



Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2022 – 06:46 AM JST

PDB ID : 7EXC
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.28.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.28.1

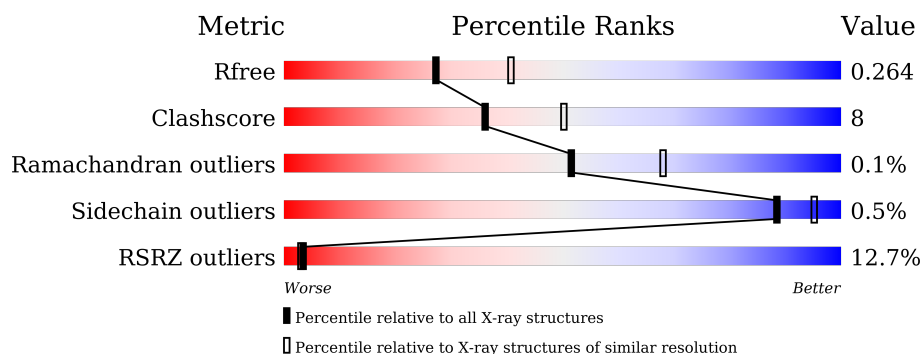
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.39 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}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (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	<div> <div>3%</div> <div>85%</div> <div>11%</div> <div>.</div> </div>
1	C	451	<div> <div>2%</div> <div>86%</div> <div>11%</div> <div>.</div> </div>
2	B	445	<div> <div>5%</div> <div>82%</div> <div>13%</div> <div>.</div> </div>
2	D	445	<div> <div>20%</div> <div>76%</div> <div>18%</div> <div>5%</div> </div>
3	E	189	<div> <div>6%</div> <div>50%</div> <div>12%</div> <div>36%</div> </div>
4	F	384	<div> <div>35%</div> <div>71%</div> <div>16%</div> <div>12%</div> </div>

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:

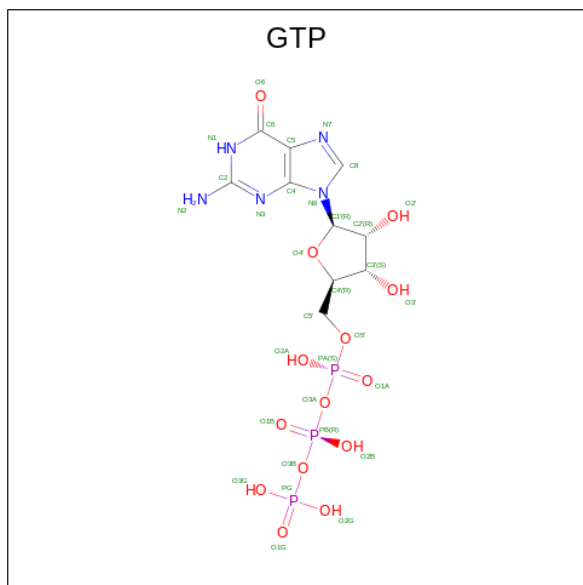
Chain	Residue	Modelled	Actual	Comment	Reference
F	379	HIS	-	expression tag	UNP E1BQ43
F	380	HIS	-	expression tag	UNP E1BQ43
F	381	HIS	-	expression tag	UNP E1BQ43
F	382	HIS	-	expression tag	UNP E1BQ43

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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 (three-letter code: 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		

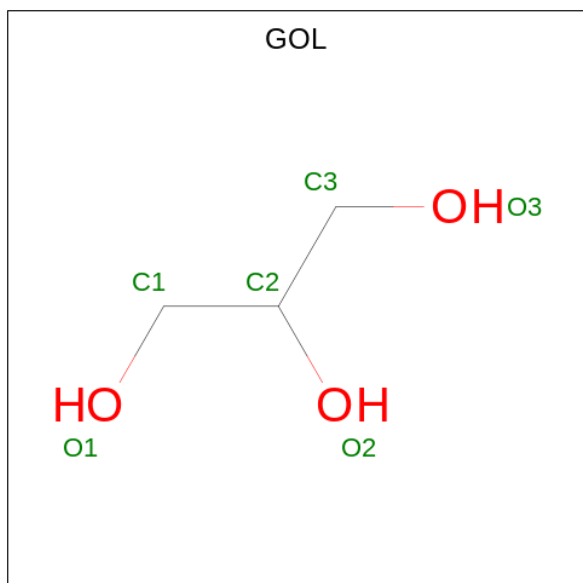
- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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 (three-letter code: CA) (formula: Ca).

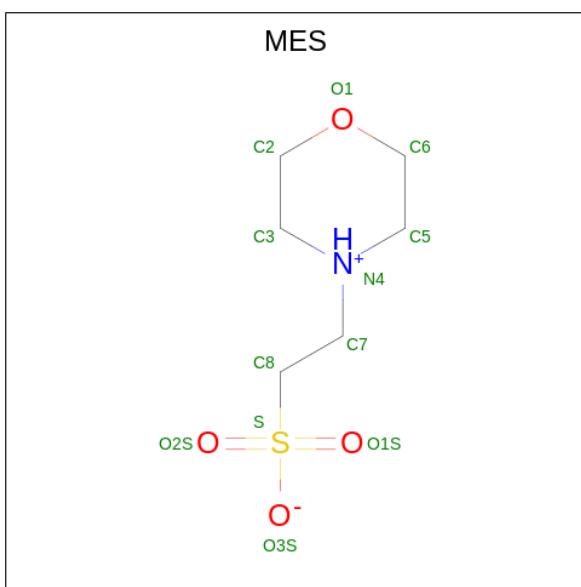
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Ca	1	0
			1	1		
7	C	1	Total	Ca	1	0
			1	1		

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



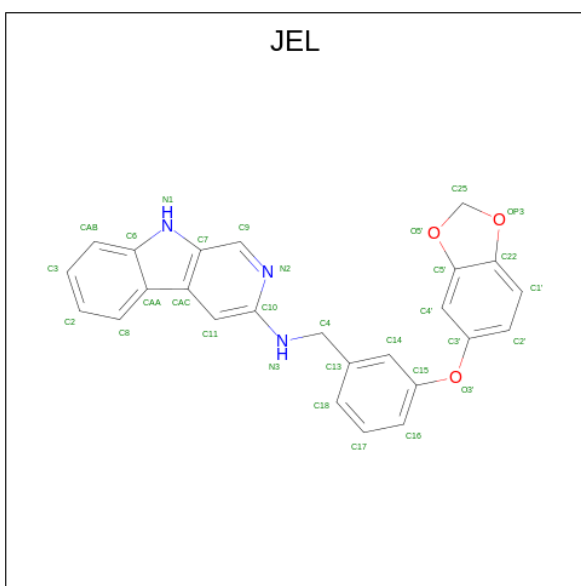
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	H	O	14	0
			14	3	8	3		

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



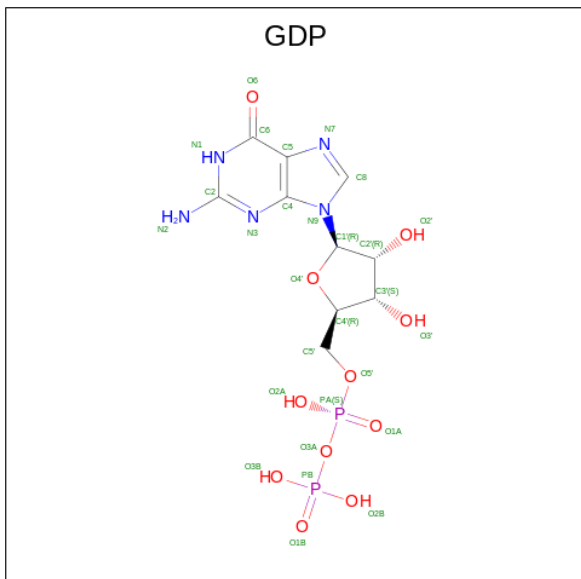
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
9	B	1	Total	C	H	N	O	S	25	0
			25	6	13	1	4	1		

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



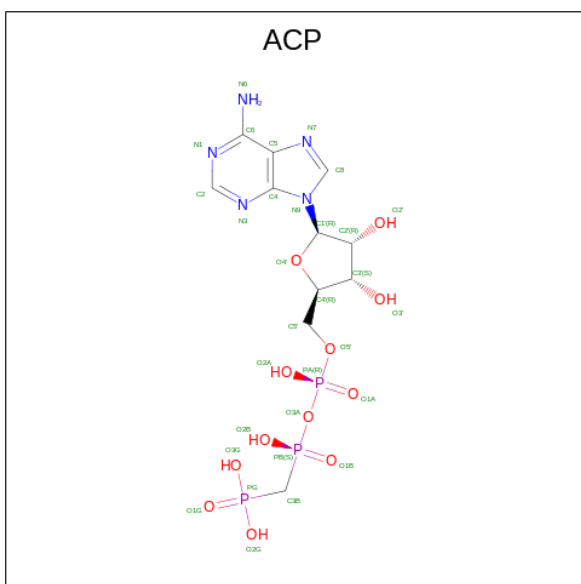
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	B	1	Total	C	H	N	O	0	0
			50	25	19	3	3		
10	D	1	Total	C	H	N	O	0	0
			50	25	19	3	3		

