



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:57 AM UTC

PDB ID : 1ETU / pdb_00001etu
Title : STRUCTURAL DETAILS OF THE BINDING OF GUANOSINE DIPHOSPHATE TO ELONGATION FACTOR TU FROM E. COLI AS STUDIED BY X-RAY CRYSTALLOGRAPHY
Authors : Clark, B.F.C.; Lacour, T.F.M.; Kjeldgaard, M.; Morikawa, K.; Nyborg, J.; Rubin, R.; Thirup, S.
Deposited on : 1988-01-15
Resolution : 2.90 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

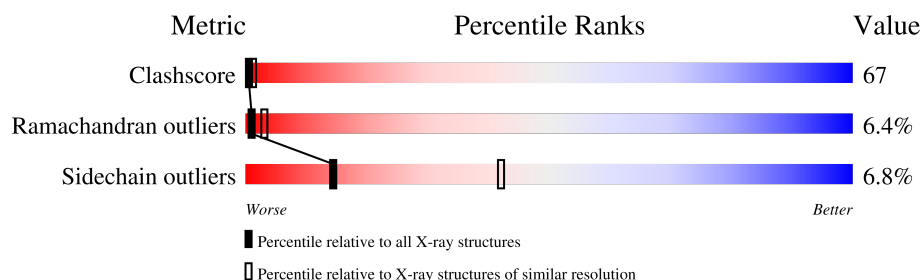
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)

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	393	9% 20% 14% . 55%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 1395 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.

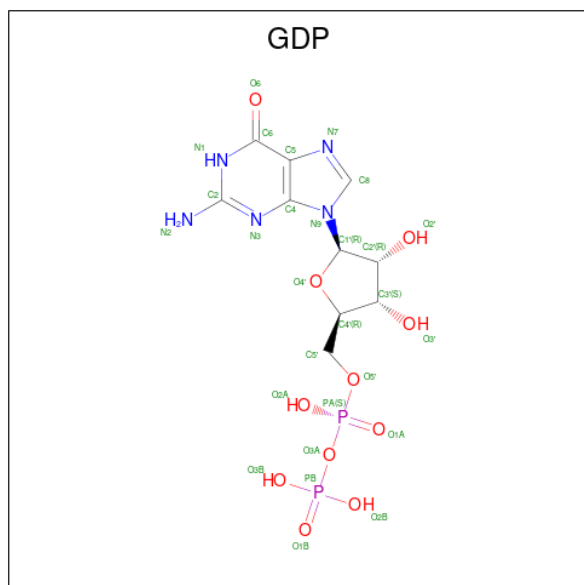
- Molecule 1 is a protein called ELONGATION FACTOR TU.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	177	Total	C	N	O	S	369	0	0
			1366	866	227	266	7			

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		

- Molecule 3 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

4 Data and refinement statistics

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

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	98.20Å 100.80Å 160.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.90	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.90)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	unknown	Depositor
R, R_{free}	(Not available) , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1395	wwPDB-VP
Average B, all atoms (Å ²)	30.0	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: GDP, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.99	49/1394 (3.5%)	2.78	143/1899 (7.5%)

