



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 08:13 AM UTC

PDB ID : 1N3S / pdb_00001n3s
Title : Biosynthesis of pteridins. Reaction mechanism of GTP cyclohydrolase I
Authors : Rebelo, J.; Auerbach, G.; Bader, G.; Bracher, A.; Nar, H.; Hoesl, C.; Schramek, N.; Kaiser, J.; Bacher, A.; Huber, R.; Fischer, M.
Deposited on : 2002-10-29
Resolution : 2.55 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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

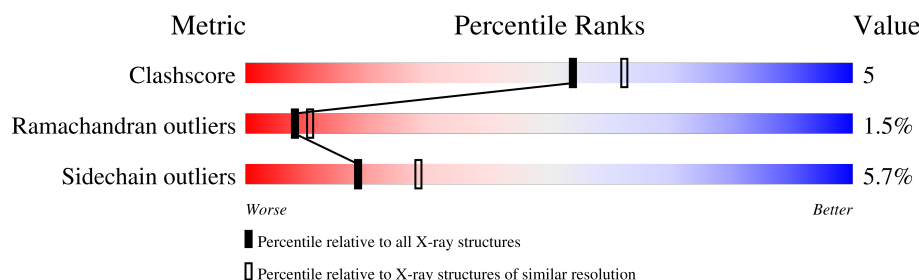
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.55 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))
Clashscore	190562	1120 (2.54-2.54)
Ramachandran outliers	187476	1106 (2.54-2.54)
Sidechain outliers	187428	1106 (2.54-2.54)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	221	77% 19% .
1	B	221	78% 20% .
1	C	221	80% 17% .
1	D	221	77% 20% .
1	E	221	77% 22%
1	F	221	74% 21% . .
1	G	221	78% 19% .
1	H	221	79% 19% .

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Mol	Chain	Length	Quality of chain
1	I	221	 81% 18% •
1	J	221	 77% 21% •

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 17795 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 GTP cyclohydrolase I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	221	Total	C	N	O	S	0	0	0
			1729	1085	307	328	9			
1	B	221	Total	C	N	O	S	0	0	0
			1729	1085	307	328	9			
1	C	221	Total	C	N	O	S	0	0	0
			1729	1085	307	328	9			
1	D	221	Total	C	N	O	S	0	0	0
			1729	1085	307	328	9			
1	E	221	Total	C	N	O	S	0	0	0
			1729	1085	307	328	9			
1	F	221	Total	C	N	O	S	0	0	0
			1729	1085	307	328	9			
1	G	221	Total	C	N	O	S	0	0	0
			1729	1085	307	328	9			
1	H	221	Total	C	N	O	S	0	0	0
			1729	1085	307	328	9			
1	I	221	Total	C	N	O	S	0	0	0
			1729	1085	307	328	9			
1	J	221	Total	C	N	O	S	0	0	0
			1729	1085	307	328	9			

There are 10 discrepancies between the modelled and reference sequences:

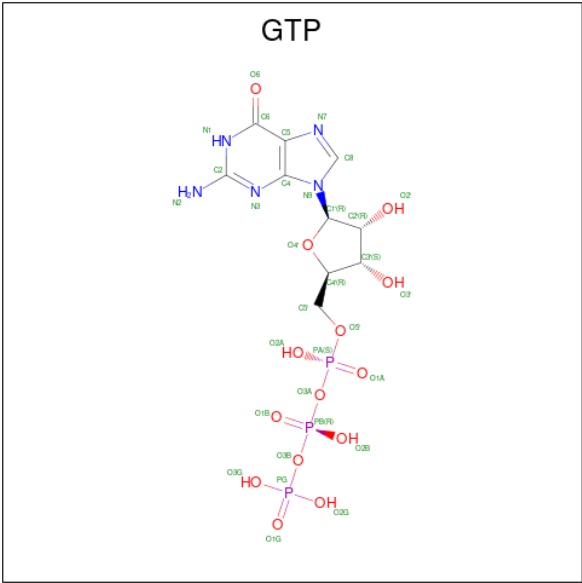
Chain	Residue	Modelled	Actual	Comment	Reference
A	113	SER	HIS	engineered mutation	UNP P0A6T5
B	113	SER	HIS	engineered mutation	UNP P0A6T5
C	113	SER	HIS	engineered mutation	UNP P0A6T5
D	113	SER	HIS	engineered mutation	UNP P0A6T5
E	113	SER	HIS	engineered mutation	UNP P0A6T5
F	113	SER	HIS	engineered mutation	UNP P0A6T5
G	113	SER	HIS	engineered mutation	UNP P0A6T5
H	113	SER	HIS	engineered mutation	UNP P0A6T5
I	113	SER	HIS	engineered mutation	UNP P0A6T5

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Chain	Residue	Modelled	Actual	Comment	Reference
J	113	SER	HIS	engineered mutation	UNP P0A6T5

- Molecule 2 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	Total 32	10	5	14	3	0	0
2	B	1	Total 32	10	5	14	3	0	0
2	C	1	Total 32	10	5	14	3	0	0
2	D	1	Total 32	10	5	14	3	0	0
2	E	1	Total 32	10	5	14	3	0	0
2	F	1	Total 32	10	5	14	3	0	0
2	G	1	Total 32	10	5	14	3	0	0
2	H	1	Total 32	10	5	14	3	0	0
2	I	1	Total 32	10	5	14	3	0	0
2	J	1	Total 32	10	5	14	3	0	0

- Molecule 3 is water.

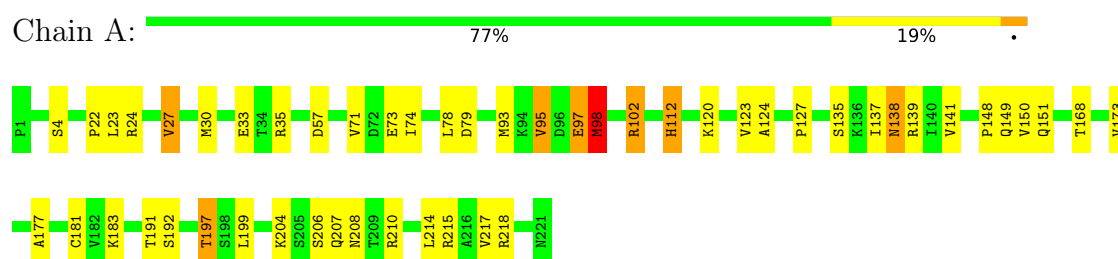
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	23	Total 23	O 23	0	0
3	B	34	Total 34	O 34	0	0
3	C	16	Total 16	O 16	0	0
3	D	24	Total 24	O 24	0	0
3	E	9	Total 9	O 9	0	0
3	F	18	Total 18	O 18	0	0
3	G	13	Total 13	O 13	0	0
3	H	9	Total 9	O 9	0	0
3	I	18	Total 18	O 18	0	0
3	J	21	Total 21	O 21	0	0

3 Residue-property plots

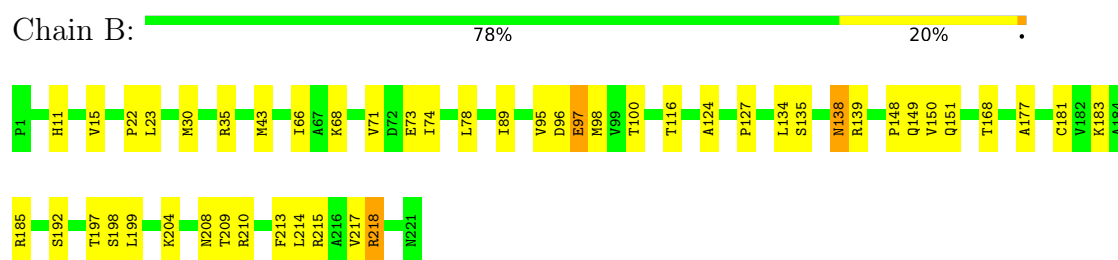
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

Note EDS was not executed.

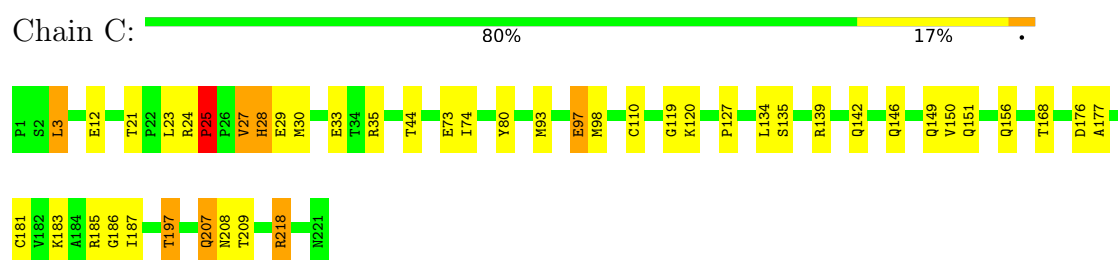
• Molecule 1: GTP cyclohydrolase I



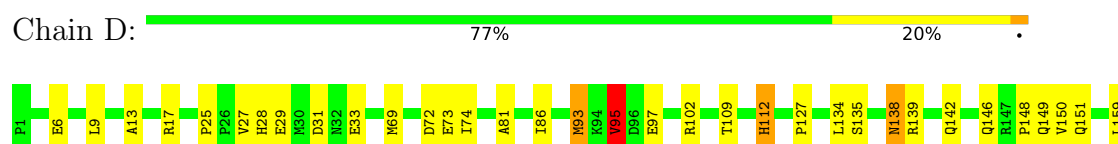
• Molecule 1: GTP cyclohydrolase I



• Molecule 1: GTP cyclohydrolase I



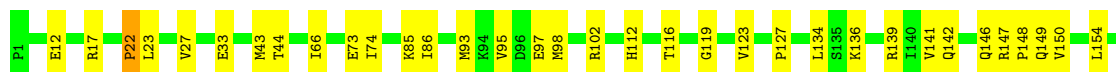
• Molecule 1: GTP cyclohydrolase I





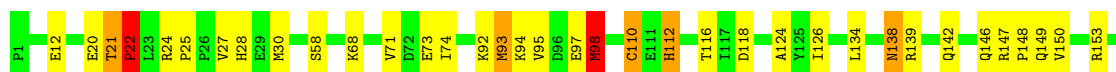
- Molecule 1: GTP cyclohydrolase I

Chain E: 77% 22%



- Molecule 1: GTP cyclohydrolase I

Chain F: 74% 21% . .



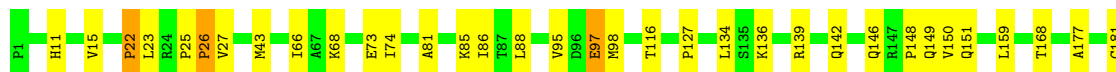
- Molecule 1: GTP cyclohydrolase I

Chain G: 78% 19% .



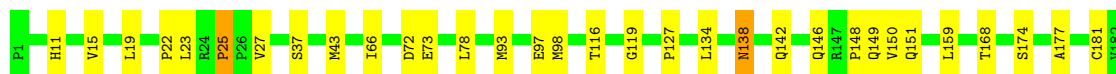
- Molecule 1: GTP cyclohydrolase I

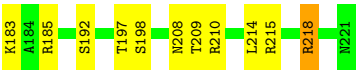
Chain H: 79% 19% .



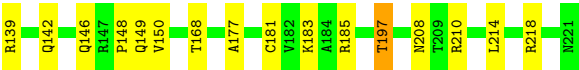
- Molecule 1: GTP cyclohydrolase I

Chain I: 81% 18% .





● Molecule 1: GTP cyclohydrolase I



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	124.30Å 124.30Å 389.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.55	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-2.55)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.262 , 0.293	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	17795	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GTP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.76	1/1756 (0.1%)	1.24	14/2377 (0.6%)
1	B	0.72	0/1756	1.23	15/2377 (0.6%)
1	C	0.87	2/1756 (0.1%)	1.84	24/2377 (1.0%)
1	D	0.70	1/1756 (0.1%)	1.25	15/2377 (0.6%)
1	E	0.73	0/1756	1.23	12/2377 (0.5%)
1	F	0.78	1/1756 (0.1%)	1.78	19/2377 (0.8%)
1	G	0.75	0/1756	1.25	17/2377 (0.7%)
1	H	0.74	0/1756	1.25	19/2377 (0.8%)
1	I	0.70	0/1756	1.23	18/2377 (0.8%)
1	J	0.77	1/1756 (0.1%)	1.26	15/2377 (0.6%)
All	All	0.75	6/17560 (0.0%)	1.37	168/23770 (0.7%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	24	ARG	CA-C	10.32	1.65	1.52
1	A	98	MET	SD-CE	-6.61	1.63	1.79
1	D	69	MET	SD-CE	-5.83	1.65	1.79
1	F	98	MET	SD-CE	-5.73	1.65	1.79
1	C	25	PRO	CA-C	5.60	1.57	1.52
1	J	126	ILE	CA-CB	5.07	1.59	1.53

