	2.45	0.52
1:C:215:ARG:NH1	1:C:299:ALA:HB1	2.24	0.52
2:D:7:ILE:O	2:D:135:LEU:HD12	2.09	0.52
2:D:51:TYR:HD2	2:D:59:TYR:HB3	1.74	0.52
4:F:135:TYR:OH	4:F:165:GLU:HA	2.10	0.52
2:B:221:THR:HG23	2:B:224:ASP:H	1.75	0.51
2:D:193:VAL:HG13	2:D:194:GLU:OE1	2.11	0.51
2:D:325:GLU:O	2:D:329:GLN:HG2	2.10	0.51
1:A:108:TYR:CE2	1:A:413:MET:HG3	2.45	0.51
2:B:317:PHE:CZ	2:B:330:MET:HE3	2.45	0.51
2:D:293:MET:HG2	2:D:367:PHE:HB2	1.93	0.51
1:A:298:PRO:HA	1:A:301:GLN:CD	2.35	0.51
2:B:252:LYS:O	2:B:256:ASN:ND2	2.44	0.51
1:A:319:TYR:HB3	1:A:323:VAL:HG21	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:104:GLY:O	2:B:109:GLY:HA3	2.11	0.51
2:D:396:HIS:CD2	2:D:397:TRP:HD1	2.29	0.51
3:E:46:SER:OG	3:E:49:GLU:HG3	2.11	0.51
2:B:238:THR:OG1	2:B:316:ILE:HG21	2.11	0.50
4:F:89:GLU:C	4:F:91:CYS:H	2.19	0.50
1:A:36:MET:HB3	1:A:61:HIS:CE1	2.47	0.50
2:B:169:VAL:HA	2:B:202:ILE:O	2.12	0.50
2:D:267:MET:O	2:D:267:MET:HG3	2.10	0.50
1:A:22:GLU:HG3	1:A:83:TYR:CE2	2.46	0.50
1:A:141:PHE:CE1	1:A:170:SER:HB3	2.46	0.50
2:B:36:TYR:CE2	2:B:44:LEU:HG	2.47	0.49
1:C:132:LEU:O	1:C:164:LYS:NZ	2.42	0.49
2:B:375:GLN:HE22	2:B:423:GLN:HE21	1.59	0.49
1:A:317:LEU:CD2	1:A:377:MET:HG3	2.43	0.49
2:B:121:ARG:HH11	2:B:158:GLU:CD	2.20	0.49
1:C:18:ASN:HD21	1:C:78:VAL:HG22	1.77	0.49
4:F:14:TYR:HA	4:F:17:VAL:HG23	1.95	0.49
1:A:346:TRP:H	1:A:346:TRP:CD1	2.31	0.49
1:A:2:ARG:HB3	1:A:131:GLY:O	2.12	0.49
1:A:234:ILE:O	1:A:238:ILE:HG13	2.13	0.49
1:A:336:LYS:HZ2	3:E:25:LYS:HE2	1.78	0.49
2:B:12:CYS:HB2	9:B:501:GDP:C8	2.47	0.48
1:C:63:PRO:O	1:C:91:GLN:NE2	2.46	0.48
2:D:109:GLY:HA3	2:D:147:MET:HG3	1.96	0.48
2:D:140:GLY:O	2:D:184:ASN:ND2	2.46	0.48
2:B:317:PHE:HE1	2:B:330:MET:HE3	1.76	0.48
2:D:211:CYS:HA	2:D:215:LEU:HB2	1.94	0.48
1:A:215:ARG:NH2	1:A:299:ALA:O	2.46	0.48
1:C:101:ASN:ND2	5:C:501:GTP:O1G	2.45	0.48
2:D:91:VAL:HG12	2:D:112:LEU:HD11	1.96	0.48
1:A:362:VAL:HG21	1:A:368:LEU:O	2.14	0.48
1:A:21:TRP:CH2	1:A:63:PRO:HB3	2.49	0.48
4:F:318:ASP:O	4:F:330:ILE:HB	2.14	0.48
1:A:22:GLU:HG3	1:A:83:TYR:HE2	1.78	0.48
1:A:54:SER:HB3	1:A:64:ARG:NH1	2.28	0.48
1:A:187:SER:CB	1:A:391:LEU:HD21	2.44	0.48
2:B:45:GLU:HB3	2:B:243:PRO:HG3	1.96	0.47
4:F:148:ILE:O	4:F:182:ILE:HD12	2.14	0.47
1:A:63:PRO:HD3	1:A:86:LEU:HG	1.97	0.47
1:C:225:THR:O	1:C:229:ARG:HG3	2.14	0.47
2:D:100:ASN:HB3	2:D:103:LYS:HE2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:324:LYS:O	2:B:328:GLU:HG3	2.14	0.47
1:C:36:MET:HB3	1:C:61:HIS:CE1	2.49	0.47
2:D:73:MET:HG3	2:D:92:PHE:CD2	2.43	0.47
1:C:209:ILE:HG22	1:C:227:LEU:HD22	1.96	0.47
2:B:310:TYR:CE1	2:B:367:PHE:HZ	2.33	0.47
1:A:172:TYR:HB3	1:A:205:ASP:HA	1.97	0.47
11:B:504:A1D8I:C08	11:B:504:A1D8I:S19	3.03	0.46
2:B:290:THR:HG23	2:B:330:MET:HE2	1.97	0.46
1:A:430:LYS:O	1:A:434:GLU:HG3	2.16	0.46
2:B:324:LYS:HE2	2:B:328:GLU:OE2	2.15	0.46
2:D:319:GLY:HA2	2:D:357:PRO:HG3	1.98	0.46
1:A:199:ASP:HB3	1:A:256:GLN:HG2	1.97	0.46
2:D:138:SER:HA	2:D:169:VAL:HB	1.97	0.46
4:F:184:LYS:HD2	4:F:185:TYR:N	2.31	0.46
1:C:151:SER:HB3	1:C:193:THR:HG21	1.98	0.46
1:C:326:LYS:HE3	1:C:327:ASP:OD1	2.16	0.46
2:D:215:LEU:HD23	2:D:215:LEU:HA	1.72	0.46
2:B:102:ALA:HA	2:B:403:MET:HE1	1.98	0.45
2:B:156:ARG:NH1	2:B:194:GLU:O	2.49	0.45
1:C:180:ALA:HB3	1:C:183:GLU:HG3	1.98	0.45
2:D:4:ILE:HG13	2:D:49:VAL:HG13	1.98	0.45
2:D:310:TYR:CE1	2:D:367:PHE:HZ	2.34	0.45
1:A:71:GLU:HG2	1:A:72:PRO:N	2.30	0.45
1:A:79:ARG:HH12	1:A:94:THR:HG21	1.81	0.45
1:A:357:TYR:CE2	3:E:17:GLY:HA2	2.51	0.45
1:C:291:ILE:HD13	1:C:373:ARG:HG3	1.96	0.45
2:D:63:ALA:C	2:D:64:ILE:HD13	2.41	0.45
4:F:185:TYR:OH	4:F:198:LYS:NZ	2.46	0.45
4:F:252:ASN:N	4:F:252:ASN:ND2	2.57	0.45
4:F:275:LEU:HD13	4:F:325:LEU:HD11	1.98	0.45
4:F:275:LEU:HD23	4:F:275:LEU:HA	1.71	0.45
1:A:38:SER:O	1:A:40:LYS:HG2	2.17	0.45
4:F:74:LYS:NZ	12:F:401:ACP:O1A	2.48	0.45
1:C:165:SER:HA	1:C:199:ASP:OD2	2.17	0.45
1:C:172:TYR:HB3	1:C:205:ASP:HA	1.99	0.45
2:D:23:VAL:HG21	2:D:230:SER:HB2	1.98	0.45
2:D:74:ASP:HA	2:D:77:ARG:HH12	1.81	0.45
4:F:320:MET:HE3	4:F:321:VAL:H	1.81	0.45
2:D:293:MET:CG	2:D:367:PHE:HB2	2.47	0.45
4:F:148:ILE:HG12	4:F:149:ALA:H	1.81	0.44
1:A:217:LEU:HB3	1:A:219:ILE:HD12	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:378:PHE:CD1	2:D:415:MET:HE2	2.52	0.44
2:B:314:ALA:HB3	2:B:368:ILE:HB	2.00	0.44
2:B:102:ALA:CB	2:B:403:MET:HE1	2.47	0.44
2:D:293:MET:SD	2:D:367:PHE:HB2	2.57	0.44
4:F:217:ARG:NH2	4:F:374:ILE:HG22	2.32	0.44
4:F:242:ASN:OD1	4:F:242:ASN:N	2.50	0.44
4:F:255:ARG:HG2	4:F:256:TYR:CD1	2.52	0.44
1:A:278:ALA:HA	1:A:369:ALA:HB2	2.00	0.44
2:B:36:TYR:HD1	2:B:37:HIS:N	2.16	0.44
2:B:61:PRO:HD3	2:B:84:ILE:HG13	2.00	0.44
2:B:336:LYS:HE3	2:B:336:LYS:HB3	1.88	0.44
1:C:210:TYR:CE1	1:C:222:PRO:HD2	2.53	0.44
1:A:3:GLU:HG2	1:A:64:ARG:CZ	2.48	0.44
4:F:186:LEU:HD12	4:F:320:MET:HG2	2.00	0.44
2:D:8:GLN:H	2:D:8:GLN:HG2	1.66	0.44
1:C:313:MET:HE3	1:C:380:ASN:ND2	2.32	0.44
