



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 07:12 AM UTC

PDB ID : 4ZI7 / pdb_00004zi7
Title : CRYSTAL STRUCTURE OF TUBULIN-STATHMIN-TTL-HTI286 COM-
PLEX
Authors : Wang, Y.; Zhang, R.
Deposited on : 2015-04-27
Resolution : 2.51 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

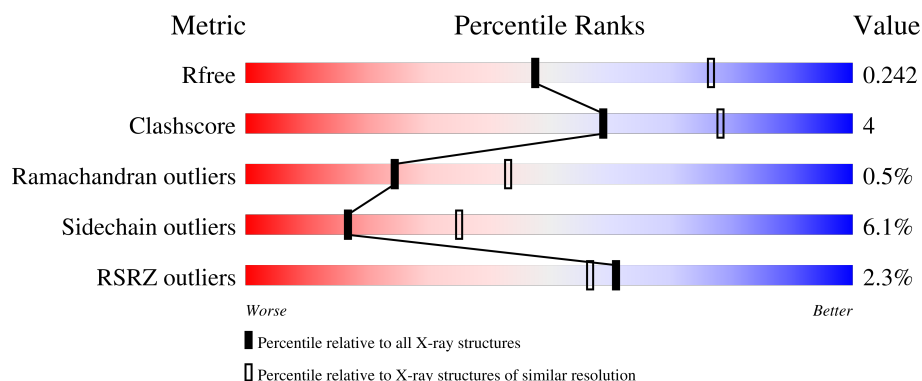
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.51 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	
1	C	451	
2	B	445	
2	D	445	
3	E	143	

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Mol	Chain	Length	Quality of chain
4	F	384	5% 74% 15% • 10%

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 17939 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Tubulin alpha-1B chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	439	Total	C	N	O	S	0	1	0
			3436	2173	584	656	23			
1	C	440	Total	C	N	O	S	0	2	0
			3452	2183	586	660	23			

- Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	430	Total	C	N	O	S	0	1	0
			3387	2129	580	652	26			
2	D	422	Total	C	N	O	S	0	0	0
			3311	2082	563	640	26			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	123	Total	C	N	O	S	0	1	0
			1024	631	186	202	5			

There are 2 discrepancies between the modelled and reference sequences:

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

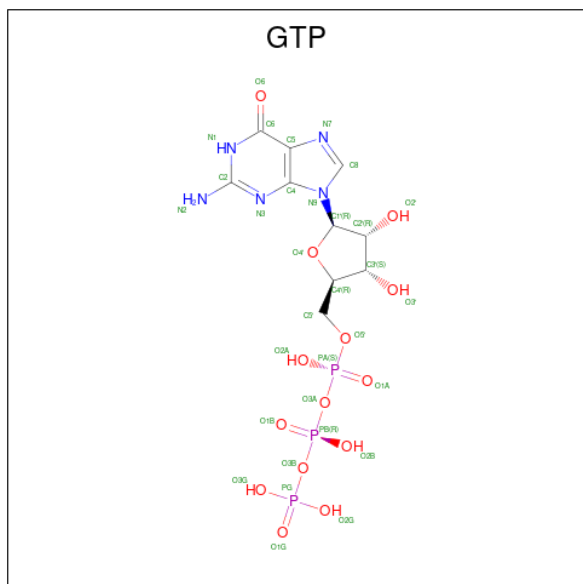
- Molecule 4 is a protein called Tubulin-Tyrosine Ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	346	Total	C	N	O	S	0	0	0
			2849	1825	492	518	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
F	383	HIS	-	expression tag	UNP E1BQ43
F	384	HIS	-	expression tag	UNP E1BQ43

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



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

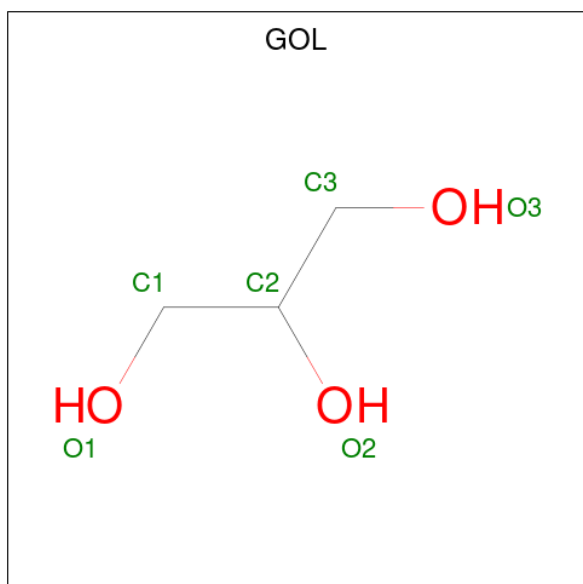
- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

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

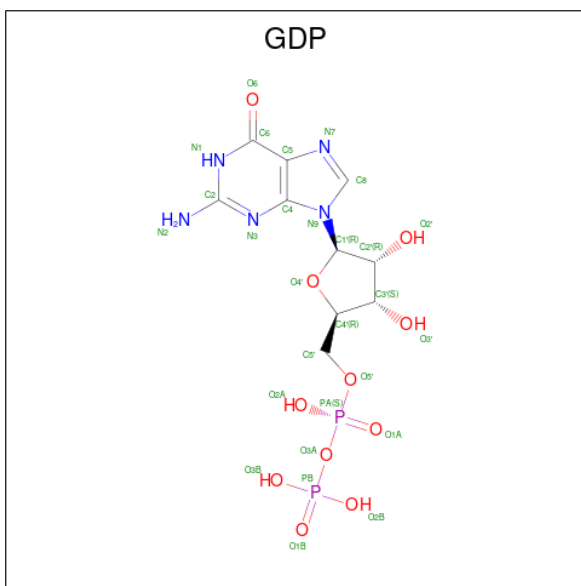
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Ca	0	0
			1	1		
7	B	1	Total	Ca	0	0
			1	1		
7	C	2	Total	Ca	0	0
			2	2		

- Molecule 8 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



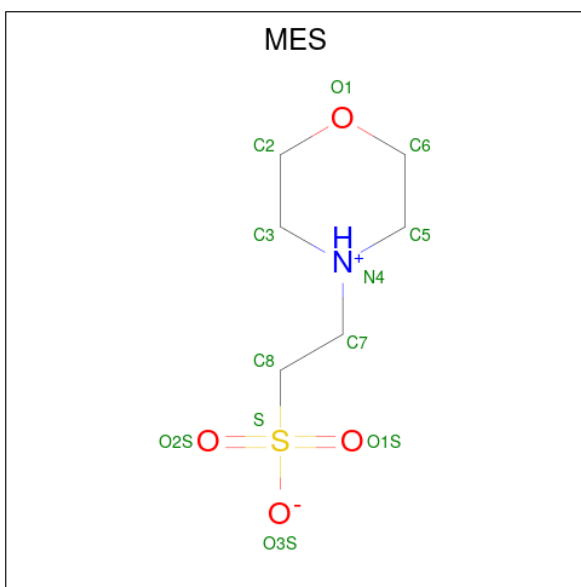
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			6	3	3		
8	A	1	Total	C	O	0	0
			6	3	3		
8	A	1	Total	C	O	0	0
			6	3	3		
8	A	1	Total	C	O	0	0
			6	3	3		
8	B	1	Total	C	O	0	0
			6	3	3		
8	C	1	Total	C	O	0	0
			6	3	3		
8	C	1	Total	C	O	0	0
			6	3	3		
8	F	1	Total	C	O	0	0
			6	3	3		

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



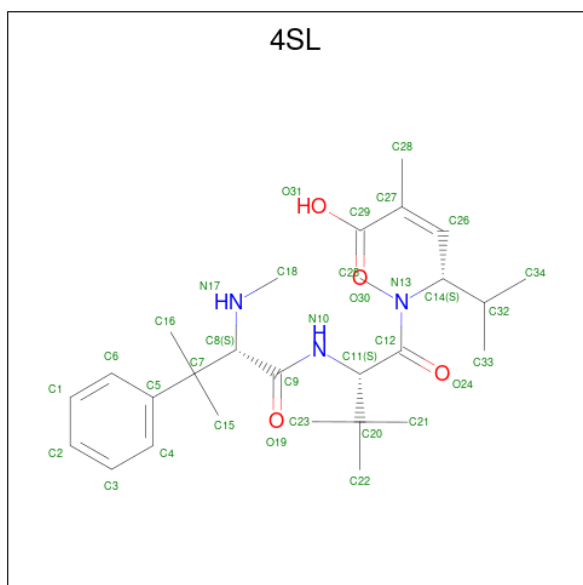
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	B	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
9	D	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- Molecule 10 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: $C_6H_{13}NO_4S$).



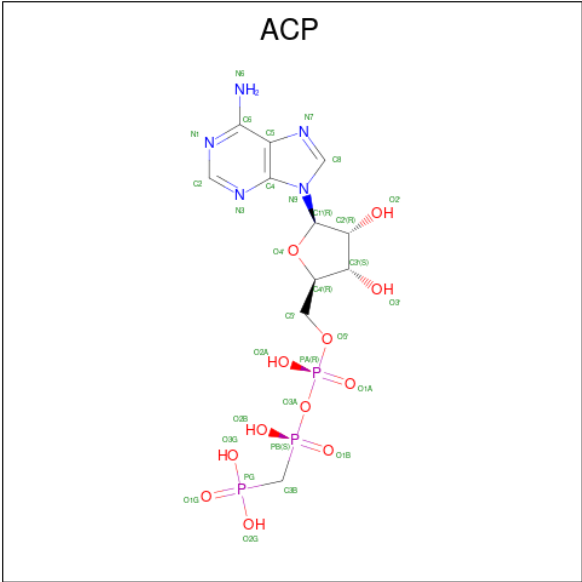
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
10	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 11 is N,beta,beta-trimethyl-L-phenylalanyl-N-[(3S,4Z)-5-carboxy-2-methylhex-4-en-3-yl]-N,3-dimethyl-L-valinamide (CCD ID: 4SL) (formula: $C_{27}H_{43}N_3O_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	B	1	Total	C	N	O	0	0
			34	27	3	4		

