



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 26, 2026 – 05:44 AM UTC

PDB ID : 9KQ9 / pdb_00009kq9
Title : The structure of the YcfA-GTP from Erwinia amylovora
Authors : Zhang, L.
Deposited on : 2024-11-25
Resolution : 2.59 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

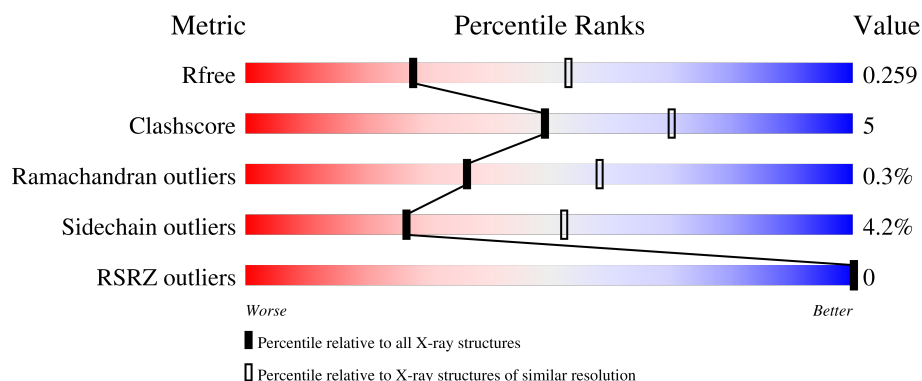
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.59 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	234	 81% 11% • 6%
1	B	234	 79% 13% • 6%
1	C	234	 75% 18% • 6%
1	D	234	 74% 17% • 6%
1	E	234	 78% 11% • 9%

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Mol	Chain	Length	Quality of chain
1	F	234	 76%13% • 7%
1	G	234	 80%9% • 9%
1	H	234	 82%10% • 6%
1	I	234	 74%14% • • 7%
1	J	234	 79%13% • 6%
1	K	234	 75%13%6%6%
1	L	234	 78%11% • 6%
1	M	234	 77%16% • 6%
1	N	234	 79%13% • 6%

2 Entry composition

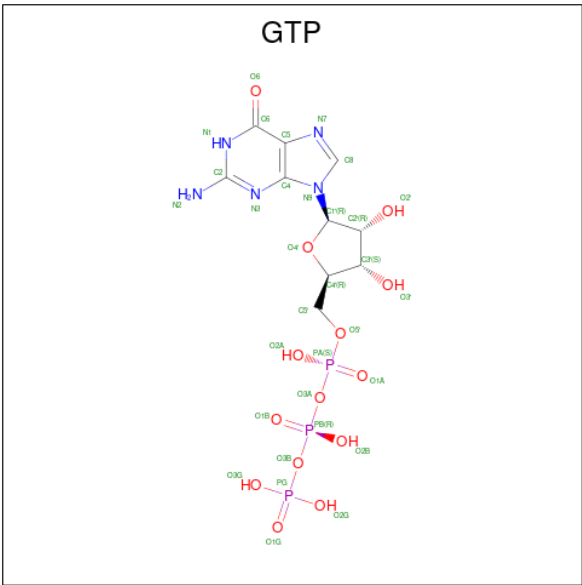
There are 3 unique types of molecules in this entry. The entry contains 24996 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Asparagine synthetase domain-containing protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	220	Total	C	N	O	S	0	0	0
			1732	1103	298	321	10			
1	C	221	Total	C	N	O	S	0	0	0
			1738	1106	299	323	10			
1	E	214	Total	C	N	O	S	0	0	0
			1686	1074	291	311	10			
1	F	217	Total	C	N	O	S	0	0	0
			1706	1088	294	315	9			
1	H	220	Total	C	N	O	S	0	0	0
			1732	1103	298	321	10			
1	L	219	Total	C	N	O	S	0	0	0
			1724	1096	297	321	10			
1	N	221	Total	C	N	O	S	0	0	0
			1738	1106	299	323	10			
1	B	220	Total	C	N	O	S	0	0	0
			1732	1103	298	321	10			
1	D	220	Total	C	N	O	S	0	0	0
			1732	1103	298	321	10			
1	G	214	Total	C	N	O	S	0	0	0
			1686	1074	291	311	10			
1	I	217	Total	C	N	O	S	0	0	0
			1708	1087	295	316	10			
1	J	220	Total	C	N	O	S	0	0	0
			1732	1103	298	321	10			
1	K	219	Total	C	N	O	S	0	0	0
			1724	1096	297	321	10			
1	M	221	Total	C	N	O	S	0	0	0
			1738	1106	299	323	10			

- Molecule 2 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	E	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
2	H	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
2	L	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
2	N	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
2	G	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
2	J	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
2	M	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	57	Total	O	0	0
			57	57		
3	C	49	Total	O	0	0
			49	49		
3	E	72	Total	O	0	0
			72	72		
3	F	32	Total	O	0	0
			32	32		
3	H	41	Total	O	0	0
			41	41		

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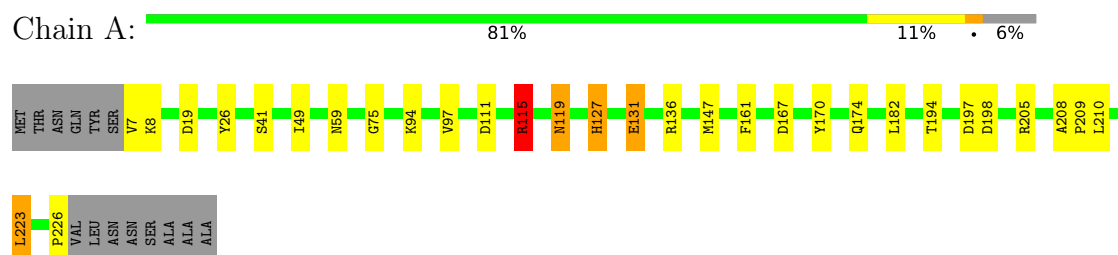
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	L	29	Total 29	O 29	0	0
3	N	57	Total 57	O 57	0	0
3	B	70	Total 70	O 70	0	0
3	D	51	Total 51	O 51	0	0
3	G	69	Total 69	O 69	0	0
3	I	24	Total 24	O 24	0	0
3	J	39	Total 39	O 39	0	0
3	K	28	Total 28	O 28	0	0
3	M	46	Total 46	O 46	0	0

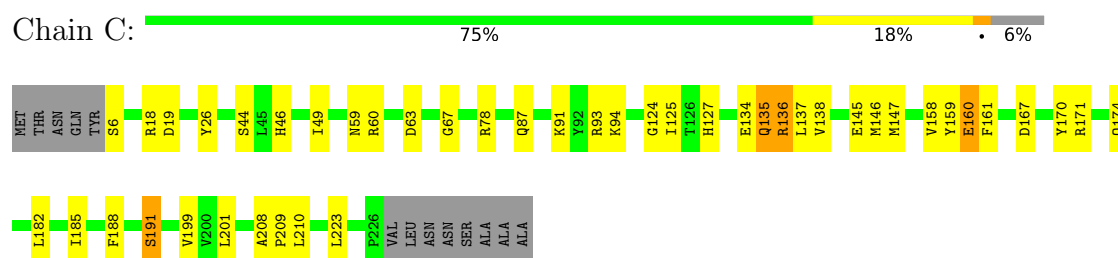
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

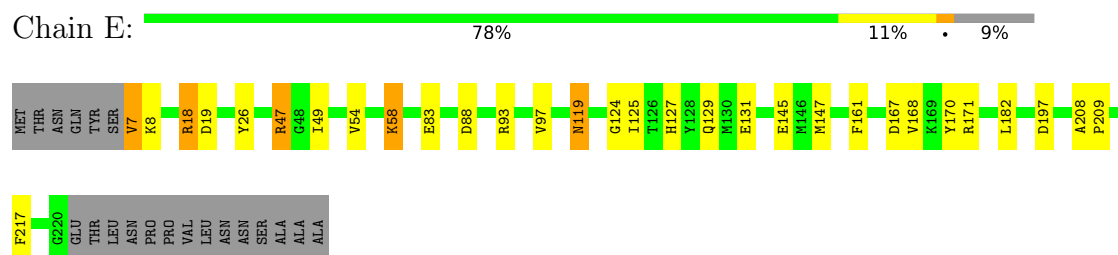
- Molecule 1: Asparagine synthetase domain-containing protein



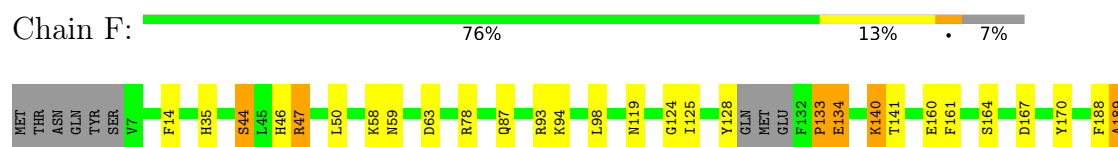
- Molecule 1: Asparagine synthetase domain-containing protein

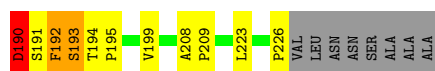


- Molecule 1: Asparagine synthetase domain-containing protein



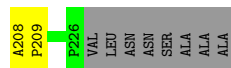
- Molecule 1: Asparagine synthetase domain-containing protein





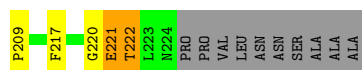
- Molecule 1: Asparagine synthetase domain-containing protein

Chain H: 82% 10% 6%



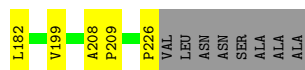
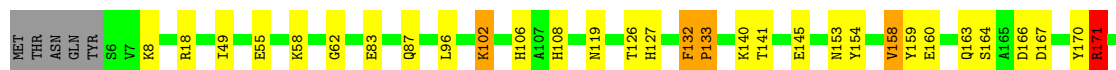
- Molecule 1: Asparagine synthetase domain-containing protein

Chain L: 78% 11% 6%



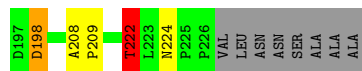
- Molecule 1: Asparagine synthetase domain-containing protein

Chain N: 79% 13% 6%



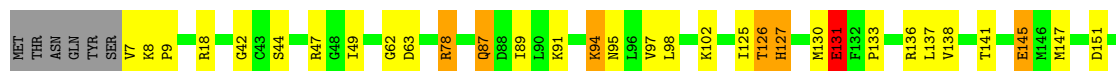
- Molecule 1: Asparagine synthetase domain-containing protein

Chain B: 79% 13% 6%



- Molecule 1: Asparagine synthetase domain-containing protein

Chain D: 74% 17% 6%





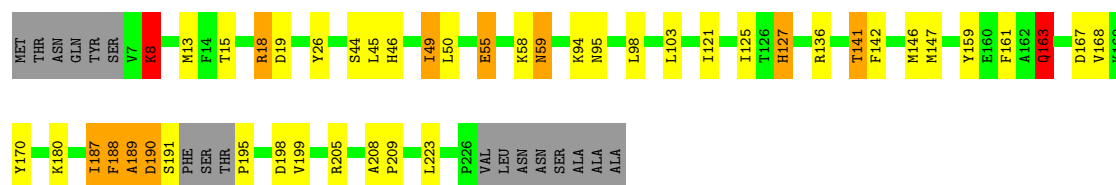
- Molecule 1: Asparagine synthetase domain-containing protein

Chain G: 80% 9% 9%



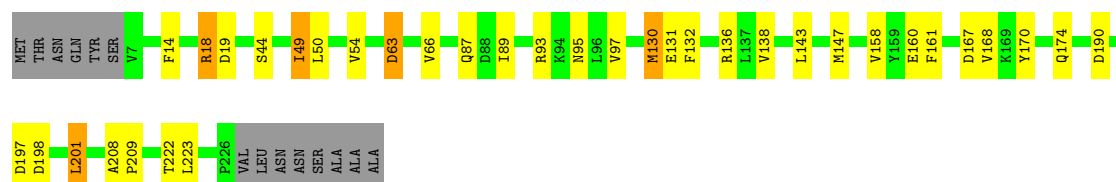
- Molecule 1: Asparagine synthetase domain-containing protein

Chain I: 74% 14% 7%



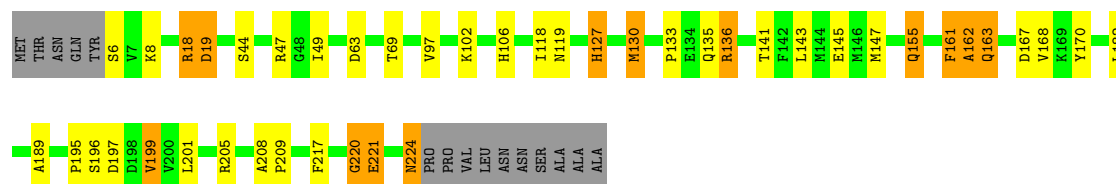
- Molecule 1: Asparagine synthetase domain-containing protein