All (168) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	24	ARG	CA-C-N	44.07	165.77	120.38
1	C	24	ARG	C-N-CA	44.07	165.77	120.38
1	F	21	THR	CA-C-N	42.06	172.42	119.84
1	F	21	THR	C-N-CA	42.06	172.42	119.84
1	D	93	MET	N-CA-C	-12.19	98.54	113.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	21	THR	C-N-CD	-11.62	77.36	125.00
1	J	98	MET	N-CA-C	11.43	128.50	110.32
1	G	98	MET	N-CA-C	11.19	128.12	110.32
1	C	24	ARG	C-N-CD	-10.84	80.55	125.00
1	E	98	MET	N-CA-C	10.78	127.45	110.32
1	H	98	MET	N-CA-C	10.53	127.11	110.17
1	H	149	GLN	N-CA-C	10.34	125.63	109.81
1	C	98	MET	N-CA-C	10.19	126.57	110.17
1	J	149	GLN	N-CA-C	10.16	125.07	110.14
1	F	149	GLN	N-CA-C	9.64	124.31	110.14
1	B	149	GLN	N-CA-C	9.56	124.19	110.14
1	I	98	MET	N-CA-C	9.49	125.46	110.17
1	I	73	GLU	N-CA-C	9.42	124.74	112.12
1	A	149	GLN	N-CA-C	9.31	123.82	110.14
1	I	149	GLN	N-CA-C	9.10	123.51	110.14
1	G	149	GLN	N-CA-C	9.09	124.21	109.85
1	C	73	GLU	N-CA-C	9.01	123.34	108.48
1	D	95	VAL	N-CA-C	8.84	120.56	108.89
1	E	149	GLN	N-CA-C	8.76	123.02	110.14
1	F	22	PRO	CA-N-CD	-8.68	99.84	112.00
1	D	149	GLN	N-CA-C	8.65	122.86	110.14
1	G	25	PRO	CA-C-N	8.42	130.37	119.84
1	G	25	PRO	C-N-CA	8.42	130.37	119.84
1	C	25	PRO	CA-N-CD	-8.37	100.28	112.00
1	H	97	GLU	N-CA-C	8.21	121.52	109.69
1	B	98	MET	N-CA-C	8.11	123.23	110.17
1	A	95	VAL	N-CA-C	7.98	119.42	108.89
1	A	93	MET	N-CA-C	-7.82	103.76	113.38
1	C	149	GLN	N-CA-C	7.82	122.53	110.42
1	G	26	PRO	N-CA-C	7.64	128.21	112.47
1	C	25	PRO	CA-C-N	7.19	144.26	127.00
1	C	25	PRO	C-N-CA	7.19	144.26	127.00
1	A	150	VAL	N-CA-C	-7.17	98.07	108.11
1	E	134	LEU	N-CA-C	7.09	119.62	111.11
1	J	150	VAL	N-CA-C	-7.01	97.40	107.77
1	F	24	ARG	N-CA-C	6.95	119.70	109.42
1	H	177	ALA	N-CA-C	6.90	119.65	109.24
1	B	134	LEU	N-CA-C	6.78	119.24	111.11
1	I	150	VAL	N-CA-C	-6.67	97.90	107.77
1	C	150	VAL	N-CA-C	-6.67	97.90	107.77
1	H	25	PRO	CA-C-N	6.54	128.02	119.84
1	H	25	PRO	C-N-CA	6.54	128.02	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	21	THR	CB-CA-C	6.52	117.33	109.31
1	G	150	VAL	N-CA-C	-6.49	98.16	107.77
1	C	134	LEU	N-CA-C	6.43	118.82	111.11
1	D	177	ALA	N-CA-C	6.42	119.18	109.23
1	E	177	ALA	N-CA-C	6.41	118.92	109.24
1	C	177	ALA	N-CA-C	6.40	119.15	109.23
1	I	134	LEU	N-CA-C	6.35	118.73	111.11
1	J	183	LYS	N-CA-C	6.34	119.14	111.40
1	I	177	ALA	N-CA-C	6.34	118.71	109.07
1	E	150	VAL	N-CA-C	-6.30	99.28	108.11
1	B	150	VAL	N-CA-C	-6.30	98.44	107.77
1	I	183	LYS	N-CA-C	6.28	118.00	111.03
1	F	134	LEU	N-CA-C	6.24	118.60	111.11
1	G	177	ALA	N-CA-C	6.20	118.73	108.99
1	G	81	ALA	N-CA-C	-6.20	105.21	112.89
1	B	183	LYS	N-CA-C	6.18	118.94	111.40
1	E	192	SER	N-CA-C	6.18	118.76	110.35
1	D	150	VAL	N-CA-C	-6.13	98.69	107.77
1	H	183	LYS	N-CA-C	6.11	118.86	111.40
1	B	177	ALA	N-CA-C	6.08	118.95	109.52
1	A	183	LYS	N-CA-C	6.08	118.82	111.40
1	J	110	CYS	CA-CB-SG	6.03	128.26	114.40
1	D	31	ASP	N-CA-C	-6.01	100.70	110.20
1	E	86	ILE	N-CA-C	5.96	116.75	109.30
1	D	134	LEU	N-CA-C	5.96	118.26	111.11
1	J	177	ALA	N-CA-C	5.91	118.17	109.24
1	E	148	PRO	N-CA-C	-5.90	100.31	112.47
1	G	148	PRO	N-CA-C	-5.87	100.37	112.47
1	F	150	VAL	N-CA-C	-5.86	99.10	107.77
1	B	181	CYS	N-CA-C	-5.85	105.97	113.23
1	F	116	THR	N-CA-C	5.84	118.47	110.24
1	J	74	ILE	N-CA-C	5.83	120.19	112.04
1	F	169	ASN	N-CA-C	-5.82	106.22	113.38
1	G	134	LEU	N-CA-C	5.81	118.08	111.11
1	H	148	PRO	N-CA-C	-5.80	101.12	110.74
1	B	148	PRO	N-CA-C	-5.79	101.12	110.74
1	J	134	LEU	N-CA-C	5.79	118.06	111.11
1	F	74	ILE	N-CA-C	5.79	120.14	112.04
1	C	74	ILE	N-CA-C	5.78	120.22	111.89
1	G	97	GLU	N-CA-C	5.78	118.65	109.81
1	D	148	PRO	N-CA-C	-5.77	101.16	110.74
1	C	25	PRO	N-CA-C	-5.76	103.67	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	110	CYS	CA-CB-SG	5.76	127.66	114.40
1	C	119	GLY	N-CA-C	5.75	119.53	111.14
1	G	182	VAL	N-CA-C	-5.74	107.25	111.90
1	A	191	THR	N-CA-C	5.74	120.55	113.50
1	B	192	SER	N-CA-C	5.72	118.56	110.50
1	I	25	PRO	CA-C-N	5.70	126.08	119.47
1	I	25	PRO	C-N-CA	5.70	126.08	119.47
1	A	148	PRO	N-CA-C	-5.65	100.83	112.47
1	C	25	PRO	C-N-CD	-5.65	108.17	120.60
1	G	119	GLY	N-CA-C	5.62	119.30	111.10
1	B	73	GLU	N-CA-C	5.61	122.75	110.80
1	E	74	ILE	N-CA-C	5.61	119.89	112.04
1	A	177	ALA	N-CA-C	5.59	117.77	108.99
1	B	151	GLN	N-CA-C	5.57	118.08	111.33
1	I	72	ASP	N-CA-C	5.57	120.21	113.41
1	H	81	ALA	N-CA-C	-5.55	106.01	112.89
1	F	73	GLU	N-CA-C	5.55	122.62	110.80
1	H	150	VAL	N-CA-C	-5.53	99.58	107.77
1	E	73	GLU	N-CA-C	5.53	122.58	110.80
1	A	74	ILE	N-CA-C	5.49	119.73	112.04
1	F	183	LYS	N-CA-C	5.49	118.10	111.40
1	G	71	VAL	N-CA-C	5.48	116.55	111.45
1	D	74	ILE	N-CA-C	5.48	120.12	113.00
1	B	97	GLU	N-CA-C	5.46	118.17	109.81
1	I	148	PRO	N-CA-C	-5.45	101.24	112.47
1	J	71	VAL	N-CA-C	5.43	117.34	111.58
1	C	151	GLN	N-CA-C	5.43	117.90	111.33
1	E	119	GLY	N-CA-C	5.43	119.06	111.14
1	B	71	VAL	N-CA-C	5.42	116.49	111.45
1	I	181	CYS	N-CA-C	-5.39	106.71	113.28
1	J	148	PRO	N-CA-C	-5.38	101.39	112.47
1	H	134	LEU	N-CA-C	5.37	117.55	111.11
1	C	28	HIS	N-CA-C	-5.33	97.83	107.75
1	J	73	GLU	N-CA-C	5.33	122.14	110.80
1	A	73	GLU	N-CA-C	5.30	122.09	110.80
1	J	116	THR	N-CA-C	5.30	117.72	110.24
1	E	116	THR	N-CA-C	5.30	118.03	110.24
1	H	208	ASN	N-CA-C	5.29	116.91	111.03
1	H	73	GLU	N-CA-C	5.29	122.07	110.80
1	H	74	ILE	N-CA-C	5.28	119.43	112.04
1	C	25	PRO	CB-CA-C	5.28	117.36	110.92
1	C	207	GLN	N-CA-C	5.26	118.96	112.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	192	SER	N-CA-C	5.26	117.47	110.53
1	F	148	PRO	N-CA-C	-5.25	102.02	110.74
1	I	192	SER	N-CA-C	5.25	118.06	110.28
1	D	72	ASP	N-CA-C	5.25	119.95	113.50
1	A	151	GLN	N-CA-C	5.24	117.00	111.28
1	H	86	ILE	N-CA-C	5.23	115.84	109.30
1	D	183	LYS	N-CA-C	5.23	117.78	111.40
1	H	181	CYS	N-CA-C	-5.22	106.91	113.28
1	H	191	THR	N-CA-C	5.22	119.92	113.50
1	D	151	GLN	N-CA-C	5.20	117.62	111.33
1	G	183	LYS	N-CA-C	5.19	117.74	111.40
1	C	97	GLU	N-CA-C	5.19	117.75	109.81
1	I	19	LEU	N-CA-C	5.19	119.30	112.92
1	F	110	CYS	CA-CB-SG	5.18	126.33	114.40
1	D	73	GLU	N-CA-C	5.17	121.81	110.80
1	I	214	LEU	N-CA-C	5.16	119.05	112.34
1	F	71	VAL	N-CA-C	5.14	117.03	111.58
1	I	116	THR	N-CA-C	5.14	117.92	110.42
1	I	151	GLN	N-CA-C	5.13	117.54	111.33
1	J	110	CYS	N-CA-C	-5.13	102.32	109.96
1	J	2	SER	N-CA-C	5.12	121.71	110.80
1	A	27	VAL	N-CA-C	5.11	119.97	109.34
1	H	182	VAL	N-CA-C	-5.11	107.42	111.81
1	H	116	THR	N-CA-C	5.11	117.64	110.23
1	G	192	SER	N-CA-C	5.10	117.27	110.53
1	B	116	THR	N-CA-C	5.10	117.43	110.24
1	D	81	ALA	N-CA-C	-5.08	106.59	112.89
1	I	119	GLY	N-CA-C	5.08	118.51	111.10
1	B	74	ILE	N-CA-C	5.07	119.14	112.04
1	G	151	GLN	N-CA-C	5.07	116.81	111.28
1	F	93	MET	N-CA-CB	5.06	119.04	110.49
1	A	57	ASP	N-CA-C	5.05	118.91	112.34
1	C	181	CYS	N-CA-C	-5.04	107.08	113.18
1	A	71	VAL	N-CA-C	5.04	116.13	111.45
1	J	181	CYS	N-CA-C	-5.03	106.40	112.54
1	F	177	ALA	N-CA-C	5.02	116.82	109.24
1	C	183	LYS	N-CA-C	5.01	117.52	111.40

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	1729	0	1766	17	0
1	B	1729	0	1766	24	0
1	C	1729	0	1764	22	0
1	D	1729	0	1766	24	0
1	E	1729	0	1766	21	0
1	F	1729	0	1764	27	0
1	G	1729	0	1766	21	0
1	H	1729	0	1766	18	0
1	I	1729	0	1766	17	0
1	J	1729	0	1764	24	0
2	A	32	0	11	1	0
2	B	32	0	11	0	0
2	C	32	0	11	2	0
2	D	32	0	11	2	0
2	E	32	0	11	3	0
2	F	32	0	11	3	0
2	G	32	0	11	1	0
2	H	32	0	11	3	0
2	I	32	0	11	1	0
2	J	32	0	11	2	0
3	A	23	0	0	0	0
3	B	34	0	0	1	0
3	C	16	0	0	0	1
3	D	24	0	0	1	1
3	E	9	0	0	0	0
3	F	18	0	0	1	0
3	G	13	0	0	0	0
3	H	9	0	0	1	0
3	I	18	0	0	0	1
3	J	21	0	0	1	1
All	All	17795	0	17764	173	2

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 5.

