



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:02 PM UTC

PDB ID : 7EXC / pdb_00007exc
Title : Crystal structure of T2R-TTL-1129A2 complex
Authors : Yang, J.H.; Yan, W.
Deposited on : 2021-05-26
Resolution : 2.39 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:

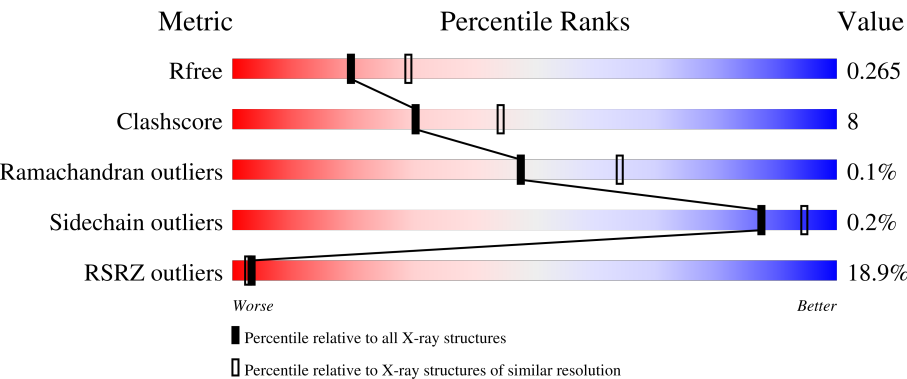
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal 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 2.39 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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

Mol	Chain	Length	Quality of chain
1	A	451	4% 85% 12% .
1	C	451	4% 86% 11% ..
2	B	445	9% 81% 14% .
2	D	445	35% 76% 18% 5%
3	E	189	19% 51% 11% .. 36%

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Mol	Chain	Length	Quality of chain
4	F	384	38% 70% 17% • 12%

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 34877 atoms, of which 16830 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	437	Total	C	H	N	O	S	0	0	0
			6733	2163	3317	581	650	22			
1	C	440	Total	C	H	N	O	S	0	0	0
			6772	2175	3335	584	656	22			

- Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	427	Total	C	H	N	O	S	0	0	0
			6560	2108	3204	576	647	25			
2	D	421	Total	C	H	N	O	S	0	0	0
			6457	2078	3153	562	638	26			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	E	121	Total	C	H	N	O	S	0	0	0
			2013	617	1013	181	197	5			

- Molecule 4 is a protein called Tubulin tyrosine ligase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	F	338	Total	C	H	N	O	S	0	0	0
			5494	1785	2709	482	504	14			

There are 6 discrepancies between the modelled and reference sequences:

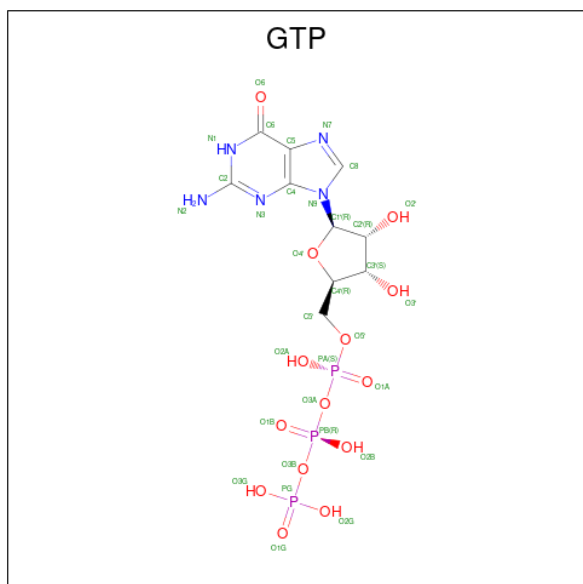
Chain	Residue	Modelled	Actual	Comment	Reference
F	379	HIS	-	expression tag	UNP E1BQ43
F	380	HIS	-	expression tag	UNP E1BQ43
F	381	HIS	-	expression tag	UNP E1BQ43
F	382	HIS	-	expression tag	UNP E1BQ43

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Chain	Residue	Modelled	Actual	Comment	Reference
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	H	N	O	P	42	0
			42	10	10	5	14	3		
5	C	1	Total	C	H	N	O	P	42	0
			42	10	10	5	14	3		
5	D	1	Total	C	H	N	O	P	42	0
			42	10	10	5	14	3		

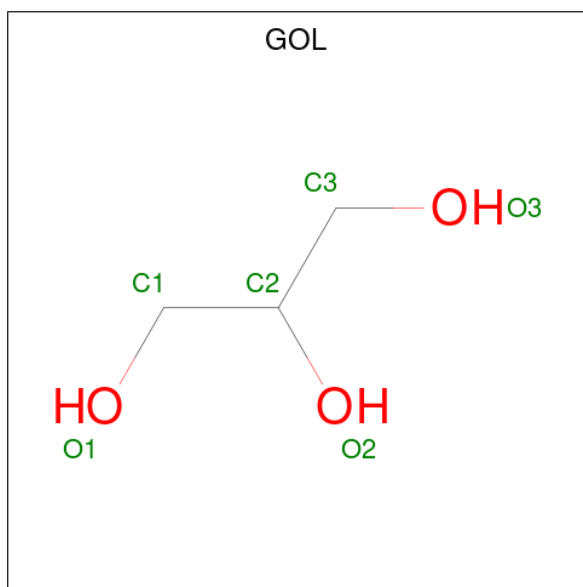
- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

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

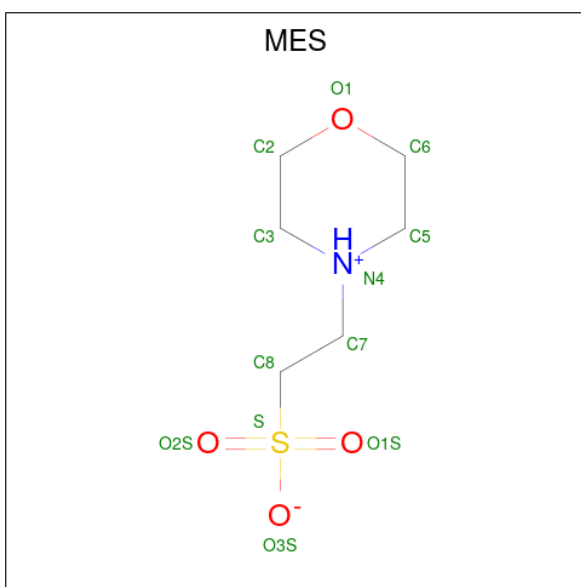
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Ca	1	0
			1	1		
7	C	1	Total	Ca	1	0
			1	1		

- Molecule 8 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



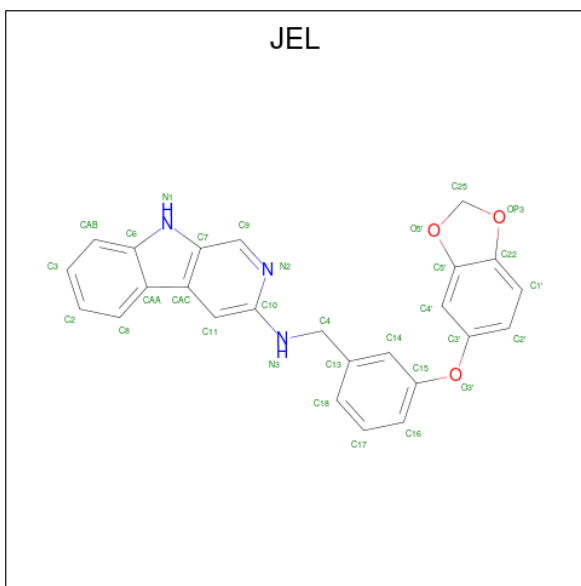
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	H	O	14	0
			14	3	8	3		

- Molecule 9 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: $C_6H_{13}NO_4S$).



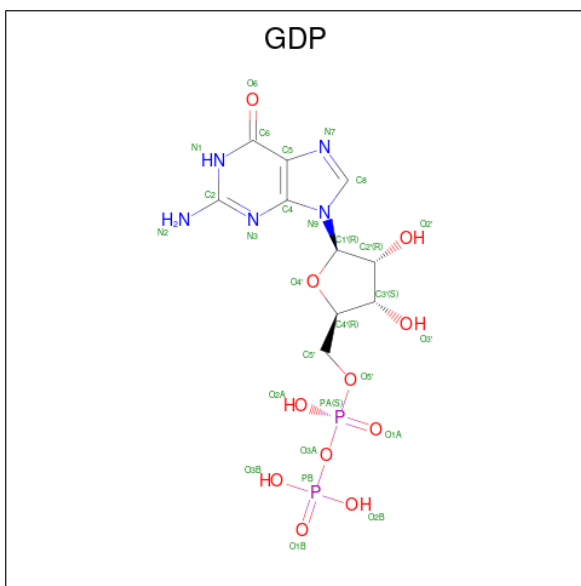
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
9	B	1	Total	C	H	N	O	S	25	0
			25	6	13	1	4	1		

- Molecule 10 is N-[[3-(1,3-benzodioxol-5-yloxy)phenyl]methyl]-9H-pyrido[3,4-b]indol-3-amine (CCD ID: JEL) (formula: C₂₅H₁₉N₃O₃) (labeled as "Ligand of Interest" by depositor).



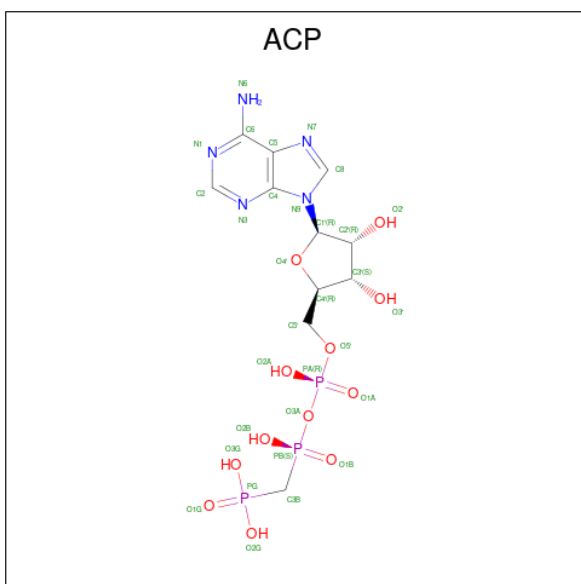
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	B	1	Total	C	H	N	O	0	0
			50	25	19	3	3		
10	D	1	Total	C	H	N	O	0	0
			50	25	19	3	3		

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
11	B	1	Total	C	H	N	O	P	38	0
			38	10	10	5	11	2		

- Molecule 12 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (CCD ID: ACP) (formula: $\text{C}_{11}\text{H}_{18}\text{N}_5\text{O}_{12}\text{P}_3$).



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

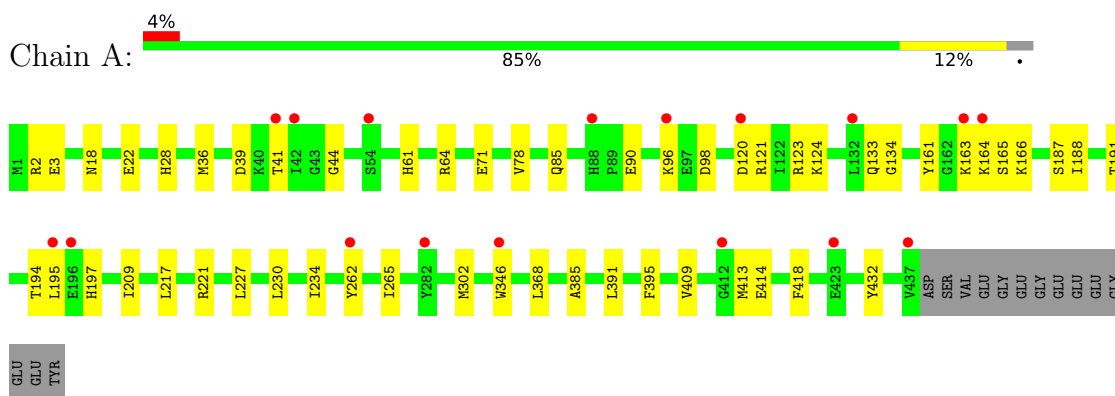
- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	125	Total 125	O 125	0	0
13	B	99	Total 99	O 99	0	0
13	C	202	Total 202	O 202	0	0
13	D	29	Total 29	O 29	0	0
13	E	19	Total 19	O 19	0	0
13	F	34	Total 34	O 34	0	0

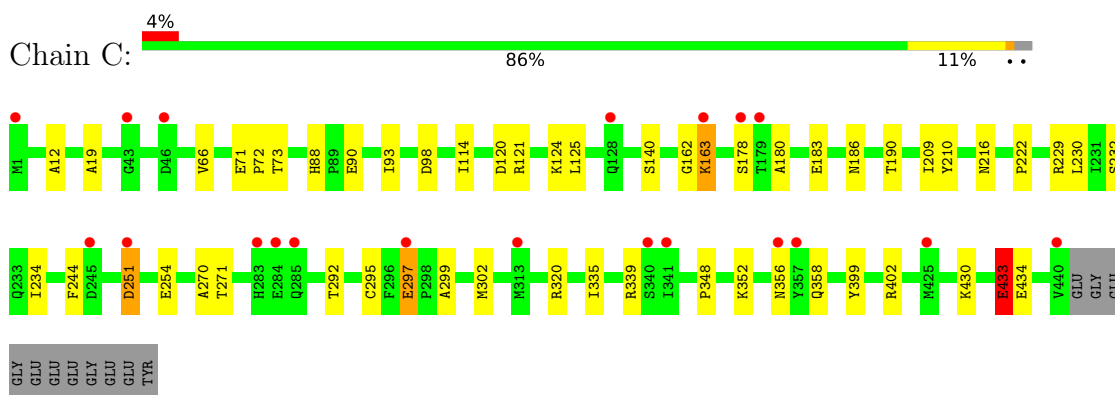
3 Residue-property plots [i](#)

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.