Chain J: 79% 13% 6%



- Molecule 1: Asparagine synthetase domain-containing protein

Chain K: 75% 13% 6% 6%



- Molecule 1: Asparagine synthetase domain-containing protein

Chain M: 77% 16% 6%



D190	T194	D197	R205	A208	P209	L210	G220	L223	P226	VAL	LEU	ASN	ASN	SER	ALA	ALA	ALA
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4 Data and refinement statistics

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	68.17Å 134.37Å 233.84Å 90.00° 98.35° 90.00°	Depositor
Resolution (Å)	47.51 – 2.59 47.51 – 2.59	Depositor EDS
% Data completeness (in resolution range)	99.8 (47.51-2.59) 99.7 (47.51-2.59)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.38 (at 2.58Å)	Xtriage
Refinement program	REFMAC 5.8.0430	Depositor
R, R_{free}	0.211 , 0.257 0.218 , 0.259	Depositor DCC
R_{free} test set	6531 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	49.1	Xtriage
Anisotropy	0.185	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 26.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	0.239 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	24996	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.20% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.93	0/1767	1.31	12/2392 (0.5%)
1	B	0.95	2/1767 (0.1%)	1.30	9/2392 (0.4%)
1	C	0.92	0/1773	1.33	15/2400 (0.6%)
1	D	0.94	0/1767	1.30	11/2392 (0.5%)
1	E	0.91	1/1719 (0.1%)	1.29	12/2324 (0.5%)
1	F	0.83	0/1740	1.30	11/2355 (0.5%)
1	G	0.94	1/1719 (0.1%)	1.33	11/2324 (0.5%)
1	H	0.84	0/1767	1.26	8/2392 (0.3%)
1	I	0.86	0/1741	1.41	21/2354 (0.9%)
1	J	0.81	0/1767	1.25	9/2392 (0.4%)
1	K	0.84	0/1757	1.27	11/2376 (0.5%)
1	L	0.83	0/1757	1.23	9/2376 (0.4%)
1	M	0.98	2/1773 (0.1%)	1.33	10/2400 (0.4%)
1	N	1.00	4/1773 (0.2%)	1.38	17/2400 (0.7%)
All	All	0.90	10/24587 (0.0%)	1.31	166/33269 (0.5%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	2
1	C	0	4
1	D	0	2
1	E	0	2
1	F	0	3
1	G	0	2
1	H	0	1
1	J	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	K	0	2
1	L	0	3
1	M	0	3
1	N	0	1
All	All	0	28

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	127	HIS	CG-CD2	-6.98	1.28	1.35
1	M	35	HIS	CE1-NE2	6.03	1.38	1.32
1	N	108	HIS	CD2-NE2	-5.76	1.31	1.37
1	B	129	GLN	C-O	-5.36	1.16	1.23
1	G	136	ARG	NE-CZ	-5.32	1.27	1.33
1	M	127	HIS	C-O	-5.27	1.16	1.23
1	E	18	ARG	CZ-NH2	-5.22	1.26	1.33
1	B	196	SER	CA-CB	-5.16	1.45	1.53
1	N	166	ASP	C-O	-5.03	1.18	1.24
1	N	133	PRO	C-O	-5.03	1.18	1.24

All (166) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	179	THR	OG1-CB-CG2	14.59	138.49	109.30
1	C	160	GLU	CB-CG-CD	11.79	132.64	112.60
1	J	63	ASP	CA-CB-CG	11.64	124.24	112.60
1	N	159	TYR	CB-CA-C	-10.82	96.49	109.80
1	G	179	THR	CA-CB-OG1	-10.66	93.61	109.60
1	A	198	ASP	CA-CB-CG	10.13	122.73	112.60
1	D	222	THR	OG1-CB-CG2	10.05	129.39	109.30
1	I	141	THR	OG1-CB-CG2	9.61	128.51	109.30
1	H	114	ARG	CB-CG-CD	9.00	132.00	111.30
1	A	115	ARG	CA-CB-CG	8.94	131.99	114.10
1	A	223	LEU	N-CA-C	-8.82	101.60	114.39
1	I	141	THR	CA-CB-OG1	-8.73	96.50	109.60
1	N	58	LYS	CB-CG-CD	8.70	131.32	111.30
1	E	18	ARG	CG-CD-NE	-8.33	93.68	112.00
1	K	155	GLN	CA-CB-CG	-8.31	97.48	114.10
1	I	163	GLN	N-CA-CB	8.27	123.10	110.28
1	I	223	LEU	N-CA-C	-8.26	102.63	114.12
1	J	18	ARG	CG-CD-NE	-8.16	94.04	112.00
1	E	127	HIS	CA-CB-CG	8.01	121.81	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	18	ARG	CG-CD-NE	-8.00	94.40	112.00
1	F	59	ASN	OD1-CG-ND2	7.95	130.55	122.60
1	K	63	ASP	CB-CA-C	-7.93	94.65	110.42
1	J	160	GLU	N-CA-CB	7.92	123.31	110.40
1	E	197	ASP	CA-CB-CG	7.89	120.49	112.60
1	B	222	THR	OG1-CB-CG2	7.88	125.06	109.30
1	H	193	SER	CA-CB-OG	-7.86	95.37	111.10
1	N	132	PHE	CB-CA-C	7.83	118.79	110.65
1	M	153	ASN	CB-CA-C	7.79	122.58	109.80
1	I	18	ARG	CG-CD-NE	-7.71	95.03	112.00
1	I	59	ASN	CA-CB-CG	-7.71	104.89	112.60
1	F	140	LYS	CG-CD-CE	7.69	128.98	111.30
1	A	197	ASP	CA-CB-CG	7.36	119.96	112.60
1	I	18	ARG	CB-CA-C	-7.31	98.61	110.74
1	E	19	ASP	CA-CB-CG	7.31	119.91	112.60
1	D	126	THR	N-CA-C	7.21	122.64	113.55
1	L	19	ASP	CA-CB-CG	7.14	119.74	112.60
1	C	60	ARG	NE-CZ-NH2	7.09	125.58	119.20
1	I	188	PHE	CA-C-O	-7.09	112.85	121.36
1	J	18	ARG	CB-CA-C	-7.07	99.49	110.81
1	C	63	ASP	CB-CA-C	-6.97	96.94	110.46
1	A	127	HIS	CA-CB-CG	6.96	120.76	113.80
1	I	46	HIS	CB-CG-CD2	-6.95	122.17	131.20
1	C	46	HIS	CB-CG-CD2	-6.92	122.21	131.20
1	G	59	ASN	CA-CB-CG	-6.86	105.74	112.60
1	D	63	ASP	CB-CA-C	-6.84	97.20	110.46
1	A	119	ASN	CA-CB-CG	6.76	119.36	112.60
1	K	18	ARG	CB-CA-C	-6.72	99.59	110.74
1	F	140	LYS	CB-CG-CD	6.71	126.72	111.30
1	C	46	HIS	CB-CG-ND1	6.68	132.73	122.70
1	N	87	GLN	CB-CG-CD	-6.68	101.25	112.60
1	K	127	HIS	CA-CB-CG	6.67	120.47	113.80
1	I	58	LYS	CG-CD-CE	6.65	126.60	111.30
1	M	126	THR	OG1-CB-CG2	-6.65	96.00	109.30
1	M	223	LEU	N-CA-C	-6.63	104.77	114.39
1	I	50	LEU	CB-CG-CD1	6.62	130.55	110.70
1	G	19	ASP	CA-CB-CG	6.60	119.20	112.60
1	C	145	GLU	CB-CG-CD	6.52	123.69	112.60
1	C	127	HIS	CB-CG-CD2	-6.52	122.73	131.20
1	F	133	PRO	CB-CA-C	6.50	122.29	111.56
1	A	19	ASP	CA-CB-CG	6.48	119.08	112.60
1	C	44	SER	CA-CB-OG	-6.46	98.17	111.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	131	GLU	CB-CG-CD	6.46	123.58	112.60
1	L	91	LYS	CG-CD-CE	6.45	126.12	111.30
1	J	19	ASP	CA-CB-CG	6.45	119.05	112.60
1	K	19	ASP	CA-CB-CG	6.42	119.02	112.60
1	E	18	ARG	CB-CA-C	-6.42	100.08	110.74
1	N	18	ARG	CB-CA-C	-6.42	100.09	110.74
1	H	19	ASP	CA-CB-CG	6.41	119.01	112.60
1	M	220	GLY	CA-C-O	-6.34	111.98	119.72
1	G	171	ARG	NE-CZ-NH2	6.34	124.91	119.20
1	M	56	GLU	CG-CD-OE2	6.31	132.92	118.40
1	G	55	GLU	CG-CD-OE1	-6.28	103.95	118.40
1	N	145	GLU	CB-CG-CD	6.27	123.26	112.60
1	C	93	ARG	CG-CD-NE	6.25	125.76	112.00
1	H	18	ARG	CB-CA-C	-6.24	100.83	110.81
1	C	127	HIS	CB-CG-ND1	6.23	132.05	122.70
1	M	56	GLU	CG-CD-OE1	-6.17	104.21	118.40
1	M	83	GLU	CB-CG-CD	-6.12	102.19	112.60
1	G	205	ARG	CG-CD-NE	6.08	125.37	112.00
1	I	163	GLN	CA-CB-CG	6.06	126.22	114.10
1	C	60	ARG	NH1-CZ-NH2	-6.04	111.45	119.30
1	D	126	THR	CA-CB-OG1	6.03	118.65	109.60
1	E	145	GLU	CB-CG-CD	5.98	122.77	112.60
1	F	63	ASP	CB-CA-C	-5.98	98.52	110.42
1	H	63	ASP	CB-CA-C	-5.98	98.86	110.46
1	C	19	ASP	CA-CB-CG	5.93	118.53	112.60
1	H	197	ASP	CA-CB-CG	5.84	118.44	112.60
1	K	8	LYS	CA-CB-CG	5.84	125.78	114.10
1	D	62	GLY	CA-C-N	5.83	128.90	120.38
1	D	62	GLY	C-N-CA	5.83	128.90	120.38
1	M	197	ASP	CA-CB-CG	5.81	118.41	112.60
1	C	59	ASN	CA-CB-CG	-5.80	106.80	112.60
1	F	46	HIS	CB-CG-CD2	-5.78	123.69	131.20
1	E	131	GLU	CB-CG-CD	5.78	122.42	112.60
1	N	170	TYR	CB-CA-C	5.77	121.43	109.95
1	D	102	LYS	CB-CG-CD	5.77	124.56	111.30
1	A	115	ARG	CD-NE-CZ	-5.74	116.37	124.40
1	B	145	GLU	CB-CG-CD	5.73	122.34	112.60
1	A	7	VAL	N-CA-CB	5.72	121.22	111.50
1	F	226	PRO	CA-C-O	-5.71	101.88	119.00
1	D	147	MET	CG-SD-CE	-5.69	88.39	100.90
1	A	59	ASN	CA-CB-CG	5.68	118.28	112.60
1	E	127	HIS	CB-CG-CD2	-5.68	123.82	131.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	87	GLN	CB-CA-C	-5.66	102.00	110.88
1	E	88	ASP	CA-CB-CG	5.64	118.24	112.60
1	L	87	GLN	OE1-CD-NE2	-5.64	116.96	122.60
1	B	196	SER	CA-CB-OG	5.60	122.30	111.10
1	K	197	ASP	CA-CB-CG	5.57	118.17	112.60
1	F	128	TYR	CA-C-O	-5.57	111.34	120.80
1	E	170	TYR	CB-CA-C	5.55	121.00	109.95
1	G	179	THR	N-CA-CB	-5.54	101.11	110.41
1	B	198	ASP	N-CA-CB	5.52	118.23	110.12
1	I	127	HIS	CA-CB-CG	5.50	119.30	113.80
1	L	87	GLN	CG-CD-NE2	5.50	124.65	116.40
1	L	160	GLU	N-CA-CB	-5.50	102.04	110.12
1	E	83	GLU	CB-CG-CD	-5.48	103.28	112.60
1	L	170	TYR	CB-CA-C	5.48	120.85	109.95
1	K	199	VAL	CA-CB-CG2	5.47	119.70	110.40
1	B	144	MET	CG-SD-CE	-5.47	88.87	100.90
1	I	180	LYS	CG-CD-CE	5.43	123.79	111.30
1	N	170	TYR	N-CA-CB	-5.42	101.31	110.41
1	B	47	ARG	CD-NE-CZ	5.40	131.96	124.40
1	D	131	GLU	CB-CG-CD	5.37	121.73	112.60
1	H	131	GLU	CB-CG-CD	5.37	121.73	112.60
1	N	58	LYS	CG-CD-CE	5.34	123.58	111.30
1	J	170	TYR	CB-CA-C	5.34	121.15	109.99
1	C	160	GLU	CG-CD-OE2	5.32	130.64	118.40
1	G	55	GLU	CG-CD-OE2	5.31	130.62	118.40
1	I	19	ASP	CA-CB-CG	5.31	117.91	112.60
1	J	198	ASP	CA-CB-CG	5.31	117.91	112.60
1	N	153	ASN	CB-CA-C	5.30	118.50	109.80
1	M	223	LEU	N-CA-CB	-5.30	103.98	110.98
1	D	145	GLU	CB-CG-CD	5.30	121.62	112.60
1	A	8	LYS	CG-CD-CE	5.30	123.50	111.30
1	I	8	LYS	CG-CD-CE	5.29	123.47	111.30
1	K	8	LYS	CB-CG-CD	5.29	123.47	111.30
1	J	222	THR	OG1-CB-CG2	5.29	119.87	109.30
1	I	55	GLU	CB-CG-CD	5.26	121.54	112.60
1	N	171	ARG	N-CA-C	-5.24	105.65	111.36
1	G	171	ARG	NH1-CZ-NH2	-5.23	112.50	119.30
1	B	127	HIS	CA-CB-CG	5.23	119.03	113.80
1	L	130	MET	CA-CB-CG	-5.22	103.66	114.10
1	H	170	TYR	CB-CA-C	5.20	120.86	109.99
1	N	141	THR	CA-CB-OG1	-5.20	101.80	109.60
1	N	226	PRO	CA-C-O	-5.20	103.41	119.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	158	VAL	N-CA-CB	-5.19	105.42	112.16
1	N	62	GLY	CA-C-N	5.18	127.95	120.38
1	N	62	GLY	C-N-CA	5.18	127.95	120.38
1	I	46	HIS	CB-CG-ND1	5.18	130.46	122.70
1	I	198	ASP	CA-CB-CG	5.18	117.78	112.60
1	E	171	ARG	N-CA-C	-5.17	105.33	111.69
1	M	194	THR	CA-CB-OG1	-5.17	101.85	109.60
1	A	205	ARG	NE-CZ-NH1	-5.15	116.35	121.50
1	B	160	GLU	CG-CD-OE2	5.14	130.22	118.40
1	I	15	THR	OG1-CB-CG2	5.12	119.55	109.30
1	K	161	PHE	CA-C-O	-5.12	115.58	121.47
1	D	170	TYR	CB-CA-C	5.09	120.63	109.99
1	F	189	ALA	N-CA-C	-5.08	105.73	112.34
1	C	170	TYR	CB-CA-C	5.08	120.61	109.99
1	G	145	GLU	CB-CG-CD	5.07	121.21	112.60
1	L	94	LYS	CB-CG-CD	5.06	122.94	111.30
1	J	197	ASP	CA-CB-CG	5.05	117.65	112.60
1	F	59	ASN	CB-CG-OD1	-5.05	110.71	120.80
1	B	63	ASP	CB-CA-C	-5.02	100.72	110.46
1	I	205	ARG	CG-CD-NE	-5.01	100.97	112.00
1	F	35	HIS	CB-CG-CD2	-5.01	124.69	131.20