All (173) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:210:ARG:HE	1:E:208:ASN:HD21	1.07	1.02
1:B:210:ARG:HE	1:C:208:ASN:HD21	1.02	0.92
1:F:93:MET:HG2	1:J:17:ARG:O	1.72	0.89
1:D:210:ARG:NE	1:E:208:ASN:HD21	1.71	0.87
1:B:210:ARG:NE	1:C:208:ASN:HD21	1.75	0.83
1:H:139:ARG:HH12	2:H:6411:GTP:PG	2.06	0.79
1:C:156:GLN:HG3	1:D:95:VAL:HG21	1.69	0.73
1:I:218:ARG:HH21	1:J:102:ARG:HH22	1.36	0.73
1:J:138:ASN:H	1:J:138:ASN:HD22	1.38	0.72
1:I:138:ASN:HD22	1:I:138:ASN:H	1.39	0.71
1:A:208:ASN:HD21	1:E:210:ARG:NE	1.90	0.69
2:F:9411:GTP:PG	1:J:185:ARG:HH22	2.16	0.68
1:F:110:CYS:SG	1:F:112:HIS:ND1	2.61	0.68
1:C:27:VAL:HG12	1:C:28:HIS:H	1.60	0.66
1:I:185:ARG:HH22	2:J:8411:GTP:PG	2.19	0.66
1:D:210:ARG:HE	1:E:208:ASN:ND2	1.87	0.64
1:G:210:ARG:NE	1:H:208:ASN:HD21	1.97	0.63
1:B:204:LYS:HA	1:B:210:ARG:HH11	1.63	0.62
1:B:97:GLU:O	1:B:127:PRO:HD2	1.99	0.62
1:H:139:ARG:NH1	2:H:6411:GTP:O2G	2.33	0.61
1:J:8:ALA:O	1:J:12:GLU:HG3	1.99	0.61
1:F:197:THR:O	1:G:97:GLU:HB3	2.01	0.61
2:A:4411:GTP:PG	1:E:185:ARG:HH22	2.23	0.60
1:E:160:ILE:HD13	1:E:163:GLN:NE2	2.15	0.60
1:J:85:LYS:O	1:J:136:LYS:HE2	2.01	0.60
1:I:23:LEU:HD11	1:I:78:LEU:HD22	1.84	0.60
1:B:23:LEU:HD11	1:B:78:LEU:HD22	1.83	0.60
1:D:93:MET:HB3	1:D:95:VAL:HG23	1.84	0.60
1:G:93:MET:HB2	1:G:95:VAL:HG23	1.82	0.60
1:H:210:ARG:NE	1:I:208:ASN:HD21	2.01	0.59
1:A:204:LYS:HA	1:A:210:ARG:HH11	1.67	0.59
1:B:185:ARG:HH22	2:C:1411:GTP:PG	2.26	0.58
1:H:159:LEU:HD22	1:H:198:SER:HB3	1.85	0.58
1:C:185:ARG:HH22	2:D:2411:GTP:PG	2.26	0.57
1:D:135:SER:O	1:D:139:ARG:HG3	2.04	0.57
1:G:199:LEU:H	1:H:97:GLU:HG3	1.68	0.57
1:J:23:LEU:HD11	1:J:78:LEU:HD22	1.86	0.57
1:E:85:LYS:O	1:E:136:LYS:HE2	2.05	0.57
1:I:159:LEU:HD22	1:I:198:SER:HB3	1.86	0.57
1:A:102:ARG:HG3	1:A:102:ARG:HH11	1.70	0.57
1:H:85:LYS:O	1:H:136:LYS:HE2	2.05	0.57
1:F:142:GLN:O	1:F:146:GLN:HG2	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:138:ASN:H	1:B:138:ASN:HD22	1.52	0.57
1:B:197:THR:O	1:C:97:GLU:HB3	2.05	0.56
1:F:28:HIS:C	1:F:30:MET:H	2.13	0.56
1:D:204:LYS:HA	1:D:210:ARG:HH11	1.70	0.56
1:D:138:ASN:HD22	1:D:138:ASN:H	1.51	0.56
1:E:154:LEU:O	1:E:158:ILE:HG12	2.05	0.55
1:H:185:ARG:HH22	2:I:7411:GTP:PG	2.29	0.55
1:G:185:ARG:HH22	2:H:6411:GTP:PG	2.30	0.55
1:A:30:MET:HB2	1:A:35:ARG:HE	1.72	0.54
1:D:159:LEU:HD22	1:D:198:SER:HB3	1.89	0.54
1:I:138:ASN:HD22	1:I:138:ASN:N	2.05	0.54
1:F:207:GLN:HE22	1:G:208:ASN:HB2	1.72	0.54
1:F:138:ASN:H	1:F:138:ASN:HD22	1.56	0.54
1:F:210:ARG:HD3	1:G:208:ASN:OD1	2.07	0.54
1:G:214:LEU:HB3	1:H:215:ARG:NH2	2.24	0.53
1:C:135:SER:O	1:C:139:ARG:HG3	2.09	0.53
1:D:197:THR:O	1:E:97:GLU:HB3	2.09	0.53
1:H:204:LYS:HA	1:H:210:ARG:HH11	1.73	0.53
1:E:159:LEU:HD22	1:E:198:SER:HB3	1.91	0.53
1:D:142:GLN:O	1:D:146:GLN:HG2	2.09	0.52
1:I:97:GLU:O	1:I:127:PRO:HD2	2.09	0.52
1:B:43:MET:HE2	1:B:66:ILE:HD13	1.91	0.52
1:G:197:THR:O	1:H:97:GLU:HB3	2.09	0.52
1:H:214:LEU:HB3	1:I:215:ARG:NH2	2.25	0.52
1:F:20:GLU:CD	1:F:147:ARG:HH12	2.17	0.52
1:I:197:THR:O	1:J:97:GLU:HB3	2.09	0.52
1:A:135:SER:O	1:A:139:ARG:HG3	2.10	0.51
1:F:118:ASP:HB3	3:F:9412:HOH:O	2.08	0.51
1:F:199:LEU:HD11	1:F:214:LEU:HD11	1.92	0.51
1:D:160:ILE:HD13	1:D:163:GLN:NE2	2.26	0.51
1:B:185:ARG:NH2	2:C:1411:GTP:O3G	2.44	0.51
1:F:139:ARG:NH1	2:F:9411:GTP:PG	2.84	0.51
1:F:160:ILE:HD13	1:F:163:GLN:NE2	2.26	0.51
1:B:30:MET:HE3	1:B:35:ARG:HG2	1.93	0.50
1:G:102:ARG:HH11	1:G:102:ARG:HG3	1.76	0.50
1:D:214:LEU:HB3	1:E:215:ARG:NH2	2.26	0.50
1:G:210:ARG:CZ	1:H:208:ASN:HD21	2.24	0.50
1:H:43:MET:HE2	1:H:66:ILE:HD13	1.94	0.50
1:A:197:THR:O	1:B:97:GLU:HB3	2.11	0.50
1:C:218:ARG:HH21	1:D:102:ARG:HH22	1.57	0.50
1:J:142:GLN:O	1:J:146:GLN:HG2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:97:GLU:O	1:D:127:PRO:HD2	2.12	0.49
1:D:185:ARG:HH22	2:E:3411:GTP:PG	2.36	0.49
1:F:208:ASN:HD21	1:J:210:ARG:NE	2.10	0.49
1:A:97:GLU:O	1:A:127:PRO:HD2	2.13	0.49
1:A:214:LEU:HB3	1:B:215:ARG:NH2	2.28	0.49
1:B:23:LEU:HD22	3:B:417:HOH:O	2.12	0.48
1:I:11:HIS:O	1:I:15:VAL:HG23	2.12	0.48
1:E:160:ILE:HD13	1:E:163:GLN:HE22	1.77	0.48
1:E:141:VAL:HA	1:E:158:ILE:HD12	1.93	0.48
1:B:11:HIS:O	1:B:15:VAL:HG23	2.14	0.48
1:J:11:HIS:O	1:J:15:VAL:HG23	2.13	0.48
1:E:139:ARG:NH1	2:E:3411:GTP:PG	2.87	0.47
1:A:123:VAL:HG22	1:A:173:VAL:HG22	1.96	0.47
1:H:11:HIS:O	1:H:15:VAL:HG23	2.14	0.47
1:J:138:ASN:HD22	1:J:138:ASN:N	2.11	0.47
1:G:135:SER:O	1:G:139:ARG:HG3	2.15	0.47
1:J:105:THR:HG21	3:J:8425:HOH:O	2.13	0.47
1:J:135:SER:O	1:J:139:ARG:HG3	2.15	0.47
1:E:142:GLN:O	1:E:146:GLN:HG2	2.15	0.47
1:F:92:LYS:O	1:F:93:MET:SD	2.73	0.47
1:A:204:LYS:HA	1:A:210:ARG:NH1	2.29	0.47
1:B:210:ARG:NE	1:C:208:ASN:ND2	2.55	0.47
1:F:198:SER:HA	1:G:97:GLU:HG3	1.97	0.47
1:A:98:MET:HE3	1:A:124:ALA:HB1	1.96	0.46
1:D:183:LYS:HG3	1:D:190:ALA:HA	1.97	0.46
1:G:13:ALA:O	1:G:17:ARG:HD2	2.16	0.46
1:C:187:ILE:HG22	3:D:2432:HOH:O	2.14	0.46
1:H:97:GLU:O	1:H:127:PRO:HD2	2.15	0.46
1:F:153:ARG:O	1:F:157:GLN:HG3	2.15	0.46
1:H:197:THR:O	1:I:97:GLU:HB3	2.16	0.46
1:C:185:ARG:NH2	2:D:2411:GTP:O3G	2.47	0.46
1:F:93:MET:HE3	1:J:18:GLY:HA3	1.97	0.45
1:J:93:MET:HB2	1:J:95:VAL:HG23	1.97	0.45
1:G:91:ASN:HD21	1:G:94:LYS:HA	1.81	0.45
1:D:210:ARG:NE	1:E:208:ASN:ND2	2.54	0.45
1:H:142:GLN:O	1:H:146:GLN:HG2	2.17	0.45
1:C:142:GLN:O	1:C:146:GLN:HG2	2.17	0.45
1:F:185:ARG:NH2	2:G:5411:GTP:O3G	2.45	0.45
1:G:159:LEU:HD22	1:G:198:SER:HB3	1.99	0.45
1:A:137:ILE:O	1:A:141:VAL:HG23	2.18	0.44
1:F:213:PHE:O	1:F:217:VAL:HG23	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:187:ILE:HG22	3:H:6416:HOH:O	2.17	0.44
1:I:142:GLN:O	1:I:146:GLN:HG2	2.17	0.44
1:J:138:ASN:H	1:J:138:ASN:ND2	2.10	0.44
1:E:147:ARG:NH1	1:E:157:GLN:HE22	2.15	0.44
1:B:199:LEU:H	1:C:97:GLU:HG3	1.82	0.44
1:B:210:ARG:O	1:B:214:LEU:HD12	2.18	0.44
1:E:97:GLU:O	1:E:127:PRO:HD2	2.18	0.44
1:J:3:LEU:HB3	1:J:4:SER:H	1.57	0.44
1:E:43:MET:HE2	1:E:66:ILE:HD13	2.00	0.44
2:J:8411:GTP:H5'	2:J:8411:GTP:O2B	2.17	0.43
1:A:23:LEU:HD21	1:A:78:LEU:HD22	2.01	0.43
1:F:98:MET:HE3	1:F:98:MET:HB2	1.91	0.43
1:C:30:MET:SD	1:C:35:ARG:HG2	2.57	0.43
1:C:185:ARG:HG2	1:C:186:GLY:N	2.33	0.43
1:C:197:THR:O	1:D:97:GLU:HB2	2.19	0.43
1:G:96:ASP:OD1	1:G:96:ASP:N	2.45	0.43
1:F:97:GLU:HB2	1:J:197:THR:O	2.18	0.43
1:I:43:MET:HE2	1:I:66:ILE:HD13	2.00	0.43
1:A:112:HIS:HE1	1:A:181:CYS:SG	2.42	0.43
1:F:215:ARG:NH2	1:J:214:LEU:HB3	2.34	0.43
1:D:6:GLU:HG2	1:D:86:ILE:HB	2.01	0.43
1:D:112:HIS:ND1	2:E:3411:GTP:H8	2.17	0.43
1:C:97:GLU:O	1:C:127:PRO:HD2	2.19	0.42
1:A:210:ARG:NE	1:B:208:ASN:HD21	2.16	0.42
1:B:198:SER:HA	1:C:97:GLU:HG3	2.01	0.42
1:A:138:ASN:HD22	1:A:138:ASN:H	1.66	0.42
1:I:210:ARG:NE	1:J:208:ASN:HD21	2.17	0.42
1:F:126:ILE:HD11	1:F:209:THR:HG21	2.02	0.42
1:F:183:LYS:HG3	1:F:190:ALA:HA	2.01	0.42
1:C:218:ARG:NH2	1:D:221:ASN:O	2.53	0.42
1:G:126:ILE:HD11	1:G:209:THR:HG21	2.02	0.42
1:I:174:SER:OG	1:I:197:THR:HG22	2.20	0.42
1:D:13:ALA:O	1:D:17:ARG:HD2	2.20	0.41
2:F:9411:GTP:O3G	1:J:185:ARG:NH2	2.51	0.41
1:I:138:ASN:N	1:I:138:ASN:ND2	2.66	0.41
1:B:213:PHE:O	1:B:217:VAL:HG23	2.20	0.41
1:F:98:MET:HE1	1:F:124:ALA:HB1	2.03	0.41
1:C:185:ARG:HG2	1:C:186:GLY:H	1.85	0.41
1:C:28:HIS:O	1:C:28:HIS:ND1	2.54	0.41
1:D:198:SER:HA	1:E:97:GLU:HG3	2.02	0.41
1:E:123:VAL:HG22	1:E:173:VAL:HG22	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:97:GLU:O	1:G:127:PRO:HD2	2.21	0.41
1:J:138:ASN:N	1:J:138:ASN:ND2	2.68	0.40
1:A:214:LEU:HB3	1:B:215:ARG:HH22	1.85	0.40
1:B:100:THR:HG23	1:B:124:ALA:HB2	2.02	0.40
1:F:176:ASP:OD2	1:G:102:ARG:NH2	2.55	0.40
1:J:98:MET:HE3	1:J:100:THR:OG1	2.21	0.40
1:B:135:SER:O	1:B:139:ARG:HG3	2.21	0.40
1:C:3:LEU:HD21	1:C:80:TYR:HB3	2.03	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:1423:HOH:O	3:J:8425:HOH:O[8_655]	2.04	0.16
3:D:2421:HOH:O	3:I:7429:HOH:O[8_655]	2.15	0.05

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	219/221 (99%)	204 (93%)	12 (6%)	3 (1%)	9	11
1	B	219/221 (99%)	203 (93%)	13 (6%)	3 (1%)	9	11
1	C	219/221 (99%)	199 (91%)	16 (7%)	4 (2%)	6	7
1	D	219/221 (99%)	199 (91%)	17 (8%)	3 (1%)	9	11
1	E	219/221 (99%)	201 (92%)	15 (7%)	3 (1%)	9	11
1	F	219/221 (99%)	194 (89%)	21 (10%)	4 (2%)	6	7
1	G	219/221 (99%)	203 (93%)	12 (6%)	4 (2%)	6	7
1	H	219/221 (99%)	201 (92%)	14 (6%)	4 (2%)	6	7
1	I	219/221 (99%)	203 (93%)	14 (6%)	2 (1%)	14	20

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	J	219/221 (99%)	201 (92%)	15 (7%)	3 (1%)	9	11
All	All	2190/2210 (99%)	2008 (92%)	149 (7%)	33 (2%)	8	10

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	27	VAL
1	C	23	LEU
1	C	25	PRO
1	C	27	VAL
1	C	29	GLU
1	D	27	VAL
1	D	28	HIS
1	F	22	PRO
1	F	25	PRO
1	F	27	VAL
1	F	94	LYS
1	G	26	PRO
1	D	29	GLU
1	G	27	VAL
1	H	27	VAL
1	I	22	PRO
1	I	27	VAL
1	A	22	PRO
1	A	218	ARG
1	B	22	PRO
1	E	22	PRO
1	E	27	VAL
1	J	22	PRO
1	J	27	VAL
1	G	28	HIS
1	H	22	PRO
1	H	26	PRO
1	B	218	ARG
1	E	95	VAL
1	J	2	SER
1	H	95	VAL
1	B	95	VAL
1	G	95	VAL