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



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

- Molecule 12 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (three-letter code: 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	C	N	O	P	31	0
			31	11	5	12	3		

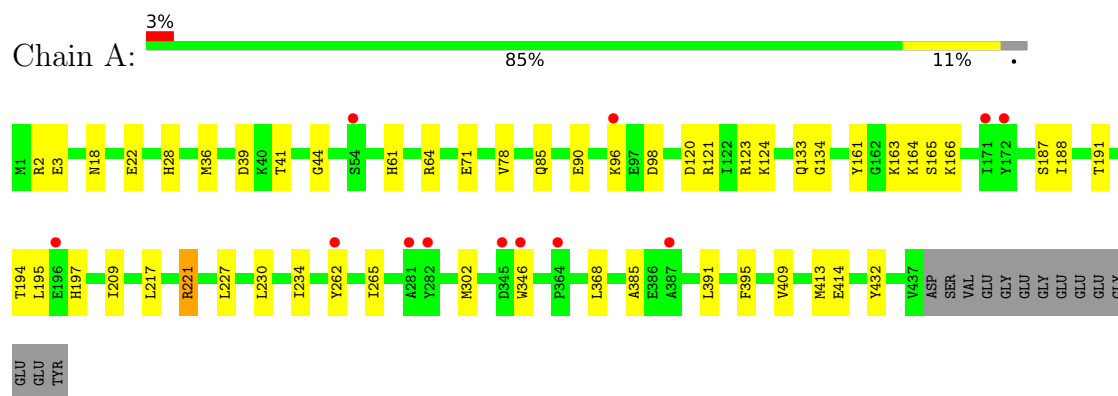
- Molecule 13 is water.

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

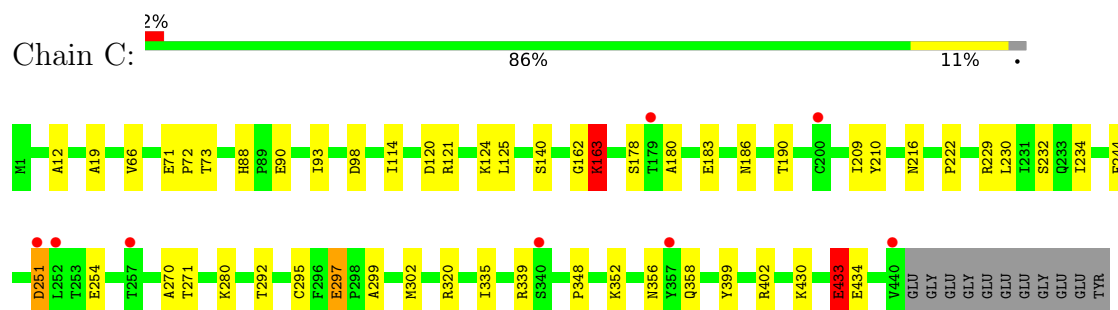
3 Residue-property plots [i](#)

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.