There are no chirality outliers.

All (28) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	115	ARG	Sidechain
1	A	136	ARG	Sidechain
1	B	136	ARG	Sidechain
1	B	18	ARG	Sidechain
1	C	136	ARG	Sidechain
1	C	171	ARG	Sidechain
1	C	18	ARG	Sidechain
1	C	78	ARG	Sidechain
1	D	18	ARG	Sidechain
1	D	78	ARG	Sidechain
1	E	47	ARG	Sidechain
1	E	93	ARG	Sidechain
1	F	47	ARG	Sidechain
1	F	78	ARG	Sidechain
1	F	93	ARG	Sidechain
1	G	47	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	G	78	ARG	Sidechain
1	H	47	ARG	Sidechain
1	J	93	ARG	Sidechain
1	K	136	ARG	Sidechain
1	K	47	ARG	Sidechain
1	L	18	ARG	Sidechain
1	L	47	ARG	Sidechain
1	L	93	ARG	Sidechain
1	M	205	ARG	Sidechain
1	M	78	ARG	Sidechain
1	M	93	ARG	Sidechain
1	N	171	ARG	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1732	0	1728	17	0
1	B	1732	0	1728	15	0
1	C	1738	0	1733	23	0
1	D	1732	0	1728	30	1
1	E	1686	0	1684	11	0
1	F	1706	0	1704	25	1
1	G	1686	0	1684	12	0
1	H	1732	0	1728	15	1
1	I	1708	0	1707	24	0
1	J	1732	0	1728	28	1
1	K	1724	0	1719	30	2
1	L	1724	0	1719	17	0
1	M	1738	0	1733	17	1
1	N	1738	0	1733	14	0
2	E	32	0	12	0	0
2	G	32	0	12	2	0
2	H	32	0	12	0	0
2	J	32	0	12	2	0
2	L	32	0	12	0	0
2	M	32	0	12	0	0
2	N	32	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	57	0	0	1	0
3	B	70	0	0	3	0
3	C	49	0	0	3	0
3	D	51	0	0	8	0
3	E	72	0	0	1	0
3	F	32	0	0	1	0
3	G	69	0	0	2	0
3	H	41	0	0	4	0
3	I	24	0	0	0	0
3	J	39	0	0	1	0
3	K	28	0	0	4	0
3	L	29	0	0	0	0
3	M	46	0	0	1	0
3	N	57	0	0	1	0
All	All	24996	0	24140	262	4