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	194/194 (100%)	175 (90%)	19 (10%)	7	9
1	B	194/194 (100%)	187 (96%)	7 (4%)	31	46
1	C	194/194 (100%)	180 (93%)	14 (7%)	13	18
1	D	194/194 (100%)	184 (95%)	10 (5%)	21	32
1	E	194/194 (100%)	182 (94%)	12 (6%)	16	24
1	F	194/194 (100%)	182 (94%)	12 (6%)	16	24
1	G	194/194 (100%)	181 (93%)	13 (7%)	15	21
1	H	194/194 (100%)	186 (96%)	8 (4%)	27	41
1	I	194/194 (100%)	187 (96%)	7 (4%)	31	46
1	J	194/194 (100%)	186 (96%)	8 (4%)	27	41
All	All	1940/1940 (100%)	1830 (94%)	110 (6%)	18	28

All (110) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	SER
1	A	24	ARG
1	A	33	GLU
1	A	79	ASP
1	A	95	VAL
1	A	97	GLU
1	A	98	MET
1	A	102	ARG
1	A	112	HIS
1	A	120	LYS
1	A	138	ASN
1	A	168	THR
1	A	192	SER
1	A	197	THR
1	A	199	LEU
1	A	206	SER

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Mol	Chain	Res	Type
1	A	207	GLN
1	A	215	ARG
1	A	217	VAL
1	B	68	LYS
1	B	89	ILE
1	B	96	ASP
1	B	138	ASN
1	B	168	THR
1	B	209	THR
1	B	218	ARG
1	C	3	LEU
1	C	12	GLU
1	C	21	THR
1	C	25	PRO
1	C	33	GLU
1	C	44	THR
1	C	93	MET
1	C	120	LYS
1	C	168	THR
1	C	176	ASP
1	C	197	THR
1	C	207	GLN
1	C	209	THR
1	C	218	ARG
1	D	9	LEU
1	D	25	PRO
1	D	33	GLU
1	D	95	VAL
1	D	109	THR
1	D	112	HIS
1	D	138	ASN
1	D	168	THR
1	D	207	GLN
1	D	218	ARG
1	E	12	GLU
1	E	17	ARG
1	E	22	PRO
1	E	23	LEU
1	E	33	GLU
1	E	44	THR
1	E	93	MET
1	E	102	ARG

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Mol	Chain	Res	Type
1	E	112	HIS
1	E	168	THR
1	E	197	THR
1	E	218	ARG
1	F	12	GLU
1	F	21	THR
1	F	22	PRO
1	F	58	SER
1	F	68	LYS
1	F	95	VAL
1	F	98	MET
1	F	112	HIS
1	F	138	ASN
1	F	168	THR
1	F	197	THR
1	F	209	THR
1	G	20	GLU
1	G	23	LEU
1	G	25	PRO
1	G	26	PRO
1	G	30	MET
1	G	68	LYS
1	G	89	ILE
1	G	102	ARG
1	G	120	LYS
1	G	146	GLN
1	G	168	THR
1	G	197	THR
1	G	209	THR
1	H	22	PRO
1	H	23	LEU
1	H	26	PRO
1	H	68	LYS
1	H	88	LEU
1	H	151	GLN
1	H	168	THR
1	H	209	THR
1	I	25	PRO
1	I	37	SER
1	I	93	MET
1	I	138	ASN
1	I	168	THR

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Mol	Chain	Res	Type
1	I	209	THR
1	I	218	ARG
1	J	9	LEU
1	J	33	GLU
1	J	68	LYS
1	J	120	LYS
1	J	138	ASN
1	J	168	THR
1	J	197	THR
1	J	218	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (64) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	112	HIS
1	A	138	ASN
1	A	156	GLN
1	A	163	GLN
1	A	208	ASN
1	B	11	HIS
1	B	138	ASN
1	B	156	GLN
1	B	163	GLN
1	C	32	ASN
1	C	112	HIS
1	C	138	ASN
1	C	156	GLN
1	C	163	GLN
1	C	208	ASN
1	C	219	HIS
1	C	220	HIS
1	D	138	ASN
1	D	146	GLN
1	D	163	GLN
1	D	211	HIS
1	D	219	HIS
1	D	220	HIS
1	E	11	HIS
1	E	146	GLN
1	E	163	GLN
1	E	207	GLN
1	E	208	ASN

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Mol	Chain	Res	Type
1	E	220	HIS
1	E	221	ASN
1	F	11	HIS
1	F	48	GLN
1	F	64	HIS
1	F	138	ASN
1	F	156	GLN
1	F	163	GLN
1	F	207	GLN
1	F	208	ASN
1	F	221	ASN
1	G	32	ASN
1	G	138	ASN
1	G	156	GLN
1	G	163	GLN
1	G	220	HIS
1	H	11	HIS
1	H	112	HIS
1	H	138	ASN
1	H	146	GLN
1	H	207	GLN
1	H	220	HIS
1	I	32	ASN
1	I	82	ASN
1	I	138	ASN
1	I	146	GLN
1	I	156	GLN
1	I	163	GLN
1	I	208	ASN
1	J	112	HIS
1	J	138	ASN
1	J	146	GLN
1	J	156	GLN
1	J	163	GLN
1	J	208	ASN
1	J	221	ASN

5.3.3 RNA ⓘ

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

10 ligands are modelled in this entry.

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$
2	GTP	D	2411	-	33,34,34	2.90	14 (42%)	50,54,54	2.87	18 (36%)
2	GTP	C	1411	-	33,34,34	2.93	14 (42%)	50,54,54	2.87	19 (38%)
2	GTP	A	4411	-	33,34,34	2.90	13 (39%)	50,54,54	2.83	18 (36%)
2	GTP	I	7411	-	33,34,34	3.01	12 (36%)	50,54,54	2.86	18 (36%)
2	GTP	E	3411	-	33,34,34	2.77	15 (45%)	50,54,54	2.79	17 (34%)
2	GTP	H	6411	-	33,34,34	2.99	12 (36%)	50,54,54	2.79	17 (34%)
2	GTP	F	9411	-	33,34,34	2.86	13 (39%)	50,54,54	2.82	19 (38%)
2	GTP	G	5411	-	33,34,34	2.82	13 (39%)	50,54,54	2.83	17 (34%)
2	GTP	J	8411	-	33,34,34	2.71	13 (39%)	50,54,54	2.91	18 (36%)
2	GTP	B	411	-	33,34,34	2.94	13 (39%)	50,54,54	2.83	19 (38%)

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
2	GTP	D	2411	-	-	4/22/38/38	0/3/3/3
2	GTP	C	1411	-	-	5/22/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GTP	A	4411	-	-	4/22/38/38	0/3/3/3
2	GTP	I	7411	-	-	4/22/38/38	0/3/3/3
2	GTP	E	3411	-	-	4/22/38/38	0/3/3/3
2	GTP	H	6411	-	-	4/22/38/38	0/3/3/3
2	GTP	F	9411	-	-	4/22/38/38	0/3/3/3
2	GTP	G	5411	-	-	5/22/38/38	0/3/3/3
2	GTP	J	8411	-	-	4/22/38/38	0/3/3/3
2	GTP	B	411	-	-	4/22/38/38	0/3/3/3

All (132) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	411	GTP	C6-N1	9.09	1.55	1.38
2	F	9411	GTP	C6-N1	8.81	1.55	1.38
2	H	6411	GTP	C6-N1	8.71	1.55	1.38
2	A	4411	GTP	C6-N1	8.61	1.55	1.38
2	I	7411	GTP	C6-N1	8.60	1.55	1.38
2	E	3411	GTP	C6-N1	8.59	1.54	1.38
2	C	1411	GTP	C6-N1	8.46	1.54	1.38
2	G	5411	GTP	C6-N1	8.45	1.54	1.38
2	D	2411	GTP	C6-N1	8.44	1.54	1.38
2	J	8411	GTP	C6-N1	8.12	1.54	1.38
2	H	6411	GTP	C2-N2	7.04	1.50	1.34
2	I	7411	GTP	C2-N2	6.97	1.50	1.34
2	A	4411	GTP	C2-N2	6.85	1.50	1.34
2	D	2411	GTP	C2-N2	6.79	1.50	1.34
2	F	9411	GTP	C2-N2	6.78	1.50	1.34
2	C	1411	GTP	C2-N2	6.77	1.50	1.34
2	I	7411	GTP	PB-O3B	6.72	1.66	1.59
2	B	411	GTP	C2-N2	6.55	1.49	1.34
2	G	5411	GTP	C2-N2	6.51	1.49	1.34
2	E	3411	GTP	C2-N2	6.40	1.49	1.34
2	H	6411	GTP	PB-O3B	6.33	1.66	1.59
2	J	8411	GTP	C2-N2	6.27	1.48	1.34
2	C	1411	GTP	PB-O3B	5.44	1.65	1.59
2	F	9411	GTP	C5-C6	-5.13	1.25	1.44
2	A	4411	GTP	PB-O3B	5.10	1.65	1.59
2	G	5411	GTP	PB-O3B	5.00	1.64	1.59
2	J	8411	GTP	C5-C6	-4.91	1.26	1.44
2	I	7411	GTP	C5-C6	-4.85	1.26	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	2411	GTP	C5-C6	-4.84	1.26	1.44
2	H	6411	GTP	C5-C6	-4.81	1.26	1.44
2	E	3411	GTP	C5-C6	-4.72	1.27	1.44
2	B	411	GTP	PB-O3B	4.63	1.64	1.59
2	B	411	GTP	O2'-C2'	-4.51	1.31	1.43
2	B	411	GTP	C5-C6	-4.49	1.28	1.44
2	A	4411	GTP	C5-C6	-4.47	1.28	1.44
2	C	1411	GTP	C5-C6	-4.46	1.28	1.44
2	D	2411	GTP	C2'-C1'	4.42	1.67	1.53
2	C	1411	GTP	C2'-C1'	4.41	1.67	1.53
2	H	6411	GTP	O2'-C2'	-4.40	1.32	1.43
2	F	9411	GTP	PB-O3A	-4.37	1.54	1.59
2	I	7411	GTP	O2'-C2'	-4.35	1.32	1.43
2	G	5411	GTP	C5-C6	-4.35	1.28	1.44
2	A	4411	GTP	O2'-C2'	-4.33	1.32	1.43
2	G	5411	GTP	O2'-C2'	-4.29	1.32	1.43
2	E	3411	GTP	O2'-C2'	-4.27	1.32	1.43
2	C	1411	GTP	O2'-C2'	-4.25	1.32	1.43
2	J	8411	GTP	O2'-C2'	-4.25	1.32	1.43
2	I	7411	GTP	C2'-C1'	4.22	1.66	1.53
2	J	8411	GTP	C2'-C1'	4.20	1.66	1.53
2	D	2411	GTP	O2'-C2'	-4.18	1.32	1.43
2	D	2411	GTP	PB-O3B	4.16	1.64	1.59
2	H	6411	GTP	C2'-C1'	4.10	1.66	1.53
2	C	1411	GTP	PB-O3A	-4.09	1.55	1.59
2	D	2411	GTP	PB-O3A	-4.04	1.55	1.59
2	F	9411	GTP	O2'-C2'	-4.02	1.33	1.43
2	E	3411	GTP	C2'-C1'	3.96	1.65	1.53
2	A	4411	GTP	C2'-C1'	3.90	1.65	1.53
2	B	411	GTP	PB-O3A	-3.84	1.55	1.59
2	B	411	GTP	C2'-C1'	3.79	1.65	1.53
2	F	9411	GTP	C2'-C1'	3.78	1.65	1.53
2	G	5411	GTP	C2'-C1'	3.69	1.65	1.53
2	E	3411	GTP	PB-O3B	3.40	1.63	1.59
2	A	4411	GTP	PA-O3A	3.36	1.63	1.59
2	F	9411	GTP	C5'-C4'	3.30	1.61	1.51
2	J	8411	GTP	PB-O3B	3.28	1.63	1.59
2	B	411	GTP	C2-N1	-3.27	1.29	1.37
2	J	8411	GTP	C2-N1	-3.18	1.29	1.37
2	G	5411	GTP	PB-O3A	-3.17	1.56	1.59
2	E	3411	GTP	C2-N1	-3.12	1.30	1.37
2	A	4411	GTP	C2-N1	-3.05	1.30	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	4411	GTP	C5'-C4'	2.95	1.60	1.51
2	F	9411	GTP	C2-N1	-2.92	1.30	1.37
2	G	5411	GTP	PG-O3G	-2.91	1.44	1.54
2	I	7411	GTP	C5'-C4'	2.89	1.60	1.51
2	H	6411	GTP	PB-O3A	-2.89	1.56	1.59
2	H	6411	GTP	C5'-C4'	2.85	1.60	1.51
2	D	2411	GTP	PA-O3A	2.84	1.62	1.59
2	C	1411	GTP	PG-O3G	-2.84	1.44	1.54
2	D	2411	GTP	C2-N1	-2.83	1.30	1.37
2	F	9411	GTP	PG-O3G	-2.83	1.44	1.54
2	A	4411	GTP	C3'-C4'	-2.81	1.45	1.53
2	H	6411	GTP	PG-O3G	-2.76	1.44	1.54
2	C	1411	GTP	C2-N1	-2.72	1.31	1.37
2	J	8411	GTP	PG-O3G	-2.70	1.44	1.54
2	B	411	GTP	PG-O3G	-2.70	1.44	1.54
2	D	2411	GTP	PG-O3G	-2.68	1.44	1.54
2	E	3411	GTP	C5'-C4'	2.67	1.59	1.51
2	B	411	GTP	C3'-C4'	-2.66	1.46	1.53
2	G	5411	GTP	C2-N1	-2.66	1.31	1.37
2	G	5411	GTP	C5'-C4'	2.64	1.59	1.51
2	I	7411	GTP	C2-N1	-2.64	1.31	1.37
2	I	7411	GTP	PB-O3A	-2.63	1.56	1.59
2	H	6411	GTP	C3'-C4'	-2.62	1.46	1.53
2	B	411	GTP	C5'-C4'	2.61	1.59	1.51
2	E	3411	GTP	PG-O3G	-2.59	1.45	1.54
2	H	6411	GTP	C2-N1	-2.58	1.31	1.37
2	I	7411	GTP	C3'-C4'	-2.58	1.46	1.53
2	J	8411	GTP	C3'-C4'	-2.58	1.46	1.53
2	D	2411	GTP	C5'-C4'	2.57	1.59	1.51
2	E	3411	GTP	PA-O3A	2.56	1.62	1.59
2	E	3411	GTP	PB-O3A	-2.55	1.56	1.59
2	C	1411	GTP	C5'-C4'	2.55	1.59	1.51
2	A	4411	GTP	PG-O3G	-2.48	1.45	1.54
2	D	2411	GTP	C5-C4	-2.47	1.31	1.38
2	I	7411	GTP	PG-O3G	-2.46	1.45	1.54
2	F	9411	GTP	C3'-C4'	-2.45	1.46	1.53
2	J	8411	GTP	PB-O3A	-2.44	1.56	1.59
2	F	9411	GTP	C5-C4	-2.43	1.31	1.38
2	F	9411	GTP	PB-O3B	2.41	1.62	1.59
2	B	411	GTP	O6-C6	2.41	1.28	1.23
2	E	3411	GTP	C3'-C4'	-2.40	1.46	1.53
2	E	3411	GTP	C5-C4	-2.27	1.32	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	8411	GTP	C5'-C4'	2.25	1.58	1.51
2	A	4411	GTP	C5-C4	-2.22	1.32	1.38
2	B	411	GTP	PB-O2B	-2.20	1.45	1.55
2	D	2411	GTP	C3'-C4'	-2.20	1.47	1.53
2	I	7411	GTP	C5-C4	-2.19	1.32	1.38
2	D	2411	GTP	PB-O2B	-2.16	1.45	1.55
2	G	5411	GTP	C3'-C4'	-2.16	1.47	1.53
2	E	3411	GTP	PB-O2B	-2.15	1.45	1.55
2	J	8411	GTP	C5-C4	-2.14	1.32	1.38
2	C	1411	GTP	C5-C4	-2.12	1.32	1.38
2	G	5411	GTP	PA-O5'	2.12	1.67	1.59
2	C	1411	GTP	O6-C6	2.11	1.27	1.23
2	G	5411	GTP	C5-C4	-2.09	1.32	1.38
2	A	4411	GTP	PA-O5'	2.09	1.67	1.59
2	C	1411	GTP	PA-O3A	2.07	1.61	1.59
2	C	1411	GTP	C3'-C4'	-2.07	1.47	1.53
2	H	6411	GTP	C5-C4	-2.05	1.32	1.38
2	F	9411	GTP	PB-O2B	-2.04	1.45	1.55
2	J	8411	GTP	PA-O3A	2.02	1.61	1.59
2	E	3411	GTP	PA-O5'	2.01	1.67	1.59