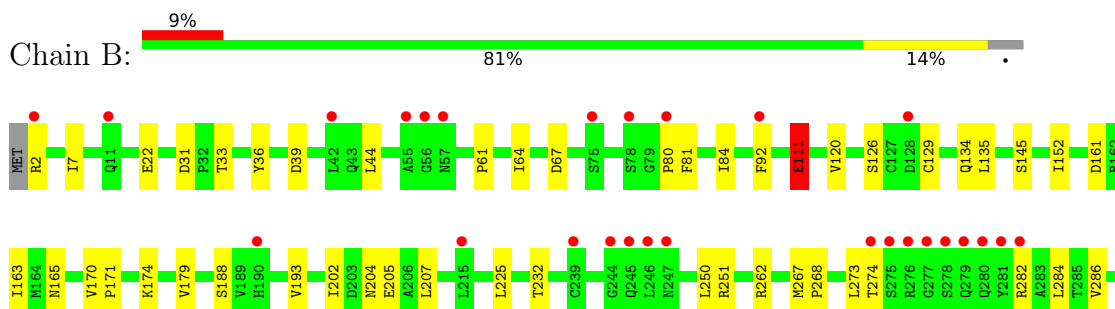
- Molecule 1: Tubulin alpha-1B chain

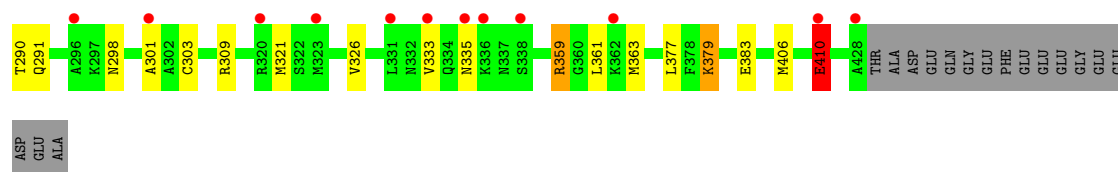


- Molecule 1: Tubulin alpha-1B chain

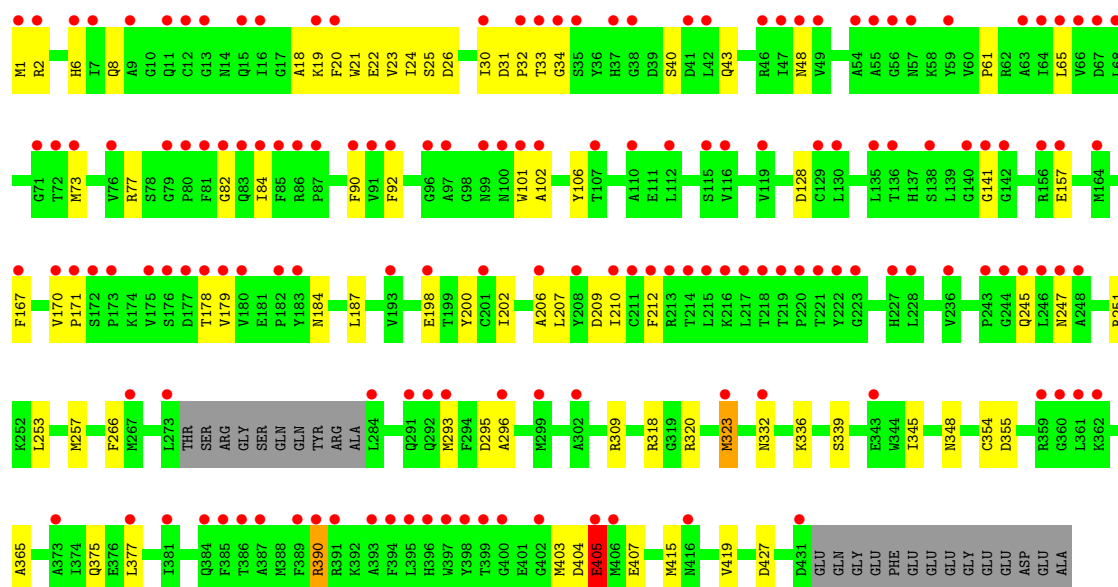
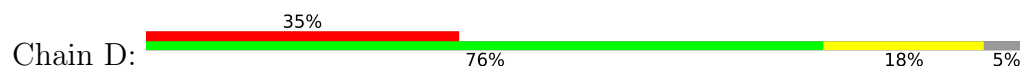


- Molecule 2: Tubulin beta chain

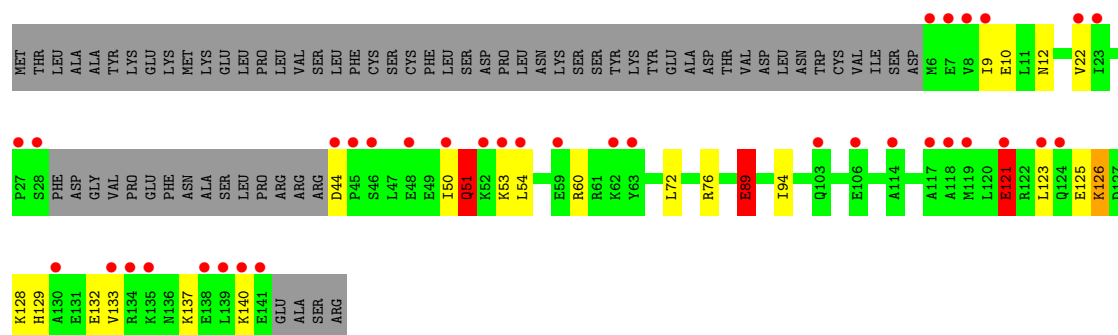




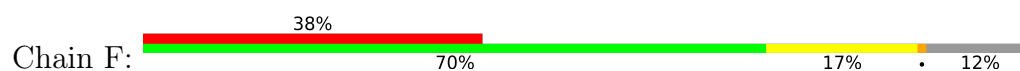
- Molecule 2: Tubulin beta chain



- Molecule 3: Stathmin-4



- Molecule 4: Tubulin tyrosine ligase



C347	C348	D352	L361	A362	ASP	THR	GLY	GLN	LYS	THR	SER	GLN	PRO	T372	S373	H379	H380	H381	H382	H383	H384																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																							</
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4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	105.25Å 157.38Å 181.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.85 – 2.39 49.85 – 2.39	Depositor EDS
% Data completeness (in resolution range)	96.9 (49.85-2.39) 96.9 (49.85-2.39)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.08 (at 2.39Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.218 , 0.264 0.220 , 0.265	Depositor DCC
R_{free} test set	2318 reflections (1.94%)	wwPDB-VP
Wilson B-factor (Å ²)	36.2	Xtriage
Anisotropy	0.057	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 42.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	34877	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.73% 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: CA, GOL, MG, GTP, JEL, ACP, GDP, MES

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	0.20	0/3494	0.42	1/4743 (0.0%)
1	C	0.50	6/3515 (0.2%)	0.61	15/4772 (0.3%)
2	B	0.25	0/3431	0.51	9/4649 (0.2%)
2	D	0.42	3/3377 (0.1%)	0.59	9/4576 (0.2%)
3	E	0.60	1/1008 (0.1%)	0.96	10/1337 (0.7%)
4	F	0.31	2/2851 (0.1%)	0.60	6/3851 (0.2%)
All	All	0.37	12/17676 (0.1%)	0.58	50/23928 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	2
2	B	0	3
2	D	0	3
3	E	0	3
4	F	0	1
All	All	0	12

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	163	LYS	CE-NZ	16.79	1.99	1.49
1	C	433	GLU	CB-CG	11.96	1.88	1.52
2	D	323	MET	CG-SD	10.38	2.06	1.80
2	D	323	MET	SD-CE	9.47	2.03	1.79
2	D	323	MET	CB-CG	8.66	1.78	1.52
1	C	163	LYS	CB-CG	8.50	1.77	1.52
1	C	433	GLU	CG-CD	7.08	1.69	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	163	LYS	CD-CE	6.99	1.73	1.52
3	E	126	LYS	CE-NZ	6.63	1.69	1.49
4	F	86	GLU	CB-CG	5.50	1.69	1.52
1	C	251	ASP	CA-C	5.44	1.59	1.52
4	F	85	PRO	C-N	-5.07	1.26	1.33

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	433	GLU	CG-CD-OE2	-13.69	86.91	118.40
4	F	86	GLU	CA-CB-CG	13.10	140.30	114.10
1	C	433	GLU	CG-CD-OE1	11.64	145.17	118.40
3	E	126	LYS	CG-CD-CE	-10.32	87.57	111.30
1	C	163	LYS	CB-CG-CD	-10.29	87.63	111.30
4	F	86	GLU	CG-CD-OE2	-10.29	94.73	118.40
4	F	86	GLU	CG-CD-OE1	10.14	141.71	118.40
3	E	126	LYS	CB-CA-C	9.86	127.61	110.85
2	B	410	GLU	OE1-CD-OE2	-9.18	100.87	122.90
1	C	433	GLU	CB-CG-CD	-8.86	97.55	112.60
2	B	359	ARG	CA-CB-CG	8.84	131.78	114.10
1	C	433	GLU	OE1-CD-OE2	-8.48	102.56	122.90
3	E	51	GLN	CA-CB-CG	8.35	130.80	114.10
2	D	405	GLU	CA-CB-CG	-8.29	97.51	114.10
4	F	86	GLU	OE1-CD-OE2	-7.82	104.14	122.90
1	C	163	LYS	CD-CE-NZ	-7.63	87.49	111.90
3	E	126	LYS	CD-CE-NZ	-7.58	87.65	111.90
2	D	390	ARG	CD-NE-CZ	7.24	134.53	124.40
2	D	390	ARG	NE-CZ-NH1	-7.15	114.35	121.50
2	B	410	GLU	CG-CD-OE1	7.01	134.52	118.40
1	C	251	ASP	CB-CA-C	6.99	121.28	109.75
1	C	163	LYS	CB-CA-C	6.98	122.52	110.72
2	D	405	GLU	OE1-CD-OE2	-6.93	106.27	122.90
2	D	323	MET	CG-SD-CE	-6.67	86.23	100.90
2	D	405	GLU	CG-CD-OE1	6.54	133.45	118.40
2	D	323	MET	CA-CB-CG	-6.50	101.11	114.10
1	C	163	LYS	CA-CB-CG	-6.20	101.69	114.10
4	F	86	GLU	CB-CG-CD	-6.10	102.23	112.60
2	B	410	GLU	CG-CD-OE2	-6.02	104.56	118.40
1	C	251	ASP	CB-CG-OD1	5.99	132.18	118.40
2	D	257	MET	CA-CB-CG	5.81	125.71	114.10
2	B	410	GLU	CA-CB-CG	5.78	125.65	114.10
4	F	305	LYS	CB-CG-CD	-5.75	98.07	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	121	GLU	CG-CD-OE1	5.74	131.60	118.40
1	C	251	ASP	CB-CG-OD2	-5.70	105.28	118.40
2	B	379	LYS	CG-CD-CE	5.69	124.39	111.30
1	A	221	ARG	CD-NE-CZ	5.64	132.29	124.40
2	B	111	GLU	CG-CD-OE2	-5.61	105.50	118.40
3	E	126	LYS	CB-CG-CD	-5.49	98.68	111.30
1	C	433	GLU	CA-CB-CG	-5.48	103.15	114.10
1	C	163	LYS	N-CA-CB	-5.47	102.25	110.73
1	C	297	GLU	CG-CD-OE1	5.45	130.93	118.40
2	B	111	GLU	CG-CD-OE1	5.43	130.89	118.40
3	E	89	GLU	CG-CD-OE1	5.41	130.84	118.40
3	E	121	GLU	OE1-CD-OE2	-5.31	110.15	122.90
2	B	410	GLU	N-CA-CB	-5.24	101.23	109.78
1	C	433	GLU	CB-CA-C	5.14	120.54	110.67
3	E	121	GLU	N-CA-CB	-5.11	102.07	110.14
3	E	89	GLU	CG-CD-OE2	-5.05	106.79	118.40
2	D	323	MET	CB-CG-SD	-5.04	97.58	112.70

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	111	GLU	Sidechain
2	B	359	ARG	Sidechain
2	B	410	GLU	Sidechain
1	C	251	ASP	Sidechain
1	C	433	GLU	Sidechain
2	D	212	PHE	Sidechain
2	D	390	ARG	Sidechain
2	D	405	GLU	Sidechain
3	E	121	GLU	Sidechain
3	E	51	GLN	Sidechain
3	E	89	GLU	Sidechain
4	F	86	GLU	Sidechain

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	3317	3330	45	0
1	C	3437	3335	3348	47	0
2	B	3356	3204	3234	46	0
2	D	3304	3153	3185	76	0
3	E	1000	1013	1018	25	0
4	F	2785	2709	2737	54	0
5	A	32	10	12	0	0
5	C	32	10	12	0	0
5	D	32	10	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
7	A	1	0	0	0	0
7	C	1	0	0	0	0
8	A	6	8	8	0	0
9	B	12	13	12	0	0
10	B	31	19	0	0	0
10	D	31	19	0	2	0
11	B	28	10	12	0	0
12	F	31	0	14	0	0
13	A	125	0	0	3	0
13	B	99	0	0	3	0
13	C	202	0	0	5	0
13	D	29	0	0	6	0
13	E	19	0	0	2	0
13	F	34	0	0	0	0
All	All	18047	16830	16934	287	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 8.