2:D:67:ASP:OD2	2:D:72:THR:OG1	2.29	0.44
2:B:67:ASP:O	2:B:92:PHE:HA	2.17	0.43
2:D:51:TYR:CD2	2:D:59:TYR:HB3	2.52	0.43
1:A:209:ILE:HG22	1:A:227:LEU:HD22	2.00	0.43
2:D:9:ALA:HA	2:D:66:VAL:O	2.19	0.43
2:B:235:GLY:O	2:B:238:THR:HG23	2.19	0.43
2:B:403:MET:HB2	2:B:403:MET:HE3	1.49	0.43
2:D:103:LYS:O	2:D:108:GLU:N	2.51	0.43
1:C:81:GLY:O	1:C:84:ARG:HG2	2.19	0.43
2:D:124:SER:O	2:D:127:CYS:HB2	2.18	0.43
1:C:2:ARG:HD2	1:C:2:ARG:HA	1.66	0.43
2:D:2:ARG:HB3	2:D:131:GLN:NE2	2.33	0.43
3:E:83:ILE:O	3:E:87:ILE:HG13	2.18	0.43
1:C:147:SER:HB2	1:C:190:THR:OG1	2.19	0.43
1:A:271:THR:HG21	1:A:295:CYS:O	2.19	0.43
2:B:290:THR:HG23	2:B:330:MET:CE	2.47	0.43
2:B:318:ARG:HA	2:B:354:CYS:O	2.18	0.43
2:D:5:VAL:HG22	2:D:62:ARG:HD3	2.01	0.43
1:C:208:ALA:HB2	1:C:304:LYS:HG2	2.00	0.43
2:D:317:PHE:CB	2:D:321:MET:HE1	2.42	0.43
2:B:36:TYR:CD2	2:B:44:LEU:HD11	2.53	0.43
2:B:65:LEU:HD22	2:B:90:PHE:CE2	2.54	0.43
1:C:7:ILE:HG21	1:C:153:LEU:HD21	2.00	0.42
1:C:344:VAL:HG21	1:C:346:TRP:CE2	2.54	0.42
1:C:97:GLU:O	1:C:110:ILE:HG21	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:21:TRP:CE3	2:D:61:PRO:HB3	2.54	0.42
2:D:100:ASN:ND2	2:D:102:ALA:HB3	2.33	0.42
2:D:156:ARG:HG2	3:E:123:LEU:HD11	2.01	0.42
2:D:160:PRO:O	3:E:119:MET:HE1	2.19	0.42
4:F:191:LEU:HD23	4:F:191:LEU:HA	1.91	0.42
2:B:2:ARG:HH11	2:B:131:GLN:CB	2.21	0.42
2:B:121:ARG:NH1	2:B:158:GLU:OE2	2.53	0.42
4:F:147:TRP:HB3	4:F:182:ILE:HD11	2.01	0.42
4:F:216:TYR:CE2	4:F:218:GLU:HB2	2.55	0.42
4:F:244:CYS:SG	4:F:245:ILE:N	2.92	0.42
4:F:325:LEU:HA	4:F:325:LEU:HD23	1.80	0.42
2:B:2:ARG:HA	2:B:129:CYS:O	2.19	0.42
2:B:12:CYS:SG	2:B:169:VAL:HG21	2.60	0.42
2:B:100:ASN:HB3	2:B:103:LYS:HG3	2.02	0.42
4:F:148:ILE:HG13	4:F:162:ILE:HG12	2.02	0.42
2:B:46:ARG:HB2	2:B:241:ARG:O	2.19	0.42
2:D:107:THR:HG22	2:D:108:GLU:N	2.33	0.42
1:A:9:VAL:HG22	1:A:68:VAL:CG1	2.50	0.42
1:A:154:MET:HG3	1:A:194:THR:HG23	2.01	0.42
2:B:36:TYR:CD1	2:B:37:HIS:N	2.88	0.42
2:B:131:GLN:OE1	2:B:249:ASP:HB2	2.19	0.42
2:B:343:GLU:OE1	2:B:343:GLU:N	2.44	0.42
4:F:284:LEU:HD12	4:F:284:LEU:HA	1.80	0.42
2:B:321:MET:HB3	2:B:363:MET:CE	2.50	0.42
1:C:93:ILE:HD11	1:C:121:ARG:HG3	2.01	0.42
1:C:292:THR:O	1:C:295:CYS:HB2	2.20	0.42
4:F:131:PHE:CE1	4:F:182:ILE:HG12	2.55	0.42
2:D:22:GLU:HG2	2:D:81:PHE:CD1	2.55	0.42
4:F:283:ILE:HD13	4:F:321:VAL:HG21	2.02	0.42
1:C:334:THR:O	1:C:335:ILE:C	2.62	0.42
4:F:216:TYR:OH	4:F:345:GLU:OE1	2.34	0.42
2:B:390:ARG:HG3	2:B:391:ARG:HG2	2.02	0.41
1:A:63:PRO:O	1:A:65:ALA:N	2.53	0.41
2:B:4:ILE:O	2:B:62:ARG:HD2	2.20	0.41
2:D:101:TRP:HE3	2:D:403:MET:HE1	1.85	0.41
4:F:13:VAL:O	4:F:17:VAL:HG23	2.20	0.41
4:F:199:PHE:CD1	4:F:199:PHE:C	2.98	0.41
1:A:100:ALA:HA	2:B:252:LYS:HG3	2.02	0.41
1:C:71:GLU:HG2	1:C:73:THR:H	1.85	0.41
4:F:164:SER:O	4:F:164:SER:OG	2.38	0.41
2:B:358:PRO:HG2	2:B:361:LEU:HD13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:284:LEU:HD23	2:D:284:LEU:HA	1.87	0.41
2:B:59:TYR:O	2:B:84:ILE:HD11	2.19	0.41
1:C:16:ILE:HG12	1:C:228:ASN:OD1	2.21	0.41
1:C:71:GLU:HB2	1:C:98:ASP:HB3	2.03	0.41
2:D:28:HIS:HA	2:D:43:GLN:HB3	2.03	0.41
2:D:100:ASN:C	2:D:100:ASN:HD22	2.29	0.41
2:D:139:LEU:HD21	2:D:168:SER:HB3	2.01	0.41
2:D:267:MET:HB3	2:D:374:ILE:HD13	2.03	0.41
1:A:155:GLU:HA	1:A:197:HIS:CE1	2.56	0.41
1:C:101:ASN:ND2	2:D:252:LYS:HE2	2.36	0.41
2:D:170:MET:HG3	2:D:377:LEU:HD11	2.03	0.41
2:B:236:VAL:HB	2:B:368:ILE:HD11	2.02	0.41
2:D:84:ILE:HG22	2:D:85:PHE:CD1	2.55	0.41
2:D:85:PHE:CD1	2:D:85:PHE:N	2.89	0.41
2:D:378:PHE:HD1	2:D:415:MET:HE2	1.85	0.41
2:B:207:LEU:HD21	2:B:300:MET:HE3	2.01	0.41
2:B:208:TYR:CE2	2:B:220:PRO:HG2	2.56	0.41
2:D:100:ASN:CB	2:D:103:LYS:HE2	2.51	0.41
2:D:163:ILE:HG21	2:D:250:LEU:HB3	2.03	0.41
2:B:164:MET:HE2	2:B:164:MET:HB2	1.78	0.41
1:C:265:ILE:HG23	1:C:432:TYR:CZ	2.56	0.41
4:F:2:TYR:CZ	4:F:359:PHE:HB3	2.56	0.41
1:A:254:GLU:HA	1:A:257:THR:OG1	2.22	0.40
2:B:268:PRO:HA	2:B:367:PHE:O	2.21	0.40
1:C:28:HIS:O	1:C:36:MET:HE3	2.22	0.40
1:C:274:PRO:HB3	1:C:286:LEU:HD13	2.03	0.40
2:D:101:TRP:NE1	2:D:146:GLY:HA2	2.36	0.40
1:A:25:CYS:HB3	1:A:30:ILE:O	2.21	0.40
1:A:317:LEU:HD23	1:A:377:MET:HG3	2.03	0.40
2:B:163:ILE:HG21	2:B:250:LEU:HB3	2.02	0.40
1:C:166:LYS:HE2	1:C:197:HIS:O	2.21	0.40
2:D:31:ASP:HB2	2:D:32:PRO:HD2	2.03	0.40
4:F:37:PHE:CZ	4:F:40:MET:HE3	2.56	0.40
1:A:103:TYR:CE1	1:A:148:GLY:HA2	2.57	0.40
1:A:146:GLY:N	5:A:501:GTP:O1B	2.51	0.40
2:B:19:LYS:HE3	2:B:19:LYS:HB3	1.82	0.40
2:D:189:VAL:HB	2:D:415:MET:HE3	2.02	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	435/450 (97%)	409 (94%)	26 (6%)	0	100	100
1	C	438/450 (97%)	424 (97%)	14 (3%)	0	100	100
2	B	425/445 (96%)	410 (96%)	15 (4%)	0	100	100
2	D	417/445 (94%)	397 (95%)	20 (5%)	0	100	100
3	E	117/143 (82%)	115 (98%)	1 (1%)	1 (1%)	14	34
4	F	324/384 (84%)	312 (96%)	12 (4%)	0	100	100
All	All	2156/2317 (93%)	2067 (96%)	88 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	E	139	LEU