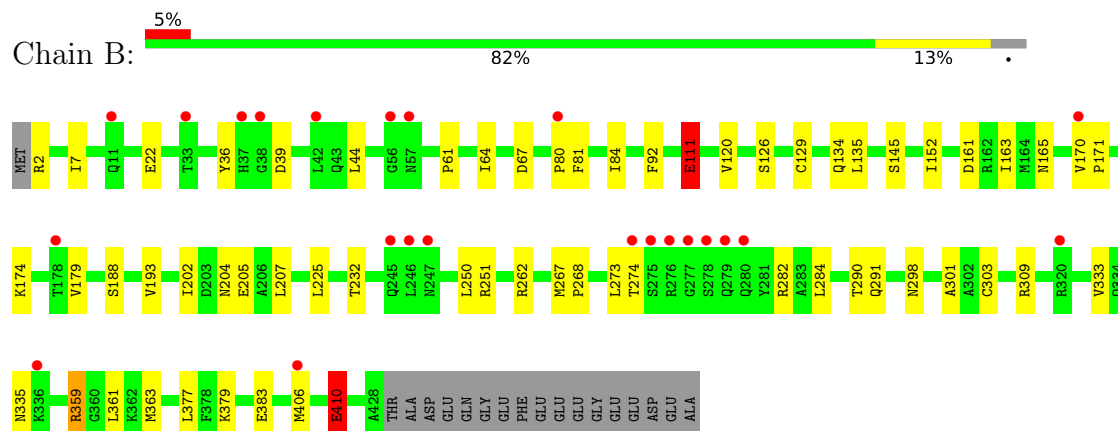
- Molecule 1: Tubulin alpha-1B chain



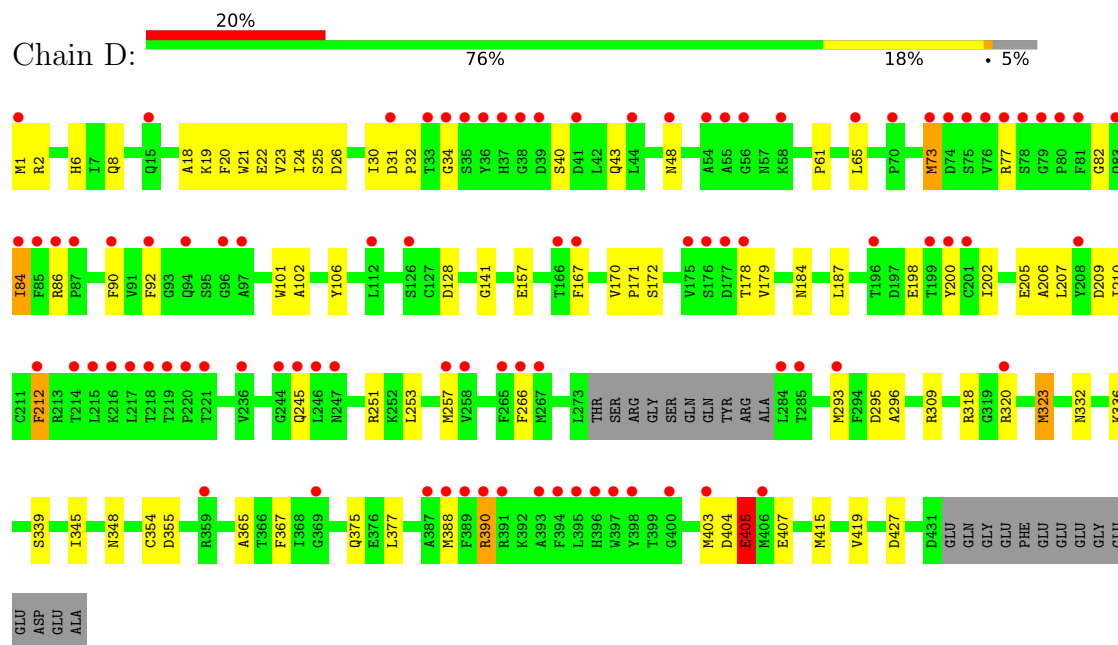
- Molecule 1: Tubulin alpha-1B chain



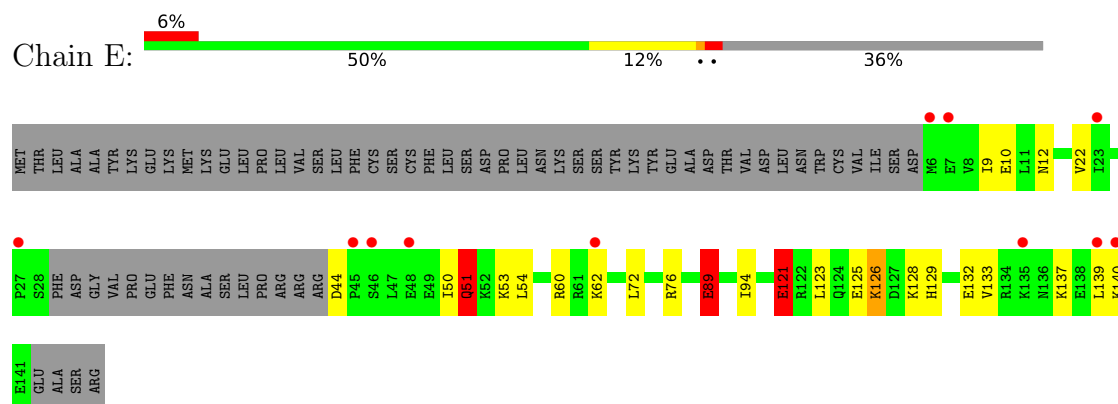
- Molecule 2: Tubulin beta chain



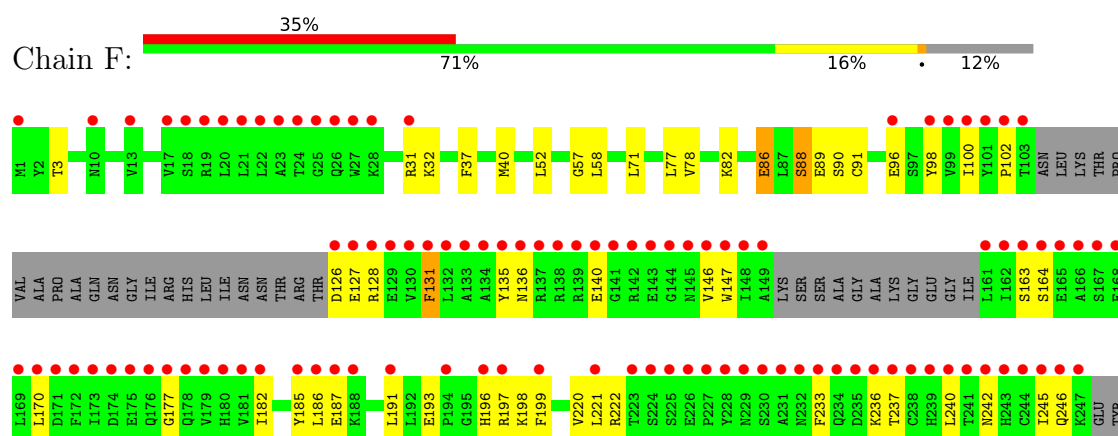
- Molecule 2: Tubulin beta chain

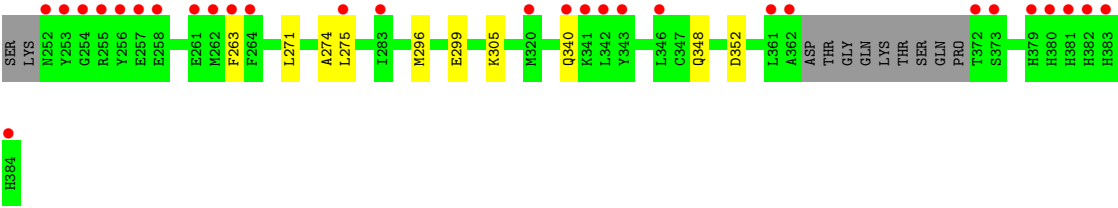


- Molecule 3: Stathmin-4



- Molecule 4: Tubulin tyrosine ligase





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 0.218 , 0.264	Depositor DCC
R_{free} test set	2318 reflections (2.00%)	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)	0.38 , 49.4	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: GTP, GOL, CA, MES, MG, GDP, JEL, ACP

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	0.30	0/3494	0.55	3/4743 (0.1%)
1	C	0.66	7/3515 (0.2%)	0.78	14/4772 (0.3%)
2	B	0.36	2/3431 (0.1%)	0.64	9/4649 (0.2%)
2	D	0.43	4/3377 (0.1%)	0.71	11/4576 (0.2%)
3	E	0.66	3/1008 (0.3%)	0.98	12/1337 (0.9%)
4	F	0.39	2/2851 (0.1%)	0.69	7/3851 (0.2%)
All	All	0.47	18/17676 (0.1%)	0.70	56/23928 (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 (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	163	LYS	CE-NZ	20.27	1.99	1.49
1	C	433	GLU	CB-CG	19.05	1.88	1.52
1	C	433	GLU	CG-CD	11.87	1.69	1.51
2	D	323	MET	CG-SD	9.83	2.06	1.81
1	C	163	LYS	CB-CG	9.41	1.77	1.52
1	C	163	LYS	CD-CE	8.87	1.73	1.51
4	F	86	GLU	CB-CG	8.84	1.69	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	323	MET	CB-CG	8.46	1.78	1.51
1	C	297	GLU	CD-OE2	-8.40	1.16	1.25
3	E	126	LYS	CE-NZ	8.08	1.69	1.49
3	E	89	GLU	CB-CG	7.81	1.67	1.52
2	B	111	GLU	CB-CG	7.49	1.66	1.52
4	F	86	GLU	CG-CD	7.24	1.62	1.51
2	D	405	GLU	CD-OE2	-7.13	1.17	1.25
1	C	297	GLU	CD-OE1	7.02	1.33	1.25
2	B	410	GLU	CD-OE1	-5.72	1.19	1.25
2	D	405	GLU	CD-OE1	-5.35	1.19	1.25
3	E	121	GLU	CD-OE2	-5.04	1.20	1.25

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	410	GLU	OE1-CD-OE2	-18.69	100.87	123.30
1	C	433	GLU	OE1-CD-OE2	-17.29	102.56	123.30
4	F	86	GLU	OE1-CD-OE2	-15.97	104.14	123.30
1	C	433	GLU	CG-CD-OE2	-15.70	86.91	118.30
1	C	251	ASP	CB-CG-OD1	15.40	132.16	118.30
1	C	251	ASP	CB-CG-OD2	-14.46	105.28	118.30
2	D	405	GLU	OE1-CD-OE2	-14.19	106.27	123.30
1	C	433	GLU	CG-CD-OE1	13.44	145.17	118.30
4	F	86	GLU	CA-CB-CG	12.24	140.34	113.40
2	D	390	ARG	NE-CZ-NH1	-11.90	114.35	120.30
4	F	86	GLU	CG-CD-OE2	-11.78	94.73	118.30
4	F	86	GLU	CG-CD-OE1	11.71	141.71	118.30
3	E	121	GLU	OE1-CD-OE2	-10.96	110.15	123.30
1	A	221	ARG	NE-CZ-NH2	-10.55	115.02	120.30
1	C	163	LYS	CD-CE-NZ	-10.53	87.49	111.70
3	E	126	LYS	CD-CE-NZ	-10.46	87.65	111.70
3	E	89	GLU	OE1-CD-OE2	-10.30	110.94	123.30
1	A	221	ARG	NE-CZ-NH1	9.82	125.21	120.30
1	C	163	LYS	CB-CG-CD	-9.22	87.63	111.60
2	D	323	MET	CG-SD-CE	-8.73	86.23	100.20
1	C	297	GLU	OE1-CD-OE2	-8.70	112.86	123.30
3	E	126	LYS	CB-CA-C	8.61	127.61	110.40
2	B	359	ARG	CA-CB-CG	8.36	131.78	113.40
2	B	410	GLU	CG-CD-OE1	8.13	134.56	118.30
3	E	126	LYS	CG-CD-CE	-8.11	87.57	111.90
3	E	51	GLN	CA-CB-CG	7.91	130.80	113.40
2	D	390	ARG	CD-NE-CZ	7.81	134.53	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	405	GLU	CG-CD-OE1	7.57	133.45	118.30
2	D	257	MET	CA-CB-CG	7.30	125.71	113.30
2	D	405	GLU	CA-CB-CG	-7.22	97.51	113.40
2	B	111	GLU	OE1-CD-OE2	-7.20	114.66	123.30
2	D	323	MET	CA-CB-CG	-7.17	101.11	113.30
2	B	410	GLU	CG-CD-OE2	-6.85	104.60	118.30
3	E	121	GLU	CG-CD-OE1	6.65	131.60	118.30
2	B	111	GLU	CG-CD-OE2	-6.41	105.48	118.30
1	C	297	GLU	CG-CD-OE1	6.31	130.93	118.30
2	B	111	GLU	CG-CD-OE1	6.29	130.89	118.30
3	E	89	GLU	CG-CD-OE1	6.27	130.84	118.30
1	A	221	ARG	CD-NE-CZ	6.21	132.29	123.60
2	D	73	MET	CG-SD-CE	6.17	110.08	100.20
1	C	433	GLU	CB-CG-CD	-6.17	97.55	114.20
1	C	163	LYS	CB-CA-C	6.06	122.52	110.40
4	F	186	LEU	CB-CG-CD2	5.85	120.94	111.00
3	E	89	GLU	CG-CD-OE2	-5.76	106.79	118.30
2	B	410	GLU	CA-CB-CG	5.57	125.65	113.40
1	C	251	ASP	CB-CA-C	5.44	121.28	110.40
3	E	62	LYS	CD-CE-NZ	-5.41	99.26	111.70
2	D	84	ILE	CG1-CB-CG2	-5.35	99.64	111.40
1	C	163	LYS	CA-CB-CG	-5.32	101.69	113.40
4	F	305	LYS	CD-CE-NZ	-5.26	99.60	111.70
2	B	410	GLU	N-CA-CB	-5.20	101.23	110.60
4	F	305	LYS	CB-CG-CD	-5.20	98.07	111.60
3	E	139	LEU	CB-CG-CD2	5.16	119.77	111.00
1	C	433	GLU	CB-CA-C	5.07	120.54	110.40
2	D	405	GLU	CG-CD-OE2	-5.06	108.18	118.30
3	E	121	GLU	CG-CD-OE2	-5.03	108.23	118.30