All (287) 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)
2:D:323:MET:CG	2:D:323:MET:CB	1.78	1.59
1:C:163:LYS:CG	1:C:163:LYS:CB	1.78	1.57
3:E:126:LYS:CE	3:E:126:LYS:NZ	1.69	1.56
1:C:433:GLU:CB	1:C:433:GLU:CG	1.88	1.50
2:D:323:MET:CE	2:D:323:MET:SD	2.03	1.47
2:D:323:MET:CG	2:D:323:MET:SD	2.06	1.42
1:C:163:LYS:CE	1:C:163:LYS:NZ	1.99	1.25

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:126:LYS:NZ	3:E:126:LYS:HG2	1.67	1.07
1:C:163:LYS:CB	1:C:163:LYS:CD	2.34	1.05
3:E:126:LYS:NZ	3:E:126:LYS:CD	2.23	1.00
3:E:126:LYS:NZ	3:E:126:LYS:CG	2.25	0.99
1:C:297:GLU:OE2	13:C:601:HOH:O	1.83	0.95
2:D:323:MET:CG	2:D:323:MET:CA	2.52	0.87
1:C:163:LYS:CG	1:C:163:LYS:CA	2.56	0.82
4:F:31:ARG:HG3	4:F:32:LYS:H	1.47	0.79
4:F:31:ARG:HG3	4:F:32:LYS:N	1.97	0.78
1:C:163:LYS:CB	1:C:163:LYS:HD2	2.14	0.77
2:D:404:ASP:OD1	2:D:405:GLU:HG2	1.85	0.76
4:F:131:PHE:CE2	4:F:182:ILE:HG12	2.20	0.76
3:E:126:LYS:HG2	3:E:126:LYS:HZ3	1.50	0.75
2:D:32:PRO:C	2:D:84:ILE:HD13	2.14	0.73
2:D:20:PHE:O	2:D:24:ILE:HG12	1.88	0.72
1:A:71:GLU:O	13:A:601:HOH:O	2.08	0.72
4:F:128:ARG:NH1	4:F:170:LEU:HD22	2.06	0.71
4:F:146:VAL:N	4:F:187:GLU:OE1	2.23	0.71
2:B:81:PHE:O	2:B:84:ILE:HG22	1.91	0.71
2:B:80:PRO:O	13:B:601:HOH:O	2.08	0.71
1:C:163:LYS:CD	1:C:163:LYS:HB3	2.21	0.70
3:E:126:LYS:CD	3:E:126:LYS:HZ2	2.05	0.70
3:E:126:LYS:HG2	3:E:126:LYS:HZ2	1.57	0.69
1:C:433:GLU:CG	1:C:433:GLU:CA	2.71	0.67
2:D:245:GLN:O	13:D:601:HOH:O	2.11	0.67
3:E:126:LYS:CG	3:E:126:LYS:HZ2	2.06	0.67
4:F:88:SER:O	4:F:90:SER:N	2.27	0.67
1:C:163:LYS:NZ	1:C:163:LYS:CD	2.58	0.67
1:A:234:ILE:HD13	1:A:302:MET:SD	2.34	0.66
3:E:12:ASN:OD1	13:E:201:HOH:O	2.12	0.66
2:D:167:PHE:CD2	2:D:202:ILE:HD11	2.30	0.66
4:F:1:MET:HE3	4:F:28:LYS:HB2	1.77	0.66
4:F:236:LYS:HB3	4:F:240:LEU:HD13	1.78	0.66
1:C:339:ARG:O	13:C:602:HOH:O	2.13	0.65
3:E:51:GLN:HE21	3:E:51:GLN:HA	1.62	0.65
4:F:348:GLN:NE2	4:F:352:ASP:OD1	2.28	0.65
1:C:71:GLU:OE2	1:C:73:THR:OG1	2.13	0.65
1:C:433:GLU:CB	1:C:433:GLU:CD	2.69	0.65
2:D:427:ASP:OD2	13:D:602:HOH:O	2.15	0.65
1:C:163:LYS:HD2	1:C:163:LYS:HB3	1.78	0.64
3:E:129:HIS:O	3:E:133:VAL:HG23	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:192:LEU:HD22	4:F:262:MET:HE1	1.80	0.64
2:D:323:MET:CG	2:D:323:MET:C	2.72	0.63
2:B:335:ASN:CG	4:F:58:LEU:HD21	2.23	0.63
2:B:335:ASN:ND2	4:F:58:LEU:HD21	2.13	0.63
2:B:179:VAL:HG12	1:C:348:PRO:HG2	1.79	0.63
2:D:106:TYR:OH	2:D:407:GLU:OE2	2.14	0.62
2:B:406:MET:HG3	2:B:410:GLU:OE1	2.00	0.61
2:B:286:VAL:HG22	2:B:321:MET:HE3	1.82	0.61
4:F:274:ALA:HB3	4:F:275:LEU:HD12	1.83	0.60
2:D:323:MET:CB	2:D:323:MET:SD	2.90	0.60
2:D:34:GLY:N	2:D:84:ILE:HD11	2.16	0.60
4:F:57:GLY:O	4:F:58:LEU:HD23	2.01	0.60
2:D:323:MET:CG	2:D:323:MET:CE	2.80	0.60
2:D:207:LEU:HA	2:D:210:ILE:CD1	2.32	0.60
2:D:320:ARG:HH21	2:D:320:ARG:HG2	1.67	0.60
2:B:202:ILE:CG2	2:B:207:LEU:HD11	2.32	0.59
2:D:1:MET:N	2:D:128:ASP:HB2	2.17	0.59
2:B:161:ASP:O	2:B:251:ARG:NH2	2.36	0.59
2:B:145:SER:HG	2:B:188:SER:HG	1.48	0.59
2:D:251:ARG:NH1	13:D:604:HOH:O	2.32	0.58
4:F:198:LYS:HE2	4:F:320:MET:HE1	1.85	0.58
2:D:206:ALA:O	2:D:210:ILE:HD12	2.02	0.58
2:B:204:ASN:OD1	2:B:225:LEU:HD23	2.04	0.57
1:C:93:ILE:HG22	1:C:114:ILE:HD11	1.87	0.57
2:D:375:GLN:HB2	2:D:419:VAL:HG13	1.87	0.57
3:E:121:GLU:O	3:E:125:GLU:HG3	2.05	0.57
1:C:71:GLU:HB2	1:C:98:ASP:HB3	1.85	0.56
1:A:22:GLU:OE1	13:A:602:HOH:O	2.18	0.56
4:F:31:ARG:CG	4:F:32:LYS:H	2.18	0.56
4:F:147:TRP:HB3	4:F:182:ILE:HD11	1.88	0.56
1:C:216:ASN:O	13:C:603:HOH:O	2.18	0.55
2:D:206:ALA:O	2:D:209:ASP:N	2.39	0.55
2:D:2:ARG:NH2	13:D:606:HOH:O	2.40	0.55
1:A:187:SER:HB3	1:A:391:LEU:HD21	1.89	0.54
1:A:163:LYS:HB3	1:A:164:LYS:HD3	1.89	0.54
4:F:128:ARG:HH11	4:F:170:LEU:HD22	1.72	0.54
1:C:162:GLY:HA2	3:E:94:ILE:HD11	1.90	0.53
4:F:163:SER:OG	4:F:164:SER:N	2.41	0.53
4:F:237:THR:O	4:F:246:GLN:NE2	2.41	0.53
2:D:1:MET:HG3	2:D:48:ASN:OD1	2.08	0.53
2:D:377:LEU:C	2:D:377:LEU:HD23	2.33	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:320:ARG:HA	1:C:356:ASN:O	2.09	0.53
2:B:309:ARG:NH1	13:B:605:HOH:O	2.36	0.53
1:A:191:THR:O	1:A:195:LEU:HB2	2.09	0.52
4:F:191:LEU:HA	4:F:197:ARG:O	2.09	0.52
1:C:163:LYS:NZ	1:C:163:LYS:HD3	2.24	0.52
4:F:102:PRO:HG2	4:F:177:GLY:O	2.10	0.52
4:F:275:LEU:HD12	4:F:275:LEU:N	2.24	0.52
2:D:30:ILE:HG13	2:D:30:ILE:O	2.09	0.52
4:F:31:ARG:CG	4:F:32:LYS:N	2.70	0.51
1:A:18:ASN:OD1	1:A:78:VAL:HG22	2.10	0.51
1:A:71:GLU:HB2	1:A:98:ASP:HB3	1.93	0.51
2:B:232:THR:HG21	2:B:268:PRO:HB2	1.92	0.51
2:D:1:MET:H3	2:D:128:ASP:HB2	1.75	0.51
2:D:179:VAL:N	13:D:605:HOH:O	2.43	0.51
2:B:2:ARG:NH1	2:B:129:CYS:SG	2.81	0.51
2:B:301:ALA:O	2:B:303:CYS:N	2.42	0.51
2:D:178:THR:HG22	13:D:605:HOH:O	2.11	0.51
1:C:120:ASP:O	1:C:124:LYS:HG2	2.11	0.50
4:F:136:ASN:O	4:F:140:GLU:N	2.40	0.50
1:A:414:GLU:OE2	3:E:60:ARG:NH1	2.44	0.50
1:A:85:GLN:OE1	13:A:603:HOH:O	2.18	0.50
1:A:166:LYS:HE2	1:A:197:HIS:O	2.11	0.50
2:B:126:SER:O	2:B:126:SER:OG	2.26	0.50
3:E:9:ILE:HD12	3:E:10:GLU:HG2	1.94	0.50
4:F:135:TYR:OH	4:F:164:SER:O	2.29	0.50
1:A:90:GLU:O	1:A:121:ARG:HD2	2.12	0.50
1:A:134:GLY:HA3	1:A:165:SER:O	2.11	0.50
2:B:170:VAL:HG11	2:B:377:LEU:HD21	1.92	0.50
2:D:21:TRP:O	2:D:25:SER:OG	2.18	0.50
2:D:141:GLY:O	2:D:184:ASN:ND2	2.45	0.50
2:D:202:ILE:CG2	2:D:207:LEU:HD11	2.41	0.50
2:D:207:LEU:HA	2:D:210:ILE:HD13	1.94	0.49
1:A:28:HIS:HB3	1:A:36:MET:HE3	1.93	0.49
4:F:40:MET:HE3	4:F:52:LEU:HD21	1.95	0.49
2:D:20:PHE:CE1	2:D:24:ILE:HD13	2.48	0.49
3:E:44:ASP:N	13:E:204:HOH:O	2.45	0.48
4:F:242:ASN:HB2	4:F:245:ILE:HG12	1.95	0.48
2:B:22:GLU:HG2	2:B:81:PHE:CD1	2.48	0.48
2:B:61:PRO:CD	2:B:84:ILE:HG12	2.43	0.48
1:A:163:LYS:C	1:A:164:LYS:HD3	2.38	0.48
2:B:290:THR:HG22	2:B:333:VAL:HG21	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:19:LYS:O	2:D:23:VAL:HG23	2.14	0.48
1:A:187:SER:CB	1:A:391:LEU:HD21	2.44	0.48
2:D:34:GLY:CA	2:D:84:ILE:HD11	2.43	0.48
2:D:293:MET:SD	2:D:365:ALA:HB1	2.54	0.48
1:A:209:ILE:HD11	1:A:302:MET:SD	2.54	0.48
1:A:39:ASP:OD1	1:A:41:THR:N	2.47	0.47
2:B:64:ILE:HD13	2:B:120:VAL:HG22	1.96	0.47
2:D:198:GLU:HG3	2:D:266:PHE:CE2	2.49	0.47
3:E:50:ILE:O	3:E:53:LYS:HG2	2.14	0.47
4:F:100:ILE:CD1	4:F:128:ARG:HA	2.44	0.47
2:B:267:MET:HG2	2:B:301:ALA:HB3	1.94	0.47
1:A:163:LYS:HG2	1:A:163:LYS:O	2.14	0.47
2:B:36:TYR:CE2	2:B:44:LEU:HD11	2.49	0.47
2:D:253:LEU:HB3	10:D:502:JEL:C9	2.45	0.47
2:D:415:MET:O	2:D:419:VAL:HG23	2.14	0.47
2:D:206:ALA:C	2:D:210:ILE:HD12	2.40	0.47
1:C:433:GLU:CG	1:C:433:GLU:C	2.88	0.47