All (180) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	7411	GTP	N9-C8-N7	-8.51	97.62	113.40
2	J	8411	GTP	N9-C8-N7	-8.37	97.87	113.40
2	D	2411	GTP	N9-C8-N7	-8.35	97.91	113.40
2	F	9411	GTP	N9-C8-N7	-8.31	97.99	113.40
2	C	1411	GTP	N9-C8-N7	-8.26	98.08	113.40
2	A	4411	GTP	N9-C8-N7	-8.19	98.22	113.40
2	H	6411	GTP	N9-C8-N7	-8.15	98.28	113.40
2	G	5411	GTP	N9-C8-N7	-8.09	98.39	113.40
2	E	3411	GTP	N9-C8-N7	-8.03	98.52	113.40
2	B	411	GTP	N9-C8-N7	-7.97	98.62	113.40
2	D	2411	GTP	C8-N7-C5	6.59	116.00	104.26
2	C	1411	GTP	C8-N7-C5	6.41	115.67	104.26
2	A	4411	GTP	C8-N7-C5	6.40	115.67	104.26
2	H	6411	GTP	C8-N7-C5	6.39	115.63	104.26
2	J	8411	GTP	C8-N7-C5	6.38	115.62	104.26
2	G	5411	GTP	C8-N7-C5	6.29	115.47	104.26
2	B	411	GTP	C8-N7-C5	6.27	115.43	104.26
2	F	9411	GTP	C8-N7-C5	6.24	115.38	104.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	3411	GTP	C8-N7-C5	6.24	115.38	104.26
2	I	7411	GTP	C8-N7-C5	6.19	115.29	104.26
2	A	4411	GTP	O6-C6-N1	-6.08	108.69	120.11
2	E	3411	GTP	O6-C6-N1	-5.93	108.97	120.11
2	G	5411	GTP	O6-C6-N1	-5.90	109.01	120.11
2	I	7411	GTP	O6-C6-N1	-5.90	109.03	120.11
2	J	8411	GTP	O6-C6-N1	-5.88	109.06	120.11
2	B	411	GTP	O6-C6-N1	-5.81	109.18	120.11
2	F	9411	GTP	C2-N1-C6	-5.60	114.96	125.11
2	C	1411	GTP	O6-C6-N1	-5.59	109.60	120.11
2	H	6411	GTP	O6-C6-N1	-5.56	109.66	120.11
2	E	3411	GTP	C2-N1-C6	-5.48	115.17	125.11
2	A	4411	GTP	C2-N1-C6	-5.43	115.26	125.11
2	B	411	GTP	C2-N1-C6	-5.41	115.29	125.11
2	J	8411	GTP	C2-N1-C6	-5.38	115.34	125.11
2	I	7411	GTP	C2-N1-C6	-5.37	115.38	125.11
2	D	2411	GTP	C2-N1-C6	-5.36	115.39	125.11
2	C	1411	GTP	N1-C2-N3	5.35	133.12	123.32
2	C	1411	GTP	C2-N1-C6	-5.35	115.40	125.11
2	J	8411	GTP	N1-C2-N3	5.32	133.06	123.32
2	H	6411	GTP	C2-N1-C6	-5.31	115.48	125.11
2	G	5411	GTP	C2-N1-C6	-5.31	115.49	125.11
2	D	2411	GTP	C6-C5-C4	5.30	126.81	118.83
2	D	2411	GTP	O6-C6-N1	-5.29	110.17	120.11
2	B	411	GTP	N1-C2-N3	5.27	132.97	123.32
2	F	9411	GTP	O6-C6-N1	-5.26	110.22	120.11
2	G	5411	GTP	N1-C2-N3	5.24	132.90	123.32
2	H	6411	GTP	C6-C5-C4	5.19	126.64	118.83
2	C	1411	GTP	C6-C5-C4	5.17	126.61	118.83
2	E	3411	GTP	N1-C2-N3	5.14	132.73	123.32
2	A	4411	GTP	N1-C2-N3	5.12	132.69	123.32
2	J	8411	GTP	C6-C5-C4	5.12	126.53	118.83
2	F	9411	GTP	N1-C2-N3	5.10	132.66	123.32
2	F	9411	GTP	C6-C5-C4	5.08	126.47	118.83
2	D	2411	GTP	N1-C2-N3	5.05	132.56	123.32
2	H	6411	GTP	N1-C2-N3	5.00	132.47	123.32
2	J	8411	GTP	O5'-C5'-C4'	-5.00	91.98	108.99
2	I	7411	GTP	C3'-C2'-C1'	-4.99	92.02	101.46
2	G	5411	GTP	O6-C6-C5	4.96	139.64	126.53
2	I	7411	GTP	N1-C2-N3	4.94	132.35	123.32
2	G	5411	GTP	C6-C5-C4	4.93	126.25	118.83
2	B	411	GTP	C6-C5-C4	4.92	126.23	118.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	411	GTP	O6-C6-C5	4.91	139.50	126.53
2	A	4411	GTP	O6-C6-C5	4.91	139.49	126.53
2	J	8411	GTP	O6-C6-C5	4.89	139.45	126.53
2	A	4411	GTP	C3'-C2'-C1'	-4.86	92.28	101.46
2	I	7411	GTP	O6-C6-C5	4.84	139.32	126.53
2	E	3411	GTP	C6-C5-C4	4.84	126.11	118.83
2	C	1411	GTP	O6-C6-C5	4.82	139.27	126.53
2	C	1411	GTP	C3'-C2'-C1'	-4.80	92.39	101.46
2	I	7411	GTP	C6-C5-C4	4.79	126.03	118.83
2	A	4411	GTP	C6-C5-C4	4.78	126.02	118.83
2	E	3411	GTP	O6-C6-C5	4.77	139.13	126.53
2	D	2411	GTP	O5'-C5'-C4'	-4.72	92.91	108.99
2	I	7411	GTP	O5'-C5'-C4'	-4.71	92.94	108.99
2	G	5411	GTP	C3'-C2'-C1'	-4.71	92.55	101.46
2	E	3411	GTP	C3'-C2'-C1'	-4.69	92.59	101.46
2	H	6411	GTP	O5'-C5'-C4'	-4.66	93.11	108.99
2	H	6411	GTP	O6-C6-C5	4.65	138.80	126.53
2	I	7411	GTP	C8-N9-C4	4.59	114.64	106.03
2	D	2411	GTP	C3'-C2'-C1'	-4.59	92.77	101.46
2	B	411	GTP	C3'-C2'-C1'	-4.59	92.78	101.46
2	J	8411	GTP	C8-N9-C4	4.59	114.62	106.03
2	D	2411	GTP	O6-C6-C5	4.50	138.42	126.53
2	F	9411	GTP	C3'-C2'-C1'	-4.50	92.95	101.46
2	D	2411	GTP	C8-N9-C4	4.50	114.46	106.03
2	F	9411	GTP	O5'-C5'-C4'	-4.44	93.89	108.99
2	G	5411	GTP	C8-N9-C4	4.43	114.33	106.03
2	F	9411	GTP	O6-C6-C5	4.42	138.21	126.53
2	F	9411	GTP	C8-N9-C4	4.42	114.30	106.03
2	J	8411	GTP	C3'-C2'-C1'	-4.41	93.13	101.46
2	C	1411	GTP	O5'-C5'-C4'	-4.40	94.00	108.99
2	H	6411	GTP	C8-N9-C4	4.39	114.25	106.03
2	A	4411	GTP	C8-N9-C4	4.35	114.19	106.03
2	C	1411	GTP	C8-N9-C4	4.31	114.11	106.03
2	E	3411	GTP	C8-N9-C4	4.30	114.08	106.03
2	F	9411	GTP	N2-C2-N3	-4.29	111.30	119.67
2	J	8411	GTP	N2-C2-N3	-4.28	111.31	119.67
2	B	411	GTP	C8-N9-C4	4.18	113.86	106.03
2	I	7411	GTP	N2-C2-N3	-4.16	111.55	119.67
2	G	5411	GTP	C4-C5-N7	-4.16	104.08	110.67
2	H	6411	GTP	C3'-C2'-C1'	-4.12	93.67	101.46
2	G	5411	GTP	N2-C2-N3	-4.11	111.64	119.67
2	A	4411	GTP	C4-C5-N7	-4.11	104.16	110.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	411	GTP	N2-C2-N3	-4.10	111.66	119.67
2	E	3411	GTP	O5'-C5'-C4'	-4.10	95.04	108.99
2	J	8411	GTP	C4-C5-N7	-4.08	104.21	110.67
2	A	4411	GTP	N2-C2-N3	-4.05	111.76	119.67
2	B	411	GTP	C4-C5-N7	-4.05	104.25	110.67
2	E	3411	GTP	N2-C2-N3	-4.01	111.84	119.67
2	I	7411	GTP	C4-C5-N7	-3.99	104.35	110.67
2	C	1411	GTP	C4-C5-N7	-3.98	104.36	110.67
2	H	6411	GTP	N2-C2-N3	-3.98	111.90	119.67
2	H	6411	GTP	C4-C5-N7	-3.98	104.37	110.67
2	C	1411	GTP	N2-C2-N3	-3.97	111.93	119.67
2	D	2411	GTP	N2-C2-N3	-3.95	111.96	119.67
2	D	2411	GTP	C4-C5-N7	-3.94	104.43	110.67
2	E	3411	GTP	C4-C5-N7	-3.84	104.58	110.67
2	G	5411	GTP	O5'-C5'-C4'	-3.79	96.08	108.99
2	B	411	GTP	O5'-C5'-C4'	-3.78	96.13	108.99
2	F	9411	GTP	C4-C5-N7	-3.74	104.74	110.67
2	G	5411	GTP	O4'-C1'-N9	3.47	116.23	108.36
2	C	1411	GTP	O4'-C1'-N9	3.41	116.09	108.36
2	A	4411	GTP	O5'-C5'-C4'	-3.41	97.39	108.99
2	D	2411	GTP	O4'-C1'-N9	3.35	115.95	108.36
2	B	411	GTP	O4'-C1'-N9	3.34	115.92	108.36
2	C	1411	GTP	C2-N3-C4	-3.34	106.55	112.30
2	J	8411	GTP	C2-N3-C4	-3.33	106.56	112.30
2	H	6411	GTP	C2-N3-C4	-3.28	106.64	112.30
2	G	5411	GTP	C2-N3-C4	-3.27	106.67	112.30
2	D	2411	GTP	C2-N3-C4	-3.17	106.83	112.30
2	F	9411	GTP	C2-N3-C4	-3.16	106.86	112.30
2	B	411	GTP	C2-N3-C4	-3.09	106.97	112.30
2	I	7411	GTP	C2-N3-C4	-3.08	106.98	112.30
2	A	4411	GTP	C2-N3-C4	-3.05	107.04	112.30
2	E	3411	GTP	C2-N3-C4	-3.04	107.06	112.30
2	J	8411	GTP	O4'-C4'-C5'	3.00	118.93	109.33
2	A	4411	GTP	O4'-C1'-N9	2.74	114.56	108.36
2	B	411	GTP	O4'-C4'-C5'	2.68	117.91	109.33
2	I	7411	GTP	O4'-C4'-C5'	2.67	117.87	109.33
2	H	6411	GTP	C2'-C3'-C4'	2.60	107.64	102.61
2	F	9411	GTP	O4'-C1'-N9	2.53	114.09	108.36
2	I	7411	GTP	C1'-N9-C4	-2.52	119.03	126.49
2	G	5411	GTP	O4'-C4'-C5'	2.51	117.39	109.33
2	I	7411	GTP	O4'-C1'-N9	2.51	114.05	108.36
2	F	9411	GTP	O2B-PB-O3A	2.47	113.96	107.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	6411	GTP	O4'-C4'-C5'	2.47	117.25	109.33
2	A	4411	GTP	O4'-C4'-C5'	2.47	117.24	109.33
2	G	5411	GTP	C2'-C3'-C4'	2.41	107.26	102.61
2	C	1411	GTP	O4'-C4'-C5'	2.40	117.04	109.33
2	J	8411	GTP	O4'-C1'-N9	2.40	113.80	108.36
2	G	5411	GTP	C1'-N9-C4	-2.39	119.43	126.49
2	J	8411	GTP	O2B-PB-O3A	2.38	113.71	107.27
2	F	9411	GTP	O4'-C4'-C5'	2.37	116.94	109.33
2	E	3411	GTP	O4'-C1'-N9	2.34	113.66	108.36
2	E	3411	GTP	O4'-C4'-C5'	2.34	116.82	109.33
2	E	3411	GTP	C2'-C3'-C4'	2.32	107.09	102.61
2	C	1411	GTP	O2B-PB-O3A	2.28	113.44	107.27
2	A	4411	GTP	O4'-C1'-C2'	-2.28	101.74	106.62
2	B	411	GTP	O4'-C1'-C2'	-2.26	101.78	106.62
2	I	7411	GTP	O4'-C1'-C2'	-2.22	101.86	106.62
2	A	4411	GTP	C2'-C3'-C4'	2.22	106.89	102.61
2	D	2411	GTP	C2'-C1'-N9	-2.21	107.09	113.25
2	A	4411	GTP	C1'-N9-C4	-2.21	119.95	126.49
2	B	411	GTP	C2'-C3'-C4'	2.20	106.86	102.61
2	J	8411	GTP	O4'-C1'-C2'	-2.19	101.93	106.62
2	D	2411	GTP	O4'-C4'-C5'	2.19	116.34	109.33
2	F	9411	GTP	C1'-N9-C4	-2.19	120.03	126.49
2	C	1411	GTP	C1'-N9-C4	-2.15	120.15	126.49
2	H	6411	GTP	O4'-C1'-N9	2.15	113.22	108.36
2	C	1411	GTP	O3A-PA-O1A	-2.13	104.31	110.70
2	D	2411	GTP	O2B-PB-O3A	2.12	113.01	107.27
2	J	8411	GTP	C1'-N9-C4	-2.11	120.25	126.49
2	B	411	GTP	O2B-PB-O3A	2.11	112.97	107.27
2	C	1411	GTP	C2'-C3'-C4'	2.09	106.65	102.61
2	F	9411	GTP	C2'-C3'-C4'	2.09	106.64	102.61
2	D	2411	GTP	C2'-C3'-C4'	2.08	106.64	102.61
2	H	6411	GTP	C1'-N9-C4	-2.07	120.36	126.49
2	B	411	GTP	C1'-N9-C4	-2.07	120.37	126.49
2	F	9411	GTP	O4'-C1'-C2'	-2.06	102.20	106.62
2	E	3411	GTP	C1'-N9-C4	-2.05	120.43	126.49
2	I	7411	GTP	C2'-C3'-C4'	2.02	106.51	102.61