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

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Mol	Chain	Res	Type	Group
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	44	0
1	C	3437	3335	3348	48	0
2	B	3356	3204	3234	42	0
2	D	3304	3153	3185	74	0
3	E	1000	1013	1018	25	0
4	F	2785	2709	2737	47	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	6	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	274	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 (274) 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
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: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
2:D:32:PRO:C	2:D:84:ILE:HD13	2.14	0.68
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:167:PHE:CD2	2:D:202:ILE:HD11	2.30	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
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
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
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
1:C:433:GLU:CB	1:C:433:GLU:CD	2.69	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:D:323:MET:CG	2:D:323:MET:C	2.72	0.58
2:B:335:ASN:CG	4:F:58:LEU:HD21	2.23	0.58
2:D:251:ARG:NH1	13:D:604:HOH:O	2.32	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
1:C:280:LYS:NZ	13:C:611:HOH:O	2.38	0.55
2:B:145:SER:OG	2:B:188:SER:OG	2.23	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:SER:HB3	1:A:391:LEU:HD21	1.89	0.54
1:A:28:HIS:HB3	1:A:36:MET:HE3	1.88	0.54
1:A:163:LYS:HB3	1:A:164:LYS:HD3	1.89	0.54
2:D:73:MET:HE1	2:D:92:PHE:HB3	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
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:B:126:SER:OG	2:B:126:SER:O	2.26	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: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
4:F:37:PHE:CZ	4:F:40:MET:HE3	2.46	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
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:1:MET:H2	2:D:128:ASP:HB2	1.75	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:207:LEU:HA	2:D:210:ILE:HD13	1.94	0.49
2:D:377:LEU:C	2:D:377:LEU:HD23	2.33	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
2:B:290:THR:HG22	2:B:333:VAL:HG21	1.94	0.48
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
2:D:293:MET:HE2	2:D:367:PHE:HB2	1.96	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
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
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
1:A:96:LYS:HD3	1:A:96:LYS:N	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
4:F:96:GLU:OE1	4:F:98:TYR:OH	2.34	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
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:B:284:LEU:O	2:B:363:MET:HE2	2.18	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
1:A:163:LYS:C	1:A:164:LYS:HD3	2.38	0.43
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:D:172:SER:HG	2:D:205:GLU:HB2	1.84	0.43
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
2:B:145:SER:HG	2:B:188:SER:HG	1.52	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: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
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:A:41:THR:OG1	1:A:41:THR:O	2.38	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
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
2:D:206:ALA:C	2:D:210:ILE:HD12	2.40	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
1:C:433:GLU:CG	1:C:433:GLU:C	2.88	0.42
2:D:170:VAL:HG13	2:D:171:PRO:HD2	2.01	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
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
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)
4:F:88:SER:C	4:F:90:SER:N	2.74	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
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
2:D:388:MET:HE2	2:D:388:MET:HB3	1.99	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
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

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%)	25	36
All	All	2160/2365 (91%)	2093 (97%)	65 (3%)	2 (0%)	51	68

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%)	367 (100%)	1 (0%)	92	97
1	C	371/379 (98%)	370 (100%)	1 (0%)	92	97
2	B	367/381 (96%)	365 (100%)	2 (0%)	88	95
2	D	362/381 (95%)	360 (99%)	2 (1%)	86	94
3	E	109/171 (64%)	108 (99%)	1 (1%)	78	90
4	F	305/342 (89%)	303 (99%)	2 (1%)	84	92
All	All	1882/2033 (93%)	1873 (100%)	9 (0%)	88	95

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	221	ARG
2	B	111	GLU
2	B	410	GLU
1	C	163	LYS
2	D	86	ARG
2	D	212	PHE
3	E	89	GLU
4	F	131	PHE
4	F	222	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	293	ASN
2	D	6	HIS
2	D	8	GLN
2	D	37	HIS
3	E	51	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 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	$\# Z > 2$
8	GOL	A	504	-	5,5,5	0.77	0	5,5,5	0.97	0
10	JEL	B	503	-	35,36,36	1.39	2 (5%)	49,51,51	1.30	7 (14%)
10	JEL	D	502	-	35,36,36	1.42	2 (5%)	49,51,51	1.38	8 (16%)
12	ACP	F	401	-	27,33,33	1.35	5 (18%)	32,52,52	1.42	4 (12%)
11	GDP	B	504	6	24,30,30	1.20	3 (12%)	31,47,47	1.97	8 (25%)
5	GTP	C	501	6	26,34,34	0.95	1 (3%)	33,54,54	1.87	7 (21%)
5	GTP	A	501	6	26,34,34	0.96	1 (3%)	33,54,54	1.87	7 (21%)
9	MES	B	502	-	12,12,12	2.22	1 (8%)	14,16,16	1.77	5 (35%)
5	GTP	D	501	6	26,34,34	0.97	1 (3%)	33,54,54	1.77	7 (21%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	GOL	A	504	-	-	2/4/4/4	-
10	JEL	B	503	-	-	0/9/15/15	0/6/6/6
10	JEL	D	502	-	-	0/9/15/15	0/6/6/6
12	ACP	F	401	-	-	4/15/38/38	0/3/3/3
11	GDP	B	504	6	-	2/12/32/32	0/3/3/3
5	GTP	C	501	6	-	5/18/38/38	0/3/3/3
5	GTP	A	501	6	-	7/18/38/38	0/3/3/3
9	MES	B	502	-	-	3/6/14/14	0/1/1/1
5	GTP	D	501	6	-	4/18/38/38	0/3/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	502	MES	C8-S	-7.45	1.66	1.77
10	D	502	JEL	C10-N3	5.69	1.44	1.36
10	B	503	JEL	C10-N3	5.42	1.44	1.36
11	B	504	GDP	C5-C6	4.30	1.48	1.41
10	D	502	JEL	CAC-CAA	-3.40	1.35	1.45
10	B	503	JEL	CAC-CAA	-3.28	1.36	1.45
5	D	501	GTP	C6-N1	3.11	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	501	GTP	C6-N1	3.11	1.38	1.33
5	C	501	GTP	C6-N1	3.02	1.38	1.33
12	F	401	ACP	PG-O3G	2.85	1.61	1.54
12	F	401	ACP	PG-O2G	2.84	1.61	1.54
12	F	401	ACP	PB-O3A	2.60	1.61	1.58
12	F	401	ACP	C5-C4	2.44	1.47	1.40
11	B	504	GDP	C5-C4	2.27	1.46	1.40
11	B	504	GDP	O4'-C1'	2.20	1.44	1.41
12	F	401	ACP	PB-O2B	2.16	1.61	1.56