4:F:126:ASP:OD1	4:F:127:GLU:N	2.48	0.47
1:A:96:LYS:HB2	1:A:96:LYS:HE2	1.54	0.46
4:F:37:PHE:CZ	4:F:40:MET:HE3	2.51	0.46
2:B:170:VAL:HG13	2:B:171:PRO:HD2	1.96	0.46
4:F:220:VAL:HG23	4:F:263:PHE:CD1	2.50	0.46
1:A:41:THR:OG1	1:A:44:GLY:O	2.33	0.46
2:B:67:ASP:O	2:B:92:PHE:HA	2.15	0.46
2:D:355:ASP:OD2	2:D:355:ASP:N	2.47	0.46
2:D:65:LEU:HD11	2:D:90:PHE:CE2	2.51	0.46
2:D:157:GLU:HG3	3:E:123:LEU:HD13	1.97	0.46
4:F:98:TYR:CG	4:F:131:PHE:HB2	2.51	0.46
2:B:39:ASP:OD1	2:B:39:ASP:N	2.47	0.46
2:D:101:TRP:CE3	2:D:187:LEU:HD13	2.50	0.46
2:D:170:VAL:HG21	2:D:377:LEU:HD11	1.98	0.46
2:B:379:LYS:O	2:B:383:GLU:HG3	2.15	0.46
1:C:19:ALA:HB1	1:C:232:SER:OG	2.16	0.46
1:C:254:GLU:HG2	1:C:352:LYS:HE2	1.98	0.46
4:F:88:SER:C	4:F:90:SER:N	2.74	0.46
1:A:96:LYS:HD3	1:A:96:LYS:N	2.31	0.46
1:A:120:ASP:O	1:A:124:LYS:HG2	2.16	0.46
1:C:292:THR:HG22	1:C:335:ILE:CD1	2.45	0.46
2:B:284:LEU:O	2:B:363:MET:CE	2.63	0.45
2:D:332:ASN:OD1	2:D:336:LYS:HE2	2.15	0.45
1:A:161:TYR:CA	1:A:164:LYS:HE2	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:32:PRO:HA	2:D:84:ILE:HD13	1.98	0.45
3:E:140:LYS:HG3	3:E:140:LYS:O	2.16	0.45
4:F:340:GLN:N	4:F:340:GLN:OE1	2.50	0.45
1:A:209:ILE:HG23	1:A:230:LEU:HD23	1.98	0.45
1:A:265:ILE:HG23	1:A:432:TYR:CE1	2.52	0.45
4:F:193:GLU:OE1	4:F:196:HIS:N	2.47	0.45
1:A:262:TYR:CE1	1:A:346:TRP:CZ2	3.05	0.45
1:C:71:GLU:HG2	1:C:72:PRO:HD2	1.99	0.45
1:C:399:TYR:O	1:C:402:ARG:NH2	2.47	0.45
2:D:102:ALA:HB2	2:D:403:MET:CE	2.47	0.45
1:A:28:HIS:O	1:A:36:MET:HE3	2.16	0.45
1:A:161:TYR:HB3	1:A:164:LYS:HB2	1.99	0.45
3:E:53:LYS:HG3	3:E:54:LEU:N	2.32	0.45
4:F:88:SER:O	4:F:91:CYS:N	2.49	0.45
2:D:65:LEU:HD11	2:D:90:PHE:CZ	2.51	0.45
4:F:3:THR:OG1	4:F:37:PHE:HA	2.17	0.45
2:D:40:SER:HB2	2:D:43:GLN:HG3	1.98	0.45
3:E:72:LEU:O	3:E:76:ARG:HG2	2.17	0.45
2:B:321:MET:HE2	2:B:326:VAL:CG2	2.47	0.44
4:F:271:LEU:HA	4:F:275:LEU:HD13	2.00	0.44
2:B:135:LEU:CD2	2:B:152:ILE:HD11	2.48	0.44
2:B:274:THR:HG21	2:B:361:LEU:HD21	1.99	0.44
2:D:20:PHE:CZ	2:D:24:ILE:HD13	2.53	0.44
2:D:61:PRO:CD	2:D:84:ILE:HG23	2.48	0.44
2:D:23:VAL:O	2:D:26:ASP:HB3	2.18	0.43
2:D:318:ARG:HA	2:D:354:CYS:O	2.18	0.43
3:E:128:LYS:O	3:E:132:GLU:HG3	2.17	0.43
1:A:188:ILE:HD12	1:A:395:PHE:HB2	2.00	0.43
2:B:7:ILE:O	2:B:135:LEU:HA	2.18	0.43
2:B:406:MET:O	2:B:410:GLU:HB2	2.18	0.43
2:D:247:ASN:O	2:D:247:ASN:CG	2.60	0.43
3:E:137:LYS:O	3:E:140:LYS:HB3	2.18	0.43
2:B:61:PRO:HD3	2:B:84:ILE:HG12	2.00	0.43
2:B:202:ILE:HG21	2:B:207:LEU:HD11	2.01	0.43
2:D:65:LEU:HD23	2:D:65:LEU:H	1.83	0.43
2:D:18:ALA:O	2:D:22:GLU:HG3	2.19	0.43
2:D:31:ASP:HB2	2:D:32:PRO:HD2	2.00	0.43
2:D:200:TYR:O	2:D:202:ILE:HD12	2.18	0.43
3:E:126:LYS:HZ2	3:E:126:LYS:HD3	1.83	0.43
4:F:340:GLN:N	4:F:340:GLN:CD	2.76	0.43
2:B:321:MET:HE2	2:B:326:VAL:HG22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:409:VAL:HA	1:A:413:MET:O	2.19	0.43
2:B:273:LEU:HD11	2:B:298:ASN:HA	2.00	0.43
4:F:78:VAL:O	4:F:82:LYS:HG2	2.18	0.43
1:C:180:ALA:HB3	1:C:183:GLU:HG3	2.00	0.43
2:D:198:GLU:OE2	10:D:502:JEL:N2	2.51	0.43
2:D:345:ILE:HG22	2:D:348:ASN:HB3	2.01	0.43
1:A:413:MET:HE2	1:A:418:PHE:CE2	2.54	0.42
1:A:36:MET:HB3	1:A:61:HIS:CE1	2.55	0.42
1:C:210:TYR:CE2	1:C:222:PRO:HD2	2.55	0.42
2:D:206:ALA:C	2:D:210:ILE:CD1	2.93	0.42
4:F:271:LEU:HD23	4:F:275:LEU:HD13	2.01	0.42
1:A:262:TYR:CZ	1:A:346:TRP:CZ2	3.08	0.42
4:F:199:PHE:CD2	4:F:221:LEU:HD23	2.54	0.42
1:C:178:SER:CB	1:C:183:GLU:OE1	2.67	0.42
1:C:270:ALA:HB3	1:C:302:MET:HG3	2.00	0.42
2:D:309:ARG:NH1	2:D:339:SER:O	2.50	0.42
4:F:296:MET:SD	4:F:299:GLU:OE1	2.78	0.42
1:A:262:TYR:CE1	1:A:346:TRP:HZ2	2.38	0.42
2:B:145:SER:OG	2:B:188:SER:OG	2.23	0.42
1:C:163:LYS:CG	1:C:163:LYS:HA	2.46	0.42
2:D:323:MET:CG	2:D:323:MET:O	2.68	0.42
4:F:40:MET:CE	4:F:52:LEU:HD21	2.49	0.42
1:A:164:LYS:HD3	1:A:164:LYS:N	2.34	0.42
1:C:234:ILE:HG12	1:C:302:MET:SD	2.59	0.42
4:F:88:SER:O	4:F:89:GLU:C	2.63	0.42
2:D:73:MET:HE2	2:D:92:PHE:HD1	1.84	0.42
2:D:170:VAL:HG13	2:D:171:PRO:HD2	2.01	0.42
2:B:284:LEU:O	2:B:363:MET:HE2	2.19	0.42
4:F:193:GLU:OE2	4:F:196:HIS:ND1	2.42	0.41
1:A:2:ARG:HB3	1:A:133:GLN:HG2	2.02	0.41
1:C:244:PHE:HB2	1:C:356:ASN:ND2	2.35	0.41
2:D:332:ASN:CG	2:D:336:LYS:HE2	2.45	0.41
4:F:185:TYR:OH	4:F:198:LYS:NZ	2.53	0.41
1:A:3:GLU:HG2	1:A:64:ARG:CZ	2.50	0.41
1:A:163:LYS:HB3	1:A:164:LYS:CD	2.50	0.41
3:E:22:VAL:O	3:E:22:VAL:HG13	2.20	0.41
4:F:71:LEU:O	4:F:77:LEU:HD13	2.21	0.41
4:F:342:LEU:O	4:F:343:TYR:C	2.63	0.41
1:C:230:LEU:O	1:C:234:ILE:HD12	2.21	0.41
1:C:244:PHE:CD1	1:C:358:GLN:HG2	2.55	0.41
2:D:207:LEU:HA	2:D:210:ILE:HD12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:33:THR:C	2:D:84:ILE:HD11	2.46	0.41
2:B:134:GLN:HA	2:B:165:ASN:O	2.20	0.41
2:B:163:ILE:HG21	2:B:250:LEU:HB3	2.02	0.41
1:C:66:VAL:HG23	1:C:125:LEU:CD1	2.51	0.41
1:C:209:ILE:HG23	1:C:230:LEU:HD23	2.02	0.41
2:D:30:ILE:O	2:D:30:ILE:CG1	2.69	0.41
4:F:198:LYS:CG	4:F:199:PHE:N	2.84	0.41
1:A:123:ARG:HG2	1:A:123:ARG:HH11	1.85	0.41
1:A:194:THR:O	1:A:194:THR:HG22	2.20	0.41
1:A:217:LEU:HD21	1:A:368:LEU:HD23	2.02	0.41
2:B:193:VAL:CG1	2:B:262:ARG:HG2	2.51	0.41
1:C:430:LYS:HE2	1:C:434:GLU:OE2	2.20	0.41
4:F:348:GLN:O	4:F:352:ASP:OD1	2.39	0.41
2:B:174:LYS:HD3	2:B:205:GLU:OE2	2.21	0.41
2:B:282:ARG:HG2	2:B:282:ARG:NH1	2.36	0.41
1:C:93:ILE:HD11	1:C:121:ARG:HG3	2.03	0.41
1:C:186:ASN:O	1:C:190:THR:HG22	2.21	0.41
1:C:271:THR:HG21	1:C:295:CYS:O	2.21	0.41
1:A:161:TYR:HA	1:A:164:LYS:HE2	2.03	0.40
2:B:31:ASP:OD2	2:B:33:THR:OG1	2.40	0.40
1:C:12:ALA:HB3	1:C:140:SER:HB3	2.03	0.40
1:C:88:HIS:CE1	1:C:90:GLU:HG3	2.57	0.40
2:D:6:HIS:HE1	2:D:8:GLN:OE1	2.04	0.40
2:D:295:ASP:OD1	2:D:296:ALA:N	2.54	0.40
4:F:146:VAL:HG21	4:F:233:PHE:CZ	2.56	0.40
2:B:291:GLN:NE2	13:B:623:HOH:O	2.54	0.40
1:C:229:ARG:NH2	13:C:610:HOH:O	2.37	0.40
2:D:293:MET:HE3	2:D:293:MET:HB2	1.93	0.40
1:A:209:ILE:HG22	1:A:227:LEU:HD22	2.04	0.40
1:A:385:ALA:HB2	1:A:432:TYR:CG	2.57	0.40
1:C:299:ALA:N	13:C:601:HOH:O	2.50	0.40
2:D:77:ARG:HA	2:D:82:GLY:HA3	2.04	0.40
2:D:207:LEU:CA	2:D:210:ILE:HD12	2.51	0.40
4:F:200:ASP:C	4:F:200:ASP:OD1	2.65	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	435/451 (96%)	427 (98%)	8 (2%)	0	100	100
1	C	438/451 (97%)	425 (97%)	13 (3%)	0	100	100
2	B	425/445 (96%)	415 (98%)	10 (2%)	0	100	100
2	D	417/445 (94%)	400 (96%)	17 (4%)	0	100	100
3	E	117/189 (62%)	112 (96%)	5 (4%)	0	100	100
4	F	328/384 (85%)	314 (96%)	12 (4%)	2 (1%)	21	32
All	All	2160/2365 (91%)	2093 (97%)	65 (3%)	2 (0%)	48	64