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



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

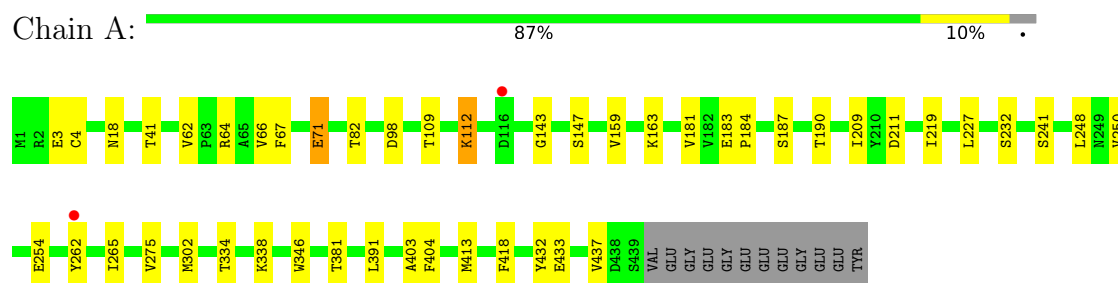
- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	51	Total	O	0	0
			51	51		
13	B	47	Total	O	0	0
			47	47		
13	C	86	Total	O	0	0
			86	86		
13	D	13	Total	O	0	0
			13	13		
13	E	2	Total	O	0	0
			2	2		
13	F	16	Total	O	0	0
			16	16		

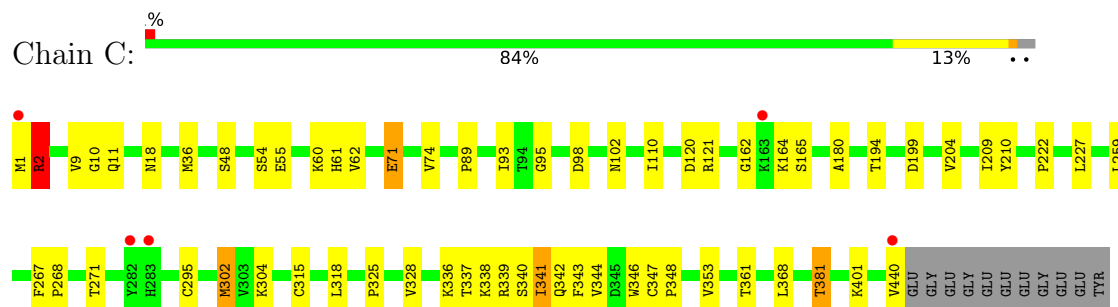
3 Residue-property plots [i](#)

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.

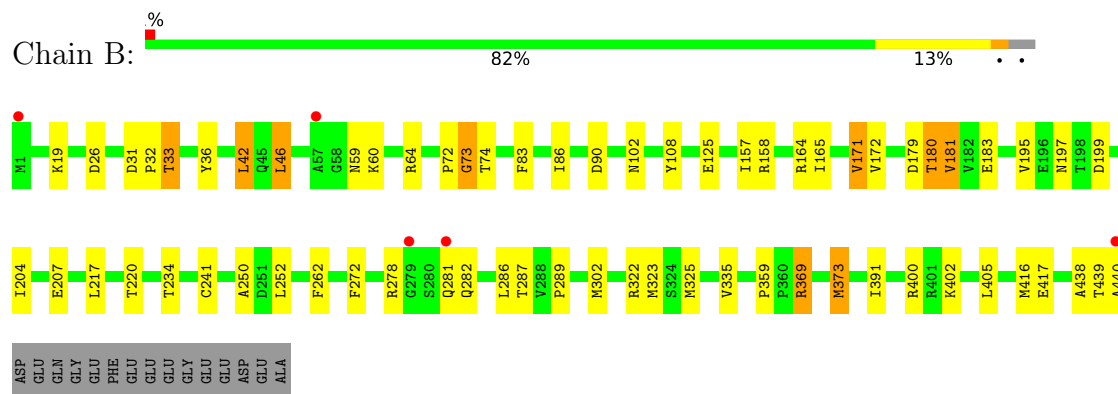
- Molecule 1: Tubulin alpha-1B chain



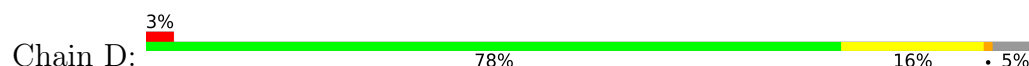
- Molecule 1: Tubulin alpha-1B chain

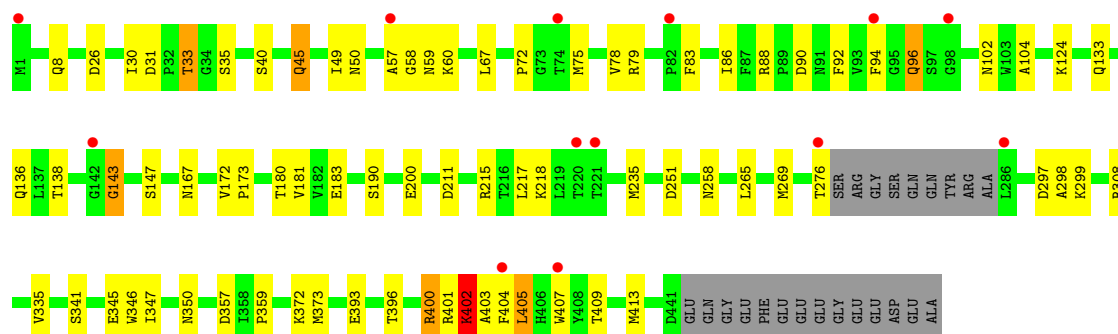


- Molecule 2: Tubulin beta chain

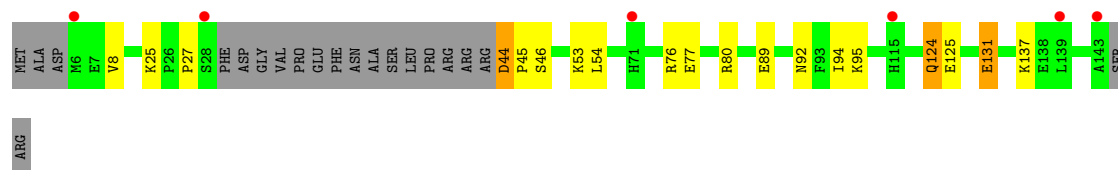
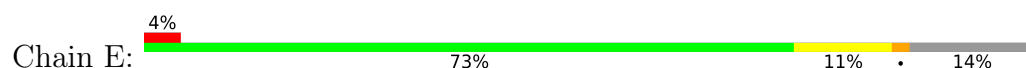


- Molecule 2: Tubulin beta chain

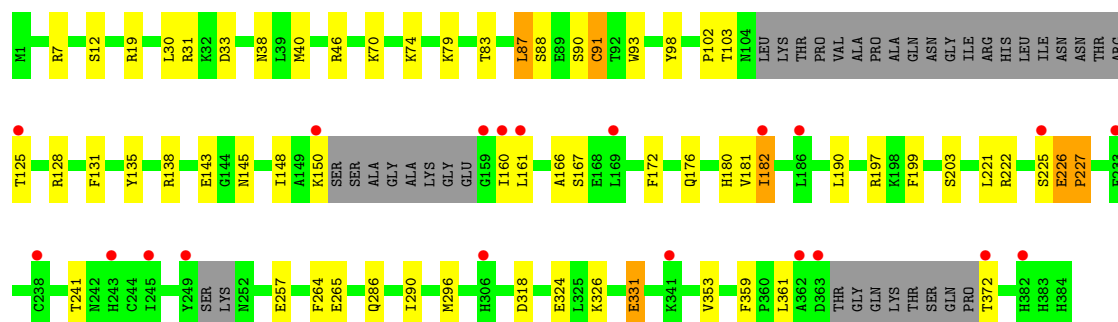
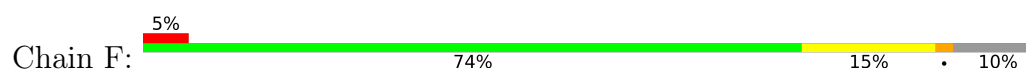




• Molecule 3: Stathmin-4



• 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	105.37Å 157.34Å 181.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.51 50.00 – 2.51	Depositor EDS
% Data completeness (in resolution range)	99.6 (50.00-2.51) 99.8 (50.00-2.51)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.42 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.183 , 0.239 0.191 , 0.242	Depositor DCC
R_{free} test set	5193 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	48.9	Xtriage
Anisotropy	0.063	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 31.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	17939	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.61% 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: MES, 4SL, GTP, CA, GDP, MG, GOL, 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	1.06	0/3514	1.08	5/4770 (0.1%)
1	C	1.16	2/3530 (0.1%)	1.11	13/4794 (0.3%)
2	B	1.14	8/3463 (0.2%)	1.10	9/4692 (0.2%)
2	D	0.99	3/3384 (0.1%)	1.08	12/4586 (0.3%)
3	E	1.07	0/1033	1.17	4/1371 (0.3%)
4	F	0.83	0/2916	0.95	1/3940 (0.0%)
All	All	1.05	13/17840 (0.1%)	1.08	44/24153 (0.2%)

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	262	PHE	CA-C	-6.40	1.47	1.52
2	D	265	LEU	CA-C	-6.31	1.46	1.53
2	B	171	VAL	C-O	-6.24	1.17	1.24
2	B	172	VAL	C-N	6.24	1.40	1.33
1	C	268	PRO	N-CA	-6.17	1.40	1.46
2	B	183	GLU	C-O	-6.02	1.18	1.24
2	D	172	VAL	C-N	5.87	1.40	1.33
2	D	173	PRO	N-CD	5.42	1.55	1.47
2	B	439	THR	CA-C	5.29	1.59	1.52
2	B	439	THR	N-CA	5.19	1.52	1.46
2	B	157	ILE	C-O	-5.17	1.18	1.24
2	B	359	PRO	C-N	5.16	1.40	1.33
1	C	328	VAL	CA-CB	-5.01	1.48	1.54