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	368/378 (97%)	354 (96%)	14 (4%)	29	54
1	C	371/378 (98%)	365 (98%)	6 (2%)	55	74
2	B	369/383 (96%)	361 (98%)	8 (2%)	45	69
2	D	364/383 (95%)	349 (96%)	15 (4%)	27	52
3	E	109/127 (86%)	105 (96%)	4 (4%)	30	55
4	F	301/342 (88%)	293 (97%)	8 (3%)	39	64

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1882/1991 (94%)	1827 (97%)	55 (3%)	37 62

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	PRO
1	A	38	SER
1	A	40	LYS
1	A	42	ILE
1	A	54	SER
1	A	55	GLU
1	A	68	VAL
1	A	71	GLU
1	A	82	THR
1	A	94	THR
1	A	97	GLU
1	A	117	LEU
1	A	177	VAL
1	A	271	THR
2	B	75	SER
2	B	88	ASP
2	B	130	LEU
2	B	135	LEU
2	B	221	THR
2	B	246	LEU
2	B	252	LYS
2	B	318	ARG
1	C	48	SER
1	C	71	GLU
1	C	190	THR
1	C	214	ARG
1	C	347	CYS
1	C	381	THR
2	D	8	GLN
2	D	100	ASN
2	D	120	VAL
2	D	126	SER
2	D	145	SER
2	D	180	VAL
2	D	194	GLU
2	D	198	GLU
2	D	205	GLU

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Mol	Chain	Res	Type
2	D	238	THR
2	D	246	LEU
2	D	316	ILE
2	D	350	LYS
2	D	383	GLU
2	D	404	ASP
3	E	19	SER
3	E	62	LYS
3	E	124	GLN
3	E	139	LEU
4	F	28	LYS
4	F	80	LEU
4	F	167	SER
4	F	242	ASN
4	F	252	ASN
4	F	311	SER
4	F	353	VAL
4	F	361	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	HIS
1	A	107	HIS
1	A	300	ASN
1	A	301	GLN
1	A	342	GLN
1	A	393	HIS
2	B	8	GLN
2	B	11	GLN
2	B	14	ASN
2	B	43	GLN
2	B	134	GLN
2	B	245	GLN
2	B	280	GLN
2	B	332	ASN
2	B	423	GLN
1	C	283	HIS
1	C	309	HIS
1	C	356	ASN
2	D	11	GLN
2	D	99	ASN

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Mol	Chain	Res	Type
2	D	100	ASN
2	D	165	ASN
2	D	191	GLN
2	D	334	GLN
3	E	12	ASN
3	E	108	ASN
3	E	136	ASN
4	F	178	GLN
4	F	232	ASN
4	F	260	ASN
4	F	380	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 14 ligands modelled in this entry, 5 are monoatomic - leaving 9 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	$\# Z > 2$
11	A1D8I	B	504	-	24,25,25	2.13	7 (29%)	31,37,37	1.89	8 (25%)
8	GOL	A	504	-	5,5,5	1.12	0	5,5,5	1.13	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	ACP	F	401	-	31,33,33	1.67	2 (6%)	47,52,52	0.79	1 (2%)
9	GDP	B	501	6	29,30,30	1.23	4 (13%)	45,47,47	1.86	10 (22%)
5	GTP	A	501	6	33,34,34	0.79	0	50,54,54	1.73	12 (24%)
9	GDP	D	501	-	29,30,30	1.67	6 (20%)	45,47,47	2.03	13 (28%)
5	GTP	C	501	6	33,34,34	0.89	0	50,54,54	1.82	11 (22%)
10	MES	B	503	-	12,12,12	2.21	1 (8%)	15,16,16	2.68	8 (53%)
11	A1D8I	D	502	-	24,25,25	2.18	7 (29%)	31,37,37	2.72	14 (45%)

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
11	A1D8I	B	504	-	-	0/8/8/8	0/4/4/4
8	GOL	A	504	-	-	3/4/4/4	-
12	ACP	F	401	-	-	9/19/38/38	0/3/3/3
9	GDP	B	501	6	-	3/16/32/32	0/3/3/3
5	GTP	A	501	6	-	5/22/38/38	0/3/3/3
9	GDP	D	501	-	-	7/16/32/32	0/3/3/3
5	GTP	C	501	6	-	7/22/38/38	0/3/3/3
10	MES	B	503	-	-	1/6/14/14	0/1/1/1
11	A1D8I	D	502	-	-	0/8/8/8	0/4/4/4

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	F	401	ACP	PA-O3A	7.28	1.67	1.59
10	B	503	MES	C8-S	-7.22	1.67	1.77
12	F	401	ACP	PB-O3A	5.65	1.64	1.58
11	D	502	A1D8I	C15-N16	-5.49	1.32	1.37
11	B	504	A1D8I	C15-N16	-5.45	1.32	1.37
11	B	504	A1D8I	C04-C21	4.39	1.48	1.42
11	D	502	A1D8I	C04-C21	4.12	1.48	1.42
9	D	501	GDP	C6-N1	-3.73	1.31	1.38
11	D	502	A1D8I	C12-C11	-3.66	1.36	1.41
11	D	502	A1D8I	C05-S19	-3.60	1.67	1.73
11	D	502	A1D8I	C06-N07	3.58	1.46	1.39
11	B	504	A1D8I	C12-C11	-3.51	1.36	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	D	501	GDP	C5-N7	-3.32	1.32	1.39
11	B	504	A1D8I	C05-S19	-3.26	1.68	1.73
9	D	501	GDP	C4-N9	-3.01	1.30	1.38
11	B	504	A1D8I	C04-C05	-2.89	1.37	1.40
11	D	502	A1D8I	C11-N16	-2.67	1.34	1.38
9	B	501	GDP	C5-C4	2.66	1.46	1.38
11	B	504	A1D8I	C11-N16	-2.44	1.34	1.38
9	D	501	GDP	O4'-C4'	-2.37	1.39	1.45
9	D	501	GDP	C8-N9	-2.21	1.32	1.37
9	B	501	GDP	C6-N1	-2.20	1.34	1.38
9	B	501	GDP	C8-N9	-2.16	1.32	1.37
11	D	502	A1D8I	C08-N07	2.12	1.47	1.42
11	B	504	A1D8I	C06-N07	2.08	1.43	1.39
9	D	501	GDP	C2-N1	-2.05	1.32	1.37
9	B	501	GDP	PA-O3A	2.02	1.61	1.59