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	F	89	GLU
4	F	88	SER

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	368/379 (97%)	368 (100%)	0	100	100
1	C	371/379 (98%)	371 (100%)	0	100	100
2	B	367/381 (96%)	365 (100%)	2 (0%)	81	91
2	D	362/381 (95%)	362 (100%)	0	100	100
3	E	109/171 (64%)	108 (99%)	1 (1%)	70	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	F	305/342 (89%)	305 (100%)	0	100	100
All	All	1882/2033 (93%)	1879 (100%)	3 (0%)	87	94

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	111	GLU
2	B	410	GLU
3	E	89	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	258	ASN
1	A	301	GLN
1	A	393	HIS
2	B	165	ASN
2	B	329	GLN
2	B	414	ASN
1	C	101	ASN
1	C	256	GLN
1	C	293	ASN
2	D	6	HIS
2	D	37	HIS
2	D	191	GLN
2	D	256	ASN
2	D	347	ASN
3	E	51	GLN
3	E	90	ASN
4	F	176	GLN
4	F	381	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 15 ligands modelled in this entry, 6 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
12	ACP	F	401	-	31,33,33	1.65	9 (29%)	47,52,52	1.80	11 (23%)
11	GDP	B	504	6	29,30,30	1.12	2 (6%)	45,47,47	1.79	8 (17%)
9	MES	B	502	-	12,12,12	2.27	1 (8%)	15,16,16	1.62	3 (20%)
8	GOL	A	504	-	5,5,5	0.79	0	5,5,5	1.05	0
10	JEL	B	503	-	36,36,36	1.42	4 (11%)	50,51,51	1.53	8 (16%)
5	GTP	A	501	6	33,34,34	0.93	1 (3%)	50,54,54	1.64	8 (16%)
5	GTP	C	501	6	33,34,34	0.95	1 (3%)	50,54,54	1.66	9 (18%)
10	JEL	D	502	-	36,36,36	1.46	4 (11%)	50,51,51	1.64	7 (14%)
5	GTP	D	501	6	33,34,34	1.01	4 (12%)	50,54,54	1.63	8 (16%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	ACP	F	401	-	-	4/19/38/38	0/3/3/3
11	GDP	B	504	6	-	1/16/32/32	0/3/3/3
9	MES	B	502	-	-	3/6/14/14	0/1/1/1
8	GOL	A	504	-	-	2/4/4/4	-
10	JEL	B	503	-	-	0/9/15/15	0/6/6/6
5	GTP	A	501	6	-	8/22/38/38	0/3/3/3
5	GTP	C	501	6	-	6/22/38/38	0/3/3/3
10	JEL	D	502	-	-	0/9/15/15	0/6/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GTP	D	501	6	-	4/22/38/38	0/3/3/3

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	502	MES	C8-S	-7.60	1.66	1.77
10	D	502	JEL	C10-N3	5.74	1.44	1.36
10	B	503	JEL	C10-N3	5.44	1.44	1.36
12	F	401	ACP	C5-C4	4.65	1.47	1.39
10	D	502	JEL	CAC-CAA	-4.29	1.35	1.46
10	B	503	JEL	CAC-CAA	-4.15	1.36	1.46
11	B	504	GDP	C5-C4	2.99	1.46	1.38
12	F	401	ACP	PG-O3G	2.90	1.61	1.55
12	F	401	ACP	PG-O2G	2.89	1.61	1.55
12	F	401	ACP	C5-C6	2.76	1.48	1.41
10	D	502	JEL	CAC-C7	-2.72	1.37	1.41
10	B	503	JEL	CAC-C7	-2.60	1.37	1.41
12	F	401	ACP	PB-O3A	2.57	1.61	1.58
12	F	401	ACP	C8-N7	2.43	1.36	1.31
5	D	501	GTP	PB-O3A	2.39	1.62	1.59
10	D	502	JEL	CAA-C6	-2.39	1.37	1.41
10	B	503	JEL	CAA-C6	-2.35	1.37	1.41
11	B	504	GDP	C6-N1	-2.32	1.34	1.38
5	D	501	GTP	C2-N3	2.27	1.38	1.33
5	C	501	GTP	C2-N3	2.26	1.38	1.33
5	A	501	GTP	C2-N3	2.25	1.38	1.33
12	F	401	ACP	C5-N7	-2.19	1.35	1.39
5	D	501	GTP	PB-O3B	2.15	1.61	1.59
5	D	501	GTP	PA-O3A	2.09	1.61	1.59
12	F	401	ACP	PB-O2B	2.07	1.61	1.56
12	F	401	ACP	C4-N9	-2.06	1.33	1.37

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	B	504	GDP	C5-C4-N3	-5.81	119.14	128.39
12	F	401	ACP	C5-C4-N3	-5.40	119.29	126.72
5	C	501	GTP	C5-C4-N3	-5.20	120.11	128.39
5	A	501	GTP	C5-C4-N3	-5.07	120.32	128.39
11	B	504	GDP	C2-N3-C4	4.96	120.84	112.30
10	D	502	JEL	C9-N2-C10	4.90	122.42	117.83
5	D	501	GTP	C5-C4-N3	-4.89	120.61	128.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	501	GTP	C2-N3-C4	4.69	120.38	112.30
10	D	502	JEL	C9-C7-N1	4.65	134.59	130.12
5	C	501	GTP	C2-N3-C4	4.63	120.27	112.30
5	D	501	GTP	C2-N3-C4	4.53	120.10	112.30
10	B	503	JEL	C9-N2-C10	4.52	122.07	117.83
10	B	503	JEL	C9-C7-N1	4.39	134.33	130.12
11	B	504	GDP	N9-C4-N3	4.35	134.66	125.95
12	F	401	ACP	N3-C4-N9	4.15	134.23	127.17
10	D	502	JEL	CAB-C6-N1	3.76	134.43	129.07
12	F	401	ACP	PB-O3A-PA	-3.70	120.28	132.37
11	B	504	GDP	C6-C5-N7	3.60	136.85	130.29
12	F	401	ACP	C4-C5-N7	-3.59	106.48	110.58
10	B	503	JEL	CAB-C6-N1	3.56	134.15	129.07
12	F	401	ACP	C2-N3-C4	3.52	120.44	111.83
5	C	501	GTP	N9-C4-N3	3.48	132.90	125.95
10	D	502	JEL	C8-CAA-C6	3.46	122.89	119.07
5	A	501	GTP	N9-C4-N3	3.45	132.85	125.95
5	D	501	GTP	N9-C4-N3	3.36	132.67	125.95
10	D	502	JEL	C9-C7-CAC	-3.33	118.38	120.02
9	B	502	MES	C5-N4-C3	3.29	115.94	108.84
5	C	501	GTP	N9-C8-N7	-3.29	107.31	113.40
10	B	503	JEL	C8-CAA-C6	3.16	122.55	119.07
5	C	501	GTP	C8-N7-C5	3.14	109.85	104.26
5	D	501	GTP	N9-C8-N7	-3.12	107.62	113.40
12	F	401	ACP	N3-C2-N1	-3.10	123.89	128.58
5	A	501	GTP	N9-C8-N7	-3.07	107.71	113.40
5	A	501	GTP	C2-N1-C6	-2.91	119.84	125.11
5	D	501	GTP	C2-N1-C6	-2.90	119.85	125.11
5	C	501	GTP	C2-N1-C6	-2.90	119.86	125.11
5	A	501	GTP	C8-N7-C5	2.79	109.22	104.26
12	F	401	ACP	C4-N9-C8	2.77	108.64	105.74
5	D	501	GTP	C8-N7-C5	2.75	109.17	104.26
10	D	502	JEL	CAB-C6-CAA	-2.75	118.82	121.68
9	B	502	MES	C6-C5-N4	-2.73	105.97	110.12
11	B	504	GDP	C4-C5-N7	-2.71	106.37	110.67
10	B	503	JEL	C9-C7-CAC	-2.69	118.70	120.02
10	D	502	JEL	C11-C10-N2	-2.55	119.58	122.92
12	F	401	ACP	C5-N7-C8	2.54	107.44	103.45
5	D	501	GTP	C5-C6-N1	2.53	119.69	113.25
5	A	501	GTP	C5-C6-N1	2.52	119.66	113.25
5	D	501	GTP	O6-C6-C5	-2.45	120.07	126.53
10	B	503	JEL	CAB-C6-CAA	-2.44	119.14	121.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	501	GTP	O6-C6-C5	-2.41	120.16	126.53
5	C	501	GTP	C5-C6-N1	2.38	119.32	113.25
5	C	501	GTP	O6-C6-C5	-2.34	120.36	126.53
12	F	401	ACP	C6-C5-N7	2.32	136.57	132.09
10	B	503	JEL	C11-C10-N2	-2.29	119.92	122.92
10	B	503	JEL	C13-C4-N3	-2.22	107.44	113.60
11	B	504	GDP	O6-C6-C5	-2.21	120.69	126.53
12	F	401	ACP	N9-C8-N7	-2.10	110.95	113.94
5	C	501	GTP	C4-C5-N7	-2.10	107.34	110.67
9	B	502	MES	O3S-S-C8	2.07	110.05	106.00
12	F	401	ACP	C3'-C2'-C1'	2.04	105.31	101.46
11	B	504	GDP	C8-N7-C5	2.03	107.88	104.26
11	B	504	GDP	C5-C6-N1	2.02	118.40	113.25

There are no chirality outliers.

All (28) torsion outliers are listed below:

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	C5'-O5'-PA-O3A
5	C	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O2A
8	A	504	GOL	O1-C1-C2-C3
9	B	502	MES	C7-C8-S-O2S
9	B	502	MES	C7-C8-S-O3S
12	F	401	ACP	C5'-O5'-PA-O1A
12	F	401	ACP	O4'-C4'-C5'-O5'
8	A	504	GOL	O1-C1-C2-O2
12	F	401	ACP	C3'-C4'-C5'-O5'
5	A	501	GTP	PB-O3B-PG-O1G
9	B	502	MES	C7-C8-S-O1S
5	D	501	GTP	C4'-C5'-O5'-PA
5	A	501	GTP	C4'-C5'-O5'-PA
5	C	501	GTP	C4'-C5'-O5'-PA
5	D	501	GTP	C5'-O5'-PA-O1A
11	B	504	GDP	C5'-O5'-PA-O3A
12	F	401	ACP	C5'-O5'-PA-O3A
5	A	501	GTP	PB-O3A-PA-O2A
5	C	501	GTP	PB-O3A-PA-O2A
5	D	501	GTP	PA-O3A-PB-O1B

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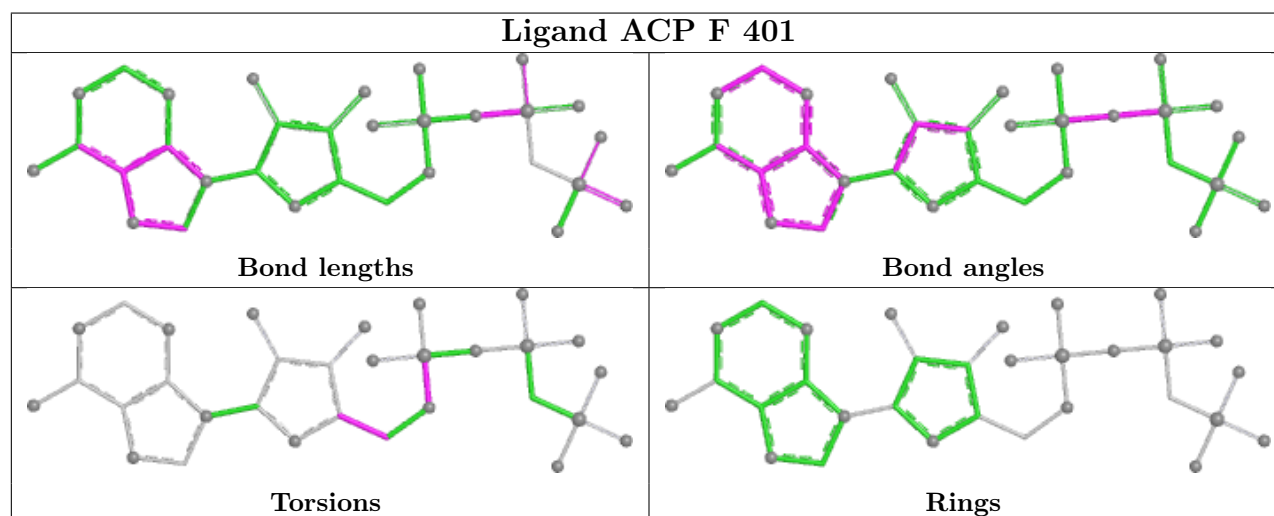
Mol	Chain	Res	Type	Atoms
5	A	501	GTP	PB-O3B-PG-O2G
5	D	501	GTP	PB-O3B-PG-O2G
5	A	501	GTP	PB-O3A-PA-O1A
5	C	501	GTP	PB-O3A-PA-O1A

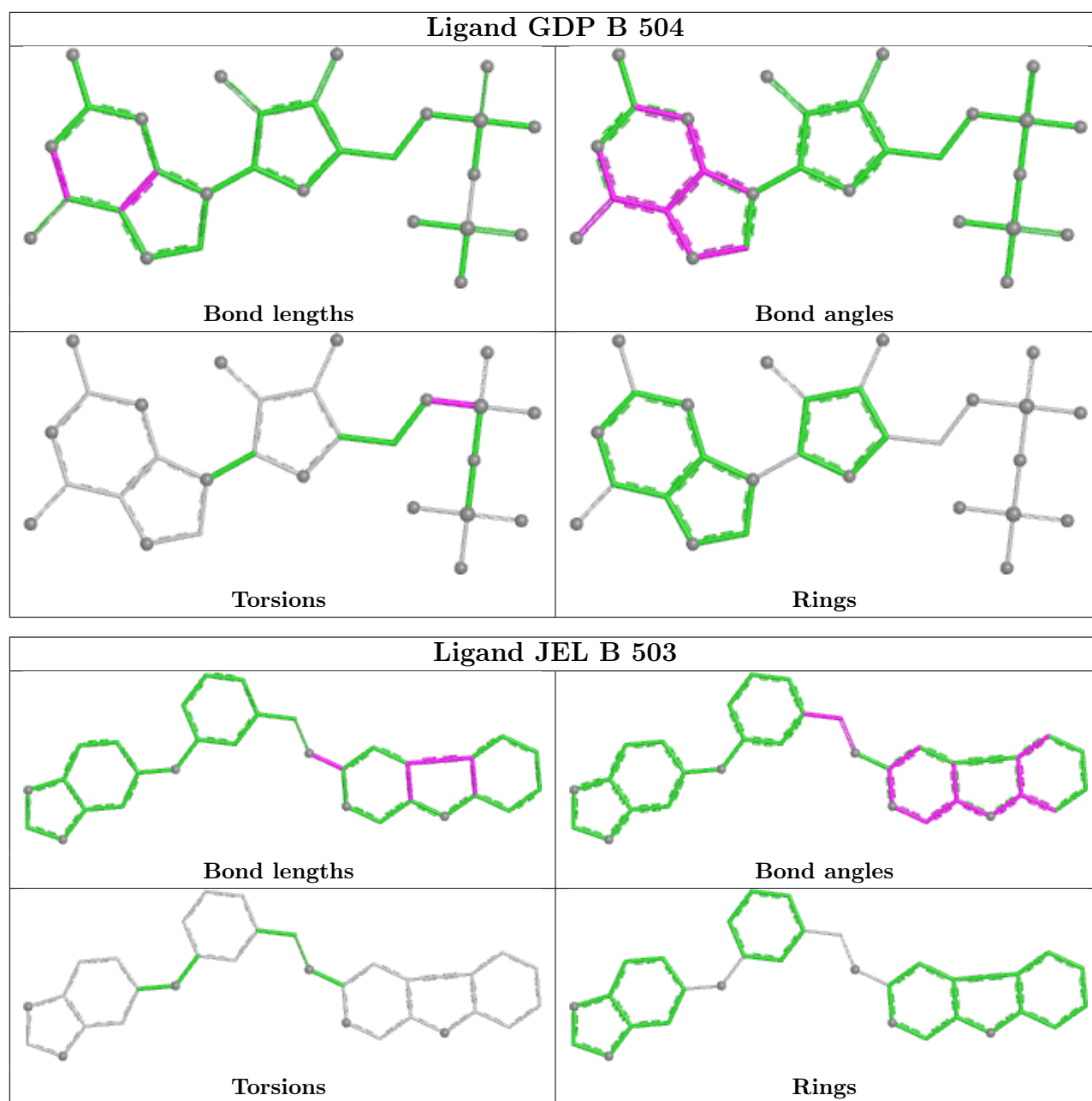
There are no ring outliers.