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 (262) 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:J:138:VAL:HG22	1:J:201:LEU:CD2	2.00	0.91
1:D:94:LYS:HE3	1:D:193:SER:OG	1.71	0.90
1:M:8:LYS:HZ3	1:M:119:ASN:HD21	1.20	0.89
1:M:8:LYS:NZ	1:M:119:ASN:HD21	1.70	0.88
1:C:146:MET:HE2	1:C:147:MET:HE3	1.56	0.86
1:N:106:HIS:HE2	1:N:154:TYR:HE2	1.23	0.85
1:D:8:LYS:HD2	1:D:9:PRO:HD2	1.58	0.85
1:J:138:VAL:HG22	1:J:201:LEU:HD22	1.60	0.84
1:I:163:GLN:HG3	1:I:167:ASP:OD2	1.76	0.84
1:N:163:GLN:HG2	1:N:167:ASP:OD2	1.79	0.83
1:C:146:MET:HE2	1:C:147:MET:CE	2.11	0.80
1:H:19:ASP:OD2	1:H:129:GLN:NE2	2.13	0.80
1:K:161:PHE:O	1:K:162:ALA:HB3	1.82	0.79
1:G:7:VAL:N	3:G:401:HOH:O	2.18	0.76
1:A:131:GLU:CD	1:A:131:GLU:H	1.95	0.74
1:D:8:LYS:CD	1:D:9:PRO:HD2	2.18	0.73
1:K:19:ASP:OD2	3:K:301:HOH:O	2.07	0.73
1:I:103:LEU:HD11	1:I:146:MET:HE1	1.73	0.71
1:K:127:HIS:O	1:K:130:MET:HG2	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:164:SER:HB2	3:F:322:HOH:O	1.92	0.69
1:L:53:ARG:NH2	1:L:180:LYS:O	2.26	0.69
1:N:140:LYS:NZ	3:N:401:HOH:O	2.25	0.69
1:F:44:SER:HB3	1:F:47:ARG:HD2	1.75	0.69
1:K:161:PHE:O	1:K:162:ALA:CB	2.41	0.68
1:M:8:LYS:NZ	1:M:119:ASN:ND2	2.40	0.68
1:F:133:PRO:HG3	1:F:195:PRO:HG3	1.74	0.67
1:K:195:PRO:HB2	1:K:199:VAL:HG23	1.76	0.67
1:K:224:ASN:C	1:K:224:ASN:OD1	2.37	0.67
1:M:106:HIS:CE1	1:M:143:LEU:HD13	2.30	0.66
1:D:133:PRO:HA	1:D:136:ARG:HG3	1.77	0.66
1:I:45:LEU:HD11	1:I:187:ILE:HD12	1.78	0.66
1:I:26:TYR:CE2	1:J:223:LEU:HD11	2.31	0.66
1:K:162:ALA:HA	1:K:167:ASP:OD2	1.96	0.65
1:F:191:SER:O	1:F:192:PHE:C	2.40	0.64
1:D:8:LYS:HD2	1:D:9:PRO:CD	2.26	0.64
1:D:141:THR:O	1:D:145:GLU:HG3	1.98	0.64
1:I:26:TYR:CD2	1:J:223:LEU:HD11	2.33	0.64
1:I:26:TYR:CZ	1:J:223:LEU:HD12	2.33	0.64
1:K:217:PHE:HA	1:K:221:GLU:O	1.97	0.63
1:A:111:ASP:O	1:A:115:ARG:HG2	1.98	0.63
1:N:49:ILE:HD12	1:N:182:LEU:HA	1.81	0.63
1:F:191:SER:O	1:F:193:SER:N	2.32	0.62
1:H:117:ASP:OD1	1:H:117:ASP:O	2.17	0.62
1:A:49:ILE:HD12	1:A:182:LEU:HA	1.81	0.62
1:A:41:SER:HB3	3:A:308:HOH:O	1.99	0.62
1:L:44:SER:HB3	1:L:47:ARG:HD2	1.81	0.62
1:M:49:ILE:HD12	1:M:182:LEU:HA	1.82	0.62
1:C:134:GLU:HG2	1:C:135:GLN:HG2	1.81	0.62
1:N:126:THR:HG22	1:N:158:VAL:HG13	1.81	0.61
2:G:301:GTP:H5'	2:G:301:GTP:H8	1.65	0.61
1:K:201:LEU:O	1:K:205:ARG:HG3	2.01	0.61
1:J:138:VAL:CG2	1:J:201:LEU:CD2	2.78	0.61
1:D:47:ARG:HD3	3:D:329:HOH:O	2.01	0.60
1:D:49:ILE:HD12	1:D:182:LEU:HA	1.83	0.60
1:I:136:ARG:NH2	1:I:195:PRO:O	2.35	0.60
1:K:162:ALA:O	1:K:163:GLN:CB	2.50	0.60
1:C:125:ILE:HG22	1:C:159:TYR:HD1	1.67	0.59
1:E:49:ILE:HD12	1:E:182:LEU:HA	1.83	0.59
1:M:102:LYS:HE3	1:M:134:GLU:HG3	1.85	0.59
1:F:190:ASP:O	1:F:192:PHE:N	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:49:ILE:HD12	1:B:182:LEU:HA	1.86	0.58
1:D:127:HIS:HA	1:D:130:MET:SD	2.43	0.58
1:L:8:LYS:NZ	1:L:119:ASN:OD1	2.36	0.58
1:D:87:GLN:CD	3:D:306:HOH:O	2.47	0.57
1:D:94:LYS:CE	1:D:193:SER:OG	2.50	0.57
1:N:8:LYS:NZ	1:N:119:ASN:OD1	2.36	0.57
1:K:130:MET:O	1:K:136:ARG:HG2	2.04	0.57
1:E:7:VAL:N	3:E:404:HOH:O	2.38	0.56
1:K:6:SER:N	3:K:304:HOH:O	2.36	0.56
1:A:210:LEU:HD13	1:A:226:PRO:HG2	1.88	0.56
1:F:190:ASP:C	1:F:192:PHE:N	2.62	0.56
1:F:190:ASP:C	1:F:192:PHE:H	2.13	0.56
1:L:53:ARG:NH1	1:L:56:GLU:OE1	2.39	0.56
1:I:26:TYR:CE2	1:J:223:LEU:CD1	2.89	0.56
1:D:7:VAL:HG22	3:D:305:HOH:O	2.05	0.56
1:M:8:LYS:HZ1	1:M:119:ASN:ND2	2.03	0.56
1:C:49:ILE:HD12	1:C:182:LEU:HA	1.87	0.56
1:J:130:MET:HG3	1:J:136:ARG:HA	1.88	0.56
1:D:126:THR:O	1:D:127:HIS:CB	2.54	0.56
1:L:7:VAL:HG22	1:L:8:LYS:H	1.68	0.56
1:G:44:SER:HB3	1:G:47:ARG:HD2	1.87	0.55
1:C:159:TYR:HD2	1:C:160:GLU:HG2	1.71	0.55
1:J:89:ILE:CD1	1:J:95:ASN:HA	2.36	0.55
1:I:26:TYR:CZ	1:J:223:LEU:CD1	2.91	0.55
1:N:163:GLN:HG2	1:N:167:ASP:CG	2.32	0.54
1:E:8:LYS:NZ	1:E:119:ASN:OD1	2.40	0.54
1:K:49:ILE:HD12	1:K:182:LEU:HA	1.88	0.54
1:H:42:GLY:CA	3:H:406:HOH:O	2.56	0.54
1:D:89:ILE:CD1	1:D:95:ASN:HA	2.38	0.54
1:B:35:HIS:HE1	1:B:69:THR:OG1	1.91	0.54
1:B:7:VAL:N	3:B:306:HOH:O	2.41	0.53
1:K:196:SER:O	1:K:199:VAL:HG22	2.08	0.53
1:K:163:GLN:NE2	3:K:303:HOH:O	2.30	0.53
1:I:190:ASP:O	1:I:191:SER:C	2.51	0.53
1:C:146:MET:CE	1:C:147:MET:CE	2.85	0.53
1:J:138:VAL:CG2	1:J:201:LEU:HD22	2.36	0.53
1:D:89:ILE:HD11	1:D:95:ASN:HA	1.91	0.53
1:D:133:PRO:HD2	3:D:304:HOH:O	2.09	0.53
1:B:125:ILE:HG22	1:B:135:GLN:HG2	1.90	0.52
1:F:160:GLU:HG3	1:F:161:PHE:N	2.23	0.52
1:D:125:ILE:HG22	1:D:159:TYR:HD1	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:220:GLY:O	1:L:221:GLU:HB2	2.09	0.52
1:C:147:MET:HA	1:C:147:MET:HE2	1.91	0.52
1:J:49:ILE:HD12	1:J:50:LEU:H	1.76	0.51
1:D:87:GLN:NE2	3:D:306:HOH:O	2.43	0.51
1:K:130:MET:HE2	1:K:135:GLN:O	2.11	0.51
1:H:89:ILE:CD1	1:H:95:ASN:HA	2.40	0.51
1:K:195:PRO:HB2	1:K:199:VAL:CG2	2.38	0.51
1:F:188:PHE:C	1:F:190:ASP:N	2.66	0.50
1:I:13:MET:HE2	1:I:121:ILE:HD12	1.92	0.50
1:G:147:MET:HE2	1:G:147:MET:HA	1.94	0.50
1:F:14:PHE:CE2	1:F:50:LEU:HD11	2.46	0.50
1:D:8:LYS:CD	1:D:9:PRO:CD	2.86	0.50
1:G:7:VAL:HG13	1:G:33:PRO:HD3	1.94	0.50
1:B:18:ARG:HG3	1:B:181:SER:OG	2.12	0.50
1:G:135:GLN:NE2	2:G:301:GTP:O6	2.44	0.50
1:I:141:THR:OG1	1:I:142:PHE:N	2.45	0.49
1:A:223:LEU:HD13	1:C:26:TYR:CD1	2.47	0.49
1:J:89:ILE:HD11	1:J:95:ASN:HA	1.94	0.49
1:F:119:ASN:OD1	1:F:119:ASN:N	2.43	0.49
1:H:18:ARG:HB3	1:H:168:VAL:HG11	1.95	0.49
1:F:191:SER:C	1:F:193:SER:N	2.71	0.49
1:J:131:GLU:OE2	3:J:401:HOH:O	2.20	0.49
2:J:301:GTP:C8	2:J:301:GTP:H5"	2.47	0.49
1:A:75:GLY:HA3	1:C:174:GLN:HA	1.95	0.48
1:N:160:GLU:OE1	1:G:205:ARG:NH2	2.47	0.48
1:K:106:HIS:CE1	1:K:143:LEU:HD13	2.48	0.48
1:J:174:GLN:HA	1:M:75:GLY:HA3	1.94	0.48
1:F:170:TYR:CD1	1:F:170:TYR:C	2.92	0.48
1:J:138:VAL:HG22	1:J:201:LEU:HD21	1.93	0.48
1:A:26:TYR:CD1	1:L:222:THR:HG23	2.48	0.47
1:H:121:ILE:CD1	1:H:147:MET:HE2	2.43	0.47
1:E:217:PHE:CZ	1:N:171:ARG:HG3	2.49	0.47
1:H:42:GLY:HA2	3:H:406:HOH:O	2.14	0.47
1:N:163:GLN:HG3	1:N:164:SER:N	2.29	0.47
1:G:170:TYR:CD1	1:G:170:TYR:C	2.92	0.47
1:I:170:TYR:CD1	1:I:170:TYR:C	2.92	0.47
1:A:208:ALA:HB3	1:A:209:PRO:HD3	1.96	0.47
1:M:163:GLN:OE1	1:M:163:GLN:HA	2.15	0.47
1:I:95:ASN:HD22	1:I:190:ASP:CB	2.28	0.47
1:H:121:ILE:HD13	1:H:147:MET:HE2	1.97	0.47
1:F:193:SER:C	1:F:195:PRO:HD3	2.40	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:106:HIS:HE2	1:M:154:TYR:HE2	1.61	0.46
1:J:158:VAL:O	1:J:158:VAL:HG12	2.16	0.46
1:B:222:THR:HG22	1:B:224:ASN:H	1.81	0.46
1:E:147:MET:HE2	1:E:147:MET:HA	1.97	0.46
1:N:208:ALA:HB3	1:N:209:PRO:HD3	1.97	0.46
1:D:138:VAL:HG22	1:D:201:LEU:HG	1.96	0.46
1:N:96:LEU:HD11	1:N:199:VAL:HG12	1.96	0.46
1:E:18:ARG:HB3	1:E:168:VAL:HG11	1.98	0.46
1:K:133:PRO:HA	1:K:136:ARG:HG3	1.98	0.46
1:I:125:ILE:HG22	1:I:159:TYR:CD1	2.51	0.46
1:J:49:ILE:HD12	1:J:50:LEU:N	2.31	0.46
1:C:208:ALA:HB3	1:C:209:PRO:HD3	1.97	0.46
1:H:42:GLY:C	3:H:406:HOH:O	2.57	0.46
1:I:18:ARG:HB3	1:I:168:VAL:HG11	1.98	0.46
1:F:208:ALA:HB3	1:F:209:PRO:HD3	1.99	0.45
1:B:91:LYS:NZ	3:B:307:HOH:O	2.50	0.45
1:J:50:LEU:HD23	1:J:54:VAL:HG23	1.98	0.45
1:K:18:ARG:HB3	1:K:168:VAL:HG11	1.98	0.45
1:H:89:ILE:HD11	1:H:95:ASN:HA	1.97	0.45
1:H:110:VAL:O	1:H:114:ARG:HG3	2.16	0.45
1:B:208:ALA:HB3	1:B:209:PRO:HD3	1.99	0.45
1:K:102:LYS:HE3	1:K:106:HIS:HE1	1.80	0.45
1:A:170:TYR:CD1	1:A:170:TYR:C	2.94	0.45
1:E:208:ALA:HB3	1:E:209:PRO:HD3	1.99	0.45
1:D:91:LYS:NZ	3:D:306:HOH:O	2.50	0.45
1:C:146:MET:CE	1:C:147:MET:HE1	2.47	0.45
1:E:54:VAL:HG12	1:E:58:LYS:HE3	1.98	0.45
1:F:192:PHE:O	1:F:193:SER:HB3	2.16	0.44
1:L:7:VAL:HG22	1:L:8:LYS:N	2.32	0.44
1:J:132:PHE:CZ	2:J:301:GTP:H3'	2.52	0.44
1:C:159:TYR:CE2	1:C:160:GLU:OE1	2.70	0.44
1:F:133:PRO:CD	1:F:192:PHE:HB3	2.47	0.44
1:N:132:PHE:HA	1:N:133:PRO:HD2	1.81	0.44
1:M:208:ALA:HB3	1:M:209:PRO:HD3	1.99	0.44
1:B:140:LYS:HE2	1:B:156:SER:HB2	1.99	0.44
1:D:126:THR:O	1:D:159:TYR:O	2.36	0.44
1:G:216:ASN:OD1	3:G:402:HOH:O	2.21	0.44
1:G:219:ALA:O	1:G:220:GLY:C	2.60	0.44
1:C:125:ILE:HD13	1:C:125:ILE:HG21	1.53	0.44
1:I:208:ALA:HB3	1:I:209:PRO:HD3	1.99	0.44
1:J:158:VAL:O	1:J:158:VAL:CG1	2.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:141:THR:O	1:K:145:GLU:HG3	2.18	0.44
1:M:8:LYS:HZ3	1:M:119:ASN:ND2	2.00	0.44
1:M:131:GLU:HG3	1:M:132:PHE:CE1	2.53	0.44
1:A:161:PHE:CZ	1:A:167:ASP:HB3	2.53	0.43
1:F:161:PHE:CZ	1:F:167:ASP:HB3	2.53	0.43
1:B:161:PHE:CZ	1:B:167:ASP:HB3	2.53	0.43
1:K:143:LEU:O	1:K:147:MET:HG2	2.18	0.43
1:C:124:GLY:O	1:C:125:ILE:C	2.61	0.43
1:L:217:PHE:HA	1:L:221:GLU:O	2.19	0.43
1:J:14:PHE:CE2	1:J:50:LEU:HD21	2.54	0.43
1:C:6:SER:CB	3:C:342:HOH:O	2.67	0.43
1:A:94:LYS:HE3	1:A:194:THR:O	2.17	0.43
1:J:14:PHE:HE2	1:J:50:LEU:HD21	1.84	0.43
1:D:131:GLU:HA	1:D:136:ARG:HD3	2.01	0.43
1:F:98:LEU:HD12	1:F:192:PHE:CE1	2.54	0.43
1:A:26:TYR:HE1	1:L:221:GLU:H	1.66	0.43
1:K:130:MET:HE2	1:K:130:MET:HA	2.01	0.43
1:J:18:ARG:HB3	1:J:168:VAL:HG11	2.00	0.43
1:K:196:SER:O	1:K:199:VAL:CG2	2.66	0.42
1:A:174:GLN:HA	1:L:75:GLY:HA3	2.01	0.42
1:K:220:GLY:O	1:K:221:GLU:HB2	2.19	0.42
1:I:8:LYS:HE3	1:I:8:LYS:CA	2.49	0.42
1:J:143:LEU:O	1:J:147:MET:HG2	2.20	0.42
1:M:121:ILE:HD13	1:M:147:MET:HE2	2.00	0.42
1:A:26:TYR:CE1	1:L:222:THR:HG23	2.55	0.42
1:A:223:LEU:HD21	1:C:158:VAL:HG12	2.02	0.42
1:C:6:SER:HA	3:C:342:HOH:O	2.19	0.42
1:A:147:MET:HA	1:A:147:MET:HE2	2.00	0.42
1:H:161:PHE:CZ	1:H:167:ASP:HB3	2.54	0.42
1:B:35:HIS:CE1	1:B:69:THR:OG1	2.72	0.42
1:K:69:THR:HG23	3:K:302:HOH:O	2.20	0.42
1:C:188:PHE:O	1:C:191:SER:HB3	2.20	0.42
1:N:102:LYS:HE3	1:N:102:LYS:HB2	1.69	0.42
1:I:49:ILE:H	1:I:49:ILE:HG13	1.65	0.42
1:I:161:PHE:CZ	1:I:167:ASP:HB3	2.55	0.42
1:M:124:GLY:O	1:M:125:ILE:C	2.62	0.42
1:M:131:GLU:O	1:M:133:PRO:HD3	2.20	0.42
1:D:138:VAL:CG2	1:D:201:LEU:HG	2.50	0.42
1:C:67:GLY:HA2	3:C:341:HOH:O	2.18	0.42
1:B:26:TYR:HE1	1:K:221:GLU:H	1.67	0.41
1:D:97:VAL:HG13	1:D:98:LEU:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:151:ASP:OD1	3:D:301:HOH:O	2.22	0.41
1:I:8:LYS:HE3	1:I:8:LYS:HA	2.01	0.41
1:I:161:PHE:CD2	1:J:223:LEU:HD23	2.55	0.41
1:D:161:PHE:CZ	1:D:167:ASP:HB3	2.56	0.41
1:C:136:ARG:O	1:C:137:LEU:C	2.63	0.41
1:F:124:GLY:O	1:F:125:ILE:C	2.62	0.41
1:G:161:PHE:CZ	1:G:167:ASP:HB3	2.55	0.41
1:I:188:PHE:O	1:I:189:ALA:HB2	2.20	0.41
1:F:133:PRO:HD2	1:F:192:PHE:HB3	2.02	0.41
1:D:42:GLY:C	3:D:317:HOH:O	2.62	0.41
1:K:161:PHE:CZ	1:K:167:ASP:HB3	2.55	0.41
1:L:7:VAL:CG2	1:L:8:LYS:H	2.33	0.41
1:D:136:ARG:O	1:D:137:LEU:C	2.63	0.41
1:J:161:PHE:CZ	1:J:167:ASP:HB3	2.56	0.41
1:C:161:PHE:CZ	1:C:167:ASP:HB3	2.56	0.41
1:E:124:GLY:O	1:E:125:ILE:C	2.62	0.41
1:H:93:ARG:HH11	1:H:93:ARG:HG2	1.86	0.41
1:H:114:ARG:NH2	3:H:403:HOH:O	2.32	0.41
1:L:147:MET:HE2	1:L:147:MET:HA	2.01	0.41
1:L:208:ALA:HB3	1:L:209:PRO:HD3	2.01	0.41
1:B:59:ASN:ND2	3:B:304:HOH:O	2.47	0.41
1:B:121:ILE:HD13	1:B:147:MET:HE2	2.02	0.41
1:D:208:ALA:HB3	1:D:209:PRO:HD3	2.03	0.41
1:I:95:ASN:HD22	1:I:190:ASP:HB3	1.86	0.41
1:J:208:ALA:HB3	1:J:209:PRO:HD3	2.02	0.41
1:F:94:LYS:NZ	1:F:195:PRO:HA	2.36	0.41
1:L:124:GLY:O	1:L:125:ILE:C	2.61	0.40
1:C:223:LEU:HG	1:E:26:TYR:CE1	2.56	0.40
1:E:161:PHE:CZ	1:E:167:ASP:HB3	2.57	0.40
1:H:208:ALA:HB3	1:H:209:PRO:HD3	2.02	0.40
1:L:161:PHE:CZ	1:L:167:ASP:HB3	2.57	0.40
1:G:208:ALA:HB3	1:G:209:PRO:HD3	2.04	0.40
1:F:133:PRO:HD2	1:F:192:PHE:CD1	2.56	0.40
1:F:133:PRO:O	1:F:134:GLU:CB	2.69	0.40
1:B:124:GLY:O	1:B:125:ILE:C	2.64	0.40
1:K:208:ALA:HB3	1:K:209:PRO:HD3	2.03	0.40
1:M:81:ALA:C	3:M:427:HOH:O	2.64	0.40
1:G:7:VAL:CG1	1:G:31:GLY:O	2.69	0.40