All (77) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	D	501	GDP	C5-C4-N3	-5.99	118.86	128.39
11	D	502	A1D8I	C05-S19-C20	5.95	99.10	91.24
10	B	503	MES	C5-N4-C3	5.52	120.74	108.84
11	D	502	A1D8I	C05-C06-N01	-5.46	115.81	122.33
9	B	501	GDP	C5-C4-N3	-5.44	119.72	128.39
11	B	504	A1D8I	N01-C06-N07	5.41	121.77	116.12
11	D	502	A1D8I	C17-N16-C11	-5.25	120.82	125.69
10	B	503	MES	O2S-S-C8	4.94	114.19	106.73
9	D	501	GDP	C2-N3-C4	4.63	120.28	112.30
5	C	501	GTP	C5-C4-N3	-4.58	121.11	128.39
9	B	501	GDP	C2-N3-C4	4.55	120.13	112.30
5	A	501	GTP	C2-N3-C4	4.52	120.09	112.30
5	C	501	GTP	C2-N3-C4	4.50	120.05	112.30
5	A	501	GTP	C5-C4-N3	-4.36	121.46	128.39
11	D	502	A1D8I	C11-N16-C15	4.35	111.07	108.35
11	D	502	A1D8I	C14-C15-N16	-4.31	106.32	110.39
9	B	501	GDP	N9-C4-N3	4.27	134.50	125.95
12	F	401	ACP	PB-O3A-PA	-4.25	118.51	132.37
9	D	501	GDP	N9-C4-N3	4.20	134.34	125.95
11	B	504	A1D8I	C11-N16-C15	3.81	110.74	108.35
11	D	502	A1D8I	C04-C05-S19	-3.67	106.98	110.75
5	C	501	GTP	C2-N1-C6	-3.60	118.58	125.11
11	B	504	A1D8I	C05-S19-C20	3.48	95.84	91.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	503	MES	C7-N4-C5	3.40	120.31	111.24
5	C	501	GTP	O2B-PB-O3A	3.40	116.45	107.27
5	C	501	GTP	N9-C8-N7	-3.30	107.27	113.40
9	D	501	GDP	C6-C5-N7	3.21	136.14	130.29
5	A	501	GTP	O2G-PG-O3B	3.21	115.41	104.64
9	B	501	GDP	C6-C5-N7	3.20	136.11	130.29
11	D	502	A1D8I	C13-C08-N07	3.19	124.78	119.79
11	D	502	A1D8I	C11-C12-C14	-3.16	103.71	106.85
11	D	502	A1D8I	N01-C06-N07	3.08	119.34	116.12
5	A	501	GTP	N9-C8-N7	-3.07	107.72	113.40
5	A	501	GTP	C8-N7-C5	3.05	109.69	104.26
5	C	501	GTP	C8-N7-C5	2.98	109.56	104.26
9	D	501	GDP	C2'-C3'-C4'	2.92	108.25	102.61
11	B	504	A1D8I	C05-C06-N01	-2.90	118.87	122.33
11	D	502	A1D8I	C12-C11-N16	2.89	110.41	107.92
9	D	501	GDP	O3B-PB-O2B	2.86	118.53	107.80
9	B	501	GDP	C4-C5-N7	-2.85	106.15	110.67
5	C	501	GTP	C4-C5-N7	-2.85	106.15	110.67
5	C	501	GTP	C5-C6-N1	2.83	120.47	113.25
11	B	504	A1D8I	C22-C02-N03	2.80	121.33	117.13
9	D	501	GDP	O3'-C3'-C2'	-2.79	102.87	111.82
11	B	504	A1D8I	C14-C15-N16	-2.79	107.76	110.39
5	C	501	GTP	C6-C5-N7	2.78	135.36	130.29
5	A	501	GTP	C4-C5-N7	-2.78	106.27	110.67
10	B	503	MES	C7-N4-C3	2.77	118.61	111.24
9	B	501	GDP	O6-C6-C5	-2.71	119.38	126.53
11	D	502	A1D8I	C21-C20-S19	-2.70	108.34	113.90
10	B	503	MES	O3S-S-O2S	-2.69	104.67	111.40
9	D	501	GDP	C4-C5-N7	-2.64	106.48	110.67
5	A	501	GTP	N2-C2-N1	2.60	122.24	116.76
11	D	502	A1D8I	C22-C02-N03	2.59	121.00	117.13
9	D	501	GDP	O6-C6-C5	-2.57	119.76	126.53
11	D	502	A1D8I	C02-N01-C06	2.54	123.74	115.02
5	C	501	GTP	O3G-PG-O3B	2.52	113.08	104.64
5	C	501	GTP	O3G-PG-O2G	2.49	117.16	107.80
10	B	503	MES	C6-O1-C2	2.48	117.89	109.88
9	D	501	GDP	O2'-C2'-C3'	-2.43	104.03	111.82
9	D	501	GDP	C2-N1-C6	-2.37	120.81	125.11
9	B	501	GDP	O4'-C4'-C5'	-2.29	102.01	109.33
9	D	501	GDP	O3'-C3'-C4'	-2.26	104.60	111.08
9	B	501	GDP	C8-N9-C4	2.25	110.25	106.03
5	A	501	GTP	C2-N1-C6	-2.21	121.10	125.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	501	GTP	O3B-PG-O1G	-2.21	99.42	111.04
5	A	501	GTP	C6-C5-N7	2.18	134.26	130.29
11	B	504	A1D8I	C10-C11-C12	-2.13	119.15	121.78
10	B	503	MES	O1-C6-C5	-2.12	107.20	111.77
11	B	504	A1D8I	C05-C06-N07	-2.10	119.37	122.14
5	A	501	GTP	O3'-C3'-C4'	-2.09	105.07	111.08
9	B	501	GDP	O4'-C1'-N9	-2.08	103.65	108.36
10	B	503	MES	C6-C5-N4	-2.07	106.97	110.12
9	B	501	GDP	C8-N7-C5	2.05	107.91	104.26
11	D	502	A1D8I	C05-C06-N07	2.04	124.85	122.14
9	D	501	GDP	C5-C6-N1	2.04	118.44	113.25
5	A	501	GTP	O4'-C4'-C3'	2.02	109.16	105.15

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	501	GTP	PB-O3B-PG-O2G
5	A	501	GTP	C5'-O5'-PA-O3A
5	A	501	GTP	C5'-O5'-PA-O1A
5	A	501	GTP	C5'-O5'-PA-O2A
8	A	504	GOL	O1-C1-C2-O2
8	A	504	GOL	O1-C1-C2-C3
9	B	501	GDP	C5'-O5'-PA-O3A
9	B	501	GDP	C5'-O5'-PA-O1A
9	B	501	GDP	C5'-O5'-PA-O2A
9	D	501	GDP	PA-O3A-PB-O2B
9	D	501	GDP	PA-O3A-PB-O3B
9	D	501	GDP	C5'-O5'-PA-O3A
9	D	501	GDP	C5'-O5'-PA-O1A
9	D	501	GDP	C5'-O5'-PA-O2A
10	B	503	MES	C8-C7-N4-C5
12	F	401	ACP	PB-C3B-PG-O1G
12	F	401	ACP	PB-C3B-PG-O2G
12	F	401	ACP	PB-C3B-PG-O3G
8	A	504	GOL	C1-C2-C3-O3
12	F	401	ACP	O4'-C4'-C5'-O5'
12	F	401	ACP	C3'-C4'-C5'-O5'
9	D	501	GDP	C3'-C4'-C5'-O5'
5	C	501	GTP	O4'-C4'-C5'-O5'
5	C	501	GTP	C5'-O5'-PA-O3A
5	C	501	GTP	C5'-O5'-PA-O1A

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Mol	Chain	Res	Type	Atoms
12	F	401	ACP	C5'-O5'-PA-O1A
12	F	401	ACP	C5'-O5'-PA-O2A
12	F	401	ACP	C5'-O5'-PA-O3A
5	C	501	GTP	C3'-C4'-C5'-O5'
5	C	501	GTP	PB-O3A-PA-O1A
12	F	401	ACP	PG-C3B-PB-O1B
5	C	501	GTP	C4'-C5'-O5'-PA
9	D	501	GDP	PA-O3A-PB-O1B
5	A	501	GTP	PB-O3B-PG-O3G
5	C	501	GTP	PB-O3A-PA-O2A

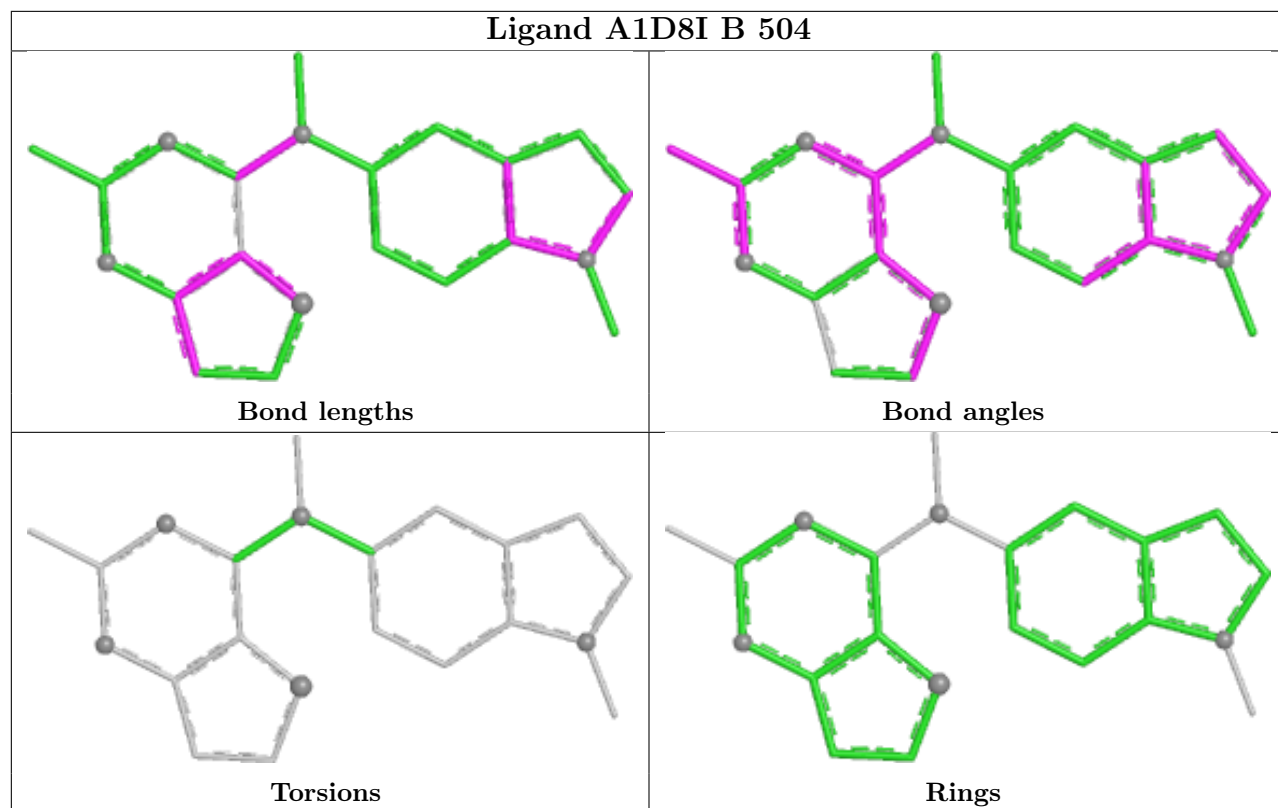
There are no ring outliers.