1 monomer is involved in 2 short contacts:

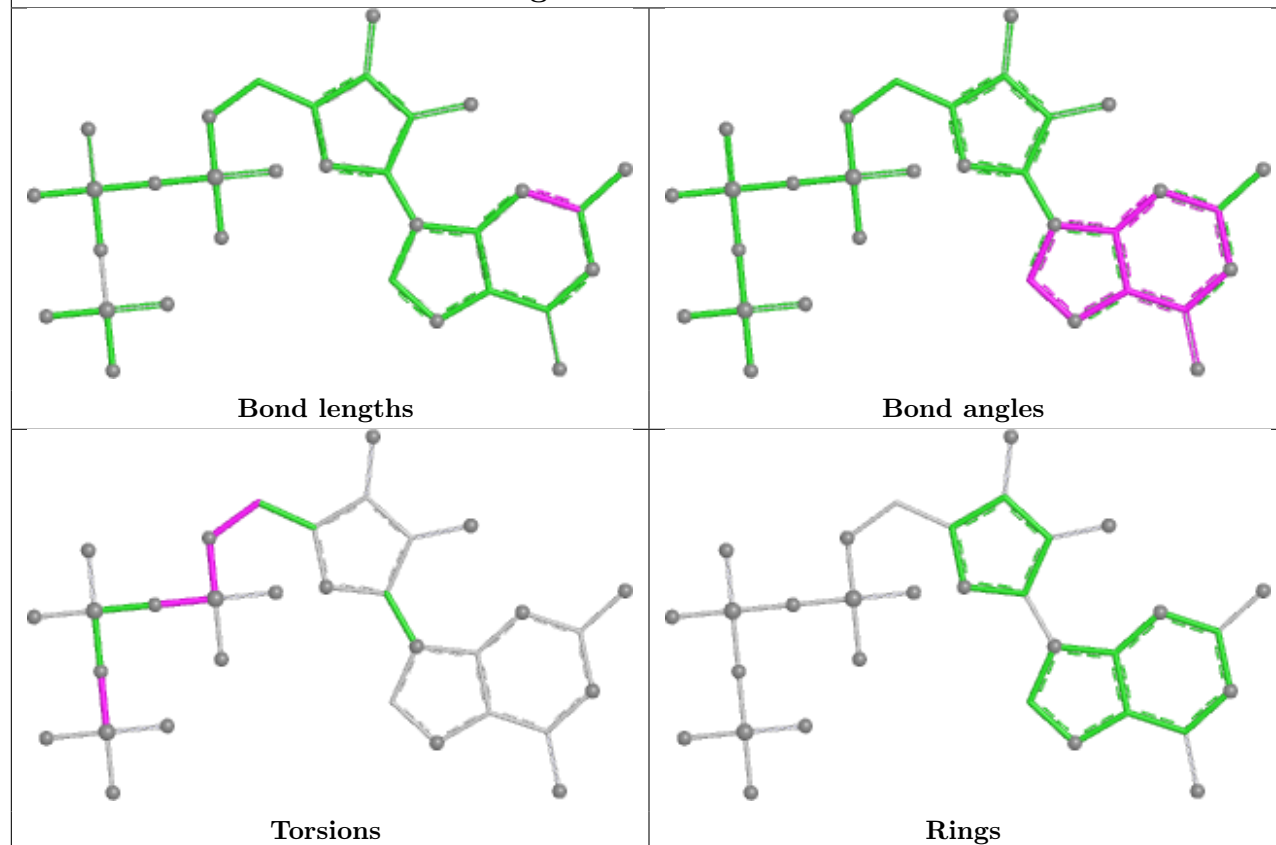
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	D	502	JEL	2	0

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

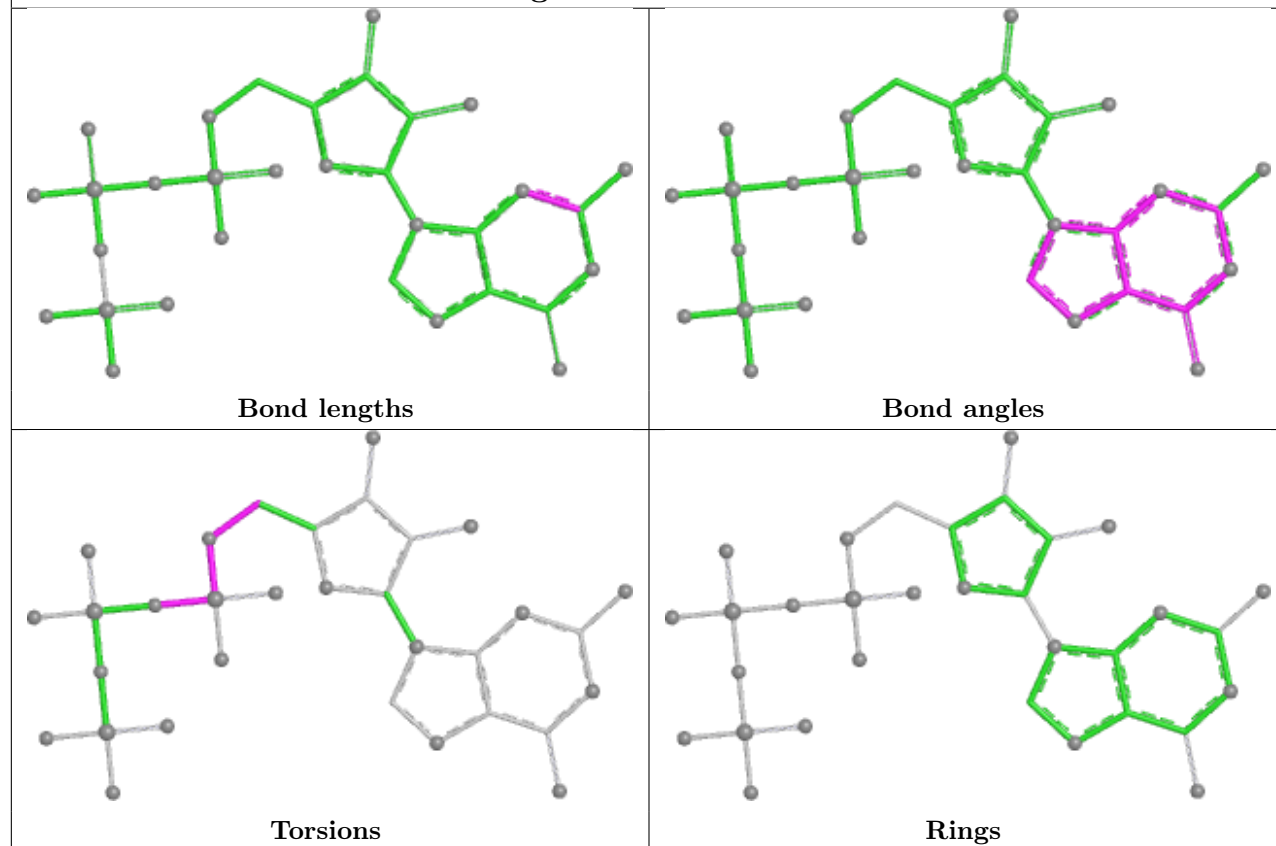


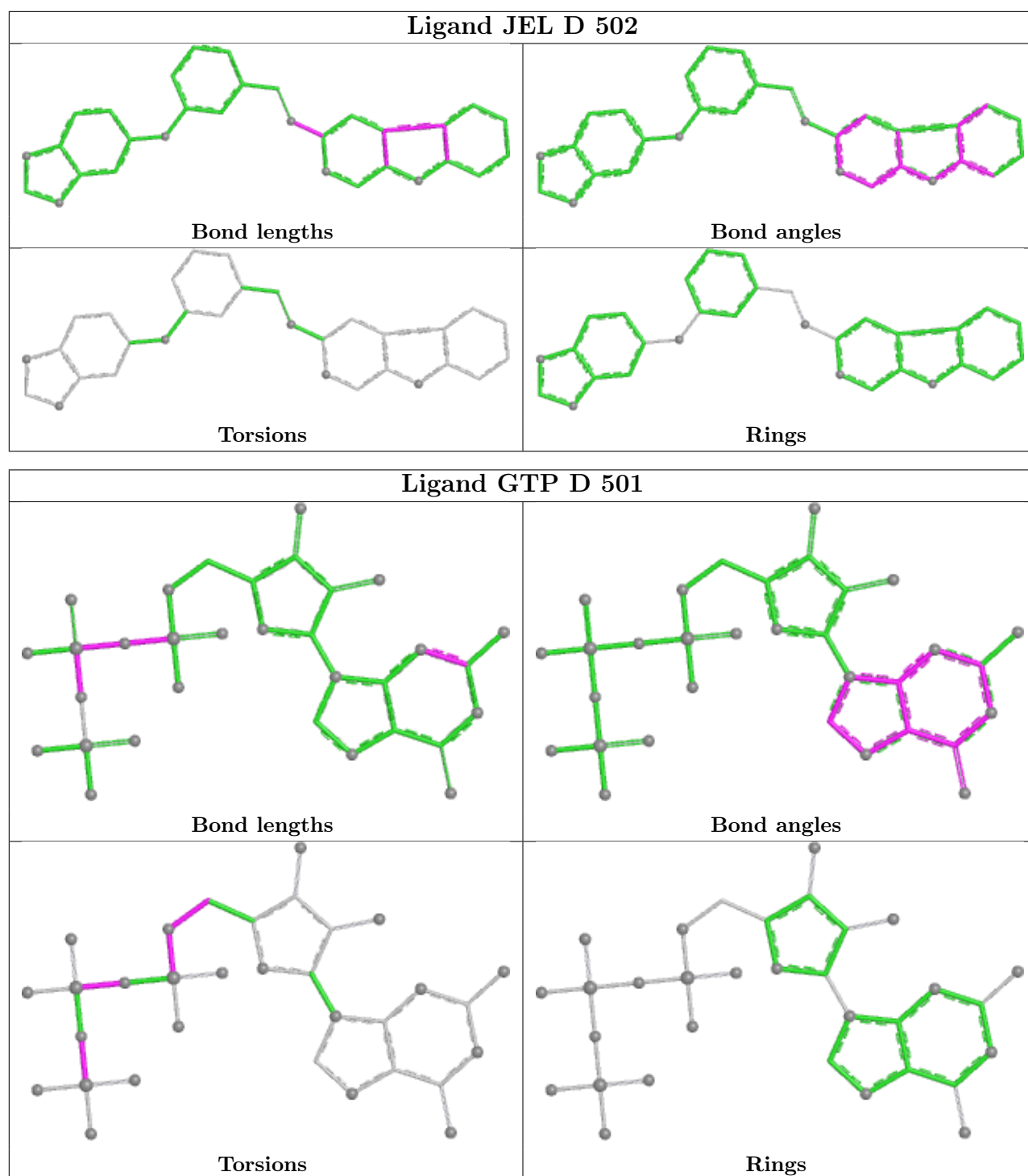


Ligand GTP A 501



Ligand GTP C 501





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	437/451 (96%)	0.44	17 (3%) 43 39	26, 45, 71, 87	0
1	C	440/451 (97%)	0.13	20 (4%) 38 34	22, 37, 63, 88	0
2	B	427/445 (95%)	0.48	39 (9%) 15 12	21, 43, 78, 119	0
2	D	421/445 (94%)	1.79	155 (36%) 1 1	38, 74, 106, 138	0
3	E	121/189 (64%)	1.35	36 (29%) 1 1	32, 67, 97, 125	0
4	F	338/384 (88%)	1.90	146 (43%) 0 0	38, 79, 137, 158	0
All	All	2184/2365 (92%)	0.92	413 (18%) 3 2	21, 53, 104, 158	0