All (4) 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)
1:F:189:ALA:CB	1:H:78:ARG:NH2[2_555]	1.96	0.24
1:K:189:ALA:O	1:M:78:ARG:NH2[2_656]	2.01	0.19
1:D:78:ARG:NH2	1:D:189:ALA:O[2_656]	2.08	0.12
1:J:190:ASP:OD2	1:K:170:TYR:OH[2_656]	2.19	0.01

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	218/234 (93%)	217 (100%)	1 (0%)	0	100	100
1	B	218/234 (93%)	216 (99%)	2 (1%)	0	100	100
1	C	219/234 (94%)	218 (100%)	1 (0%)	0	100	100
1	D	218/234 (93%)	214 (98%)	3 (1%)	1 (0%)	24	46
1	E	212/234 (91%)	212 (100%)	0	0	100	100
1	F	213/234 (91%)	204 (96%)	5 (2%)	4 (2%)	6	13
1	G	212/234 (91%)	211 (100%)	1 (0%)	0	100	100
1	H	218/234 (93%)	217 (100%)	1 (0%)	0	100	100
1	I	213/234 (91%)	211 (99%)	1 (0%)	1 (0%)	24	46
1	J	218/234 (93%)	217 (100%)	1 (0%)	0	100	100
1	K	217/234 (93%)	212 (98%)	2 (1%)	3 (1%)	9	19
1	L	217/234 (93%)	213 (98%)	3 (1%)	1 (0%)	24	46
1	M	219/234 (94%)	216 (99%)	3 (1%)	0	100	100
1	N	219/234 (94%)	215 (98%)	4 (2%)	0	100	100
All	All	3031/3276 (92%)	2993 (99%)	28 (1%)	10 (0%)	36	58

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	134	GLU

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Mol	Chain	Res	Type
1	L	221	GLU
1	D	127	HIS
1	I	189	ALA
1	K	162	ALA
1	K	221	GLU
1	F	192	PHE
1	F	193	SER
1	F	190	ASP
1	K	220	GLY

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	189/200 (94%)	185 (98%)	4 (2%)	47	73
1	B	189/200 (94%)	183 (97%)	6 (3%)	34	62
1	C	190/200 (95%)	180 (95%)	10 (5%)	20	43
1	D	189/200 (94%)	181 (96%)	8 (4%)	26	52
1	E	183/200 (92%)	177 (97%)	6 (3%)	33	61
1	F	186/200 (93%)	177 (95%)	9 (5%)	23	47
1	G	183/200 (92%)	177 (97%)	6 (3%)	33	61
1	H	189/200 (94%)	182 (96%)	7 (4%)	30	57
1	I	186/200 (93%)	173 (93%)	13 (7%)	14	31
1	J	189/200 (94%)	181 (96%)	8 (4%)	26	52
1	K	188/200 (94%)	180 (96%)	8 (4%)	26	51
1	L	188/200 (94%)	174 (93%)	14 (7%)	13	29
1	M	190/200 (95%)	183 (96%)	7 (4%)	30	57
1	N	190/200 (95%)	186 (98%)	4 (2%)	47	73
All	All	2629/2800 (94%)	2519 (96%)	110 (4%)	26	52

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

Mol	Chain	Res	Type
1	A	97	VAL
1	A	119	ASN
1	A	127	HIS
1	A	131	GLU
1	C	87	GLN
1	C	91	LYS
1	C	94	LYS
1	C	135	GLN
1	C	138	VAL
1	C	185	ILE
1	C	191	SER
1	C	199	VAL
1	C	201	LEU
1	C	210	LEU
1	E	7	VAL
1	E	47	ARG
1	E	58	LYS
1	E	97	VAL
1	E	119	ASN
1	E	129	GLN
1	F	44	SER
1	F	58	LYS
1	F	87	GLN
1	F	140	LYS
1	F	141	THR
1	F	190	ASP
1	F	194	THR
1	F	199	VAL
1	F	223	LEU
1	H	66	VAL
1	H	97	VAL
1	H	127	HIS
1	H	131	GLU
1	H	185	ILE
1	H	193	SER
1	H	199	VAL
1	L	18	ARG
1	L	44	SER
1	L	49	ILE
1	L	83	GLU
1	L	91	LYS
1	L	97	VAL
1	L	98	LEU

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Mol	Chain	Res	Type
1	L	119	ASN
1	L	131	GLU
1	L	160	GLU
1	L	161	PHE
1	L	185	ILE
1	L	199	VAL
1	L	222	THR
1	N	55	GLU
1	N	83	GLU
1	N	102	LYS
1	N	171	ARG
1	B	44	SER
1	B	97	VAL
1	B	127	HIS
1	B	196	SER
1	B	198	ASP
1	B	222	THR
1	D	44	SER
1	D	87	GLN
1	D	94	LYS
1	D	131	GLU
1	D	160	GLU
1	D	178	SER
1	D	185	ILE
1	D	199	VAL
1	G	7	VAL
1	G	44	SER
1	G	119	ASN
1	G	179	THR
1	G	185	ILE
1	G	210	LEU
1	I	8	LYS
1	I	44	SER
1	I	49	ILE
1	I	55	GLU
1	I	59	ASN
1	I	94	LYS
1	I	98	LEU
1	I	127	HIS
1	I	147	MET
1	I	163	GLN
1	I	187	ILE

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Mol	Chain	Res	Type
1	I	190	ASP
1	I	199	VAL
1	J	44	SER
1	J	49	ILE
1	J	63	ASP
1	J	66	VAL
1	J	87	GLN
1	J	97	VAL
1	J	130	MET
1	J	201	LEU
1	K	44	SER
1	K	97	VAL
1	K	118	ILE
1	K	119	ASN
1	K	130	MET
1	K	155	GLN
1	K	163	GLN
1	K	224	ASN
1	M	44	SER
1	M	59	ASN
1	M	90	LEU
1	M	102	LYS
1	M	130	MET
1	M	190	ASP
1	M	210	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	127	HIS
1	A	163	GLN
1	C	116	ASN
1	C	155	GLN
1	E	30	GLN
1	E	52	HIS
1	F	30	GLN
1	F	35	HIS
1	F	46	HIS
1	F	87	GLN
1	F	153	ASN
1	F	216	ASN
1	H	116	ASN

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Mol	Chain	Res	Type
1	H	129	GLN
1	H	163	GLN
1	L	10	GLN
1	L	106	HIS
1	L	108	HIS
1	L	122	ASN
1	L	127	HIS
1	N	108	HIS
1	B	35	HIS
1	B	52	HIS
1	B	119	ASN
1	B	163	GLN
1	D	155	GLN
1	G	30	GLN
1	G	52	HIS
1	I	108	HIS
1	K	10	GLN
1	K	30	GLN
1	K	106	HIS
1	K	108	HIS
1	K	122	ASN
1	K	153	ASN
1	K	155	GLN
1	K	163	GLN
1	M	95	ASN
1	M	119	ASN
1	M	135	GLN
1	M	153	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

7 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	L	301	-	33,34,34	0.59	0	50,54,54	0.53	0
2	GTP	H	301	-	33,34,34	0.60	0	50,54,54	0.58	0
2	GTP	G	301	-	33,34,34	0.64	0	50,54,54	0.62	0
2	GTP	E	301	-	33,34,34	0.58	0	50,54,54	0.56	0
2	GTP	J	301	-	33,34,34	0.58	0	50,54,54	0.57	0
2	GTP	N	301	-	33,34,34	0.57	0	50,54,54	0.61	0
2	GTP	M	301	-	33,34,34	0.57	0	50,54,54	0.57	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
2	GTP	L	301	-	-	4/22/38/38	0/3/3/3
2	GTP	H	301	-	-	3/22/38/38	0/3/3/3
2	GTP	G	301	-	-	3/22/38/38	0/3/3/3
2	GTP	E	301	-	-	2/22/38/38	0/3/3/3
2	GTP	J	301	-	-	7/22/38/38	0/3/3/3
2	GTP	N	301	-	-	4/22/38/38	0/3/3/3
2	GTP	M	301	-	-	4/22/38/38	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	H	301	GTP	C5'-O5'-PA-O3A
2	H	301	GTP	C5'-O5'-PA-O2A
2	L	301	GTP	C5'-O5'-PA-O3A
2	N	301	GTP	C5'-O5'-PA-O1A
2	G	301	GTP	C5'-O5'-PA-O1A
2	J	301	GTP	C5'-O5'-PA-O3A
2	J	301	GTP	C5'-O5'-PA-O1A
2	J	301	GTP	C5'-O5'-PA-O2A
2	M	301	GTP	C5'-O5'-PA-O3A
2	J	301	GTP	C3'-C4'-C5'-O5'
2	J	301	GTP	O4'-C4'-C5'-O5'
2	E	301	GTP	O4'-C4'-C5'-O5'
2	M	301	GTP	PB-O3B-PG-O3G
2	J	301	GTP	C4'-C5'-O5'-PA
2	L	301	GTP	C5'-O5'-PA-O1A
2	L	301	GTP	C5'-O5'-PA-O2A
2	N	301	GTP	C5'-O5'-PA-O3A
2	N	301	GTP	C5'-O5'-PA-O2A
2	G	301	GTP	C5'-O5'-PA-O2A
2	M	301	GTP	C5'-O5'-PA-O1A
2	L	301	GTP	O4'-C4'-C5'-O5'
2	M	301	GTP	C4'-C5'-O5'-PA
2	J	301	GTP	PB-O3A-PA-O2A
2	N	301	GTP	O4'-C4'-C5'-O5'
2	E	301	GTP	C3'-C4'-C5'-O5'
2	H	301	GTP	PA-O3A-PB-O2B
2	G	301	GTP	O4'-C4'-C5'-O5'