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	359	PRO	O-C-N	8.99	125.38	121.15
1	C	36	MET	CA-C-N	6.99	128.58	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	36	MET	C-N-CA	6.99	128.58	119.84
2	D	269	MET	CA-C-N	-6.74	113.71	120.31
2	D	269	MET	C-N-CA	-6.74	113.71	120.31
1	C	95	GLY	N-CA-C	-6.73	104.72	112.79
1	C	267	PHE	CA-C-N	-6.51	113.56	120.66
1	C	267	PHE	C-N-CA	-6.51	113.56	120.66
2	B	359	PRO	CA-C-N	-6.42	113.37	119.85
2	B	359	PRO	C-N-CA	-6.42	113.37	119.85
2	B	391	ILE	CB-CA-C	-6.37	103.82	111.97
2	B	172	VAL	CA-C-N	-6.23	114.20	120.31
2	B	172	VAL	C-N-CA	-6.23	114.20	120.31
1	C	302	MET	CB-CG-SD	-6.19	94.12	112.70
4	F	190	LEU	N-CA-C	-6.13	101.21	110.28
3	E	44	ASP	CA-C-N	5.97	126.32	119.93
3	E	44	ASP	C-N-CA	5.97	126.32	119.93
1	A	262	TYR	CA-C-N	5.90	127.21	119.84
1	A	262	TYR	C-N-CA	5.90	127.21	119.84
2	D	33	THR	N-CA-C	-5.79	105.04	111.36
1	A	4	CYS	CA-C-N	-5.73	116.08	123.19
1	A	4	CYS	C-N-CA	-5.73	116.08	123.19
2	D	373	MET	N-CA-C	5.68	118.45	108.75
3	E	45	PRO	N-CA-C	5.67	120.50	111.26
2	D	58	GLY	N-CA-C	-5.60	108.13	115.47
1	C	110	ILE	N-CA-C	-5.60	107.00	111.81
1	C	62	VAL	N-CA-C	5.52	113.91	107.89
2	D	359	PRO	CA-C-N	-5.50	112.97	119.84
2	D	359	PRO	C-N-CA	-5.50	112.97	119.84
1	C	381	THR	CB-CA-C	-5.45	98.60	109.33
2	D	88	ARG	CA-C-N	5.43	125.25	119.28
2	D	88	ARG	C-N-CA	5.43	125.25	119.28
2	B	195	VAL	CB-CA-C	-5.37	104.89	112.14
1	A	109	THR	N-CA-C	5.22	116.83	111.03
3	E	8	VAL	CB-CA-C	-5.21	103.95	111.34
2	B	179	ASP	CA-C-N	-5.19	113.68	120.95
2	B	179	ASP	C-N-CA	-5.19	113.68	120.95
2	B	335	VAL	CB-CA-C	-5.15	105.38	111.97
1	C	18	ASN	CB-CA-C	-5.12	102.62	110.81
1	C	259	LEU	N-CA-C	5.10	119.21	112.89
2	D	172	VAL	CA-C-N	-5.06	114.13	120.51
2	D	172	VAL	C-N-CA	-5.06	114.13	120.51
1	C	353	VAL	N-CA-C	5.05	115.39	108.12
1	C	9	VAL	N-CA-C	5.03	115.15	108.11

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3436	0	3344	18	0
1	C	3452	0	3359	29	0
2	B	3387	0	3266	37	0
2	D	3311	0	3192	35	0
3	E	1024	0	1035	9	0
4	F	2849	0	2796	28	0
5	A	32	0	12	1	0
5	C	32	0	12	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	C	2	0	0	0	0
8	A	24	0	32	1	0
8	B	6	0	8	0	0
8	C	12	0	16	2	0
8	F	6	0	8	1	0
9	B	28	0	12	2	0
9	D	28	0	12	3	0
10	B	24	0	26	2	0
11	B	34	0	0	0	0
12	F	31	0	14	2	0
13	A	51	0	0	0	0
13	B	47	0	0	4	0
13	C	86	0	0	2	0
13	D	13	0	0	2	0
13	E	2	0	0	0	0
13	F	16	0	0	0	0
All	All	17939	0	17144	153	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 4.

All (153) 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:40:SER:O	2:D:45:GLN:HG3	1.60	1.02
2:D:33:THR:OG1	2:D:60:LYS:NZ	2.05	0.90
2:D:40:SER:O	2:D:45:GLN:CG	2.20	0.89
1:C:336:LYS:HE2	13:C:676:HOH:O	1.71	0.88
2:B:26:ASP:OD1	2:B:369:ARG:NH1	2.09	0.85
2:D:33:THR:CB	2:D:60:LYS:NZ	2.40	0.85
2:B:36:TYR:CE1	2:B:46:LEU:HD21	2.12	0.84
9:B:501:GDP:O3B	13:B:601:HOH:O	1.96	0.82
3:E:124:GLN:HE21	3:E:124:GLN:HA	1.44	0.82
9:D:501:GDP:O3B	13:D:601:HOH:O	1.99	0.80
2:D:33:THR:HB	2:D:60:LYS:NZ	1.98	0.79
4:F:197:ARG:NH1	4:F:257:GLU:OE1	2.16	0.77
2:B:36:TYR:CE1	2:B:46:LEU:CD2	2.68	0.75
2:D:33:THR:HB	2:D:60:LYS:HZ2	1.51	0.75
2:B:26:ASP:CG	2:B:369:ARG:NH1	2.46	0.74
4:F:88:SER:HG	4:F:90:SER:HG	1.28	0.70
9:D:501:GDP:O3B	13:D:602:HOH:O	2.12	0.67
2:D:401:ARG:O	2:D:403:ALA:N	2.28	0.65
2:B:26:ASP:CG	2:B:369:ARG:HH11	2.05	0.64
3:E:124:GLN:HE21	3:E:124:GLN:CA	2.10	0.64
2:B:72:PRO:O	2:B:73:GLY:C	2.41	0.64
1:A:209:ILE:HG22	1:A:227:LEU:HD22	1.80	0.63
2:B:83:PHE:O	2:B:86:ILE:HG22	1.99	0.63
2:B:36:TYR:CD1	2:B:46:LEU:HD21	2.33	0.63
2:D:75:MET:HG3	2:D:94:PHE:HB3	1.81	0.63
2:B:199:ASP:OD2	10:B:504:MES:H52	1.99	0.63
2:B:36:TYR:CZ	2:B:46:LEU:CD2	2.83	0.62
2:B:272[B]:PHE:CD2	2:B:302:MET:HE3	2.34	0.62
2:D:136:GLN:HA	2:D:167:ASN:O	2.00	0.62
2:B:36:TYR:CZ	2:B:46:LEU:HD21	2.35	0.61
2:B:26:ASP:OD2	2:B:369:ARG:NH1	2.33	0.61
2:D:297:ASP:OD1	2:D:298:ALA:N	2.34	0.61
3:E:131:GLU:HA	3:E:131:GLU:OE2	2.01	0.60
1:C:204:VAL:HG22	1:C:302:MET:CE	2.31	0.59
4:F:7:ARG:HD3	4:F:40:MET:HE3	1.83	0.59
2:B:323:MET:HB3	2:B:373:MET:HE1	1.85	0.58
1:C:1:MET:O	1:C:2:ARG:HB2	2.04	0.58
1:C:165:SER:HA	1:C:199:ASP:OD2	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:209:ILE:HG22	1:C:227:LEU:HD22	1.88	0.56
2:B:234:THR:HG1	2:B:272[B]:PHE:HD2	1.55	0.54
2:D:31:ASP:OD1	2:D:31:ASP:C	2.49	0.54
2:B:33:THR:O	2:B:60:LYS:HE3	2.07	0.54
4:F:148:ILE:HD11	4:F:160:ILE:HD11	1.90	0.54
2:B:164:ARG:HD2	13:B:641:HOH:O	2.06	0.54
4:F:87:LEU:O	4:F:88:SER:OG	2.26	0.54
9:B:501:GDP:O1A	13:B:602:HOH:O	2.19	0.54
4:F:38:ASN:HB3	4:F:359:PHE:CZ	2.43	0.53
4:F:318:ASP:OD2	12:F:401:ACP:O3G	2.26	0.53
1:C:339:ARG:O	1:C:339:ARG:HG3	2.08	0.53
1:C:346:TRP:CZ3	1:C:347[A]:CYS:SG	3.01	0.53
2:D:40:SER:O	2:D:45:GLN:HG2	2.07	0.53
4:F:135:TYR:CE2	4:F:166:ALA:HB2	2.45	0.52
2:B:241:CYS:O	2:B:250:ALA:HA	2.10	0.52
1:C:204:VAL:HG22	1:C:302:MET:HE1	1.91	0.52
1:A:147:SER:HB2	1:A:190:THR:HB	1.92	0.51
1:C:194:THR:O	1:C:194:THR:HG22	2.10	0.51
4:F:331:GLU:OE2	12:F:401:ACP:O1B	2.28	0.51
1:A:413:MET:HE2	1:A:418:PHE:CE2	2.46	0.50
1:C:71:GLU:HB2	1:C:98:ASP:HB3	1.94	0.50
3:E:124:GLN:CA	3:E:124:GLN:NE2	2.73	0.50
4:F:199:PHE:CD2	4:F:221:LEU:HD23	2.45	0.50
4:F:264:PHE:O	4:F:265:GLU:C	2.53	0.50
4:F:296:MET:HE2	8:F:402:GOL:H2	1.94	0.50
1:C:271:THR:HG21	1:C:295:CYS:O	2.11	0.50
2:D:33:THR:CB	2:D:60:LYS:HZ1	2.22	0.49
2:D:83:PHE:O	2:D:86:ILE:HG22	2.12	0.49
1:A:183:GLU:N	1:A:184:PRO:CD	2.74	0.49
2:B:440:ALA:HB3	4:F:31:ARG:HH22	1.78	0.49
1:C:210:TYR:CZ	1:C:222:PRO:HD2	2.47	0.49
2:D:33:THR:CB	2:D:60:LYS:HZ2	2.15	0.48
4:F:128:ARG:O	4:F:131:PHE:HB3	2.13	0.48
1:C:304:LYS:HE3	8:C:505:GOL:H31	1.96	0.48
1:C:162:GLY:HA2	3:E:94:ILE:HD11	1.96	0.48
4:F:222:ARG:O	4:F:241:THR:HB	2.13	0.48
2:D:67:LEU:N	2:D:67:LEU:HD12	2.29	0.48
4:F:88:SER:OG	4:F:90:SER:OG	2.11	0.47
1:C:194:THR:O	1:C:194:THR:CG2	2.62	0.47
2:D:102:ASN:OD1	2:D:102:ASN:C	2.58	0.47
2:D:143:GLY:HA3	9:D:501:GDP:O3A	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:211:ASP:O	2:D:215:ARG:HB2	2.14	0.47
4:F:98:TYR:HB2	4:F:182:ILE:HG22	1.97	0.47
1:A:241:SER:HB2	1:A:248:LEU:O	2.15	0.47
4:F:19:ARG:HB3	4:F:19:ARG:NH1	2.29	0.47
1:C:10:GLY:O	1:C:11:GLN:C	2.58	0.47
2:B:171:VAL:HA	2:B:204:ILE:O	2.14	0.47
1:A:209:ILE:HD11	1:A:302:MET:SD	2.55	0.46
1:A:403:ALA:O	1:A:404:PHE:HB2	2.15	0.46
2:B:181:VAL:HG23	1:C:348:PRO:CG	2.45	0.46
2:B:36:TYR:CE1	2:B:46:LEU:HD22	2.51	0.46
2:B:19:LYS:HB2	2:B:19:LYS:HE2	1.70	0.46
1:C:204:VAL:HG13	1:C:302:MET:HE2	1.96	0.46
3:E:131:GLU:OE2	3:E:131:GLU:CA	2.63	0.46
2:D:393:GLU:O	2:D:396:THR:HG22	2.16	0.46
1:C:102:ASN:C	1:C:102:ASN:OD1	2.58	0.46
1:C:304:LYS:HG3	8:C:505:GOL:H12	1.97	0.46
1:C:93:ILE:HD11	1:C:121:ARG:HG3	1.97	0.46
4:F:172:PHE:O	4:F:176:GLN:HG2	2.17	0.45
2:B:102:ASN:OD1	2:B:102:ASN:C	2.60	0.45
1:C:344:VAL:HG21	1:C:346:TRP:CE2	2.51	0.45
1:A:143:GLY:HA3	5:A:501:GTP:O3A	2.17	0.45
1:A:265:ILE:HG23	1:A:432:TYR:CE1	2.52	0.45
1:C:180:ALA:HA	2:D:258:ASN:OD1	2.16	0.45
1:A:187:SER:HB3	1:A:391:LEU:HD21	1.98	0.45
2:D:57:ALA:C	2:D:59:ASN:H	2.25	0.45
2:D:72:PRO:HG3	2:D:96:GLN:HA	1.99	0.45
1:C:341:ILE:HD11	1:C:343:PHE:CE1	2.52	0.45
2:D:75:MET:HE3	2:D:92:PHE:HD2	1.81	0.45
2:B:165:ILE:HG21	2:B:252:LEU:HB3	1.99	0.45
1:A:250:VAL:HG22	1:A:254:GLU:OE1	2.17	0.44
3:E:137:LYS:O	3:E:137:LYS:HG2	2.16	0.44
1:A:433:GLU:OE2	4:F:46:ARG:NH1	2.49	0.44
2:D:347:ILE:HG22	2:D:350:ASN:HB3	1.99	0.44
1:A:71:GLU:HB3	1:A:98:ASP:HB3	1.99	0.44
2:B:180:THR:HB	13:C:619:HOH:O	2.18	0.44
2:D:217:LEU:C	2:D:218:LYS:HG2	2.43	0.43
2:B:108:TYR:OH	2:B:417:GLU:OE2	2.22	0.43
2:B:286:LEU:HD12	2:B:286:LEU:N	2.33	0.43
2:B:31:ASP:OD1	2:B:31:ASP:C	2.61	0.43
2:D:67:LEU:CD2	2:D:78:VAL:HG11	2.48	0.43
1:C:11:GLN:HG3	1:C:74:VAL:HG21	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:138:THR:HG21	2:D:235:MET:HE1	2.01	0.43
4:F:286:GLN:O	4:F:290:ILE:HG13	2.17	0.43
2:D:251:ASP:OD1	2:D:251:ASP:C	2.62	0.43
4:F:74:LYS:HB3	4:F:181:VAL:HG21	2.00	0.43
1:A:275:VAL:O	8:A:505:GOL:H12	2.18	0.43
2:B:42:LEU:HD12	2:B:42:LEU:HA	1.81	0.43
4:F:197:ARG:NH1	4:F:257:GLU:CD	2.77	0.42
2:B:369:ARG:CZ	2:B:369:ARG:HB2	2.48	0.42
2:B:74:THR:HB	13:B:607:HOH:O	2.20	0.42
4:F:79:LYS:O	4:F:83:THR:OG1	2.32	0.42
2:B:287:THR:HB	2:B:289:PRO:HD2	2.01	0.42
4:F:150:LYS:N	4:F:181:VAL:O	2.50	0.42
2:B:64:ARG:HG3	2:B:125:GLU:OE1	2.20	0.42
1:A:112:LYS:HG3	3:E:54:LEU:HD13	2.02	0.42
1:C:55:GLU:HA	1:C:60:LYS:O	2.19	0.42
1:C:1:MET:O	1:C:2:ARG:CB	2.67	0.42
2:B:31:ASP:HB2	2:B:32:PRO:CD	2.51	0.41
4:F:138:ARG:HB2	4:F:145:ASN:ND2	2.35	0.41
1:C:401:LYS:HG3	2:D:346:TRP:CE3	2.56	0.41
1:A:3:GLU:HG2	1:A:64:ARG:CZ	2.50	0.41
4:F:226:GLU:O	4:F:227:PRO:C	2.63	0.41
1:A:346:TRP:CD1	1:A:346:TRP:H	2.38	0.41
2:B:158:ARG:NH1	2:B:197:ASN:OD1	2.52	0.41
2:D:400:ARG:HG3	2:D:401:ARG:N	2.36	0.41
2:D:104:ALA:HB2	2:D:413:MET:SD	2.61	0.40
2:D:147:SER:HB2	2:D:190:SER:OG	2.21	0.40
1:C:54:SER:O	1:C:61:HIS:HA	2.21	0.40
2:D:402:LYS:O	2:D:405:LEU:HB2	2.20	0.40
4:F:91:CYS:SG	4:F:93:TRP:CE2	3.15	0.40
1:A:67:PHE:CD1	1:A:67:PHE:N	2.90	0.40
3:E:76:ARG:O	3:E:80:ARG:HG3	2.21	0.40
2:D:180:THR:HB	2:D:183:GLU:HG3	2.04	0.40
2:B:199:ASP:OD1	10:B:504:MES:H32	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	438/451 (97%)	422 (96%)	16 (4%)	0	100	100
1	C	440/451 (98%)	431 (98%)	8 (2%)	1 (0%)	43	63
2	B	429/445 (96%)	418 (97%)	9 (2%)	2 (0%)	24	43
2	D	418/445 (94%)	396 (95%)	19 (4%)	3 (1%)	18	34
3	E	120/143 (84%)	114 (95%)	5 (4%)	1 (1%)	16	31
4	F	336/384 (88%)	304 (90%)	29 (9%)	3 (1%)	14	27
All	All	2181/2319 (94%)	2085 (96%)	86 (4%)	10 (0%)	24	43