All (413) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	179	THR	10.6
2	D	55	ALA	6.4
4	F	161	LEU	6.4
2	B	246	LEU	6.4
4	F	134	ALA	6.3
4	F	133	ALA	6.1
2	D	397	TRP	6.0
2	B	55	ALA	5.9
4	F	132	LEU	5.8
4	F	381	HIS	5.7
1	A	41	THR	5.5
4	F	186	LEU	5.5
4	F	233	PHE	5.4
4	F	166	ALA	5.3
4	F	169	LEU	5.2
4	F	130	VAL	5.2
2	D	170	VAL	5.1
4	F	103	THR	5.0
2	B	247	ASN	4.9

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Mol	Chain	Res	Type	RSRZ
4	F	173	ILE	4.7
4	F	383	HIS	4.7
2	D	30	ILE	4.6
4	F	170	LEU	4.6
4	F	199	PHE	4.6
2	D	214	THR	4.6
2	D	394	PHE	4.6
4	F	177	GLY	4.5
2	D	212	PHE	4.5
4	F	149	ALA	4.5
4	F	137	ARG	4.5
2	D	136	THR	4.4
4	F	182	ILE	4.4
4	F	245	ILE	4.4
4	F	382	HIS	4.4
3	E	28	SER	4.4
4	F	131	PHE	4.3
4	F	144	GLY	4.3
2	D	37	HIS	4.3
2	B	280	GLN	4.3
1	C	357	TYR	4.2
4	F	362	ALA	4.2
2	D	65	LEU	4.2
2	D	284	LEU	4.2
2	D	142	GLY	4.2
3	E	6	MET	4.2
4	F	253	TYR	4.2
4	F	263	PHE	4.2
2	B	245	GLN	4.1
2	D	92	PHE	4.1
4	F	172	PHE	4.1
2	D	80	PRO	4.1
2	D	81	PHE	4.1
4	F	98	TYR	4.1
2	D	246	LEU	4.0
2	D	90	PHE	4.0
2	D	42	LEU	3.9
4	F	167	SER	3.9
2	D	217	LEU	3.9
4	F	283	ILE	3.9
4	F	146	VAL	3.9
4	F	101	TYR	3.8

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Mol	Chain	Res	Type	RSRZ
2	B	279	GLN	3.8
2	B	277	GLY	3.8
2	D	112	LEU	3.8
4	F	179	VAL	3.7
2	D	1	MET	3.7
2	D	54	ALA	3.7
2	D	141	GLY	3.7
4	F	99	VAL	3.7
4	F	231	ALA	3.7
4	F	330	ILE	3.6
2	D	244	GLY	3.6
2	D	215	LEU	3.6
3	E	140	LYS	3.6
4	F	224	SER	3.6
2	D	245	GLN	3.6
4	F	237	THR	3.6
2	D	396	HIS	3.6
2	D	210	ILE	3.6
2	D	293	MET	3.6
2	D	173	PRO	3.6
4	F	257	GLU	3.6
4	F	256	TYR	3.6
4	F	138	ARG	3.6
4	F	178	GLN	3.5
4	F	135	TYR	3.5
2	D	220	PRO	3.5
2	D	176	SER	3.5
4	F	384	HIS	3.5
1	A	437	VAL	3.5
4	F	225	SER	3.5
4	F	141	GLY	3.5
4	F	235	ASP	3.5
2	B	278	SER	3.4
2	D	85	PHE	3.4
2	B	57	ASN	3.4
4	F	136	ASN	3.4
2	D	72	THR	3.4
1	C	340	SER	3.4
4	F	234	GLN	3.4
2	D	73	MET	3.4
4	F	372	THR	3.4
2	B	276	ARG	3.4

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Mol	Chain	Res	Type	RSRZ
2	D	248	ALA	3.4
4	F	142	ARG	3.3
1	A	262	TYR	3.3
2	D	16	ILE	3.3
2	D	399	THR	3.3
4	F	164	SER	3.3
2	D	228	LEU	3.3
2	D	395	LEU	3.3
4	F	380	HIS	3.3
4	F	228	TYR	3.3
2	D	76	VAL	3.3
2	D	175	VAL	3.3
4	F	254	GLY	3.2
4	F	171	ASP	3.2
4	F	275	LEU	3.2
1	C	440	VAL	3.2
2	D	6	HIS	3.2
4	F	264	PHE	3.2
2	B	75	SER	3.2
2	D	208	TYR	3.2
2	D	387	ALA	3.2
4	F	12	SER	3.2
1	A	96	LYS	3.1
1	A	196	GLU	3.1
2	D	56	GLY	3.1
2	D	79	GLY	3.1
2	D	393	ALA	3.1
2	D	46	ARG	3.1
2	D	323	MET	3.1
1	C	163	LYS	3.1
2	D	296	ALA	3.1
4	F	145	ASN	3.1
2	D	49	VAL	3.1
2	D	64	ILE	3.1
2	D	219	THR	3.1
4	F	143	GLU	3.1
2	B	239	CYS	3.1
4	F	232	ASN	3.1
4	F	242	ASN	3.1
2	D	11	GLN	3.1
2	D	135	LEU	3.1
1	A	88	HIS	3.1

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Mol	Chain	Res	Type	RSRZ
2	D	390	ARG	3.1
4	F	240	LEU	3.1
2	D	138	SER	3.0
2	D	15	GLN	3.0
1	A	412	GLY	3.0
3	E	117	ALA	3.0
2	D	130	LEU	3.0
4	F	379	HIS	3.0
2	D	247	ASN	3.0
2	D	180	VAL	3.0
4	F	162	ILE	3.0
4	F	243	HIS	3.0
4	F	139	ARG	3.0
2	D	377	LEU	3.0
4	F	17	VAL	3.0
4	F	20	LEU	3.0
4	F	22	LEU	3.0
2	B	2	ARG	3.0
2	D	221	THR	3.0
3	E	135	LYS	2.9
4	F	168	GLU	2.9
2	B	215	LEU	2.9
2	D	13	GLY	2.9
2	D	177	ASP	2.9
4	F	163	SER	2.9
4	F	192	LEU	2.9
4	F	127	GLU	2.9
4	F	140	GLU	2.9
2	D	115	SER	2.9
3	E	22	VAL	2.9
4	F	238	CYS	2.9
3	E	7	GLU	2.9
3	E	121	GLU	2.9
2	D	391	ARG	2.8
1	A	346	TRP	2.8
2	D	222	TYR	2.8
2	B	92	PHE	2.8
3	E	8	VAL	2.8
2	D	218	THR	2.8
2	D	71	GLY	2.8
2	D	402	GLY	2.8
2	D	32	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
4	F	75	ALA	2.8
1	C	341	ILE	2.8
2	D	84	ILE	2.8
2	D	57	ASN	2.8
4	F	147	TRP	2.8
2	D	360	GLY	2.8
2	D	216	LYS	2.8
2	B	296	ALA	2.8
2	D	406	MET	2.8
2	D	156	ARG	2.8
4	F	181	VAL	2.8
2	D	227	HIS	2.7
3	E	9	ILE	2.7
4	F	252	ASN	2.7
1	C	284	GLU	2.7
4	F	255	ARG	2.7
2	D	91	VAL	2.7
4	F	176	GLN	2.7
1	C	178	SER	2.7
2	D	2	ARG	2.7
4	F	191	LEU	2.7
4	F	279	LEU	2.7
3	E	45	PRO	2.7
4	F	27	TRP	2.7
1	A	282	TYR	2.7
4	F	185	TYR	2.7
2	D	405	GLU	2.7
2	D	38	GLY	2.7
4	F	244	CYS	2.7
2	D	9	ALA	2.6
2	D	167	PHE	2.6
4	F	343	TYR	2.6
3	E	141	GLU	2.6
2	D	381	ILE	2.6
1	A	54	SER	2.6
2	D	172	SER	2.6
4	F	373	SER	2.6
4	F	196	HIS	2.6
2	D	291	GLN	2.6
2	D	59	TYR	2.6
2	D	99	ASN	2.6
2	D	86	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
4	F	197	ARG	2.6
2	D	100	ASN	2.6
2	D	400	GLY	2.6
4	F	262	MET	2.6
4	F	230	SER	2.6
4	F	221	LEU	2.6
4	F	5	VAL	2.6
4	F	189	PRO	2.6
2	D	183	TYR	2.6
2	D	83	GLN	2.5
3	E	139	LEU	2.5
4	F	261	GLU	2.5
1	C	313	MET	2.5
2	B	128	ASP	2.5
3	E	62	LYS	2.5
4	F	11	SER	2.5
4	F	148	ILE	2.5
4	F	239	HIS	2.5
2	B	281	TYR	2.5
4	F	340	GLN	2.5
4	F	86	GLU	2.5
3	E	123	LEU	2.5
4	F	320	MET	2.5
1	C	46	ASP	2.5
2	D	97	ALA	2.5
2	B	11	GLN	2.5
2	D	179	VAL	2.5
2	D	7	ILE	2.5
4	F	187	GLU	2.5
1	C	1	MET	2.5
1	C	425	MET	2.5
2	B	301	ALA	2.5
2	B	428	ALA	2.5
4	F	236	LYS	2.5
2	B	190	HIS	2.5
4	F	194	PRO	2.5
2	D	33	THR	2.5
2	D	386	THR	2.5
3	E	114	ALA	2.5
1	C	285	GLN	2.5
2	D	35	SER	2.4
2	B	42	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
2	D	68	LEU	2.4
4	F	361	LEU	2.4
3	E	53	LYS	2.4
4	F	229	ASN	2.4
2	D	102	ALA	2.4
2	B	56	GLY	2.4
2	B	410	GLU	2.4
2	D	182	PRO	2.4
2	D	223	GLY	2.4
4	F	165	GLU	2.4
2	B	78	SER	2.4
2	B	275	SER	2.4
1	A	42	ILE	2.4
2	D	362	LYS	2.4
2	D	101	TRP	2.4
2	D	48	ASN	2.4
4	F	174	ASP	2.4
4	F	260	ASN	2.4
2	D	140	GLY	2.4
3	E	130	ALA	2.4
2	D	19	LYS	2.4
2	D	243	PRO	2.4
2	D	178	THR	2.4
2	D	20	PHE	2.4
1	A	195	LEU	2.4
4	F	128	ARG	2.4
2	D	171	PRO	2.3
4	F	339	ALA	2.3
2	D	107	THR	2.3
4	F	241	THR	2.3
2	D	164	MET	2.3
2	D	47	ILE	2.3
2	B	282	ARG	2.3
2	D	359	ARG	2.3
2	D	332	ASN	2.3
4	F	10	ASN	2.3
2	D	206	ALA	2.3
2	D	302	ALA	2.3
2	D	116	VAL	2.3
4	F	180	HIS	2.3
4	F	129	GLU	2.3
4	F	267	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
2	D	12	CYS	2.3
1	C	251	ASP	2.3
2	B	80	PRO	2.3
4	F	102	PRO	2.3
4	F	24	THR	2.3
4	F	100	ILE	2.3
2	D	129	CYS	2.3
2	D	41	ASP	2.3
2	D	67	ASP	2.3
4	F	336	PRO	2.3
2	D	267	MET	2.3
3	E	118	ALA	2.3
4	F	274	ALA	2.3
2	D	343	GLU	2.3
3	E	124	GLN	2.3
1	C	43	GLY	2.2
2	B	274	THR	2.2
4	F	14	TYR	2.2
2	B	338	SER	2.2
3	E	46	SER	2.2
4	F	246	GLN	2.2
4	F	21	LEU	2.2
2	D	385	PHE	2.2
2	B	323	MET	2.2
2	D	87	PRO	2.2
3	E	138	GLU	2.2
4	F	175	GLU	2.2
1	C	128	GLN	2.2
2	B	336	LYS	2.2
2	B	362	LYS	2.2
4	F	247	LYS	2.2
3	E	54	LEU	2.2
2	D	119	VAL	2.2
2	D	236	VAL	2.2
3	E	44	ASP	2.2
2	D	96	GLY	2.2
4	F	347	CYS	2.2
4	F	341	LYS	2.2
4	F	83	THR	2.2
4	F	223	THR	2.2
4	F	344	ALA	2.2
1	C	245	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
4	F	13	VAL	2.2
4	F	333	ASN	2.2
4	F	227	PRO	2.2
4	F	280	GLU	2.2
2	D	292	GLN	2.2
2	D	398	TYR	2.1
2	B	333	VAL	2.1
2	D	193	VAL	2.1
2	D	431	ASP	2.1
4	F	8	ASP	2.1
3	E	106	GLU	2.1
2	D	384	GLN	2.1
2	D	82	GLY	2.1
2	D	201	CYS	2.1
2	D	211	CYS	2.1
2	D	110	ALA	2.1
1	A	163	LYS	2.1
2	B	331	LEU	2.1
1	C	356	ASN	2.1
1	C	283	HIS	2.1
3	E	133	VAL	2.1
2	D	389	PHE	2.1
3	E	27	PRO	2.1
4	F	332	VAL	2.1
2	D	34	GLY	2.1
2	D	213	ARG	2.1
3	E	134	ARG	2.1
1	A	164	LYS	2.1
4	F	184	LYS	2.1
2	D	157	GLU	2.1
2	D	273	LEU	2.1
4	F	226	GLU	2.1
2	B	335	ASN	2.1
2	D	66	VAL	2.1
2	B	244	GLY	2.1
1	A	423	GLU	2.1
4	F	9	GLU	2.1
3	E	103	GLN	2.1
4	F	126	ASP	2.1
2	B	320	ARG	2.1
4	F	204	TRP	2.1
3	E	52	LYS	2.0