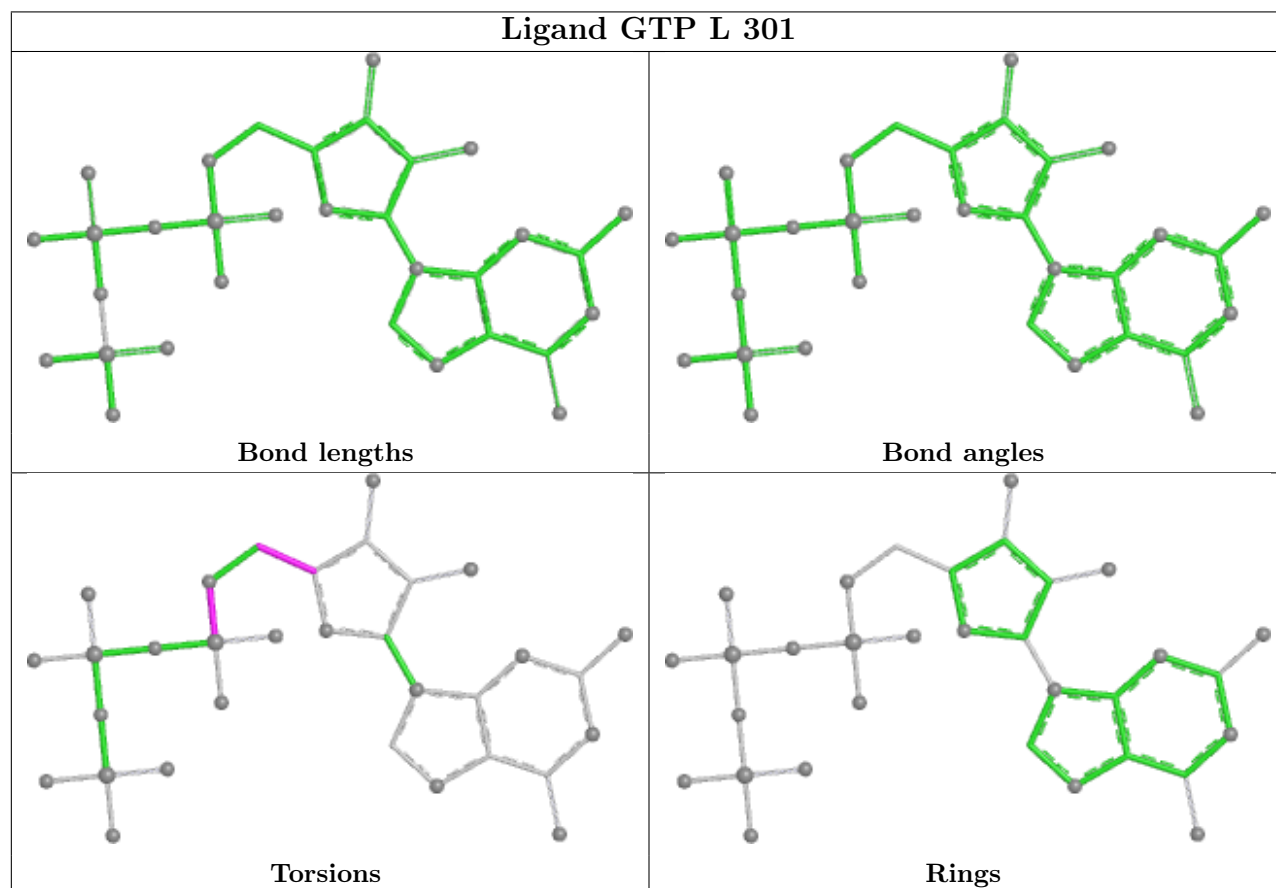
There are no ring outliers.

2 monomers are involved in 4 short contacts:

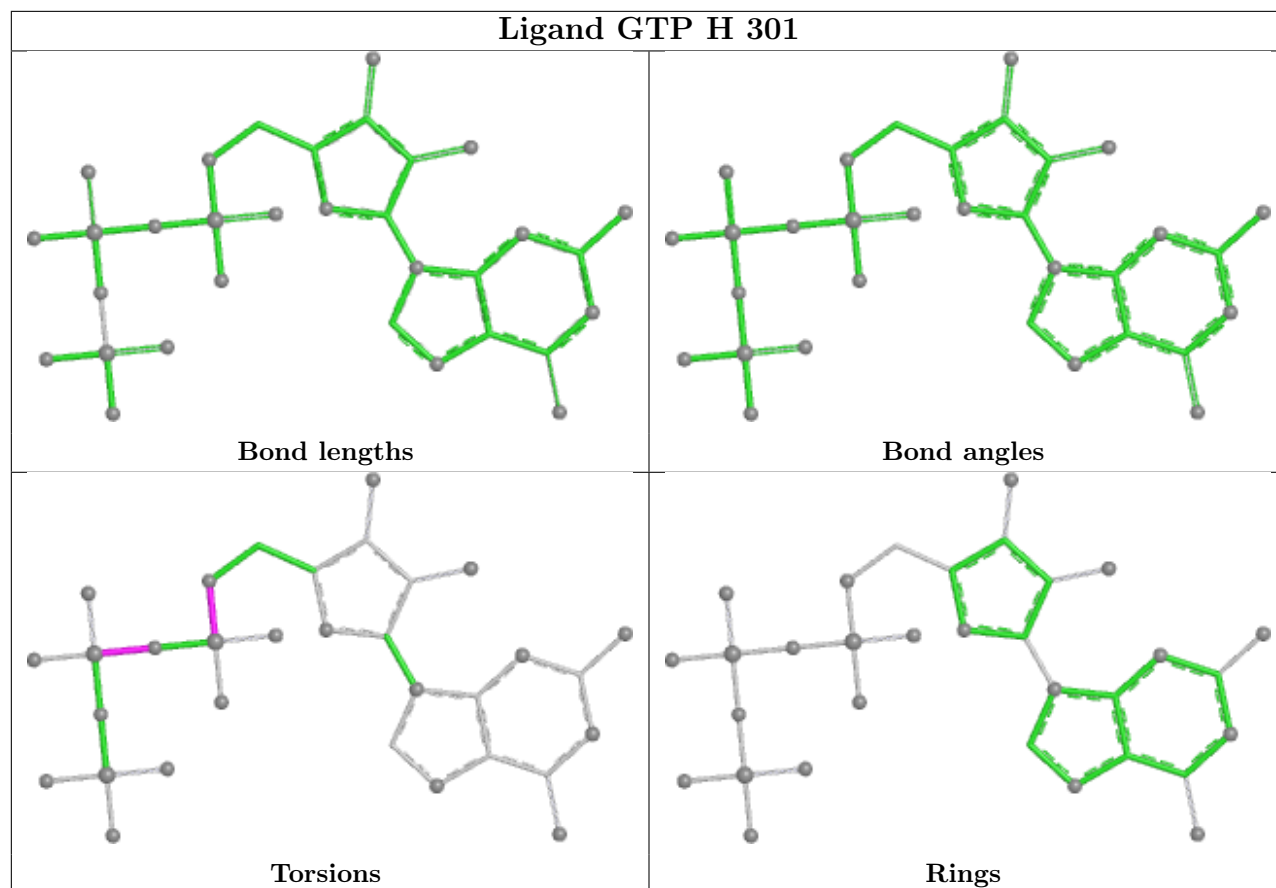
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	301	GTP	2	0
2	J	301	GTP	2	0

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

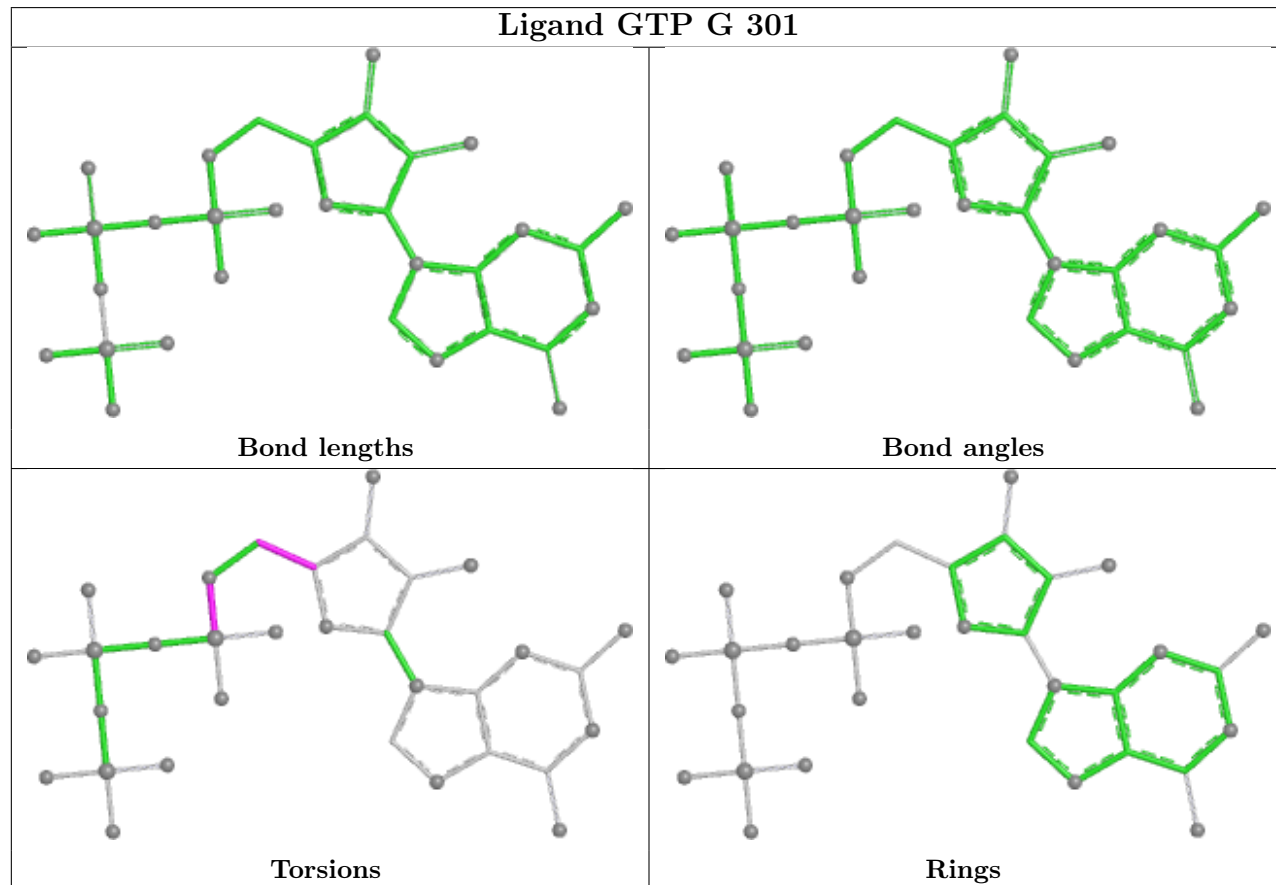
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