There are no chirality outliers.

All (42) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	1411	GTP	PB-O3B-PG-O3G

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Mol	Chain	Res	Type	Atoms
2	H	6411	GTP	O4'-C4'-C5'-O5'
2	A	4411	GTP	O4'-C4'-C5'-O5'
2	B	411	GTP	O4'-C4'-C5'-O5'
2	C	1411	GTP	O4'-C4'-C5'-O5'
2	D	2411	GTP	O4'-C4'-C5'-O5'
2	E	3411	GTP	O4'-C4'-C5'-O5'
2	F	9411	GTP	O4'-C4'-C5'-O5'
2	G	5411	GTP	O4'-C4'-C5'-O5'
2	I	7411	GTP	O4'-C4'-C5'-O5'
2	J	8411	GTP	O4'-C4'-C5'-O5'
2	B	411	GTP	C3'-C4'-C5'-O5'
2	D	2411	GTP	C3'-C4'-C5'-O5'
2	F	9411	GTP	C3'-C4'-C5'-O5'
2	G	5411	GTP	C3'-C4'-C5'-O5'
2	H	6411	GTP	C3'-C4'-C5'-O5'
2	I	7411	GTP	C3'-C4'-C5'-O5'
2	A	4411	GTP	C3'-C4'-C5'-O5'
2	C	1411	GTP	C3'-C4'-C5'-O5'
2	E	3411	GTP	C3'-C4'-C5'-O5'
2	J	8411	GTP	C3'-C4'-C5'-O5'
2	A	4411	GTP	PA-O3A-PB-O2B
2	B	411	GTP	PA-O3A-PB-O2B
2	C	1411	GTP	PA-O3A-PB-O2B
2	D	2411	GTP	PA-O3A-PB-O2B
2	E	3411	GTP	PA-O3A-PB-O2B
2	F	9411	GTP	PA-O3A-PB-O2B
2	G	5411	GTP	PA-O3A-PB-O2B
2	H	6411	GTP	PA-O3A-PB-O2B
2	I	7411	GTP	PA-O3A-PB-O2B
2	J	8411	GTP	PA-O3A-PB-O2B
2	G	5411	GTP	PB-O3B-PG-O3G
2	A	4411	GTP	PA-O3A-PB-O1B
2	B	411	GTP	PA-O3A-PB-O1B
2	E	3411	GTP	PA-O3A-PB-O1B
2	F	9411	GTP	PA-O3A-PB-O1B
2	G	5411	GTP	PA-O3A-PB-O1B
2	H	6411	GTP	PA-O3A-PB-O1B
2	I	7411	GTP	PA-O3A-PB-O1B
2	J	8411	GTP	PA-O3A-PB-O1B
2	C	1411	GTP	PA-O3A-PB-O1B
2	D	2411	GTP	PA-O3A-PB-O1B

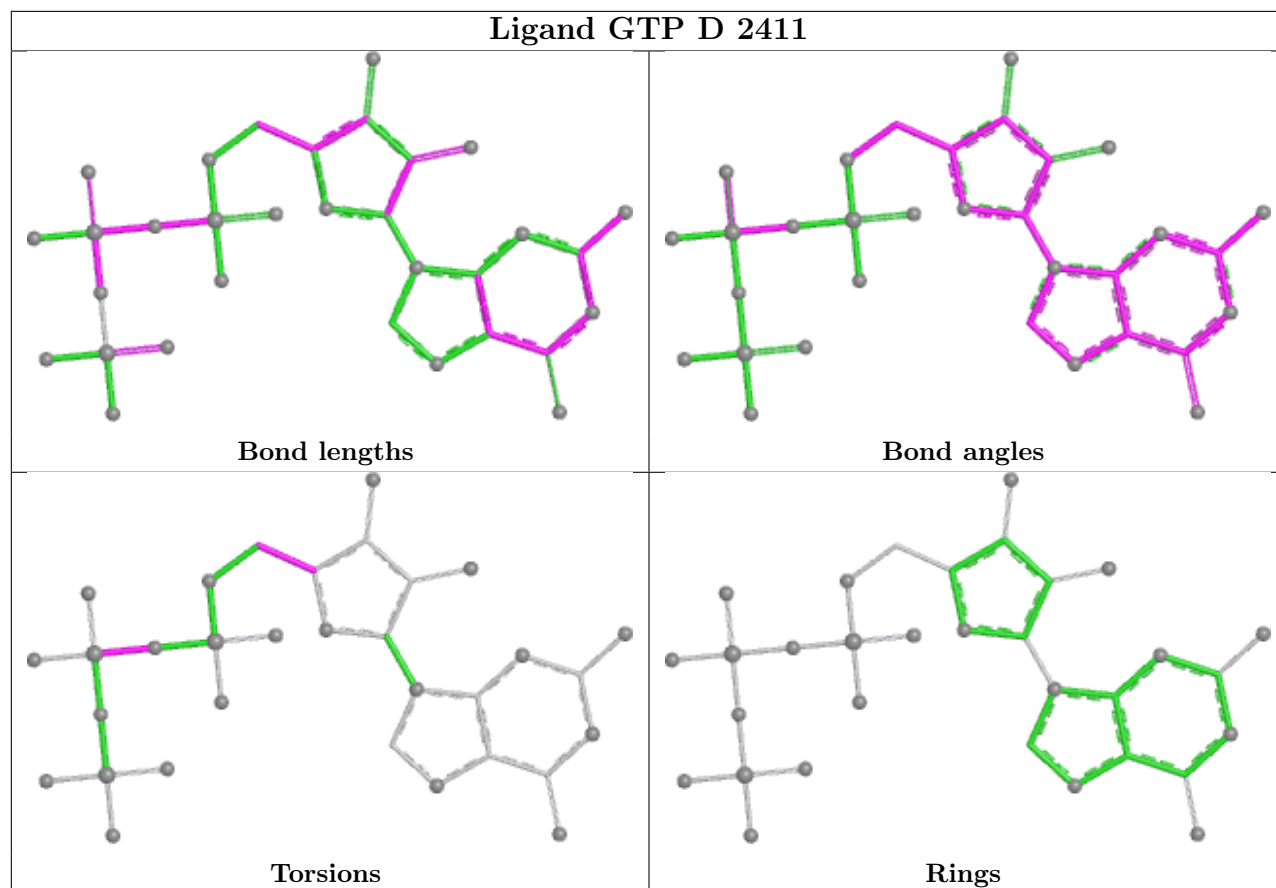
There are no ring outliers.

9 monomers are involved in 18 short contacts:

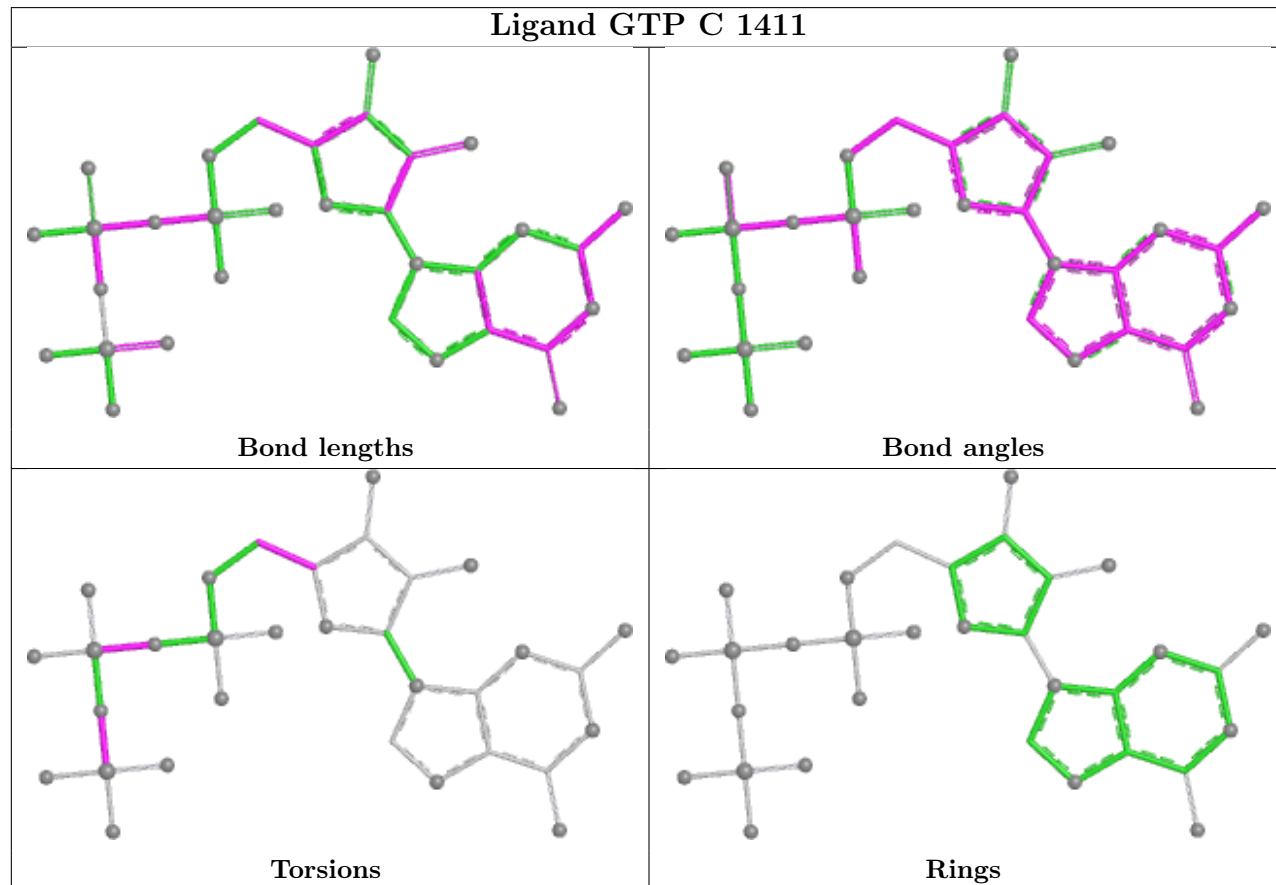
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	2411	GTP	2	0
2	C	1411	GTP	2	0
2	A	4411	GTP	1	0
2	I	7411	GTP	1	0
2	E	3411	GTP	3	0
2	H	6411	GTP	3	0
2	F	9411	GTP	3	0
2	G	5411	GTP	1	0
2	J	8411	GTP	2	0