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	73	GLY
2	D	402	LYS
3	E	27	PRO
1	C	2	ARG
2	D	404	PHE
4	F	102	PRO
4	F	91	CYS
4	F	227	PRO
2	B	438	ALA
2	D	143	GLY

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	371/379 (98%)	354 (95%)	17 (5%)	24	48
1	C	373/379 (98%)	355 (95%)	18 (5%)	23	46
2	B	370/381 (97%)	349 (94%)	21 (6%)	18	39
2	D	363/381 (95%)	336 (93%)	27 (7%)	13	27
3	E	111/127 (87%)	100 (90%)	11 (10%)	7	16
4	F	312/342 (91%)	291 (93%)	21 (7%)	15	31
All	All	1900/1989 (96%)	1785 (94%)	115 (6%)	17	35

All (115) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	ASN
1	A	41	THR
1	A	62	VAL
1	A	66	VAL
1	A	71	GLU
1	A	82	THR
1	A	112	LYS
1	A	159	VAL
1	A	163	LYS
1	A	181	VAL
1	A	211	ASP
1	A	219	ILE
1	A	232	SER
1	A	334	THR
1	A	338	LYS
1	A	381	THR
1	A	437	VAL
2	B	33	THR
2	B	42	LEU
2	B	46	LEU
2	B	59	ASN
2	B	90	ASP
2	B	180	THR
2	B	181	VAL
2	B	207	GLU
2	B	217	LEU
2	B	220	THR
2	B	278	ARG
2	B	281	GLN
2	B	282	GLN

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Mol	Chain	Res	Type
2	B	322	ARG
2	B	325	MET
2	B	369	ARG
2	B	373	MET
2	B	400	ARG
2	B	402	LYS
2	B	405	LEU
2	B	416	MET
1	C	2	ARG
1	C	48	SER
1	C	71	GLU
1	C	89	PRO
1	C	120	ASP
1	C	164	LYS
1	C	315	CYS
1	C	318	LEU
1	C	325	PRO
1	C	337	THR
1	C	338	LYS
1	C	340	SER
1	C	341	ILE
1	C	342	GLN
1	C	361	THR
1	C	368	LEU
1	C	381	THR
1	C	440	VAL
2	D	8	GLN
2	D	26	ASP
2	D	30	ILE
2	D	35	SER
2	D	45	GLN
2	D	49	ILE
2	D	50	ASN
2	D	79	ARG
2	D	90	ASP
2	D	96	GLN
2	D	124	LYS
2	D	133	GLN
2	D	181	VAL
2	D	200	GLU
2	D	276	THR
2	D	299	LYS

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Mol	Chain	Res	Type
2	D	308	ARG
2	D	335	VAL
2	D	341	SER
2	D	345	GLU
2	D	357	ASP
2	D	372	LYS
2	D	400	ARG
2	D	402	LYS
2	D	405	LEU
2	D	407	TRP
2	D	409	THR
3	E	25	LYS
3	E	44	ASP
3	E	46	SER
3	E	53	LYS
3	E	77	GLU
3	E	89	GLU
3	E	92	ASN
3	E	95	LYS
3	E	124	GLN
3	E	125	GLU
3	E	131	GLU
4	F	12	SER
4	F	30	LEU
4	F	33	ASP
4	F	70	LYS
4	F	87	LEU
4	F	103	THR
4	F	125	THR
4	F	143	GLU
4	F	161	LEU
4	F	167	SER
4	F	180	HIS
4	F	182	ILE
4	F	203	SER
4	F	225	SER
4	F	226	GLU
4	F	324	GLU
4	F	326	LYS
4	F	331	GLU
4	F	353	VAL
4	F	361	LEU