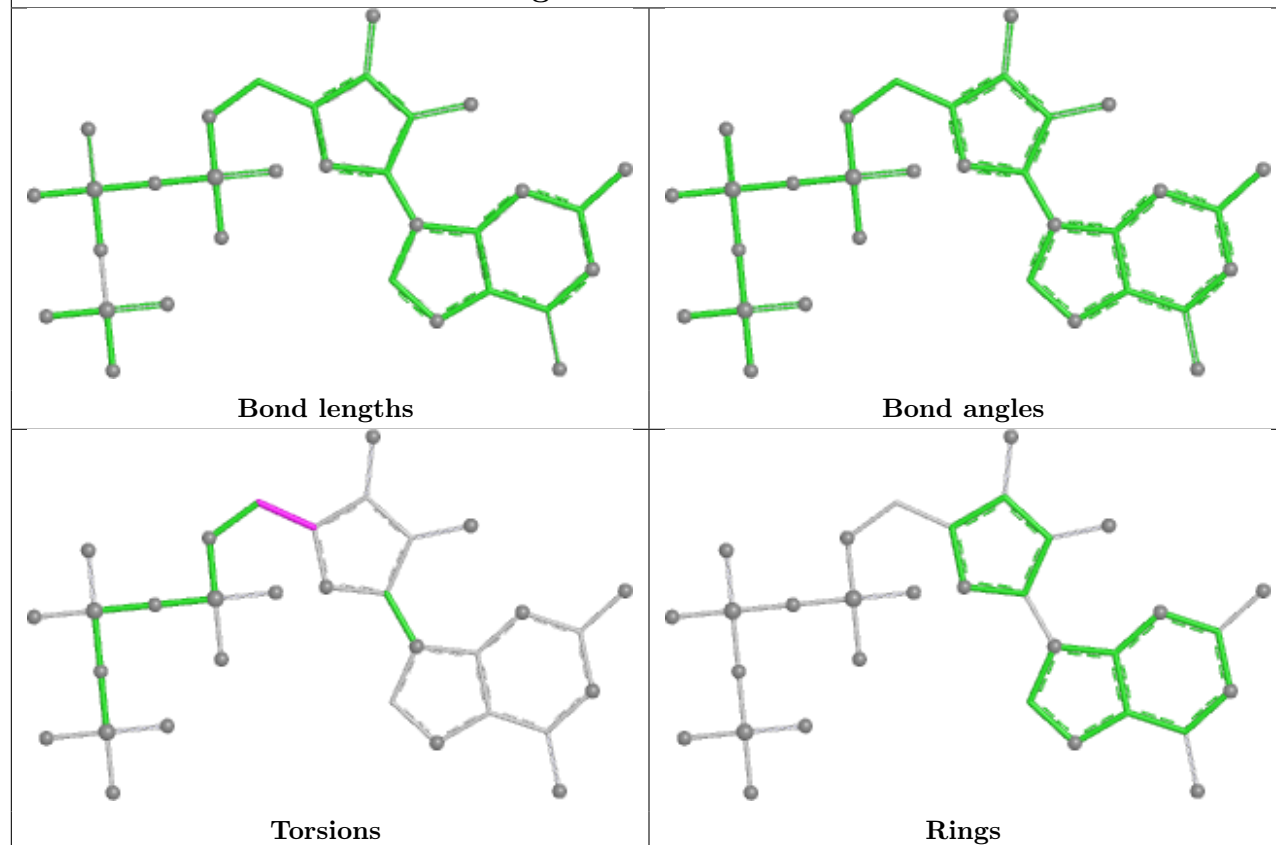
Ligand GTP H 301



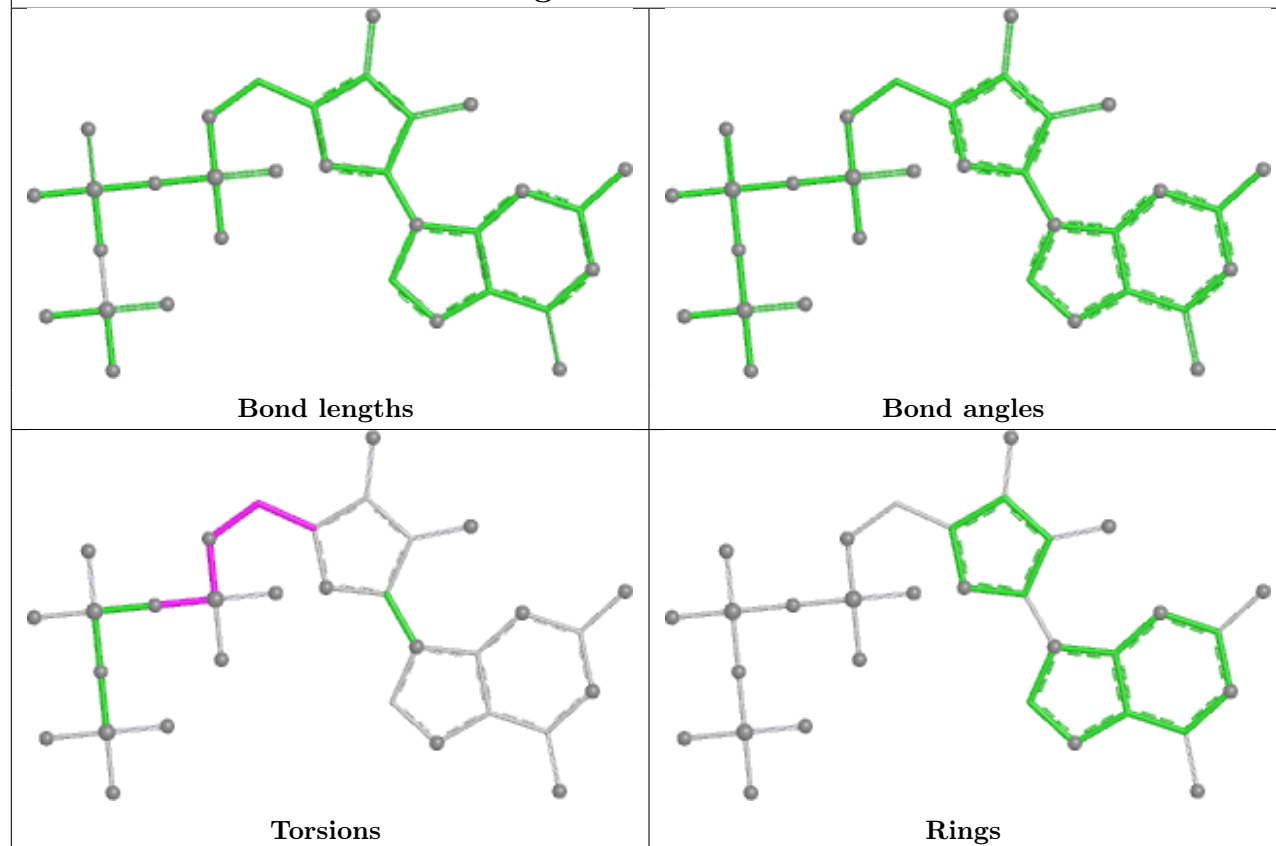
Ligand GTP G 301



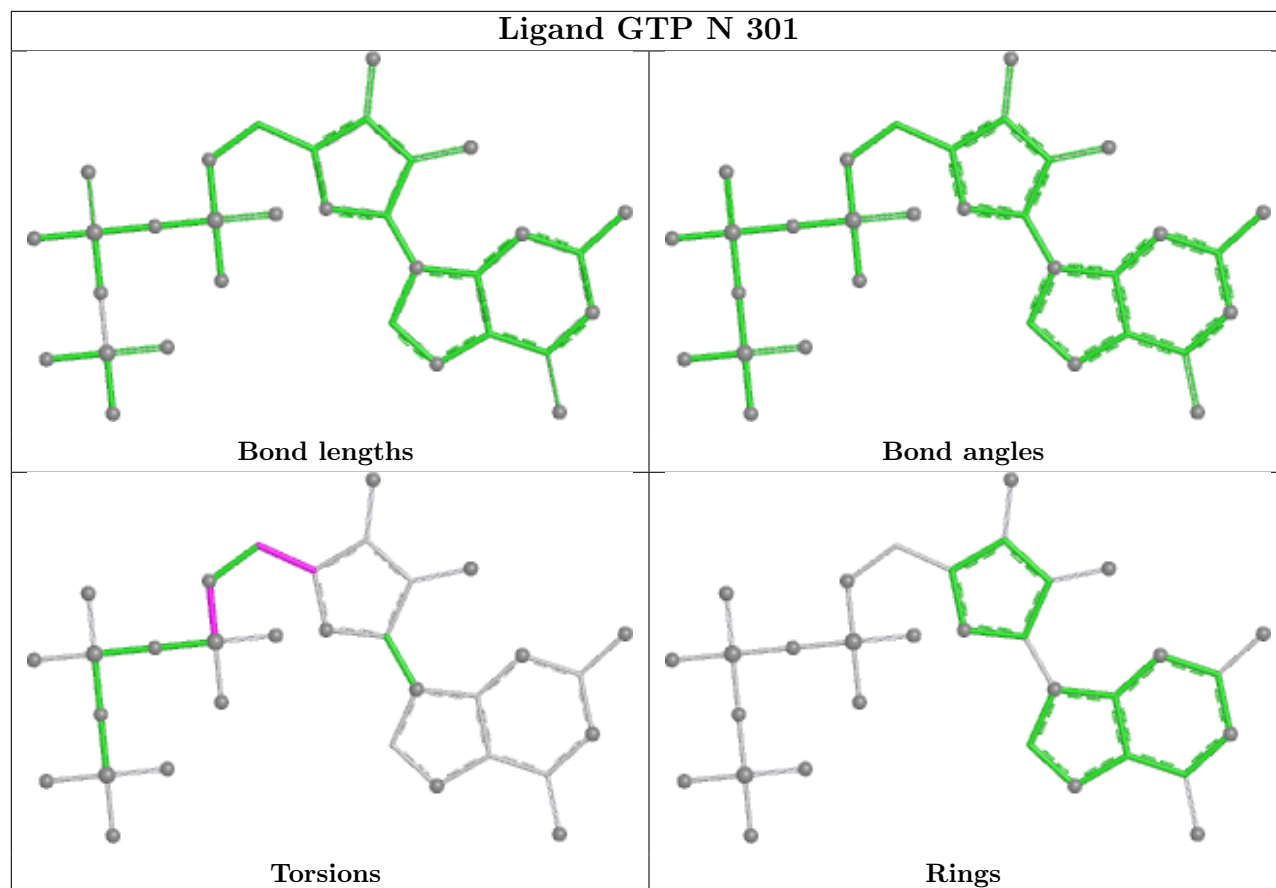
Ligand GTP E 301



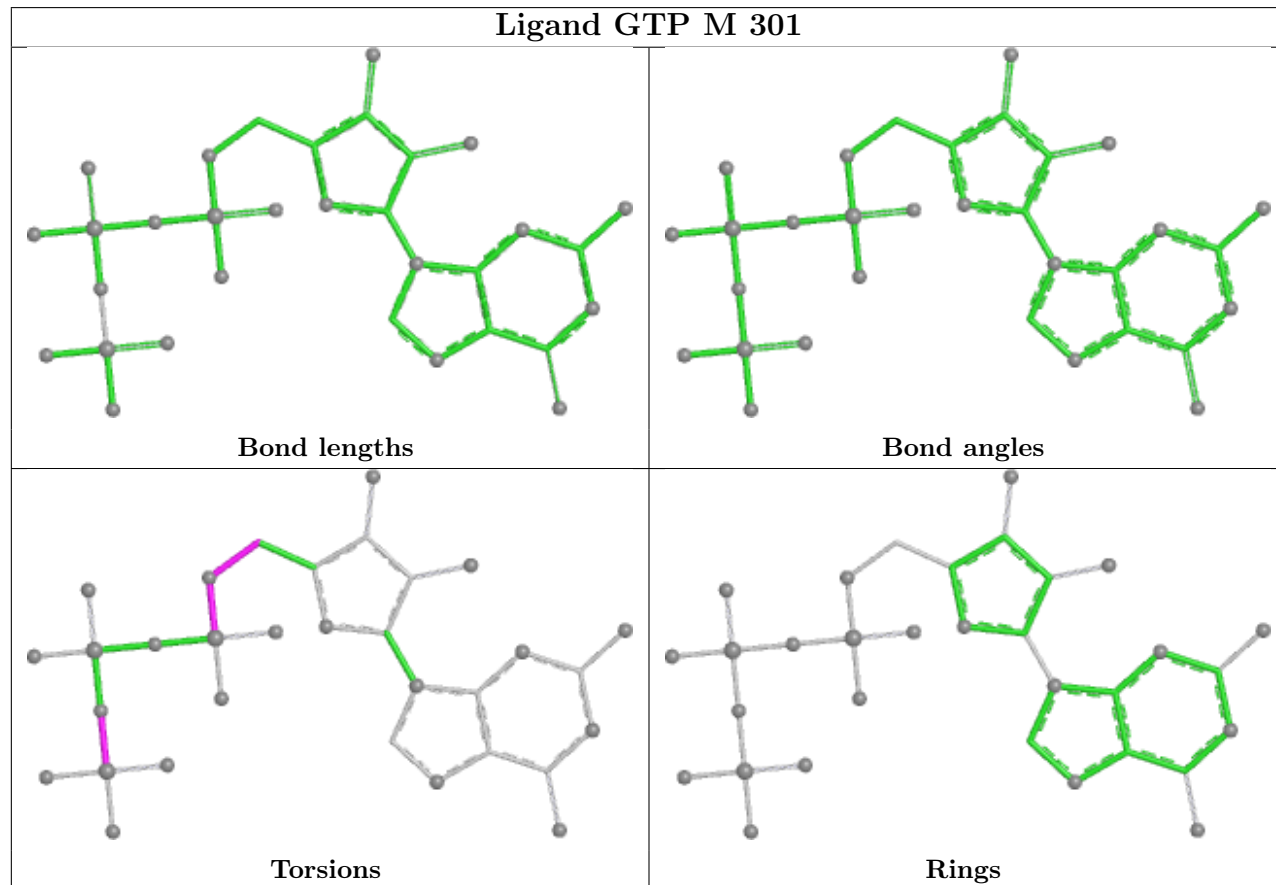
Ligand GTP J 301



Ligand GTP N 301



Ligand GTP M 301



5.7 Other polymers

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	220/234 (94%)	-1.44	0 100 100	30, 43, 57, 73	0
1	B	220/234 (94%)	-1.45	0 100 100	30, 45, 63, 84	0
1	C	221/234 (94%)	-1.38	0 100 100	29, 47, 76, 109	0
1	D	220/234 (94%)	-1.37	0 100 100	32, 48, 83, 119	0
1	E	214/234 (91%)	-1.49	0 100 100	31, 42, 57, 70	0
1	F	217/234 (92%)	-1.25	0 100 100	40, 57, 85, 140	0
1	G	214/234 (91%)	-1.44	0 100 100	31, 41, 55, 82	0
1	H	220/234 (94%)	-1.38	0 100 100	39, 55, 70, 89	0
1	I	217/234 (92%)	-1.30	0 100 100	43, 60, 84, 122	0
1	J	220/234 (94%)	-1.36	0 100 100	42, 56, 77, 98	0
1	K	219/234 (93%)	-1.31	0 100 100	40, 64, 96, 126	0
1	L	219/234 (93%)	-1.37	0 100 100	37, 55, 80, 105	0
1	M	221/234 (94%)	-1.43	0 100 100	35, 50, 67, 86	0
1	N	221/234 (94%)	-1.43	0 100 100	33, 46, 63, 94	0
All	All	3063/3276 (93%)	-1.39	0 100 100	29, 51, 77, 140	0

There are no RSRZ outliers to report.