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	501	GTP	N3-C2-N1	-5.38	120.05	127.22
5	D	501	GTP	N3-C2-N1	-5.32	120.13	127.22
5	C	501	GTP	N3-C2-N1	-5.30	120.15	127.22
11	B	504	GDP	C2-N3-C4	4.80	120.84	115.36
10	D	502	JEL	C9-N2-C10	4.56	122.43	117.81
5	A	501	GTP	C2-N3-C4	4.40	120.38	115.36
5	C	501	GTP	C2-N3-C4	4.30	120.27	115.36
11	B	504	GDP	C4-C5-C6	-4.21	116.78	120.80
10	B	503	JEL	C9-N2-C10	4.21	122.07	117.81
5	D	501	GTP	C2-N3-C4	4.15	120.10	115.36
12	F	401	ACP	PB-O3A-PA	-3.87	120.28	132.56
5	A	501	GTP	PB-O3B-PG	-3.78	119.85	132.83
5	C	501	GTP	PB-O3B-PG	-3.74	120.00	132.83
11	B	504	GDP	C2-N1-C6	3.71	121.82	115.93
11	B	504	GDP	C5-C6-N1	-3.68	118.40	123.43
10	D	502	JEL	C8-CAA-C6	3.56	122.89	118.17
5	C	501	GTP	PA-O3A-PB	-3.45	121.00	132.83
5	A	501	GTP	PA-O3A-PB	-3.36	121.31	132.83
10	B	503	JEL	C8-CAA-C6	3.31	122.55	118.17
9	B	502	MES	C5-N4-C3	3.16	115.94	108.83
11	B	504	GDP	N3-C2-N1	-3.15	123.03	127.22
12	F	401	ACP	N3-C2-N1	-3.06	123.89	128.68
11	B	504	GDP	PA-O3A-PB	-3.06	122.34	132.83
5	C	501	GTP	C5-C6-N1	-3.00	119.33	123.43
11	B	504	GDP	C4-C5-N7	-2.90	106.37	109.40
5	D	501	GTP	PB-O3B-PG	-2.89	122.90	132.83
12	F	401	ACP	C3'-C2'-C1'	2.88	105.31	100.98
11	B	504	GDP	C3'-C2'-C1'	2.83	105.24	100.98
12	F	401	ACP	C4-C5-N7	-2.80	106.48	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	501	GTP	C5-C6-N1	-2.76	119.65	123.43
5	D	501	GTP	C5-C6-N1	-2.74	119.69	123.43
9	B	502	MES	C6-C5-N4	-2.73	105.97	110.10
10	D	502	JEL	C11-CAC-C7	2.69	121.94	118.26
9	B	502	MES	O3S-S-C8	2.65	110.05	105.77
5	D	501	GTP	PA-O3A-PB	-2.52	124.18	132.83
5	C	501	GTP	C3'-C2'-C1'	2.49	104.73	100.98
5	A	501	GTP	C3'-C2'-C1'	2.49	104.72	100.98
5	C	501	GTP	C2-N1-C6	2.47	119.86	115.93
5	D	501	GTP	C2-N1-C6	2.47	119.85	115.93
5	A	501	GTP	C2-N1-C6	2.46	119.84	115.93
10	B	503	JEL	C13-C4-N3	-2.43	107.44	113.77
10	B	503	JEL	C11-CAC-C7	2.42	121.57	118.26
5	D	501	GTP	C3'-C2'-C1'	2.38	104.57	100.98
9	B	502	MES	O1S-S-C8	2.27	109.65	106.92
10	D	502	JEL	C11-C10-N2	-2.27	119.57	122.75
10	B	503	JEL	CAC-CAA-C6	2.24	108.54	106.09
10	D	502	JEL	CAA-CAC-C7	2.22	108.52	106.09
10	D	502	JEL	CAC-CAA-C6	2.22	108.52	106.09
10	D	502	JEL	C9-C7-CAC	-2.16	118.38	121.16
10	B	503	JEL	CAA-CAC-C7	2.14	108.43	106.09
10	D	502	JEL	C8-CAA-CAC	-2.07	128.59	133.15
9	B	502	MES	O2S-S-C8	2.04	109.38	106.92
10	B	503	JEL	C11-C10-N2	-2.02	119.92	122.75

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	501	GTP	C5'-O5'-PA-O1A
5	A	501	GTP	C5'-O5'-PA-O2A
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'
12	F	401	ACP	C3'-C4'-C5'-O5'
8	A	504	GOL	O1-C1-C2-O2
5	A	501	GTP	PB-O3B-PG-O1G
5	D	501	GTP	C4'-C5'-O5'-PA

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Mol	Chain	Res	Type	Atoms
5	A	501	GTP	C4'-C5'-O5'-PA
5	C	501	GTP	C4'-C5'-O5'-PA
12	F	401	ACP	C5'-O5'-PA-O3A
9	B	502	MES	C7-C8-S-O1S
5	A	501	GTP	PB-O3A-PA-O2A
5	C	501	GTP	PB-O3A-PA-O2A
5	D	501	GTP	PA-O3A-PB-O1B
5	A	501	GTP	PB-O3B-PG-O2G
5	D	501	GTP	PB-O3B-PG-O2G
5	A	501	GTP	C5'-O5'-PA-O3A
5	C	501	GTP	C5'-O5'-PA-O3A
11	B	504	GDP	C5'-O5'-PA-O3A
5	D	501	GTP	C5'-O5'-PA-O1A
11	B	504	GDP	C5'-O5'-PA-O2A

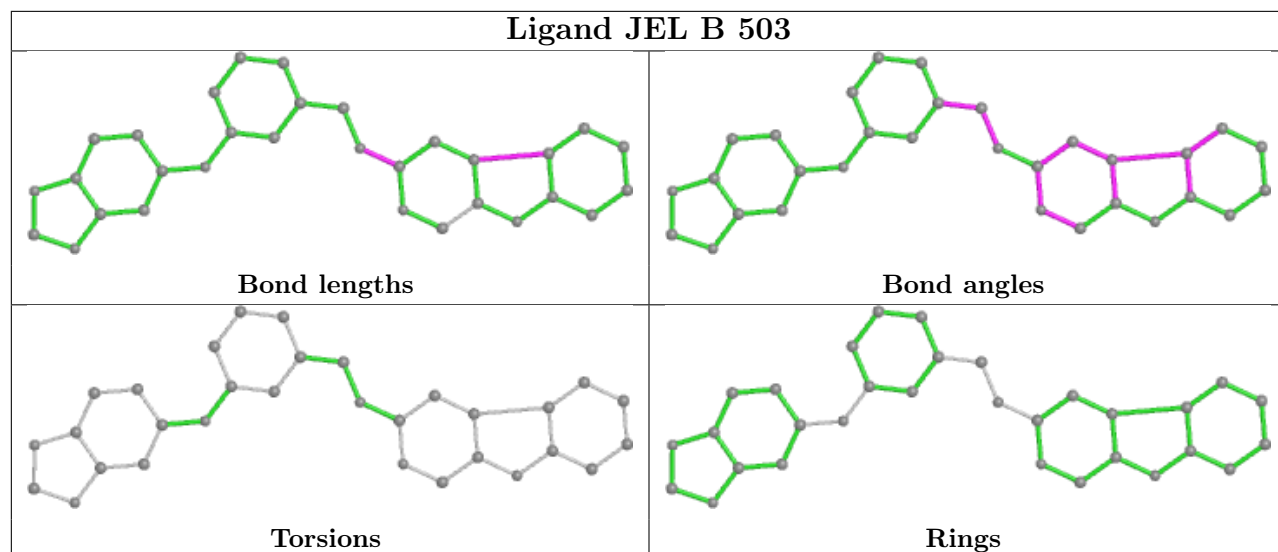
There are no ring outliers.

1 monomer is involved in 2 short contacts:

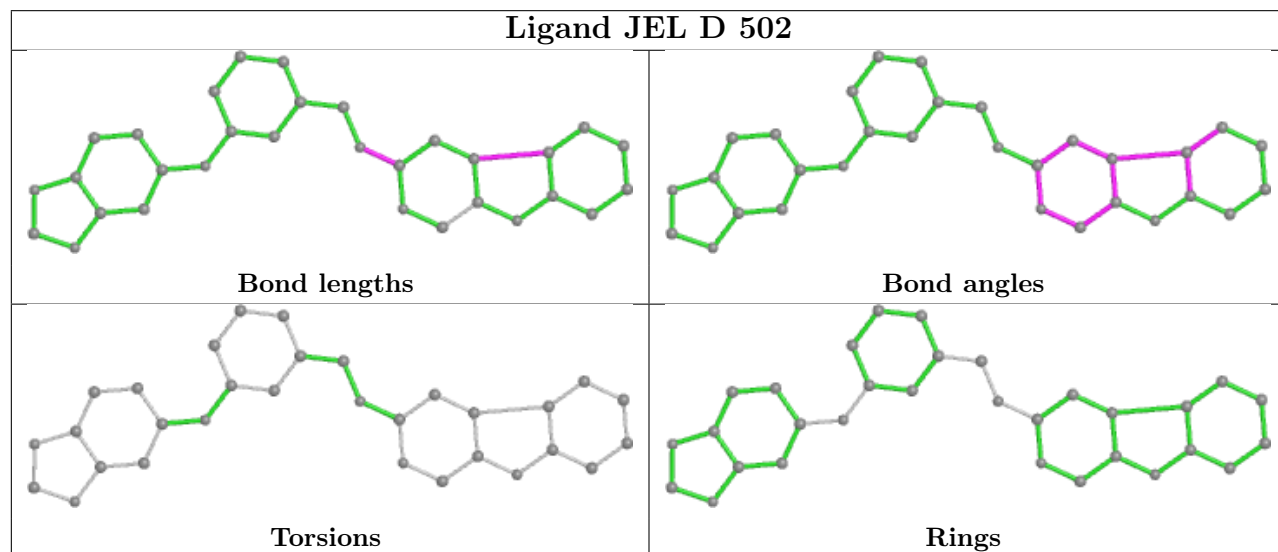
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	D	502	JEL	2	0

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.