7 monomers are involved in 11 short contacts:

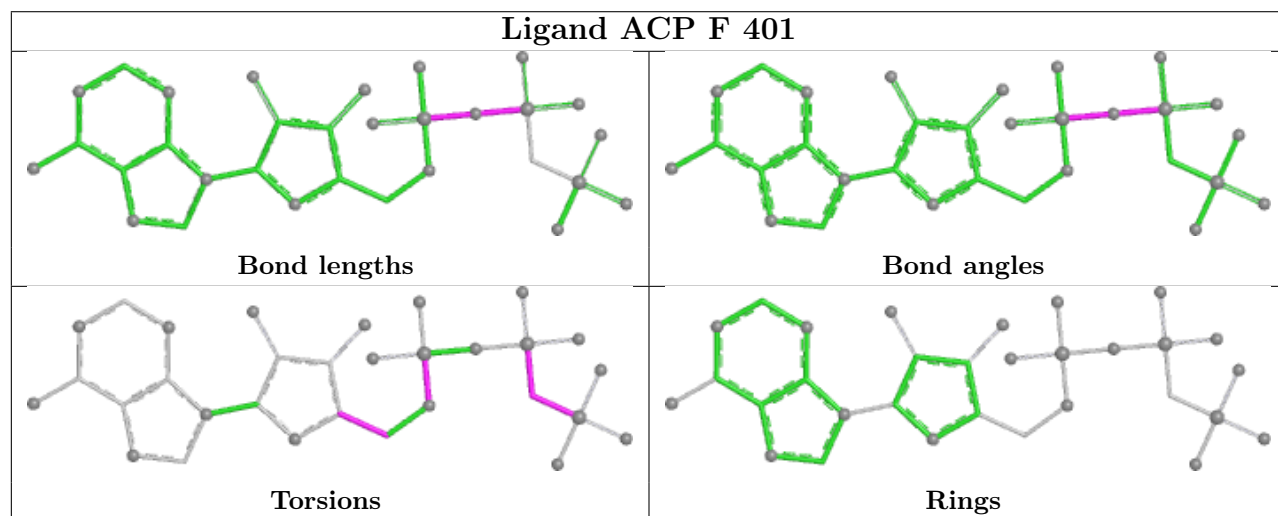
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	B	504	A1D8I	1	0
12	F	401	ACP	1	0
9	B	501	GDP	1	0
5	A	501	GTP	1	0
9	D	501	GDP	5	0
5	C	501	GTP	1	0
10	B	503	MES	1	0

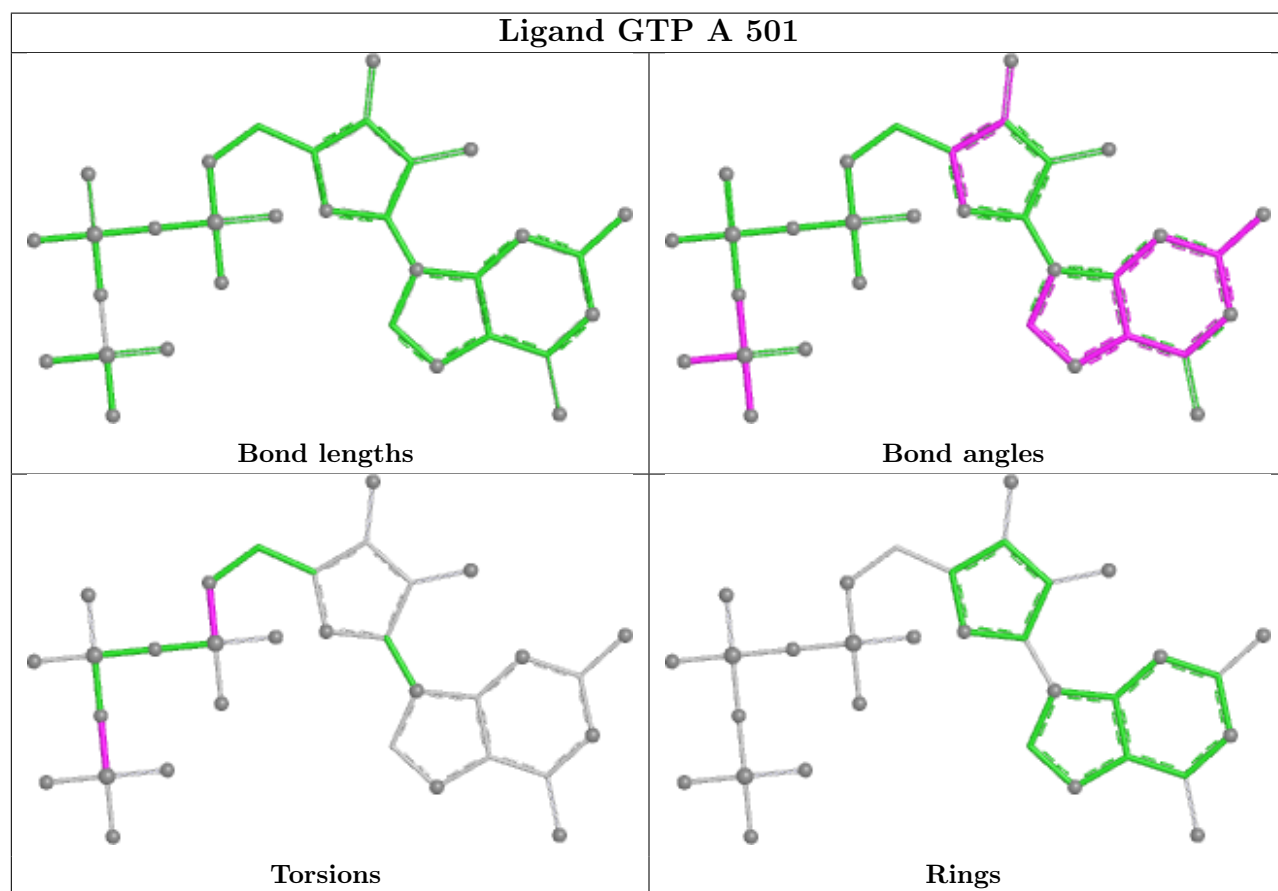
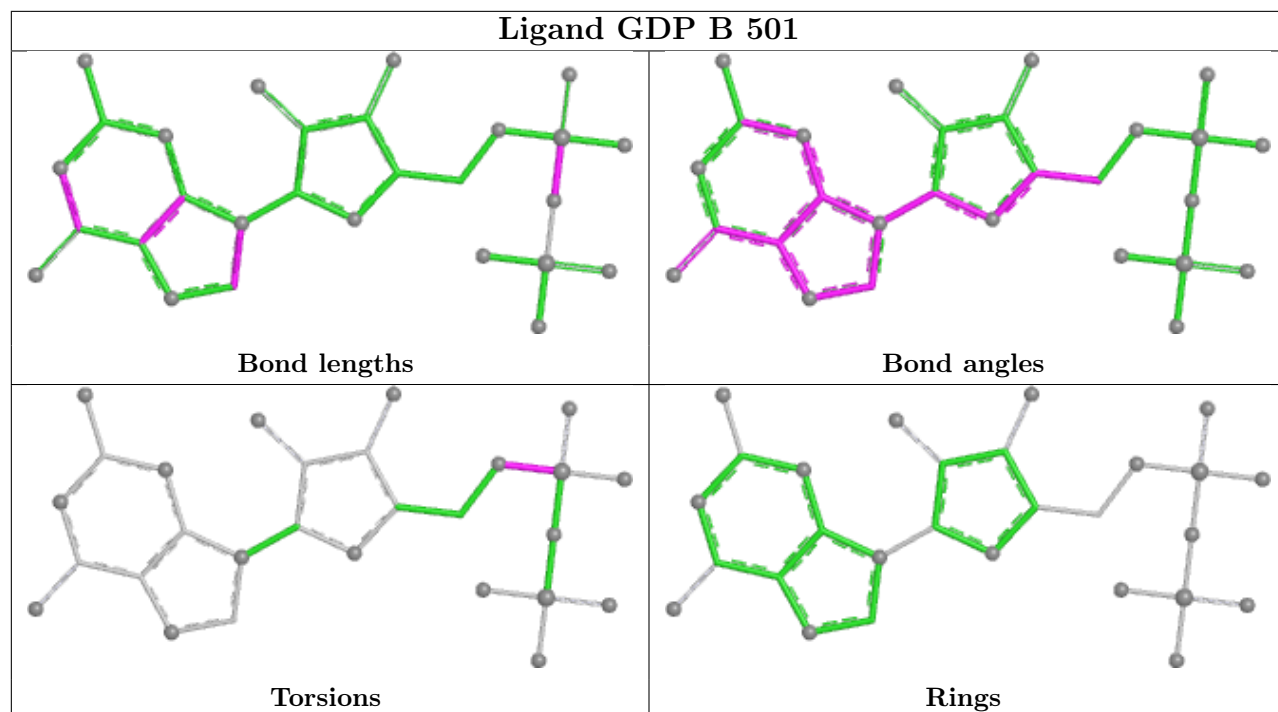
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