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Mol	Chain	Res	Type
4	F	372	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	128	GLN
1	A	309	HIS
2	B	8	GLN
2	B	96	GLN
2	B	101	ASN
2	B	136	GLN
2	B	334	ASN
2	B	434	GLN
1	C	11	GLN
1	C	256	GLN
2	D	247	GLN
3	E	12	ASN
3	E	18	GLN
3	E	78	HIS
3	E	124	GLN
3	E	136	ASN
4	F	136	ASN
4	F	183	GLN
4	F	260	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 24 ligands modelled in this entry, 8 are monoatomic - leaving 16 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
5	GTP	A	501	6	33,34,34	1.40	5 (15%)	50,54,54	1.69	11 (22%)
8	GOL	C	505	-	5,5,5	0.81	0	5,5,5	0.87	0
8	GOL	B	506	-	5,5,5	0.50	0	5,5,5	0.40	0
10	MES	B	505	-	12,12,12	2.35	1 (8%)	15,16,16	1.55	3 (20%)
8	GOL	A	507	-	5,5,5	0.77	0	5,5,5	1.04	0
8	GOL	F	402	-	5,5,5	0.82	0	5,5,5	0.48	0
8	GOL	A	504	-	5,5,5	0.40	0	5,5,5	0.09	0
10	MES	B	504	-	12,12,12	2.05	2 (16%)	15,16,16	5.68	10 (66%)
12	ACP	F	401	-	31,33,33	2.27	11 (35%)	47,52,52	1.66	8 (17%)
9	GDP	B	501	6	29,30,30	1.49	6 (20%)	45,47,47	1.80	10 (22%)
11	4SL	B	507	-	31,34,34	3.35	6 (19%)	43,50,50	1.43	8 (18%)
8	GOL	A	506	-	5,5,5	0.58	0	5,5,5	0.22	0
9	GDP	D	501	6	29,30,30	1.35	5 (17%)	45,47,47	1.94	13 (28%)
5	GTP	C	502	6	33,34,34	1.27	5 (15%)	50,54,54	1.76	12 (24%)
8	GOL	A	505	-	5,5,5	0.42	0	5,5,5	1.07	0
8	GOL	C	506	-	5,5,5	0.39	0	5,5,5	0.54	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GTP	A	501	6	-	3/22/38/38	0/3/3/3
8	GOL	C	505	-	-	2/4/4/4	-
8	GOL	B	506	-	-	2/4/4/4	-
10	MES	B	505	-	-	4/6/14/14	0/1/1/1
8	GOL	A	507	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	GOL	F	402	-	-	1/4/4/4	-
8	GOL	A	504	-	-	2/4/4/4	-
10	MES	B	504	-	-	4/6/14/14	0/1/1/1
12	ACP	F	401	-	-	3/19/38/38	0/3/3/3
9	GDP	B	501	6	-	4/16/32/32	0/3/3/3
11	4SL	B	507	-	-	7/52/52/52	0/1/1/1
8	GOL	A	506	-	-	2/4/4/4	-
9	GDP	D	501	6	-	4/16/32/32	0/3/3/3
5	GTP	C	502	6	-	7/22/38/38	0/3/3/3
8	GOL	A	505	-	-	0/4/4/4	-
8	GOL	C	506	-	-	2/4/4/4	-

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	B	507	4SL	C26-C27	14.54	1.52	1.33
11	B	507	4SL	C7-C5	-8.43	1.39	1.54
10	B	505	MES	C8-S	-7.46	1.67	1.77
12	F	401	ACP	PG-O1G	5.99	1.62	1.50
10	B	504	MES	C8-S	-5.77	1.69	1.77
12	F	401	ACP	C5-C4	5.41	1.48	1.39
12	F	401	ACP	PB-O3A	4.94	1.63	1.58
11	B	507	4SL	C29-C27	-4.69	1.38	1.49
9	B	501	GDP	PA-O3A	4.45	1.64	1.59
9	D	501	GDP	PA-O3A	4.06	1.63	1.59
12	F	401	ACP	PA-O3A	3.69	1.63	1.59
5	A	501	GTP	C6-N1	-3.26	1.32	1.38
5	A	501	GTP	PA-O3A	3.16	1.62	1.59
12	F	401	ACP	PG-O3G	3.15	1.62	1.55
10	B	504	MES	O2S-S	3.06	1.53	1.45
5	C	502	GTP	C6-N1	-3.05	1.33	1.38
5	C	502	GTP	PA-O3A	3.03	1.62	1.59
11	B	507	4SL	C11-C12	2.90	1.58	1.53
11	B	507	4SL	C32-C14	2.86	1.57	1.54
9	D	501	GDP	C5-N7	-2.83	1.33	1.39
12	F	401	ACP	C8-N7	2.74	1.36	1.31
12	F	401	ACP	C5-C6	2.61	1.48	1.41
9	B	501	GDP	C6-N1	-2.58	1.34	1.38
9	D	501	GDP	C5-C4	2.58	1.45	1.38
12	F	401	ACP	PG-O2G	-2.57	1.49	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	501	GDP	C5-C4	2.51	1.45	1.38
5	A	501	GTP	C5-C4	2.50	1.45	1.38
5	A	501	GTP	C5-N7	-2.41	1.34	1.39
9	B	501	GDP	C5-N7	-2.35	1.34	1.39
9	B	501	GDP	C2-N1	-2.34	1.31	1.37
12	F	401	ACP	PB-O2B	2.34	1.62	1.56
12	F	401	ACP	C5-N7	-2.33	1.34	1.39
11	B	507	4SL	O30-C29	2.27	1.28	1.22
5	C	502	GTP	O6-C6	2.22	1.27	1.23
12	F	401	ACP	C4-N9	-2.17	1.33	1.37
9	D	501	GDP	C8-N7	2.13	1.38	1.32
5	A	501	GTP	C2-N1	-2.12	1.32	1.37
5	C	502	GTP	C4-N9	-2.11	1.32	1.38
5	C	502	GTP	C5-C4	2.08	1.44	1.38
9	B	501	GDP	C4-N9	-2.03	1.32	1.38
9	D	501	GDP	C6-N1	-2.02	1.35	1.38

All (75) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	504	MES	O3S-S-O1S	-12.51	80.09	111.40
10	B	504	MES	O3S-S-O2S	-11.17	83.45	111.40
10	B	504	MES	O2S-S-C8	7.86	118.61	106.73
10	B	504	MES	O1S-S-C8	7.09	117.45	106.73
10	B	504	MES	O3S-S-C8	-6.38	93.52	106.00
9	D	501	GDP	C5-C4-N3	-5.65	119.40	128.39
12	F	401	ACP	C5-C4-N3	-5.41	119.27	126.72
9	B	501	GDP	C5-C4-N3	-5.21	120.10	128.39
5	A	501	GTP	C5-C4-N3	-5.08	120.31	128.39
9	B	501	GDP	C2-N3-C4	4.87	120.69	112.30
9	D	501	GDP	C2-N3-C4	4.73	120.44	112.30
5	C	502	GTP	C5-C4-N3	-4.72	120.87	128.39
12	F	401	ACP	N3-C4-N9	4.35	134.56	127.17
5	C	502	GTP	C2-N3-C4	4.33	119.77	112.30
5	A	501	GTP	N9-C4-N3	4.20	134.36	125.95
9	D	501	GDP	N9-C4-N3	4.00	133.95	125.95
9	B	501	GDP	N9-C4-N3	3.87	133.69	125.95
5	C	502	GTP	C6-C5-N7	3.78	137.16	130.29
10	B	504	MES	C6-C5-N4	3.71	115.75	110.12
11	B	507	4SL	O30-C29-C27	-3.54	112.96	122.09
5	C	502	GTP	O3B-PB-O1B	3.52	121.30	110.70
9	D	501	GDP	C6-C5-N7	3.50	136.67	130.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	501	GTP	C2-N3-C4	3.47	118.27	112.30
12	F	401	ACP	C2-N3-C4	3.40	120.13	111.83
12	F	401	ACP	N3-C2-N1	-3.37	123.48	128.58
9	B	501	GDP	C6-C5-N7	3.37	136.42	130.29
10	B	505	MES	O1S-S-C8	3.32	111.75	106.73
10	B	504	MES	C2-C3-N4	3.32	115.16	110.12
5	A	501	GTP	C6-C5-N7	3.24	136.18	130.29
9	B	501	GDP	O6-C6-C5	-3.10	118.34	126.53
5	C	502	GTP	C4-C5-N7	-2.99	105.94	110.67
5	C	502	GTP	O2A-PA-O3A	2.93	115.20	107.27
10	B	505	MES	C2-C3-N4	-2.87	105.77	110.12
12	F	401	ACP	C4-C5-N7	-2.86	107.31	110.58
10	B	504	MES	C5-N4-C3	2.86	115.00	108.84
9	D	501	GDP	O3B-PB-O1B	2.85	121.93	110.83
5	C	502	GTP	N9-C4-N3	2.84	131.63	125.95
12	F	401	ACP	O2G-PG-C3B	2.83	113.25	106.40
5	A	501	GTP	O6-C6-C5	-2.76	119.26	126.53
9	B	501	GDP	O3B-PB-O2B	2.75	118.13	107.80
10	B	504	MES	C6-O1-C2	2.72	118.68	109.88
11	B	507	4SL	C33-C32-C14	2.70	114.02	110.50
5	C	502	GTP	O3A-PB-O1B	-2.68	102.63	110.70
5	A	501	GTP	N9-C8-N7	-2.68	108.44	113.40
9	B	501	GDP	C5-C6-N1	2.67	120.06	113.25
9	B	501	GDP	C6-C5-C4	-2.63	114.87	118.83
11	B	507	4SL	C34-C32-C14	2.59	113.87	110.50
11	B	507	4SL	C16-C7-C15	2.57	110.56	107.43
5	A	501	GTP	C8-N9-C4	2.57	110.83	106.03
10	B	504	MES	O2S-S-O1S	2.56	122.16	113.82
9	D	501	GDP	C4-C5-N7	-2.55	106.63	110.67
11	B	507	4SL	C32-C14-N13	-2.47	108.23	112.89
5	C	502	GTP	O3'-C3'-C4'	-2.45	104.03	111.08
12	F	401	ACP	C4-N9-C8	2.44	108.30	105.74
5	C	502	GTP	N9-C8-N7	-2.43	108.89	113.40
12	F	401	ACP	C2-N1-C6	2.43	122.72	118.73
9	D	501	GDP	C8-N7-C5	2.41	108.56	104.26
11	B	507	4SL	C28-C27-C29	-2.39	112.05	115.69
9	D	501	GDP	O6-C6-C5	-2.37	120.29	126.53
9	D	501	GDP	O2A-PA-O3A	2.36	113.66	107.27
5	A	501	GTP	C1'-N9-C4	-2.36	119.51	126.49
9	D	501	GDP	N9-C8-N7	-2.36	109.03	113.40
9	D	501	GDP	C5-C6-N1	2.33	119.20	113.25
5	C	502	GTP	O2'-C2'-C3'	2.30	119.20	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	D	501	GDP	C2'-C3'-C4'	2.28	107.01	102.61
5	C	502	GTP	C8-N7-C5	2.24	108.26	104.26
11	B	507	4SL	C26-C27-C29	2.24	122.40	119.35
5	A	501	GTP	C5-C6-N1	2.21	118.87	113.25
9	D	501	GDP	C2-N1-C6	-2.18	121.16	125.11
5	A	501	GTP	O3G-PG-O3B	-2.18	97.32	104.64
11	B	507	4SL	C4-C5-C7	-2.16	117.62	121.38
10	B	505	MES	C7-N4-C3	-2.09	105.66	111.24
9	B	501	GDP	O3A-PA-O1A	2.04	116.85	110.70
5	A	501	GTP	C8-N7-C5	2.02	107.86	104.26
9	B	501	GDP	C2-N1-C6	-2.01	121.46	125.11

There are no chirality outliers.