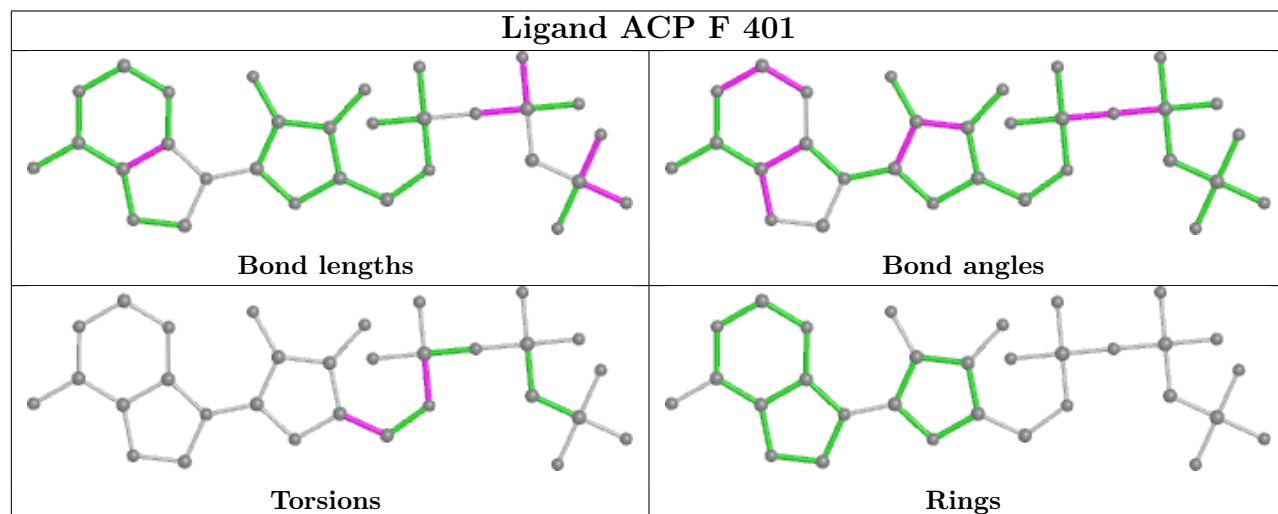
Ligand JEL B 503

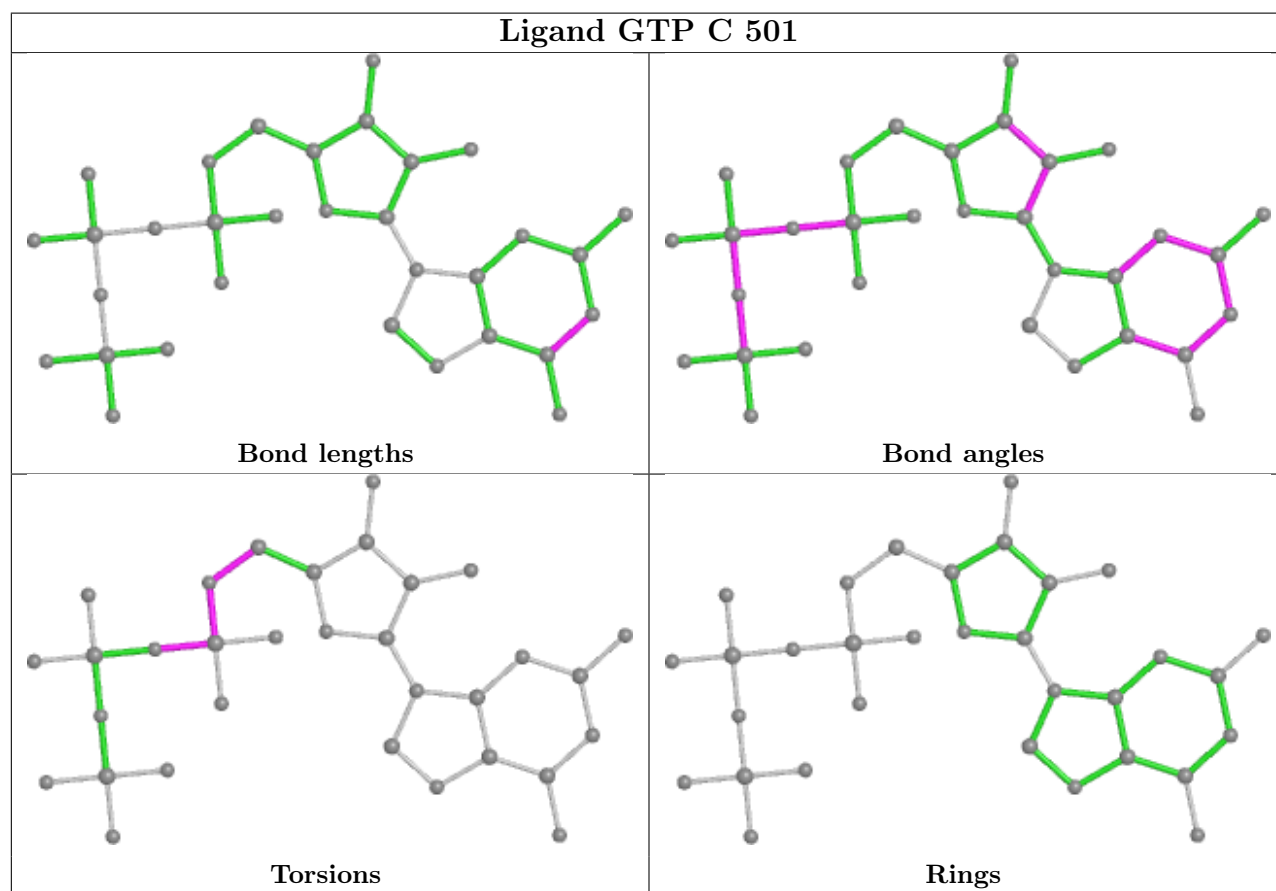
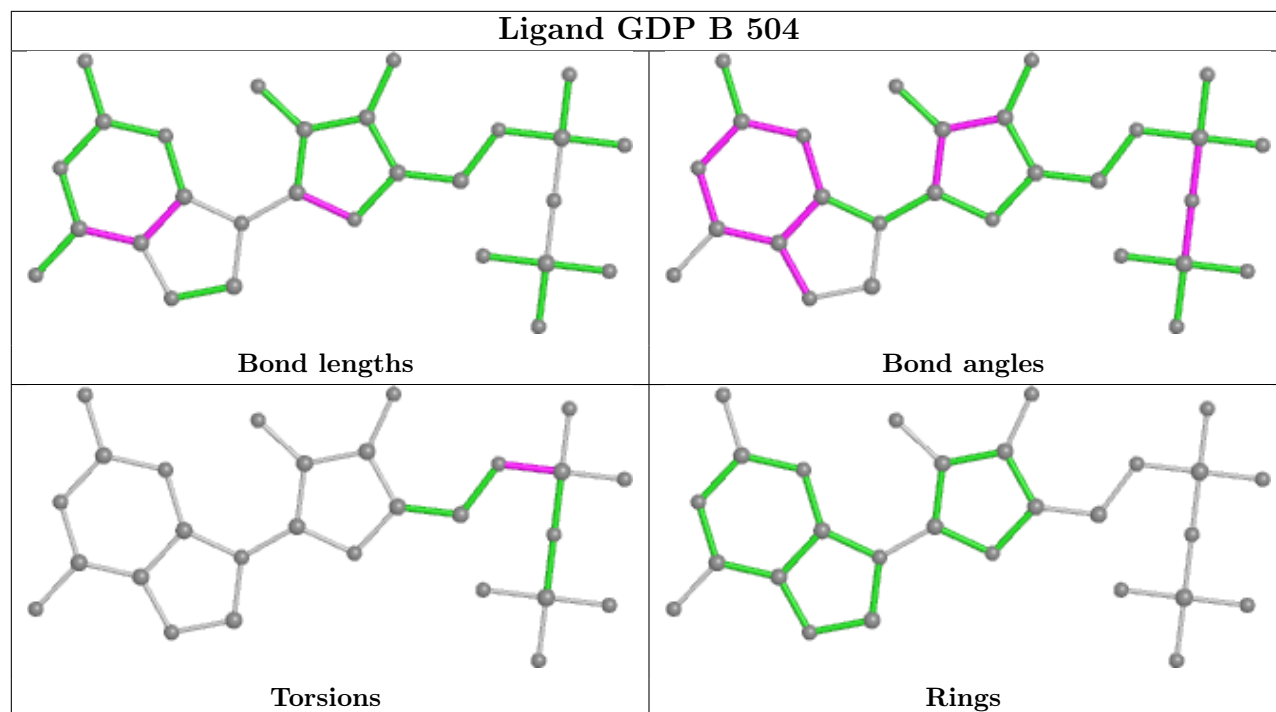