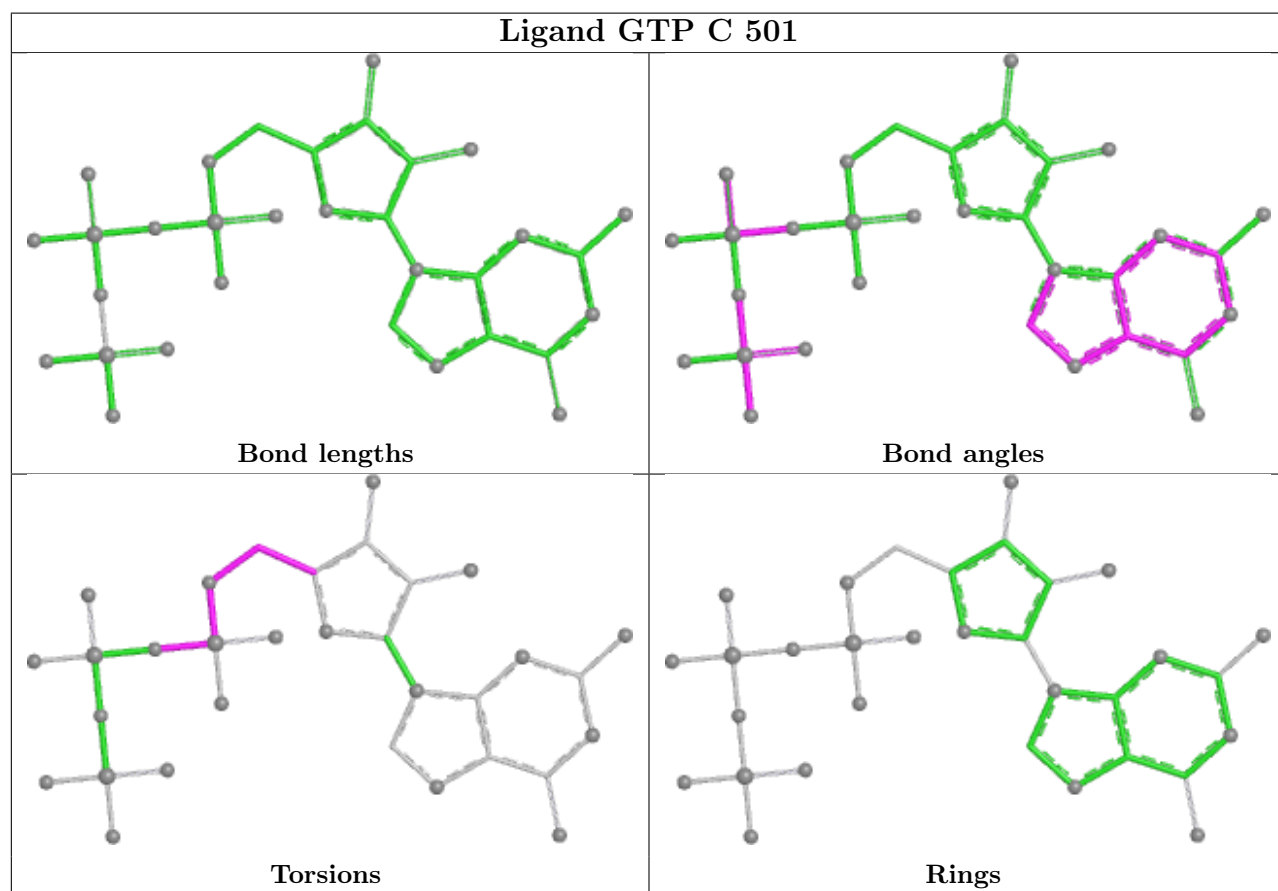
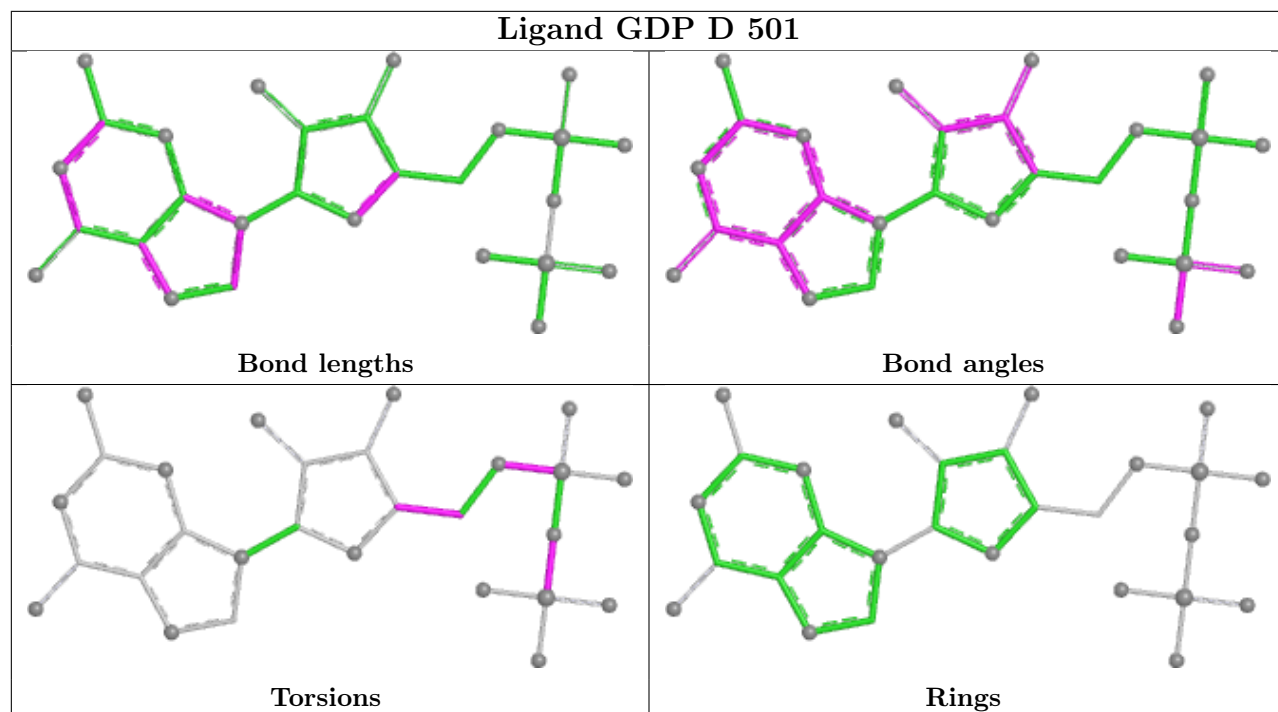
Ligand A1D8I B 504