All (49) 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	502	GTP	C5'-O5'-PA-O3A
5	C	502	GTP	C5'-O5'-PA-O1A
5	C	502	GTP	C5'-O5'-PA-O2A
8	A	504	GOL	O1-C1-C2-C3
9	B	501	GDP	C5'-O5'-PA-O3A
9	B	501	GDP	C5'-O5'-PA-O1A
9	D	501	GDP	C5'-O5'-PA-O3A
9	D	501	GDP	C5'-O5'-PA-O1A
10	B	504	MES	C8-C7-N4-C5
10	B	504	MES	C7-C8-S-O1S
10	B	505	MES	C7-C8-S-O2S
11	B	507	4SL	C26-C14-C32-C34
11	B	507	4SL	C26-C14-C32-C33
11	B	507	4SL	N13-C14-C32-C34
11	B	507	4SL	C26-C14-N13-C12
11	B	507	4SL	C26-C14-N13-C25
12	F	401	ACP	PG-C3B-PB-O1B
12	F	401	ACP	PG-C3B-PB-O2B
12	F	401	ACP	PG-C3B-PB-O3A
8	A	504	GOL	O1-C1-C2-O2
10	B	505	MES	C7-C8-S-O3S
8	A	506	GOL	O1-C1-C2-C3
8	A	507	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
8	B	506	GOL	O1-C1-C2-C3
8	C	505	GOL	O1-C1-C2-C3
8	C	506	GOL	C1-C2-C3-O3
8	A	506	GOL	O1-C1-C2-O2
10	B	504	MES	N4-C7-C8-S
8	B	506	GOL	O1-C1-C2-O2
10	B	505	MES	C8-C7-N4-C3
8	F	402	GOL	O2-C2-C3-O3
10	B	504	MES	C7-C8-S-O2S
9	D	501	GDP	C3'-C4'-C5'-O5'
8	C	505	GOL	O1-C1-C2-O2
11	B	507	4SL	N13-C14-C32-C33
9	B	501	GDP	C5'-O5'-PA-O2A
9	D	501	GDP	C5'-O5'-PA-O2A
8	A	507	GOL	O1-C1-C2-O2
8	C	506	GOL	O2-C2-C3-O3
5	C	502	GTP	PB-O3B-PG-O1G
10	B	505	MES	C8-C7-N4-C5
5	C	502	GTP	PB-O3B-PG-O2G
5	C	502	GTP	PB-O3B-PG-O3G
11	B	507	4SL	C32-C14-N13-C25
9	B	501	GDP	PB-O3A-PA-O1A
5	C	502	GTP	PB-O3A-PA-O1A

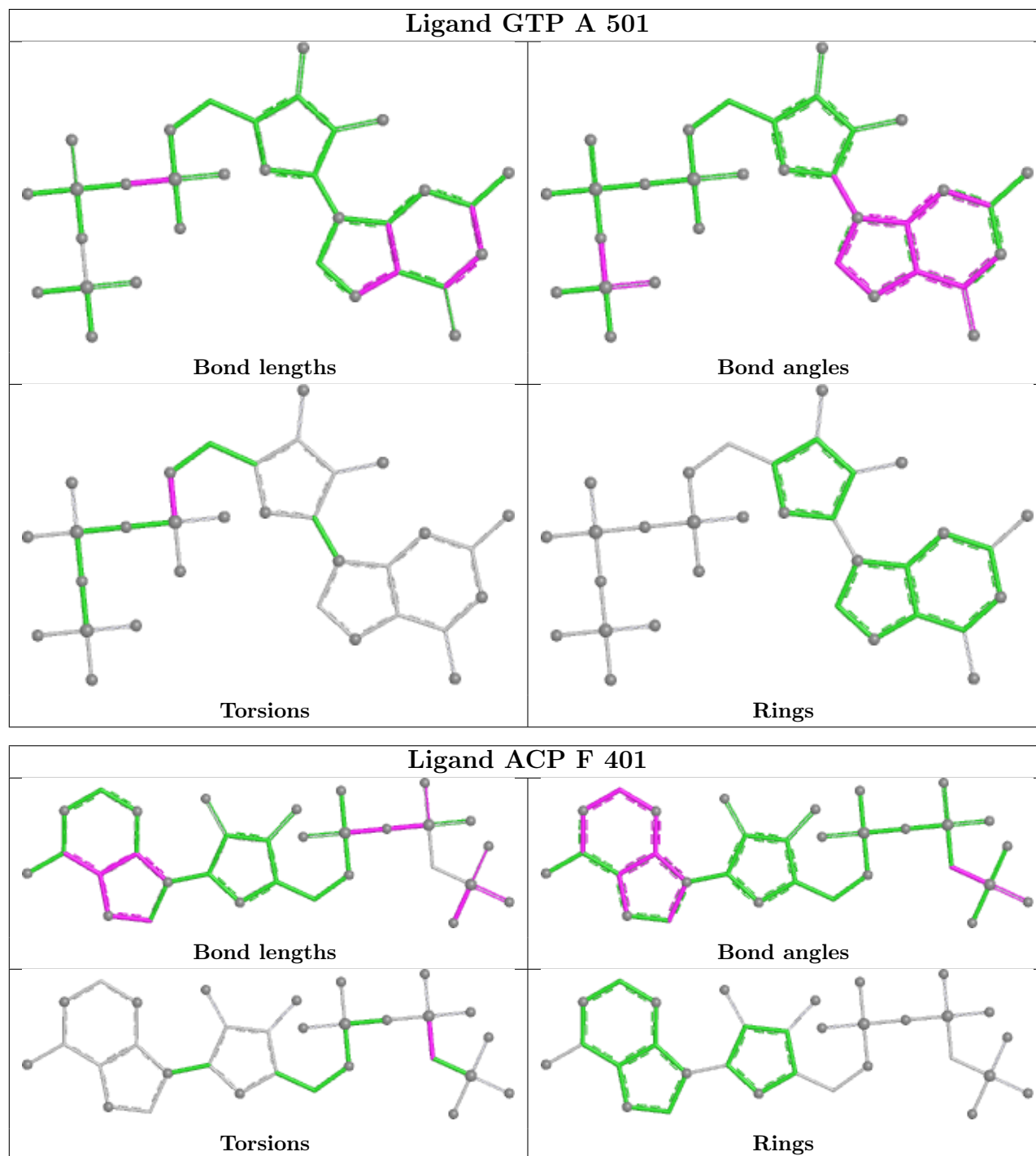
There are no ring outliers.

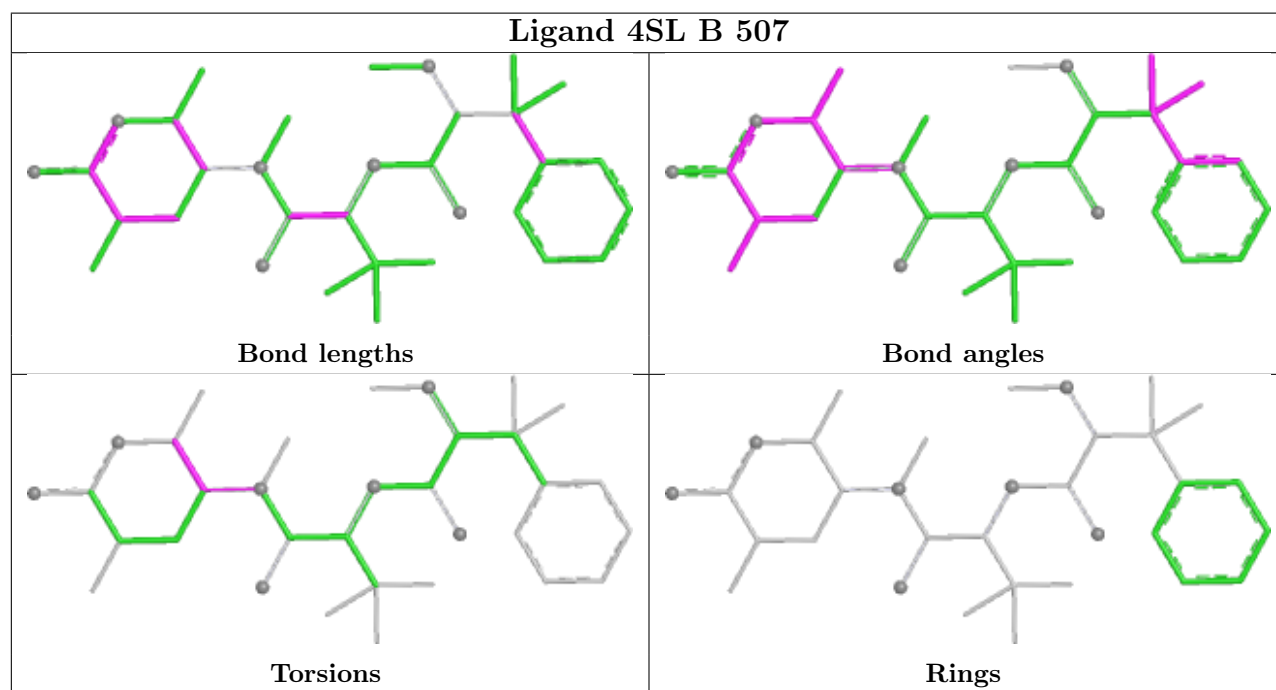
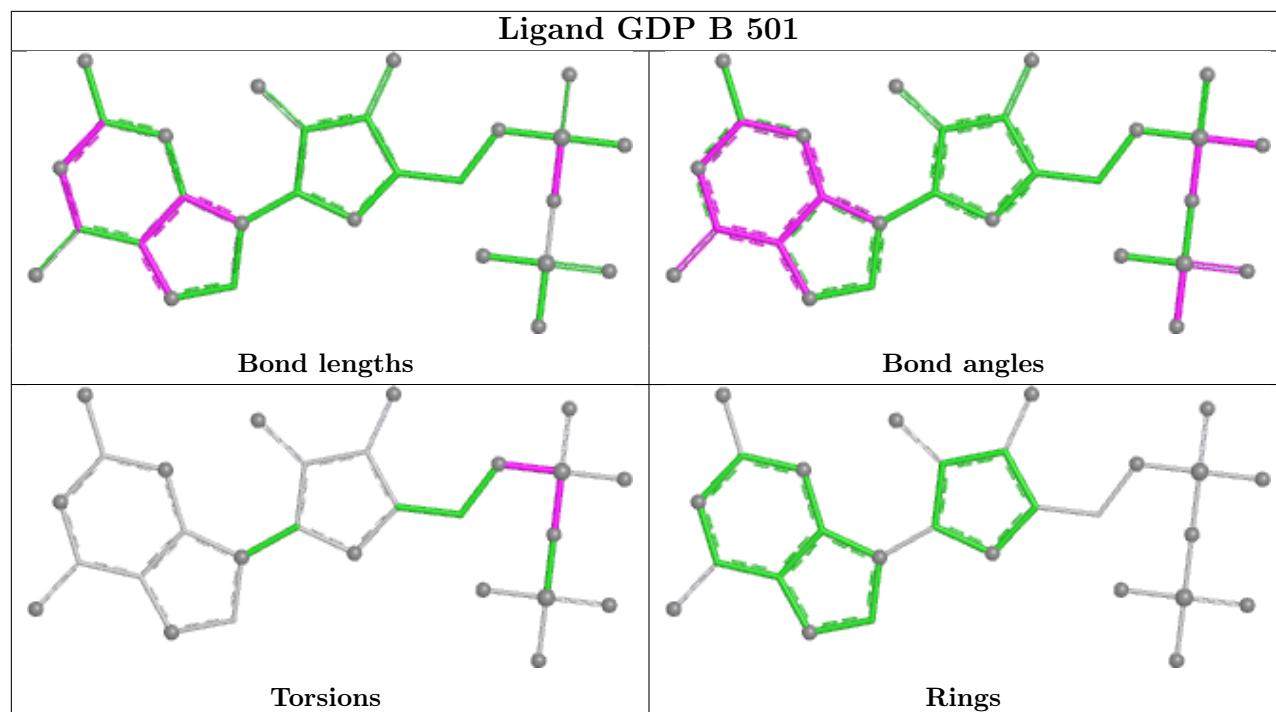
8 monomers are involved in 14 short contacts:

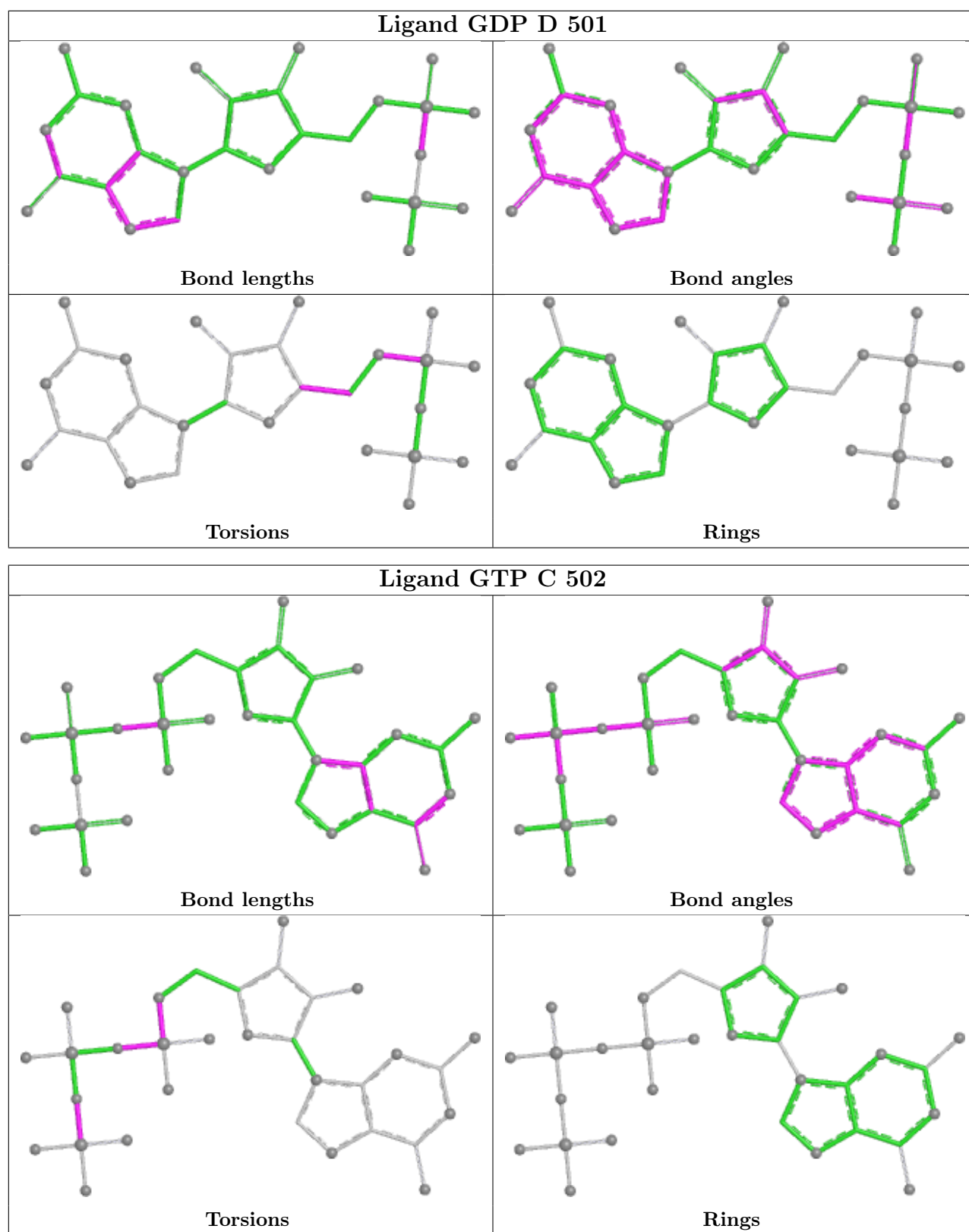
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	501	GTP	1	0
8	C	505	GOL	2	0
8	F	402	GOL	1	0
10	B	504	MES	2	0
12	F	401	ACP	2	0
9	B	501	GDP	2	0
9	D	501	GDP	3	0
8	A	505	GOL	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







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	439/451 (97%)	-0.17	2 (0%) 87 85	21, 46, 78, 114	1 (0%)
1	C	440/451 (97%)	-0.31	5 (1%) 78 75	23, 41, 66, 111	2 (0%)
2	B	430/445 (96%)	-0.16	5 (1%) 76 73	21, 43, 78, 117	1 (0%)
2	D	422/445 (94%)	0.31	13 (3%) 51 47	33, 59, 94, 117	0
3	E	123/143 (86%)	0.38	6 (4%) 35 31	24, 61, 98, 127	1 (0%)
4	F	346/384 (90%)	0.50	20 (5%) 29 25	33, 67, 127, 148	0
All	All	2200/2319 (94%)	0.03	51 (2%) 61 57	21, 51, 96, 148	5 (0%)

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	279	GLY	5.7
4	F	161	LEU	4.8
4	F	125	THR	4.0
4	F	245	ILE	3.7
1	C	163	LYS	3.7
2	D	276	THR	3.6
4	F	169	LEU	3.5
2	B	1	MET	3.5
4	F	150	LYS	3.3
2	D	407	TRP	3.3
2	D	1	MET	3.3
1	C	440	VAL	3.3
4	F	160	ILE	3.2
2	D	98	GLY	3.2
4	F	233	PHE	3.1
2	D	82	PRO	3.1
2	D	286	LEU	3.1
2	D	74	THR	3.0
1	C	283	HIS	2.9

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Mol	Chain	Res	Type	RSRZ
3	E	143	ALA	2.9
4	F	249	TYR	2.8
1	A	262	TYR	2.8
4	F	372	THR	2.7
4	F	362	ALA	2.7
2	B	281	GLN	2.7
2	B	440	ALA	2.6
2	D	94	PHE	2.6
4	F	186	LEU	2.6
2	D	404	PHE	2.5
1	C	1	MET	2.5
3	E	6	MET	2.5
2	B	57	ALA	2.4
4	F	238	CYS	2.4
3	E	139	LEU	2.4
4	F	182	ILE	2.3
2	D	57	ALA	2.3
2	D	142	GLY	2.3
1	C	282	TYR	2.3
2	D	221	THR	2.2
4	F	159	GLY	2.2
4	F	382	HIS	2.2
3	E	28	SER	2.2
1	A	116	ASP	2.1
4	F	363	ASP	2.1
3	E	115	HIS	2.1
2	D	220	THR	2.1
4	F	341	LYS	2.1
4	F	243	HIS	2.1
4	F	306	HIS	2.1
4	F	225	SER	2.0
3	E	71[A]	HIS	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 ⓘ

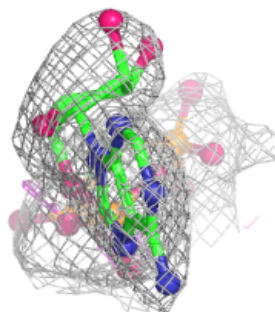
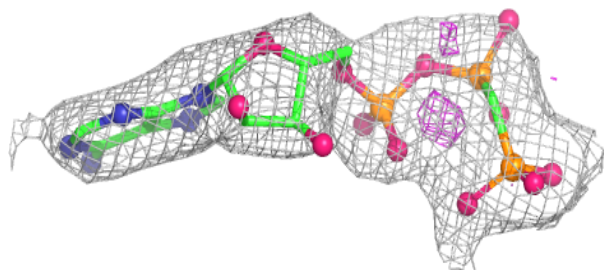
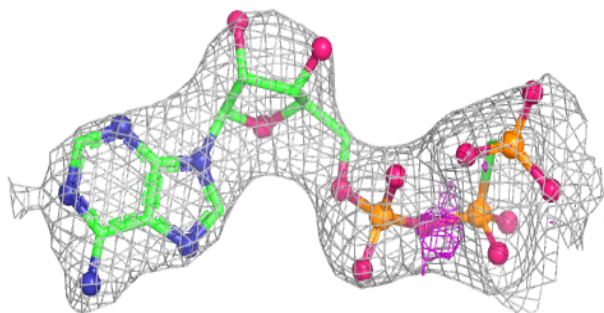
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
8	GOL	F	402	6/6	0.77	0.18	63,81,85,86	0
8	GOL	B	506	6/6	0.82	0.17	82,87,88,94	0
8	GOL	A	507	6/6	0.84	0.16	50,61,66,71	0
7	CA	C	501	1/1	0.86	0.18	96,96,96,96	0
8	GOL	A	504	6/6	0.87	0.15	89,98,101,104	0
7	CA	B	503	1/1	0.89	0.10	89,89,89,89	0
8	GOL	A	505	6/6	0.90	0.14	62,66,74,84	0
12	ACP	F	401	31/31	0.90	0.10	77,88,105,117	0
8	GOL	A	506	6/6	0.91	0.13	65,72,84,89	0
10	MES	B	504	12/12	0.92	0.12	55,68,82,83	0
8	GOL	C	505	6/6	0.92	0.14	54,69,71,76	0
6	MG	D	502	1/1	0.93	0.06	72,72,72,72	0
11	4SL	B	507	34/34	0.94	0.09	32,40,45,49	0
6	MG	B	502	1/1	0.94	0.11	57,57,57,57	0
9	GDP	D	501	28/28	0.95	0.07	40,49,60,66	0
10	MES	B	505	12/12	0.95	0.11	51,62,64,66	0
7	CA	A	503	1/1	0.96	0.05	62,62,62,62	0
8	GOL	C	506	6/6	0.97	0.07	47,51,56,62	0
5	GTP	C	502	32/32	0.98	0.05	27,30,34,36	0
9	GDP	B	501	28/28	0.99	0.04	26,32,34,38	0
5	GTP	A	501	32/32	0.99	0.04	26,31,33,37	0
7	CA	C	504	1/1	1.00	0.06	48,48,48,48	0
6	MG	A	502	1/1	1.00	0.03	35,35,35,35	0
6	MG	C	503	1/1	1.00	0.01	37,37,37,37	0