Ligand JEL D 502

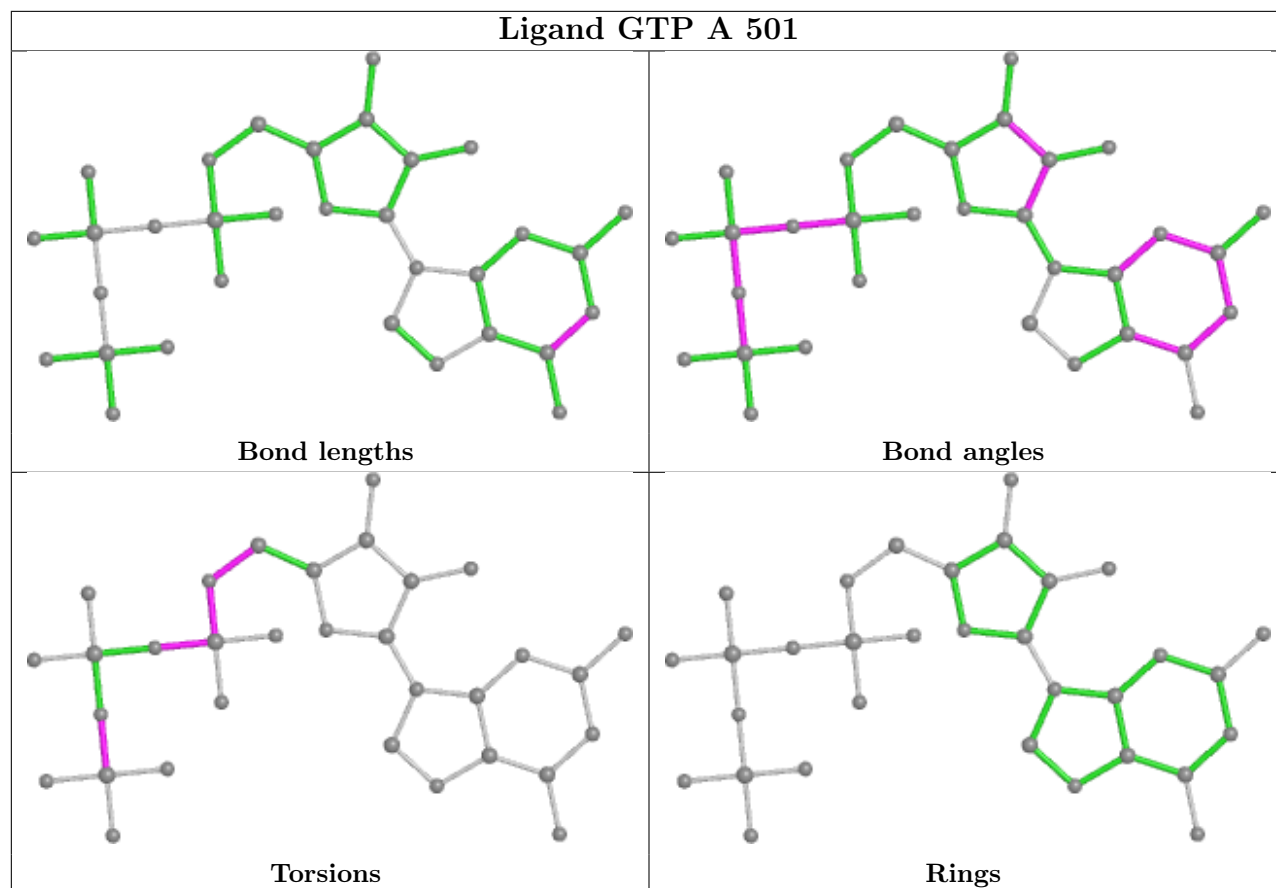


Ligand ACP F 401

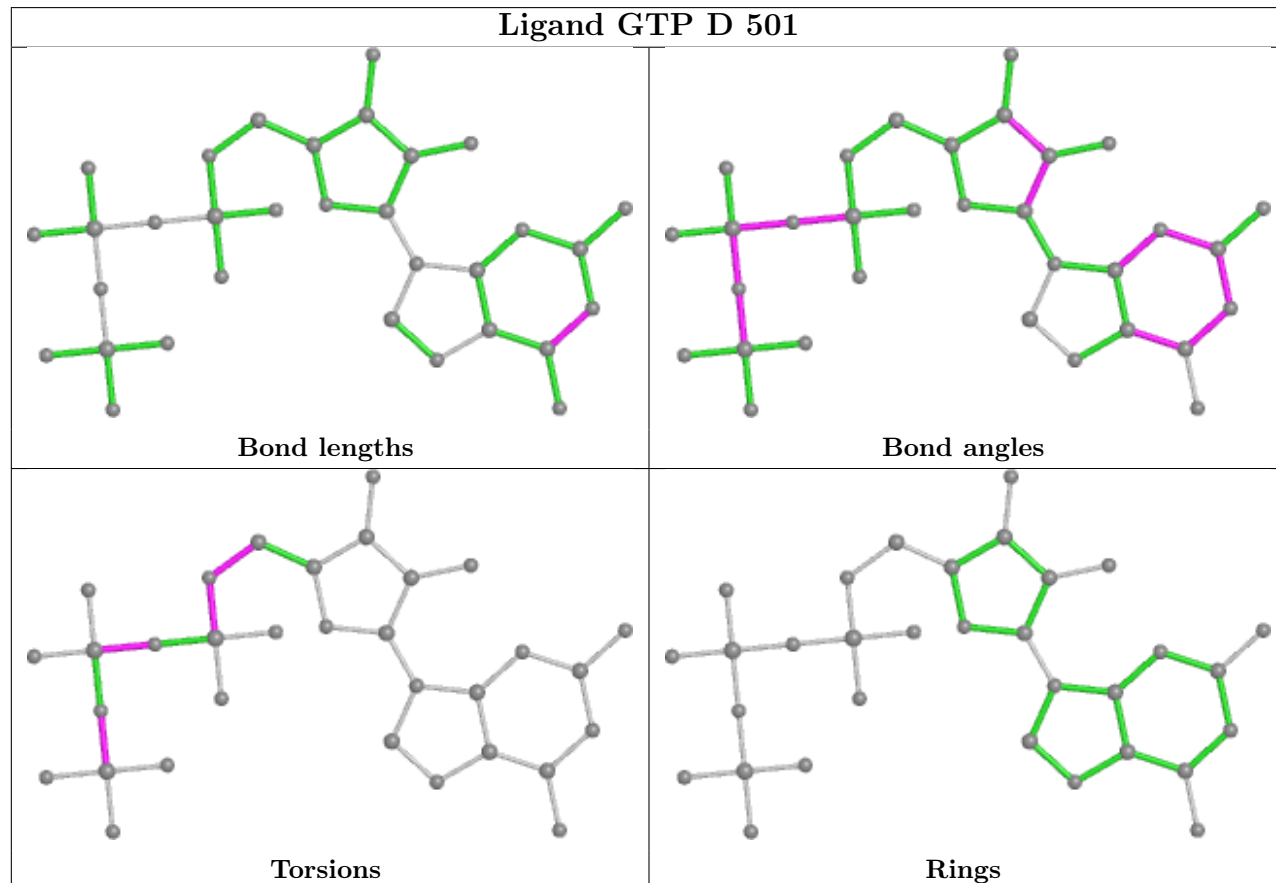




Ligand GTP A 501



Ligand GTP D 501



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	437/451 (96%)	0.37	12 (2%) 54 52	25, 41, 64, 79	0
1	C	440/451 (97%)	0.27	8 (1%) 68 66	21, 34, 57, 79	0
2	B	427/445 (95%)	0.48	23 (5%) 25 24	20, 40, 71, 118	0
2	D	421/445 (94%)	1.23	90 (21%) 0 0	33, 67, 97, 132	0
3	E	121/189 (64%)	0.79	11 (9%) 9 8	29, 62, 88, 109	0
4	F	338/384 (88%)	1.92	133 (39%) 0 0	36, 72, 125, 141	0
All	All	2184/2365 (92%)	0.80	277 (12%) 3 3	20, 49, 95, 141	0

All (277) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	161	LEU	12.9
4	F	169	LEU	12.3
4	F	233	PHE	12.1
4	F	173	ILE	12.0
4	F	130	VAL	11.0
4	F	134	ALA	9.6
4	F	139	ARG	9.4
4	F	166	ALA	8.9
4	F	234	GLN	8.5
4	F	178	GLN	8.2
4	F	170	LEU	8.0
4	F	244	CYS	8.0
4	F	253	TYR	7.7
4	F	101	TYR	7.6
4	F	103	THR	7.4
2	D	37	HIS	7.1
2	D	175	VAL	6.6
1	C	179	THR	6.6
4	F	252	ASN	6.5