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Mol	Chain	Res	Type	RSRZ
2	D	63	ALA	2.0
2	D	373	ALA	2.0
3	E	119	MET	2.0
2	D	198	GLU	2.0
3	E	59	GLU	2.0
1	A	120	ASP	2.0
1	A	132	LEU	2.0
2	D	361	LEU	2.0
2	D	416	ASN	2.0
3	E	23	ILE	2.0
3	E	50	ILE	2.0
3	E	63	TYR	2.0
1	C	297	GLU	2.0
2	D	299	MET	2.0
3	E	48	GLU	2.0
4	F	190	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no 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
5	GTP	A	501	32/32	-	-	29,31,38,40	42
5	GTP	C	501	32/32	-	-	25,29,39,44	42
5	GTP	D	501	32/32	-	-	66,70,84,86	42
6	MG	A	502	1/1	-	-	35,35,35,35	1
6	MG	B	501	1/1	-	-	33,33,33,33	1
6	MG	C	502	1/1	-	-	31,31,31,31	1
6	MG	D	503	1/1	-	-	75,75,75,75	1

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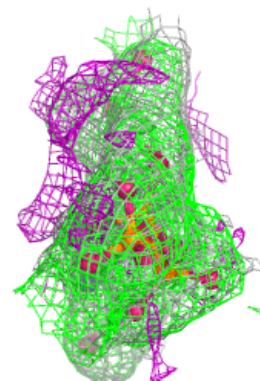
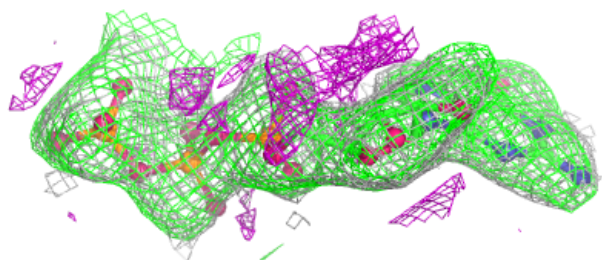
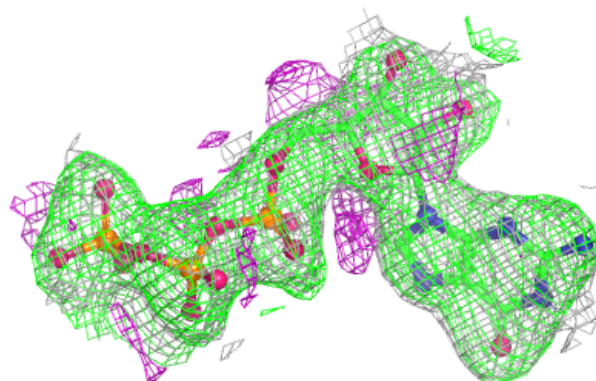
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	CA	A	503	1/1	-	-	60,60,60,60	1
7	CA	C	503	1/1	-	-	48,48,48,48	1
8	GOL	A	504	6/6	-	-	32,39,42,43	14
9	MES	B	502	12/12	-	-	34,40,46,46	25
10	JEL	D	502	31/31	0.89	0.14	42,66,82,84	0
10	JEL	B	503	31/31	0.97	0.07	23,31,40,47	0
11	GDP	B	504	28/28	-	-	23,32,41,41	38
12	ACP	F	401	31/31	-	-	69,86,90,90	31

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.

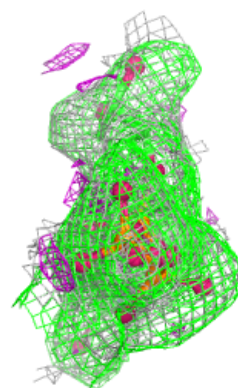
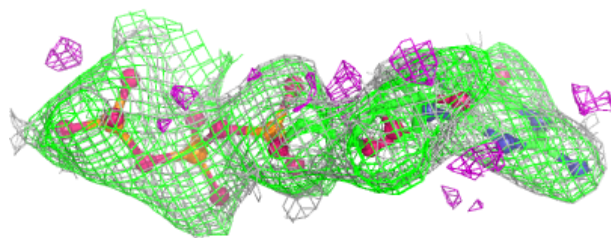
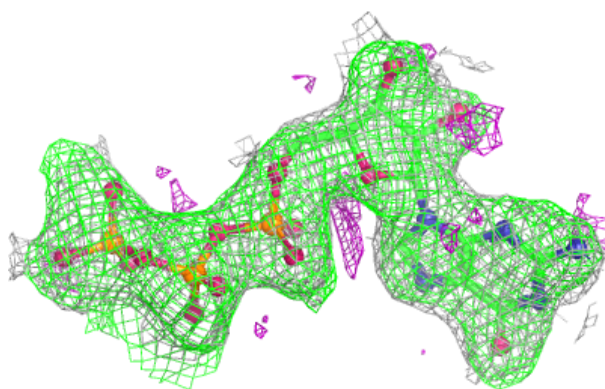
Electron density around GTP A 501:

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

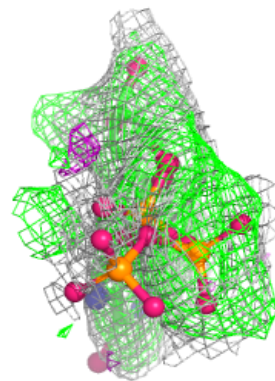
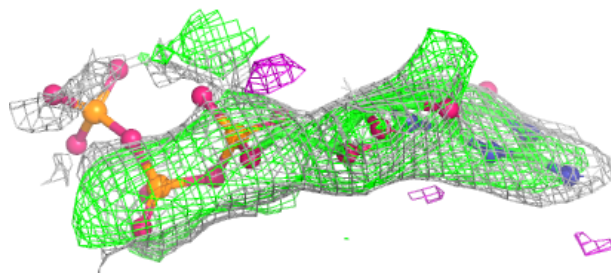
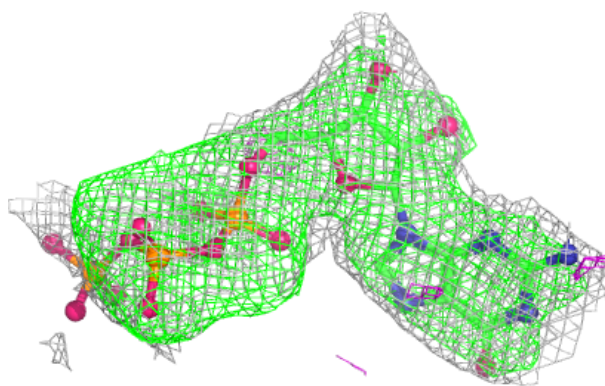


Electron density around GTP C 501:

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

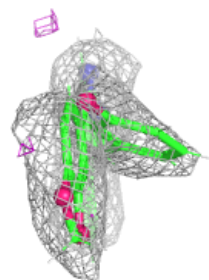
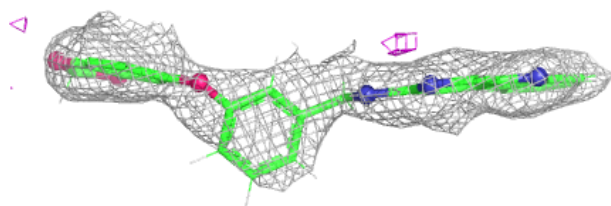
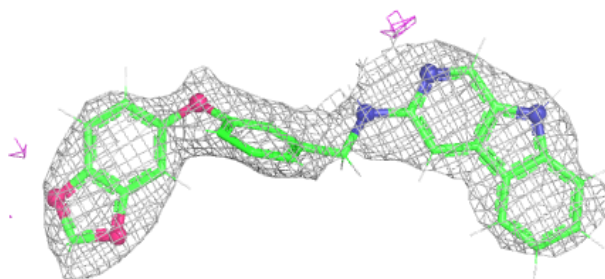
**Electron density around GTP D 501:**

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and green (positive)

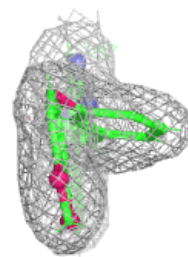
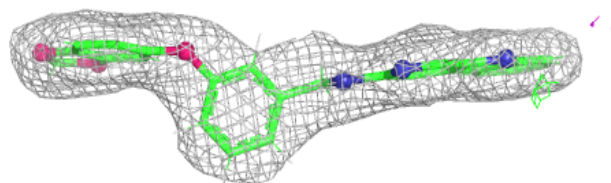
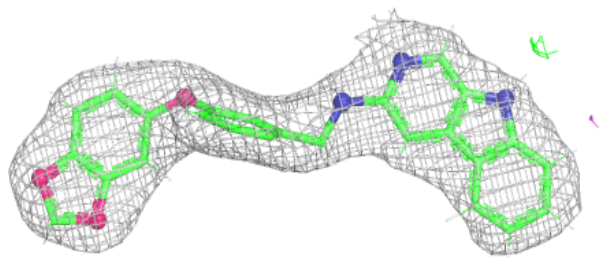


Electron density around JEL D 502:

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and green (positive)

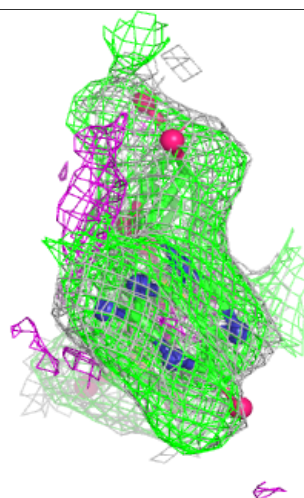
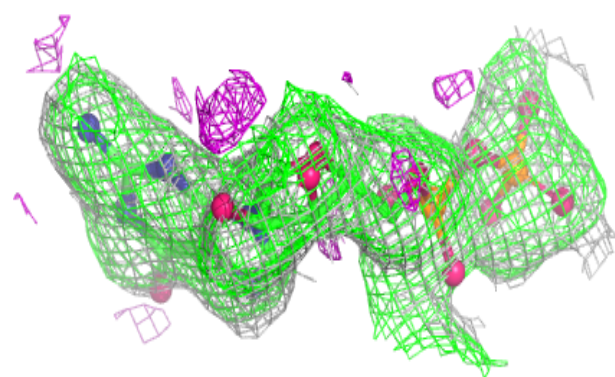
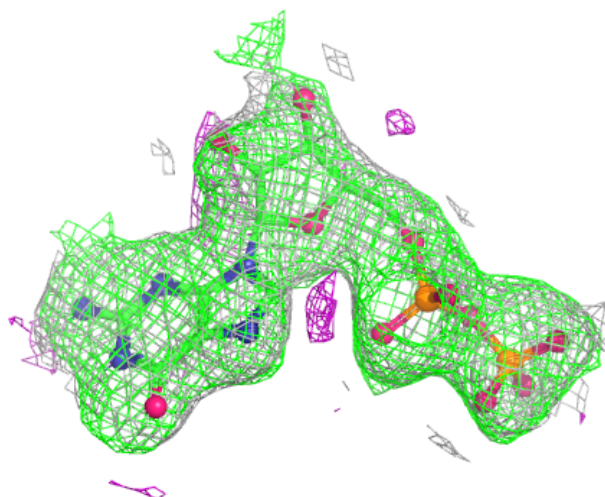
**Electron density around JEL B 503:**

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



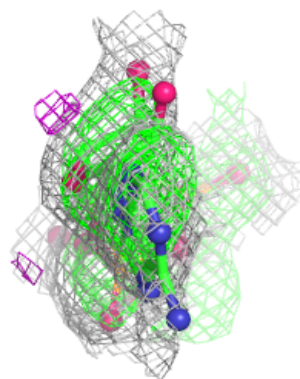
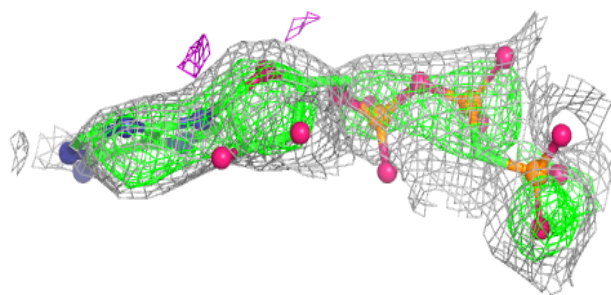
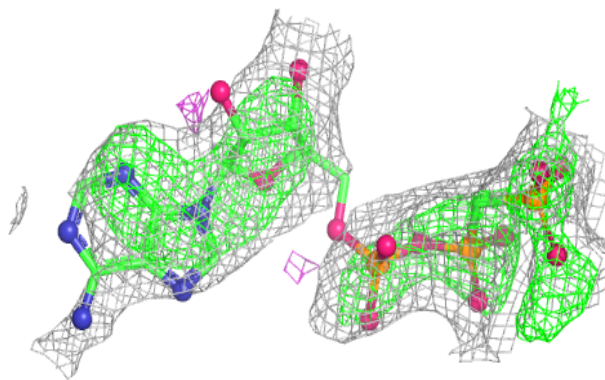
Electron density around GDP B 504:

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



Electron density around 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.