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

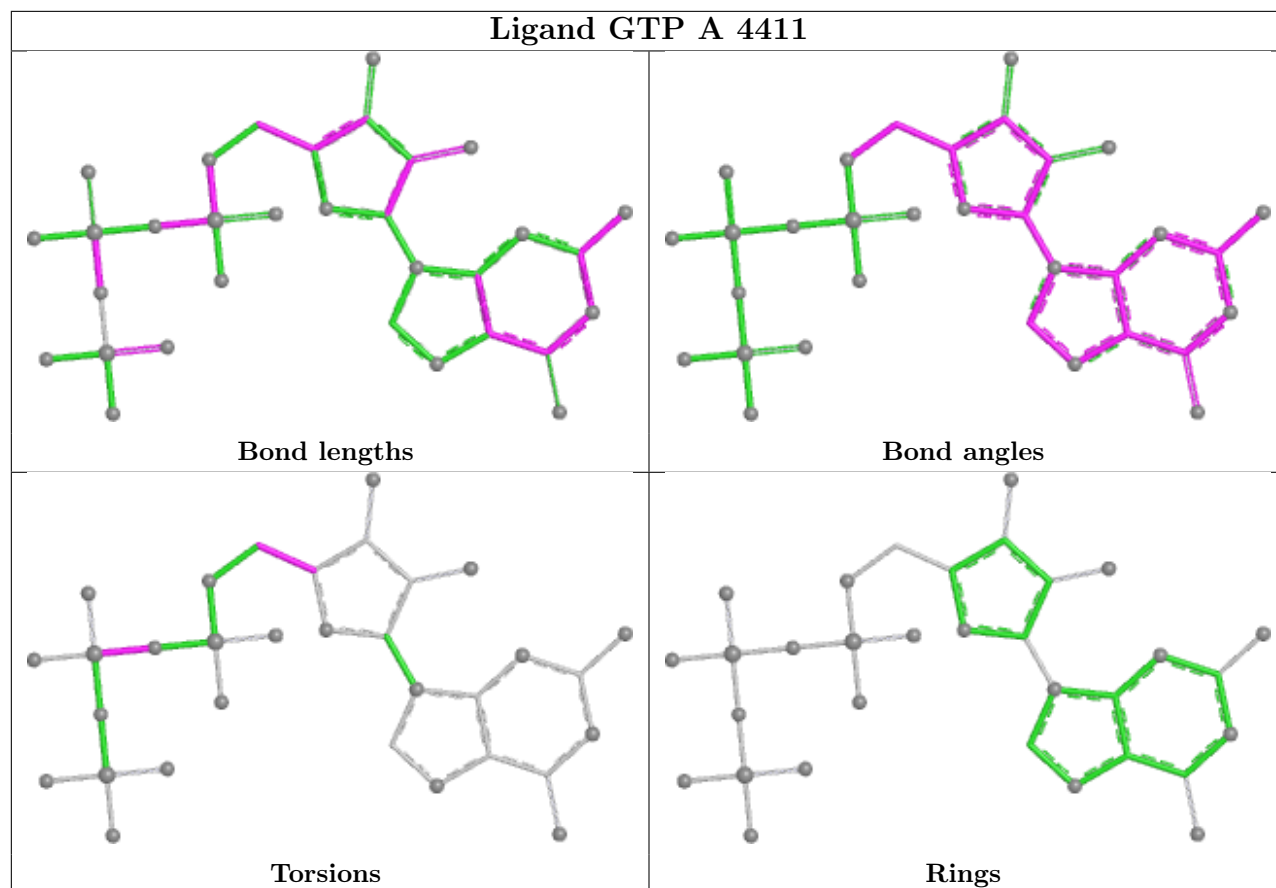
Ligand GTP D 2411



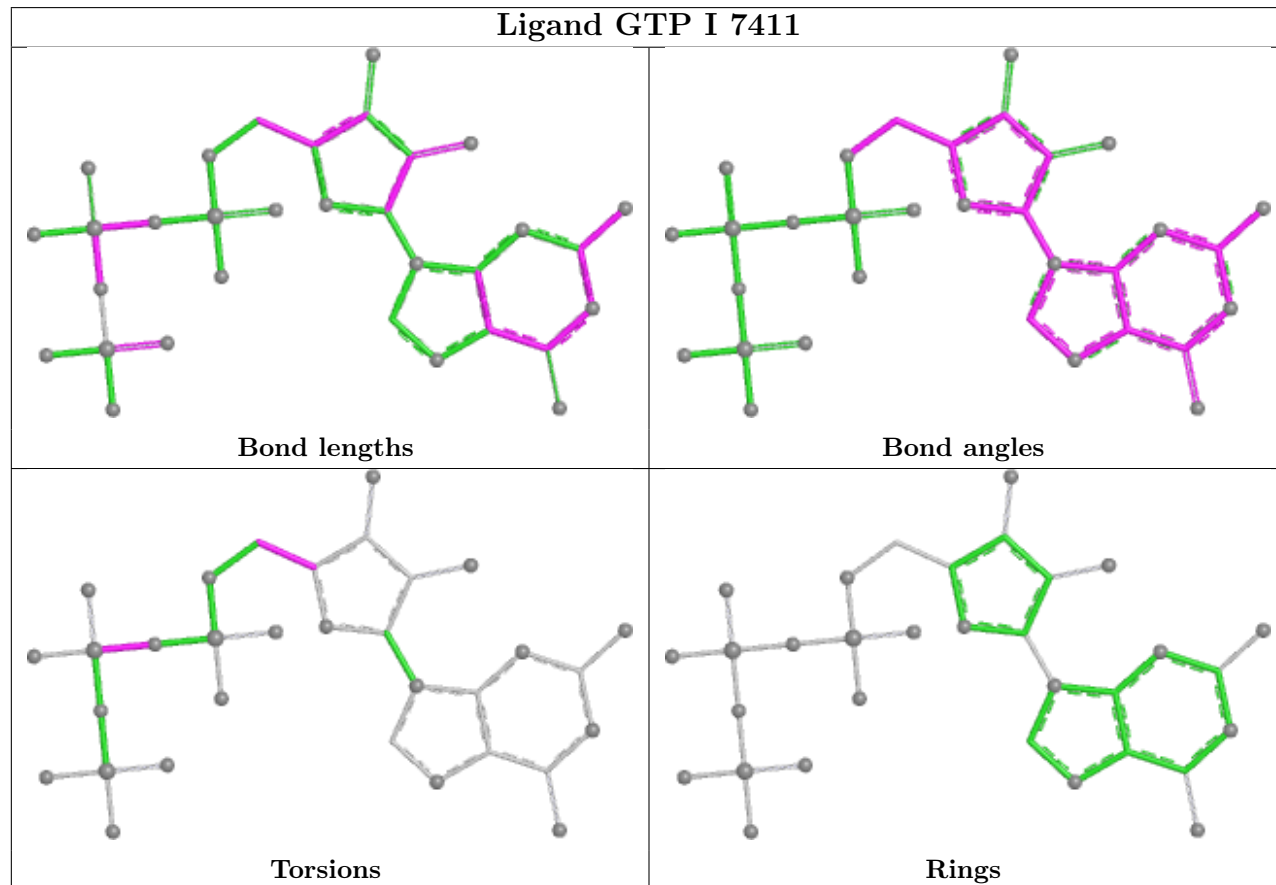
Ligand GTP C 1411



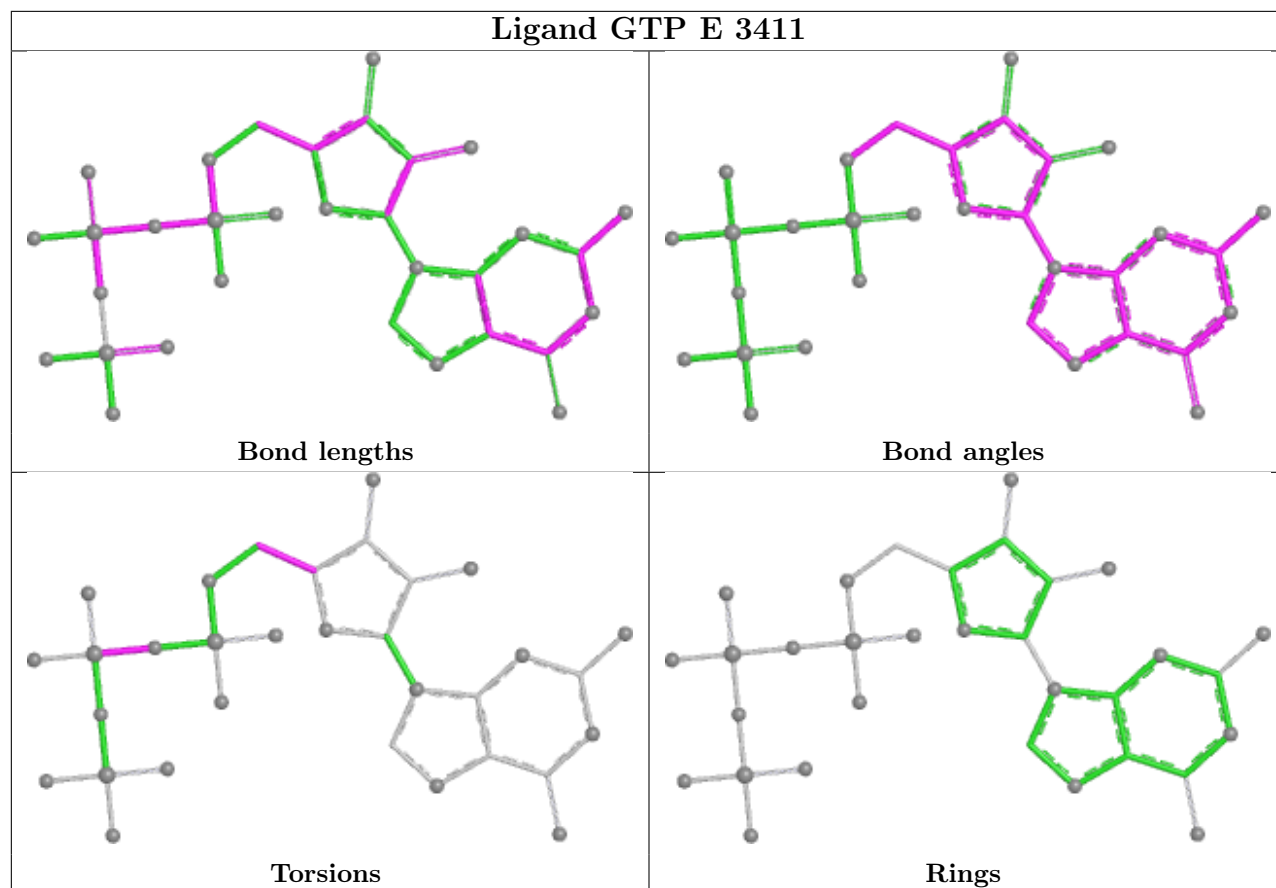
Ligand GTP A 4411



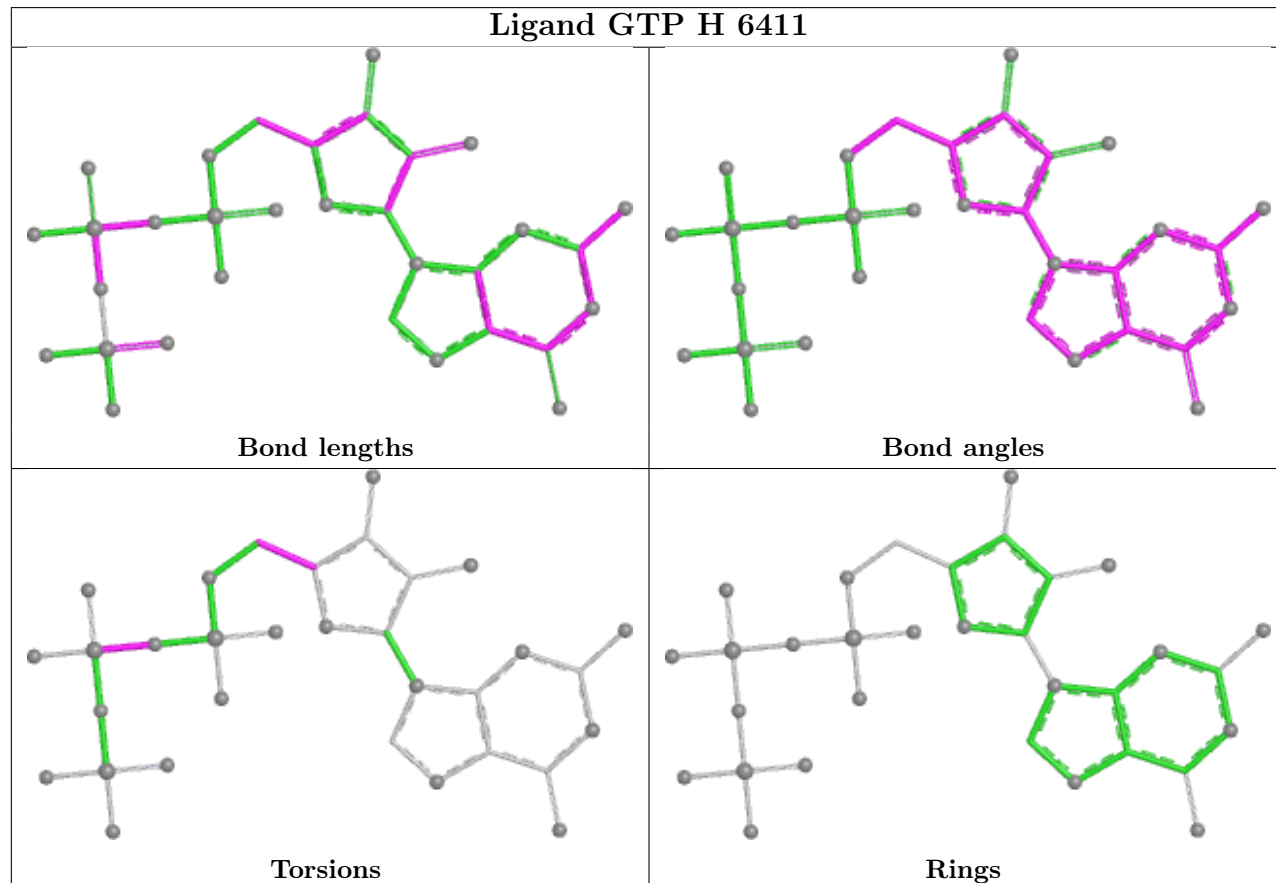
Ligand GTP I 7411



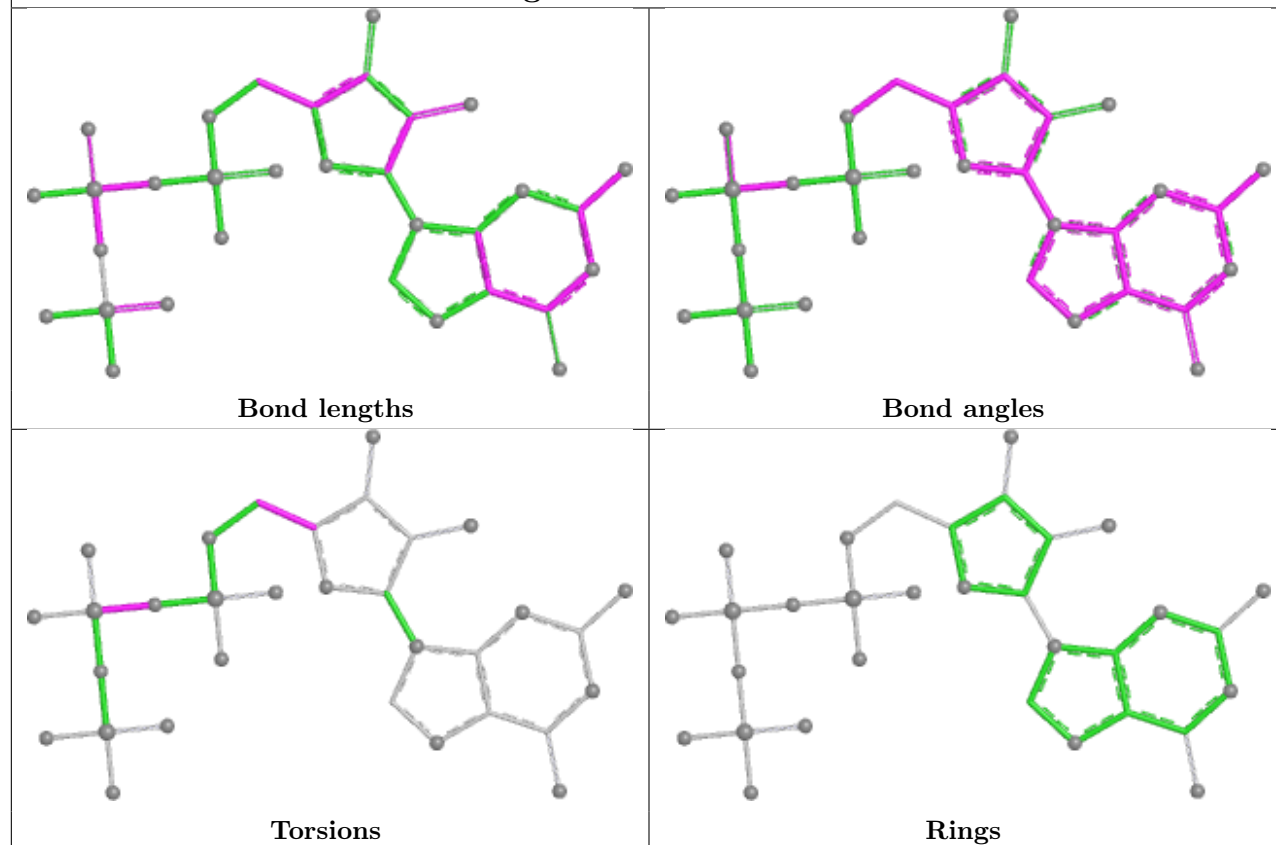