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Mol	Chain	Res	Type	RSRZ
4	F	182	ILE	6.4
2	D	245	GLN	6.3
2	D	55	ALA	6.2
4	F	137	ARG	6.2
4	F	245	ILE	6.0
4	F	255	ARG	6.0
4	F	256	TYR	5.9
4	F	186	LEU	5.8
4	F	133	ALA	5.8
2	D	391	ARG	5.8
3	E	140	LYS	5.7
4	F	236	LYS	5.7
4	F	168	GLU	5.6
4	F	179	VAL	5.6
2	D	81	PHE	5.6
4	F	132	LEU	5.6
4	F	162	ILE	5.6
4	F	127	GLU	5.5
2	D	80	PRO	5.5
4	F	231	ALA	5.5
4	F	381	HIS	5.5
2	D	177	ASP	5.4
4	F	172	PHE	5.4
4	F	142	ARG	5.2
4	F	372	THR	5.1
4	F	20	LEU	5.0
4	F	149	ALA	5.0
4	F	22	LEU	4.9
4	F	136	ASN	4.9
4	F	165	GLU	4.9
2	D	390	ARG	4.9
2	D	219	THR	4.8
3	E	7	GLU	4.8
2	B	246	LEU	4.8
2	D	217	LEU	4.8
4	F	225	SER	4.7
4	F	167	SER	4.6
4	F	240	LEU	4.6
2	D	41	ASP	4.6
4	F	242	ASN	4.6
4	F	164	SER	4.6
4	F	143	GLU	4.5

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Mol	Chain	Res	Type	RSRZ
4	F	362	ALA	4.5
2	B	57	ASN	4.5
4	F	146	VAL	4.5
2	B	279	GLN	4.4
2	D	73	MET	4.4
2	D	396	HIS	4.4
3	E	46	SER	4.4
4	F	135	TYR	4.4
4	F	361	LEU	4.3
2	D	214	THR	4.3
4	F	138	ARG	4.3
2	D	54	ALA	4.3
4	F	100	ILE	4.3
2	D	394	PHE	4.3
2	D	74	ASP	4.3
2	B	278	SER	4.2
4	F	379	HIS	4.2
4	F	141	GLY	4.2
2	D	92	PHE	4.2
4	F	99	VAL	4.1
2	B	56	GLY	4.1
4	F	175	GLU	4.1
4	F	232	ASN	4.1
2	D	1	MET	4.1
2	D	215	LEU	4.1
3	E	6	MET	4.1
4	F	174	ASP	4.0
2	D	33	THR	4.0
4	F	129	GLU	3.9
2	D	176	SER	3.9
4	F	131	PHE	3.9
2	B	280	GLN	3.8
3	E	135	LYS	3.8
2	B	80	PRO	3.8
4	F	148	ILE	3.7
4	F	243	HIS	3.7
2	D	85	PHE	3.7
4	F	185	TYR	3.7
2	B	276	ARG	3.7
4	F	228	TYR	3.7
4	F	140	GLU	3.7
2	D	35	SER	3.7

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Mol	Chain	Res	Type	RSRZ
4	F	17	VAL	3.6
2	D	39	ASP	3.6
2	D	393	ALA	3.6
4	F	145	ASN	3.5
4	F	163	SER	3.5
2	D	70	PRO	3.5
4	F	230	SER	3.5
2	B	245	GLN	3.5
2	D	87	PRO	3.5
2	B	42	LEU	3.4
4	F	19	ARG	3.4
2	D	200	TYR	3.4
2	D	84	ILE	3.4
4	F	199	PHE	3.4
4	F	98	TYR	3.4
3	E	139	LEU	3.4
2	D	77	ARG	3.4
2	D	83	GLN	3.4
2	D	221	THR	3.4
4	F	254	GLY	3.4
4	F	224	SER	3.4
2	D	244	GLY	3.3
2	D	359	ARG	3.3
4	F	176	GLN	3.3
4	F	191	LEU	3.3
4	F	227	PRO	3.3
2	B	275	SER	3.3
2	D	76	VAL	3.3
4	F	187	GLU	3.3
2	D	400	GLY	3.2
1	C	200	CYS	3.2
2	D	36	TYR	3.2
1	A	262	TYR	3.2
1	A	346	TRP	3.2
2	B	37	HIS	3.2
4	F	171	ASP	3.2
2	D	112	LEU	3.2
4	F	257	GLU	3.2
4	F	24	THR	3.1
1	C	340	SER	3.1
2	B	247	ASN	3.1
4	F	13	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
4	F	181	VAL	3.1
1	C	357	TYR	3.0
2	D	94	GLN	3.0
4	F	237	THR	3.0
4	F	25	GLY	3.0
4	F	264	PHE	3.0
2	D	48	ASN	3.0
2	B	336	LYS	3.0
2	D	216	LYS	3.0
4	F	180	HIS	3.0
4	F	239	HIS	3.0
4	F	380	HIS	3.0
4	F	221	LEU	3.0
4	F	128	ARG	3.0
4	F	194	PRO	3.0
4	F	188	LYS	3.0
4	F	147	TRP	2.9
4	F	1	MET	2.9
4	F	223	THR	2.9
4	F	21	LEU	2.9
4	F	226	GLU	2.9
4	F	102	PRO	2.9
2	D	167	PHE	2.9
4	F	320	MET	2.9
4	F	373	SER	2.9
2	D	79	GLY	2.9
3	E	45	PRO	2.9
2	D	387	ALA	2.9
4	F	177	GLY	2.8
4	F	23	ALA	2.8
4	F	246	GLN	2.8
4	F	258	GLU	2.8
2	D	397	TRP	2.8
4	F	247	LYS	2.8
4	F	263	PHE	2.7
1	A	172	TYR	2.7
3	E	48	GLU	2.7
4	F	275	LEU	2.7
2	D	96	GLY	2.7
1	C	440	VAL	2.7
4	F	27	TRP	2.7
2	D	56	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
2	D	246	LEU	2.7
1	A	281	ALA	2.6
2	B	170	VAL	2.6
2	D	86	ARG	2.6
2	D	212	PHE	2.6
2	D	266	PHE	2.6
2	D	284	LEU	2.6
2	D	196	THR	2.6
3	E	27	PRO	2.6
2	B	277	GLY	2.6
4	F	241	THR	2.6
2	D	208	TYR	2.6
4	F	262	MET	2.5
2	D	78	SER	2.5
1	A	364	PRO	2.5
3	E	62	LYS	2.5
4	F	197	ARG	2.5
4	F	10	ASN	2.5
2	D	201	CYS	2.5
2	D	403	MET	2.5
4	F	235	ASP	2.5
4	F	382	HIS	2.5
1	A	387	ALA	2.4
4	F	196	HIS	2.4
2	D	369	GLY	2.4
4	F	343	TYR	2.4
4	F	283	ILE	2.4
2	D	126	SER	2.4
4	F	18	SER	2.4
2	D	38	GLY	2.4
1	C	252	LEU	2.4
4	F	346	LEU	2.4
2	D	199	THR	2.4
4	F	261	GLU	2.4
4	F	126	ASP	2.3
2	D	90	PHE	2.3
4	F	96	GLU	2.3
2	B	38	GLY	2.3
1	C	251	ASP	2.3
2	D	267	MET	2.3
2	B	11	GLN	2.3
4	F	28	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
2	D	178	THR	2.3
2	D	395	LEU	2.2
4	F	342	LEU	2.2
2	D	34	GLY	2.2
4	F	341	LYS	2.2
4	F	26	GLN	2.2
2	D	58	LYS	2.2
2	D	97	ALA	2.2
2	B	178	THR	2.2
2	D	236	VAL	2.2
2	D	31	ASP	2.2
2	B	274	THR	2.2
1	A	171	ILE	2.1
2	D	75	SER	2.1
2	D	220	PRO	2.1
2	D	406	MET	2.1
2	B	320	ARG	2.1
2	D	320	ARG	2.1
2	D	218	THR	2.1
2	D	265	PHE	2.1
4	F	238	CYS	2.1
2	B	33	THR	2.1
2	D	166	THR	2.1
2	D	285	THR	2.1
4	F	31	ARG	2.1
2	B	406	MET	2.1
2	D	293	MET	2.1
4	F	384	HIS	2.1
4	F	340	GLN	2.1
1	C	257	THR	2.1
2	D	247	ASN	2.1
2	D	258	VAL	2.1
1	A	96	LYS	2.1
1	A	282	TYR	2.1
2	D	15	GLN	2.1
4	F	229	ASN	2.1
2	D	389	PHE	2.1
2	D	398	TYR	2.1
2	D	257	MET	2.0
2	D	388	MET	2.0
1	A	196	GLU	2.0
4	F	383	HIS	2.0

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Mol	Chain	Res	Type	RSRZ
2	D	44	LEU	2.0
2	D	65	LEU	2.0
3	E	23	ILE	2.0
1	A	54	SER	2.0
4	F	144	GLY	2.0
1	A	345	ASP	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

LIGAND-RSR INFOmissingINFO

6.5 Other polymers [i](#)

There are no such residues in this entry.