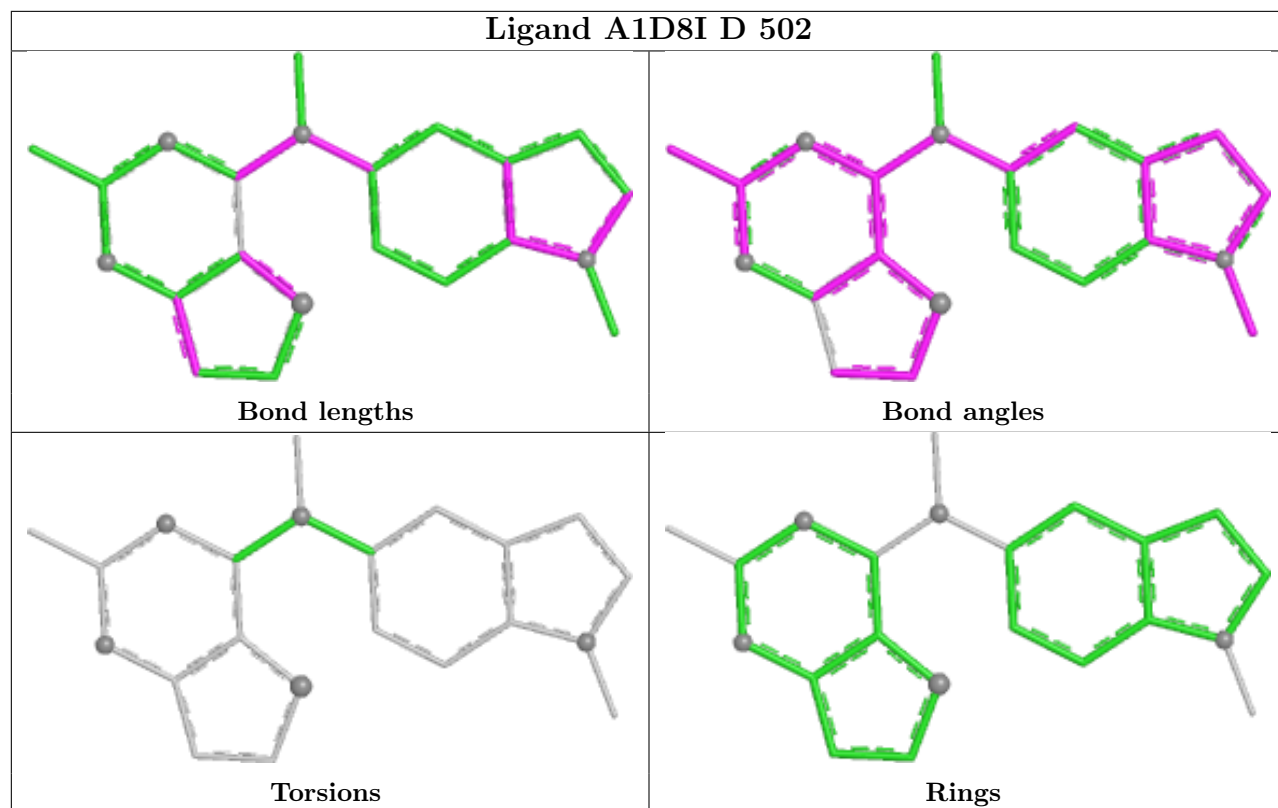


Ligand ACP F 401









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	437/450 (97%)	-0.25	3 (0%) 84 79	37, 53, 77, 93	0
1	C	440/450 (97%)	-0.47	3 (0%) 84 79	26, 44, 67, 81	0
2	B	427/445 (95%)	-0.26	0 100 100	32, 52, 84, 126	0
2	D	421/445 (94%)	0.18	5 (1%) 76 70	38, 71, 100, 121	0
3	E	121/143 (84%)	0.14	3 (2%) 58 49	44, 66, 98, 113	0
4	F	334/384 (86%)	0.32	17 (5%) 33 27	43, 75, 129, 147	0
All	All	2180/2317 (94%)	-0.11	31 (1%) 73 66	26, 58, 100, 147	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	161	LEU	4.2
4	F	149	ALA	4.1
2	D	72	THR	3.4
4	F	130	VAL	3.1
1	A	88	HIS	3.0
2	D	1	MET	2.9
3	E	6	MET	2.9
4	F	134	ALA	2.9
4	F	372	THR	2.9
4	F	182	ILE	2.8
4	F	331	GLU	2.7
2	D	284	LEU	2.7
3	E	141	GLU	2.7
4	F	240	LEU	2.6
2	D	55	THR	2.5
4	F	380	HIS	2.2
3	E	139	LEU	2.2
4	F	231	ALA	2.2
4	F	245	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
4	F	169	LEU	2.2
4	F	362	ALA	2.2
4	F	233	PHE	2.2
2	D	245	GLN	2.1
1	C	357	TYR	2.1
4	F	253	TYR	2.1
4	F	173	ILE	2.1
1	A	437	VAL	2.1
4	F	135	TYR	2.1
1	C	163	LYS	2.1
1	C	1	MET	2.0
1	A	282	TYR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	MG	B	502	1/1	0.83	0.29	57,57,57,57	0
12	ACP	F	401	31/31	0.86	0.10	85,93,112,124	0
6	MG	C	502	1/1	0.87	0.28	41,41,41,41	0
8	GOL	A	504	6/6	0.88	0.10	53,56,58,60	0
6	MG	A	502	1/1	0.89	0.23	46,46,46,46	0
7	CA	A	503	1/1	-	-	80,80,80,80	1
7	CA	C	503	1/1	-	-	62,62,62,62	1
9	GDP	D	501	28/28	0.91	0.09	60,68,82,88	0
10	MES	B	503	12/12	0.94	0.09	43,52,68,70	0
5	GTP	A	501	32/32	0.95	0.07	40,44,52,63	0
11	A1D8I	D	502	22/22	0.96	0.09	47,53,59,70	0

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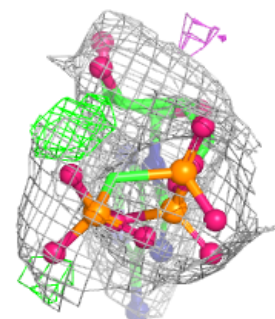
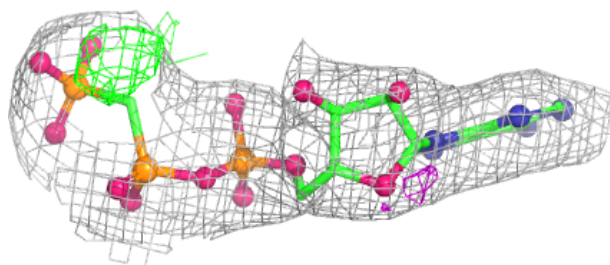
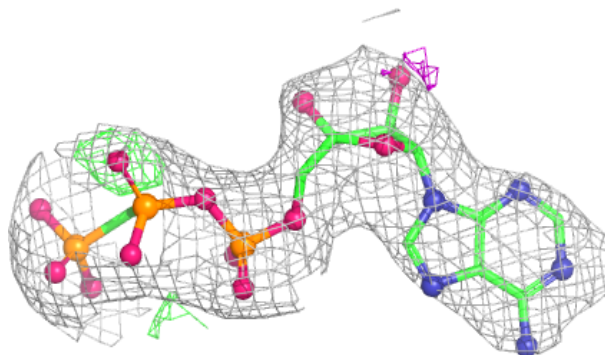
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	GTP	C	501	32/32	0.96	0.06	32,39,43,46	0
9	GDP	B	501	28/28	0.97	0.06	35,41,47,48	0
11	A1D8I	B	504	22/22	0.97	0.09	35,44,50,52	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.

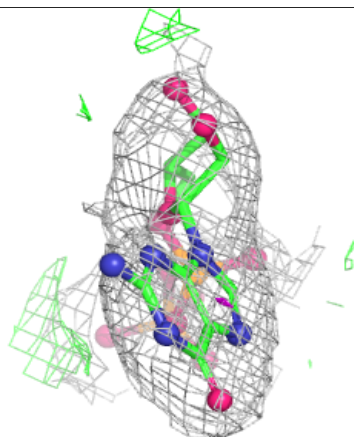
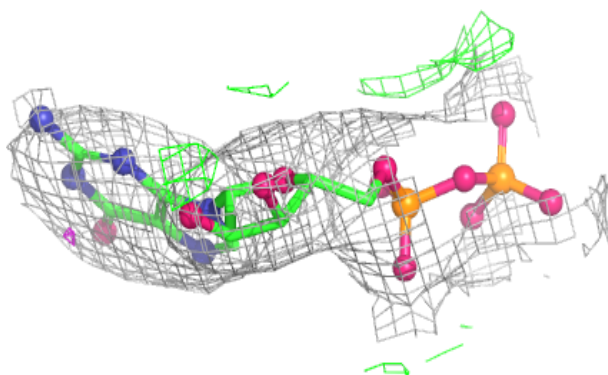
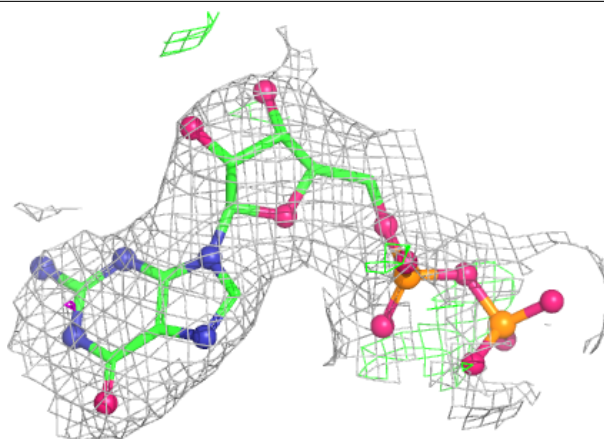
Electron density around ACP F 401:

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



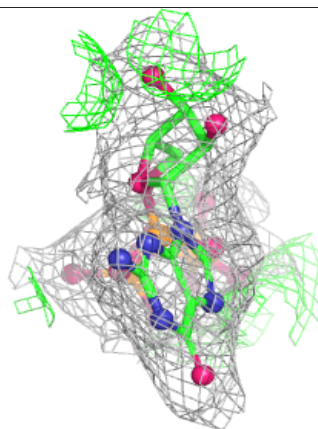
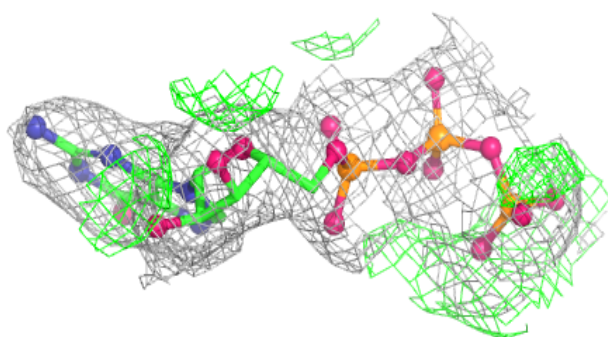
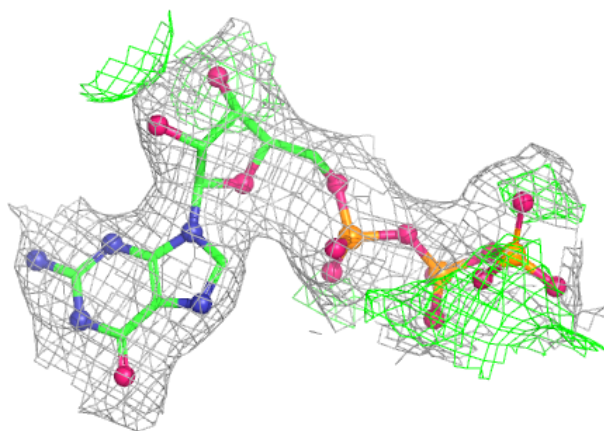
Electron density around GDP D 501:

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

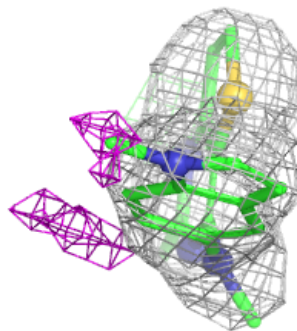
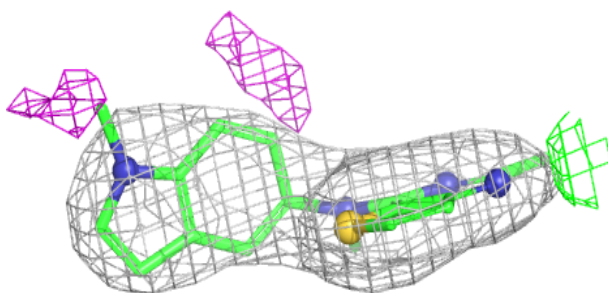
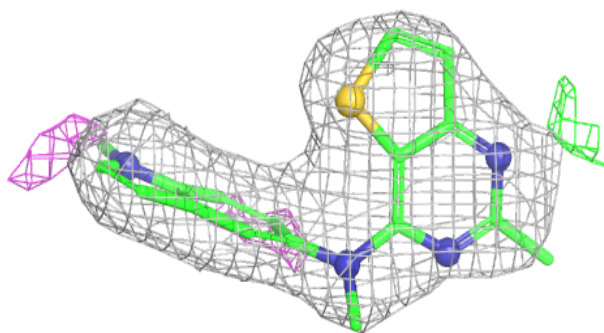


Electron density around GTP A 501:

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

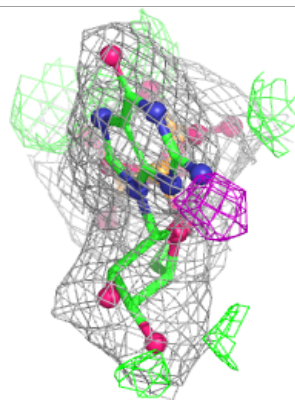
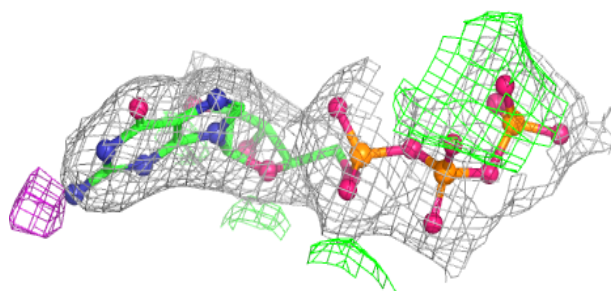
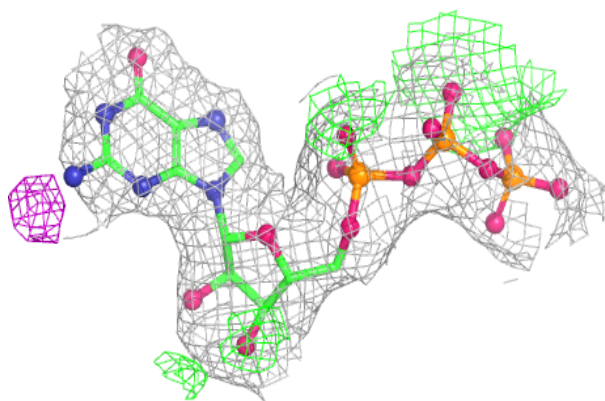
**Electron density around A1D8I D 502:**

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



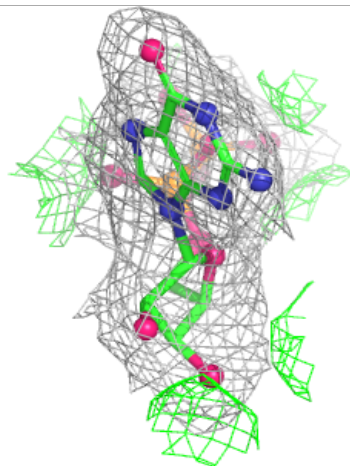
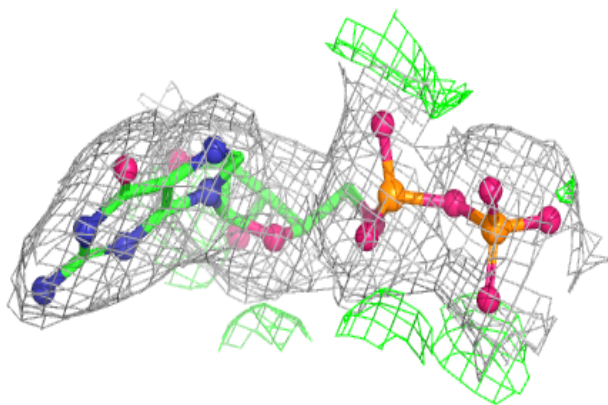
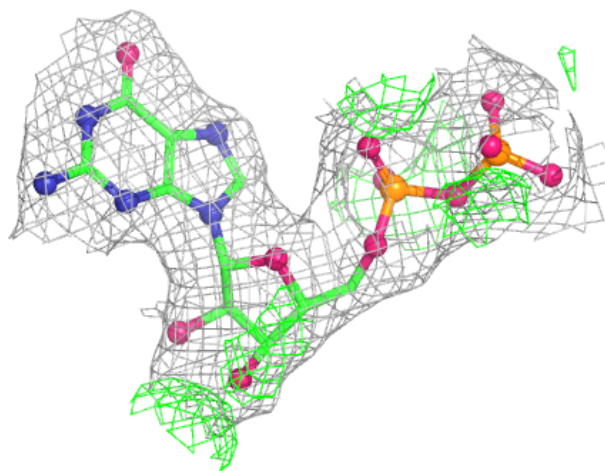
Electron density around GTP C 501:

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



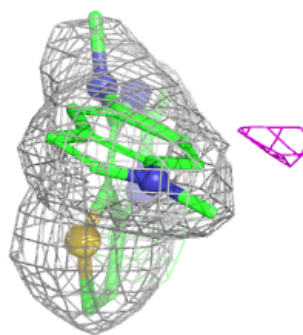
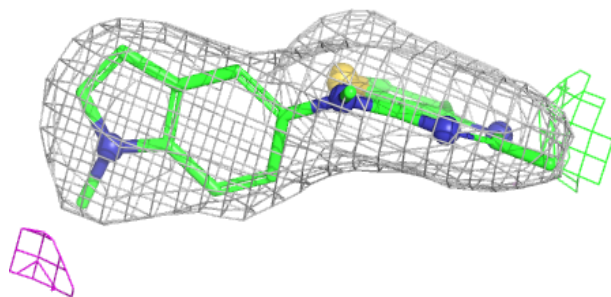
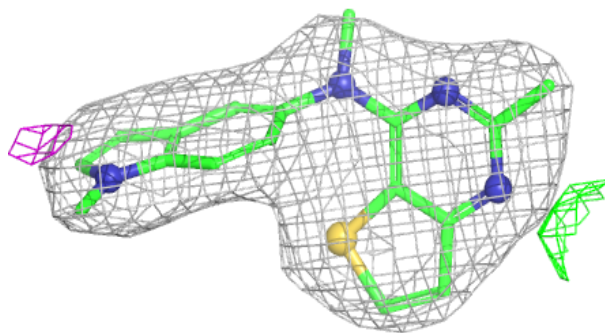
Electron density around GDP B 501:

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



Electron density around A1D8I 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.