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 ⓘ

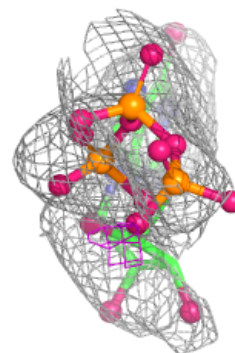
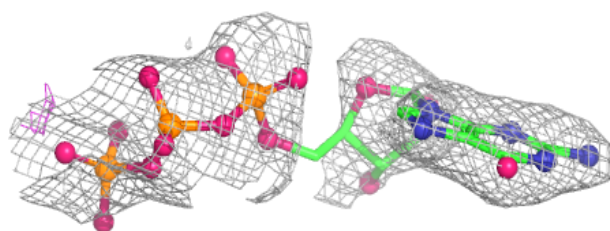
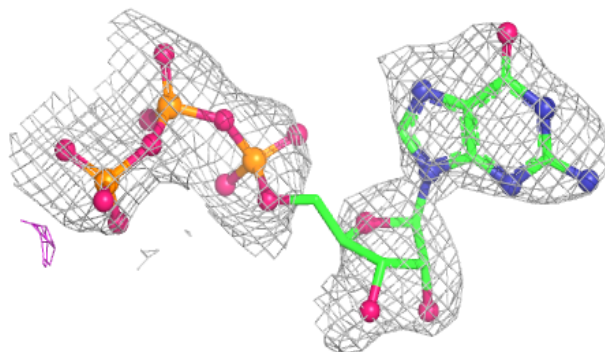
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	GTP	J	301	32/32	0.98	0.04	56,91,132,135	0
2	GTP	H	301	32/32	0.99	0.04	58,83,111,119	0
2	GTP	L	301	32/32	0.99	0.04	58,93,141,174	0
2	GTP	N	301	32/32	0.99	0.04	50,66,99,103	0
2	GTP	G	301	32/32	0.99	0.04	43,68,96,111	0
2	GTP	E	301	32/32	0.99	0.03	43,67,115,121	0
2	GTP	M	301	32/32	0.99	0.03	54,73,87,109	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.

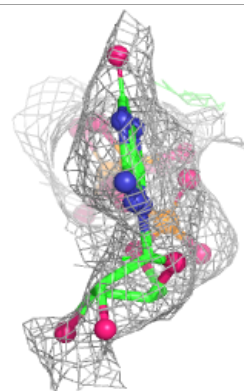
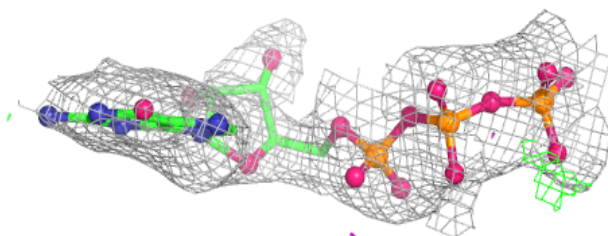
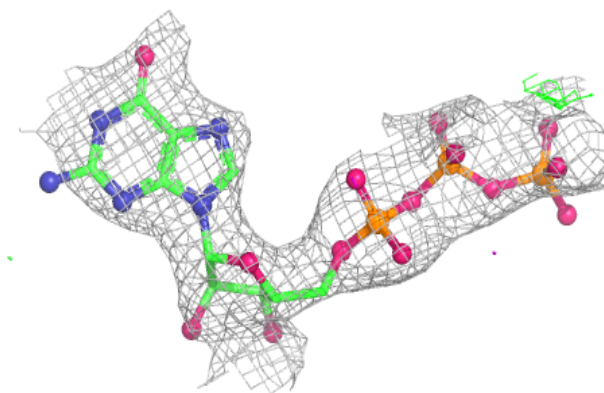
Electron density around GTP J 301:

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

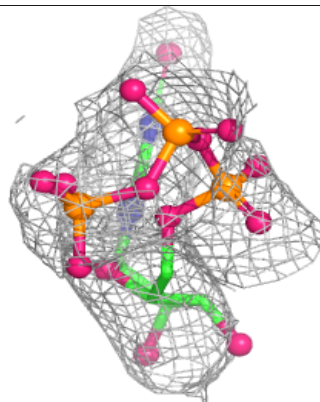
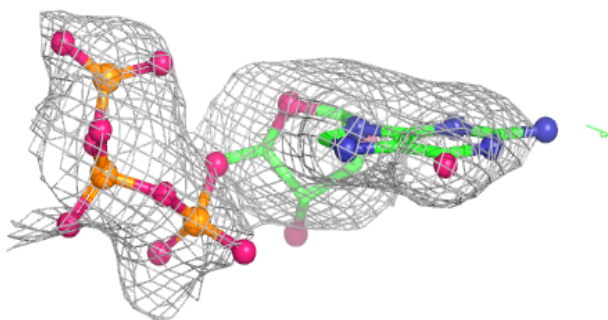
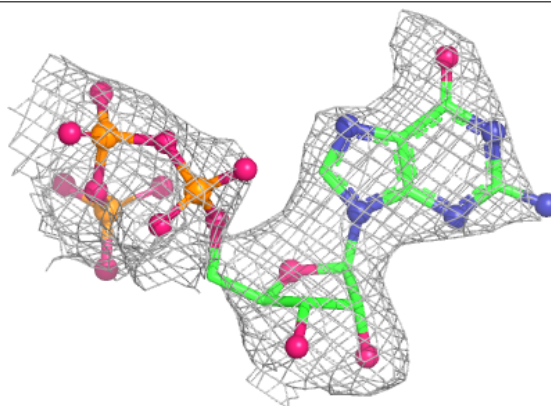


Electron density around GTP H 301:

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

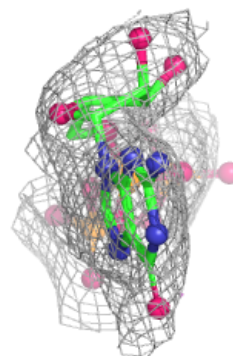
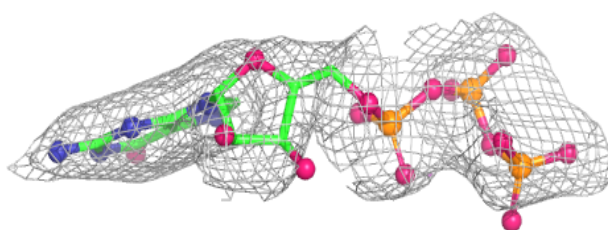
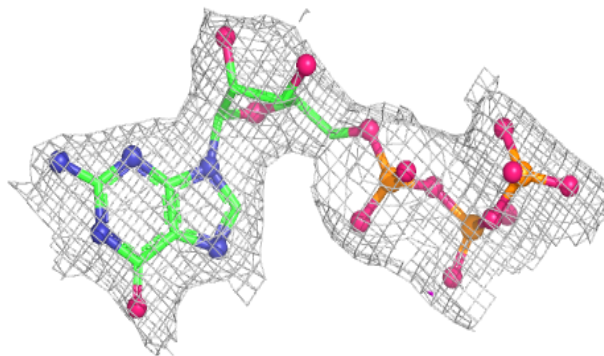
**Electron density around GTP L 301:**

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

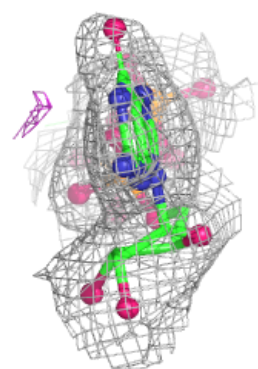
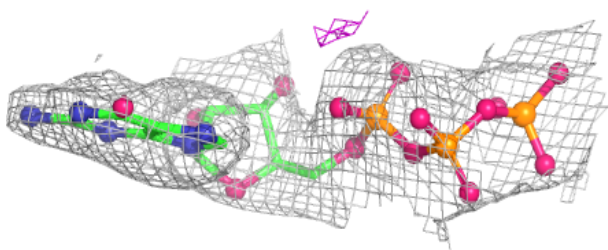
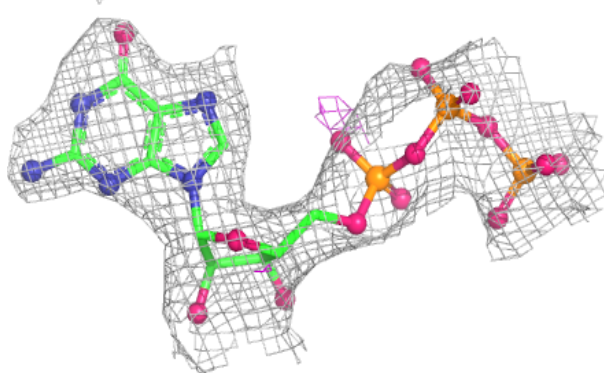


Electron density around GTP N 301:

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

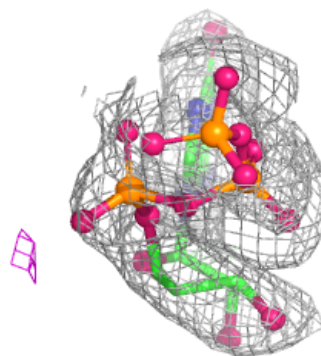
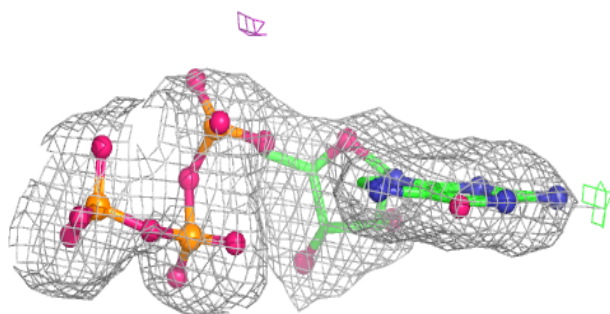
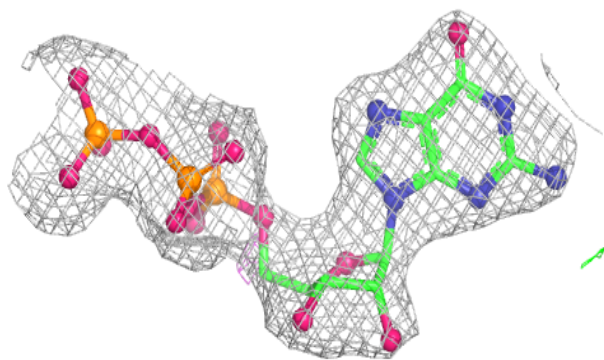
**Electron density around GTP G 301:**

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

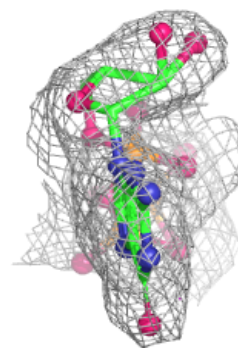
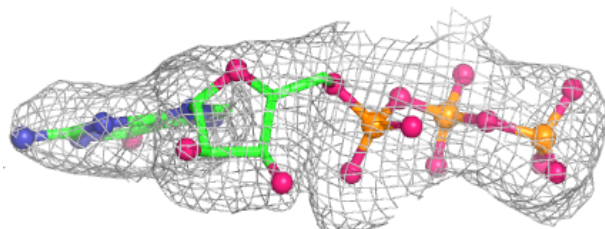
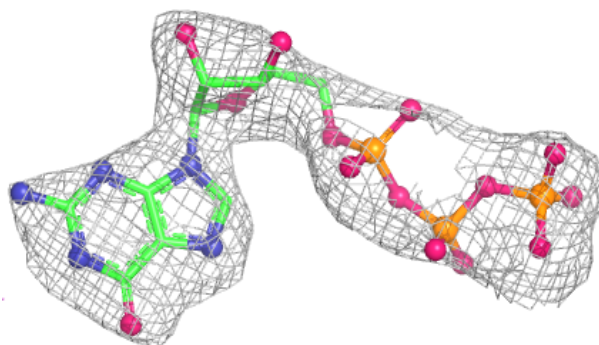


Electron density around GTP E 301:

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

**Electron density around GTP M 301:**

$2mF_o-DF_c$ (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.