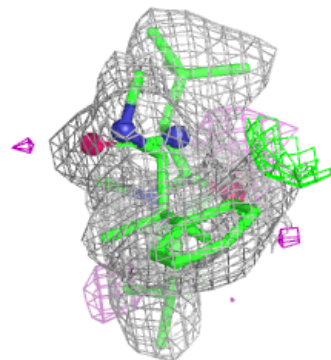
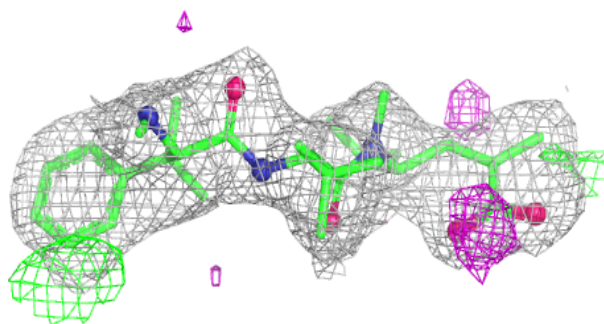
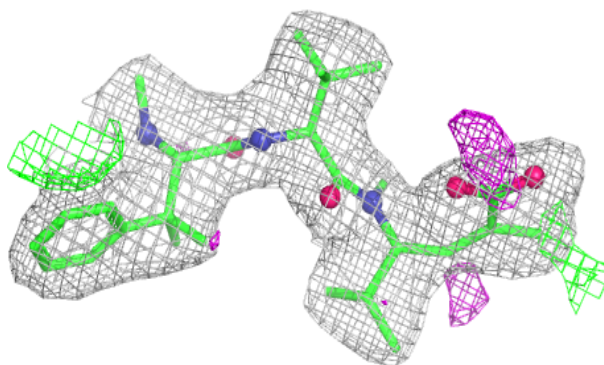
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ACP F 401:

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

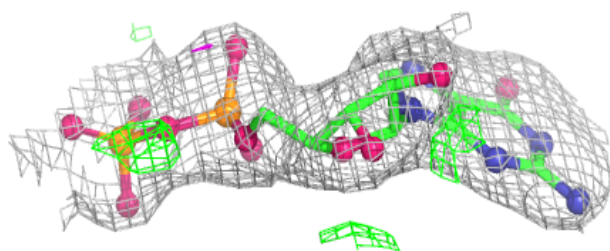
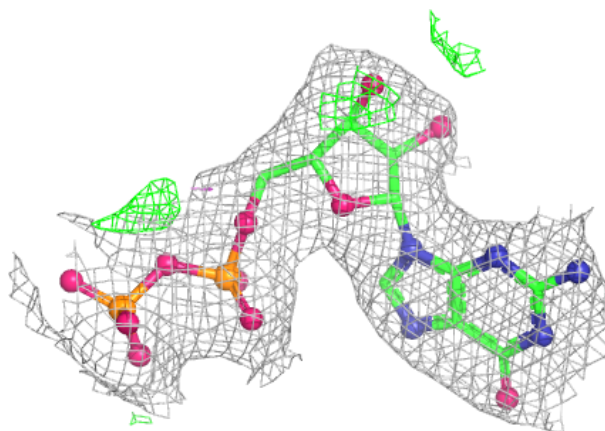
**Electron density around 4SL B 507:**

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



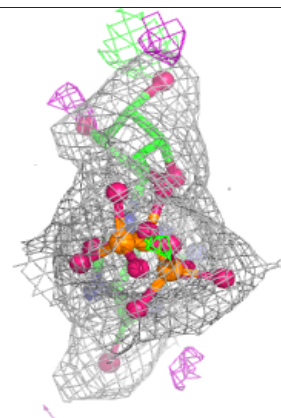
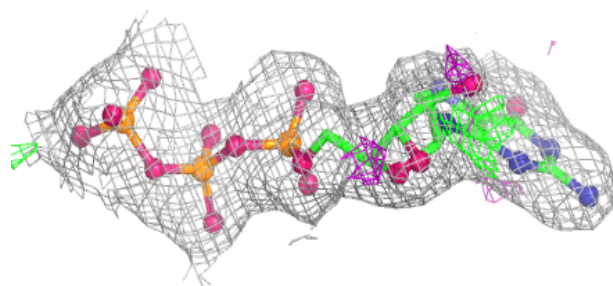
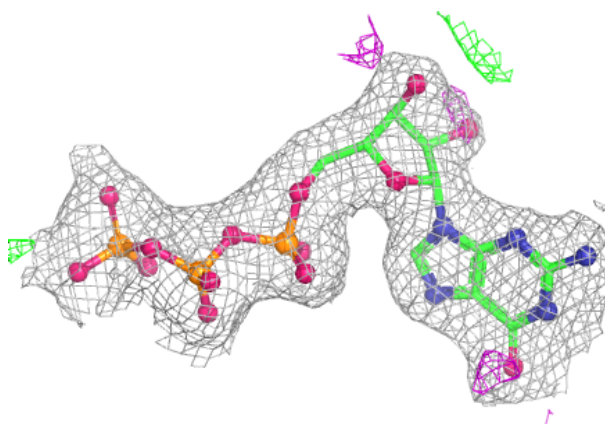
Electron density around GDP D 501:

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

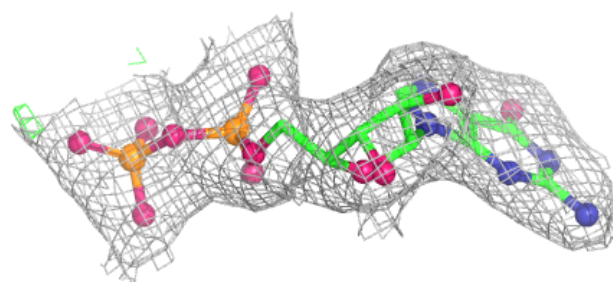
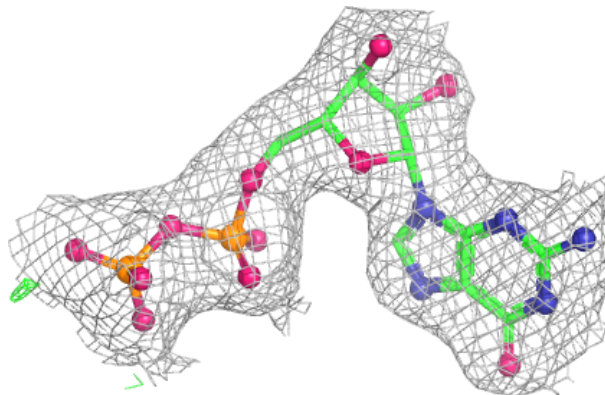


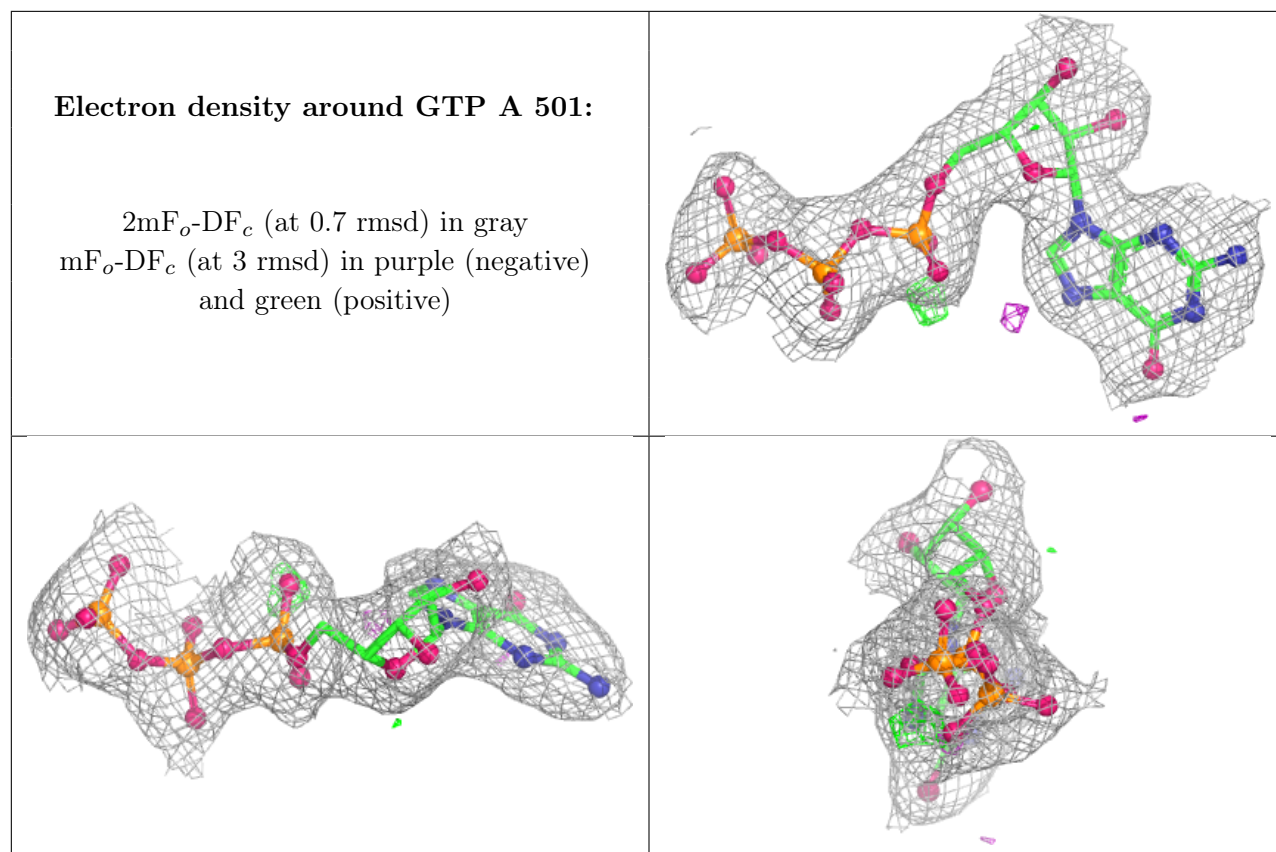
Electron density around GTP C 502:

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

**Electron density around GDP B 501:**

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





6.5 Other polymers [i](#)

There are no such residues in this entry.