Ligand GTP E 3411



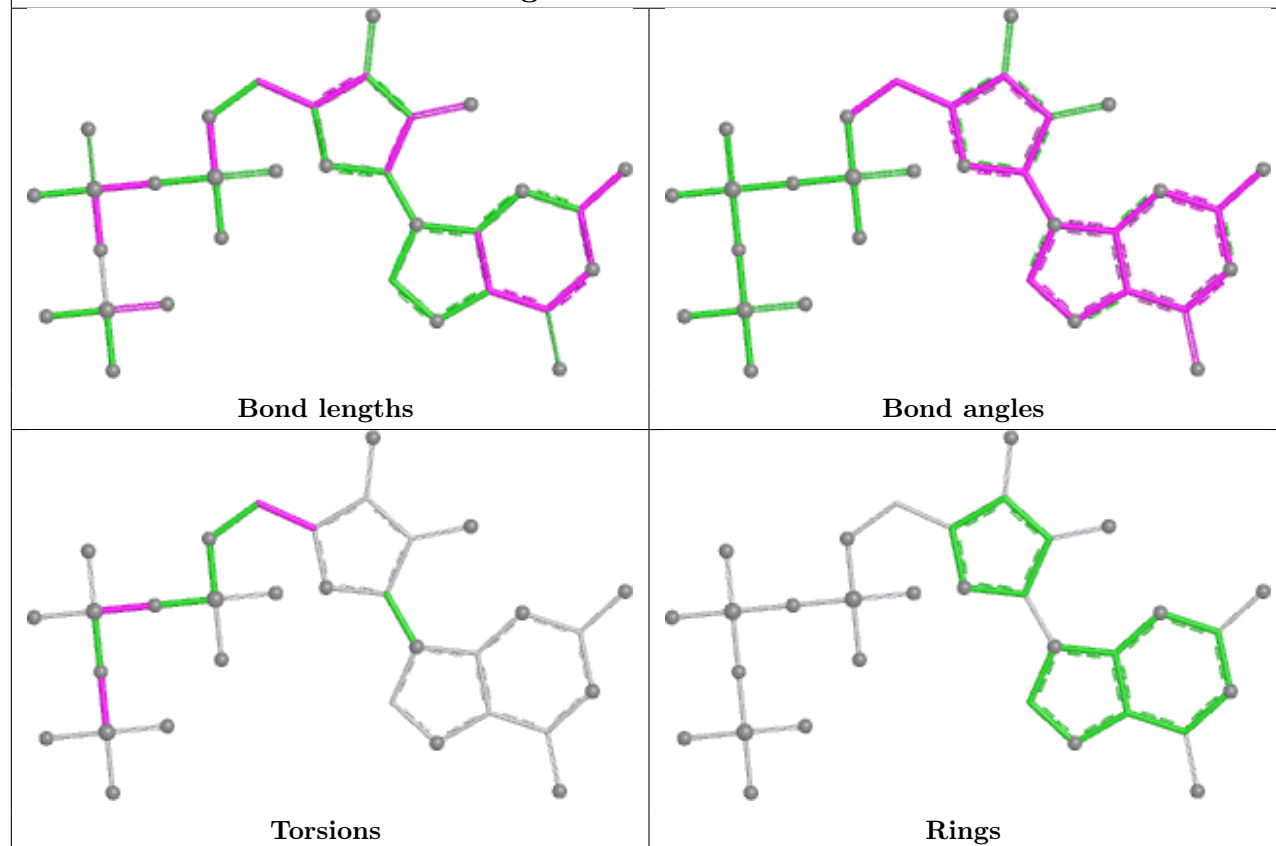
Ligand GTP H 6411



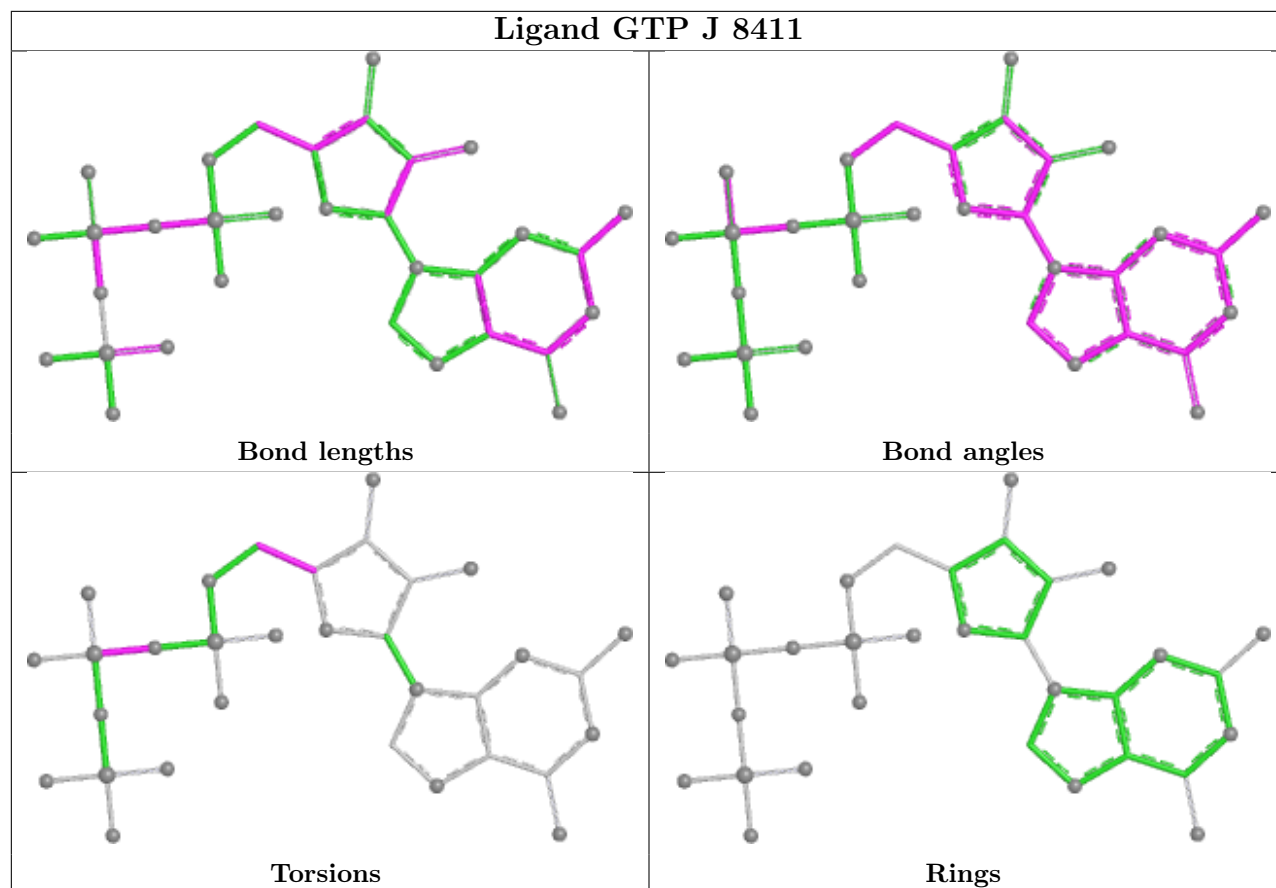
Ligand GTP F 9411



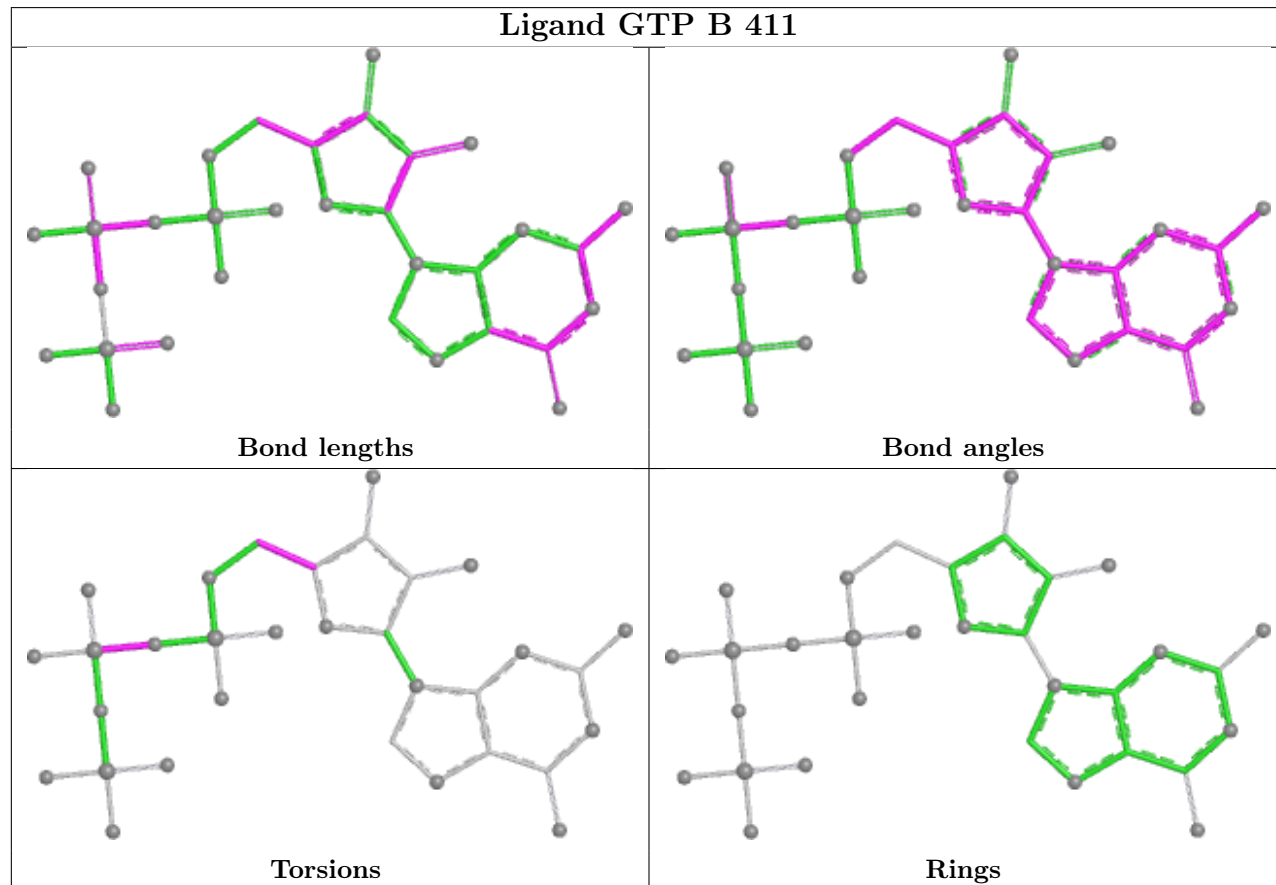
Ligand GTP G 5411



Ligand GTP J 8411



Ligand GTP B 411



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 ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.