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	1

All (49) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	7	ARG	N-CA	12.80	1.61	1.46
1	A	71	THR	C-N	10.17	1.44	1.34
1	A	9	LYS	N-CA	-9.69	1.32	1.46
1	A	152	GLU	C-N	-9.50	1.22	1.33
1	A	7	ARG	CA-C	9.24	1.64	1.52
1	A	153	VAL	C-N	-9.05	1.22	1.33
1	A	6	GLU	CA-C	9.03	1.64	1.52
1	A	60	ILE	C-N	8.77	1.47	1.33
1	A	70	ASP	CA-C	8.23	1.62	1.52
1	A	102	ILE	C-N	-7.51	1.23	1.33
1	A	11	HIS	N-CA	7.13	1.55	1.46
1	A	61	THR	N-CA	7.05	1.54	1.46
1	A	71	THR	N-CA	7.02	1.56	1.46
1	A	139	MET	N-CA	-6.92	1.41	1.47
1	A	24	LYS	C-N	-6.85	1.25	1.33
1	A	142	ASP	C-N	-6.69	1.25	1.33
1	A	139	MET	CA-C	-6.60	1.47	1.52
1	A	103	LEU	C-N	-6.59	1.25	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	6	GLU	C-N	6.57	1.42	1.33
1	A	171	ARG	N-CA	6.51	1.54	1.46
1	A	172	GLY	C-N	-6.51	1.24	1.33
1	A	170	VAL	CA-C	6.43	1.60	1.52
1	A	102	ILE	N-CA	6.27	1.54	1.46
1	A	8	THR	CA-C	-6.21	1.44	1.52
1	A	169	ILE	C-N	-6.10	1.25	1.33
1	A	38	THR	N-CA	-6.09	1.39	1.46
1	A	170	VAL	C-N	6.07	1.43	1.33
1	A	76	TYR	C-N	-5.88	1.25	1.33
1	A	153	VAL	CA-C	-5.88	1.45	1.52
1	A	103	LEU	CA-C	-5.84	1.45	1.52
1	A	112	MET	C-N	5.79	1.41	1.34
1	A	113	PRO	C-N	-5.66	1.26	1.33
1	A	170	VAL	CA-CB	-5.64	1.47	1.54
1	A	145	LEU	N-CA	5.63	1.53	1.46
1	A	175	LEU	C-N	-5.50	1.26	1.33
1	A	193	GLY	N-CA	5.49	1.52	1.45
1	A	184	TRP	NE1-CE2	-5.41	1.31	1.37
1	A	112	MET	N-CA	5.39	1.53	1.46
1	A	112	MET	CA-C	5.38	1.59	1.52
1	A	77	ALA	N-CA	-5.32	1.39	1.46
1	A	138	ASP	N-CA	-5.21	1.40	1.46
1	A	144	GLU	CA-C	5.20	1.59	1.52
1	A	175	LEU	N-CA	5.19	1.52	1.46
1	A	120	LEU	N-CA	5.10	1.52	1.46
1	A	101	ALA	CA-C	5.05	1.58	1.52
1	A	115	THR	CA-C	5.04	1.59	1.52
1	A	181	ASP	N-CA	-5.04	1.39	1.45
1	A	196	ASP	N-CA	-5.02	1.40	1.46
1	A	93	THR	CA-CB	-5.01	1.45	1.53

All (143) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	180	GLY	O-C-N	15.07	134.59	123.14
1	A	60	ILE	CB-CA-C	14.55	140.71	111.60
1	A	39	TYR	N-CA-C	13.61	125.84	111.14
1	A	179	GLU	CA-C-N	-13.54	111.74	122.16
1	A	179	GLU	C-N-CA	-13.54	111.74	122.16
1	A	7	ARG	N-CA-C	11.65	123.54	111.07
1	A	152	GLU	CB-CA-C	11.47	129.84	110.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	71	THR	O-C-N	-11.47	108.13	121.32
1	A	60	ILE	O-C-N	11.46	141.34	123.00
1	A	63	ASN	O-C-N	11.37	137.23	123.36
1	A	7	ARG	CA-C-N	11.36	135.50	120.28
1	A	7	ARG	C-N-CA	11.36	135.50	120.28
1	A	137	CYS	O-C-N	11.01	136.48	121.83
1	A	6	GLU	O-C-N	-10.86	110.80	122.09
1	A	106	ALA	O-C-N	10.85	136.79	123.13
1	A	178	LEU	O-C-N	10.81	133.20	122.07
1	A	182	ALA	O-C-N	10.73	136.86	122.59
1	A	197	SER	N-CA-C	10.72	122.93	111.03
1	A	140	VAL	O-C-N	10.52	135.72	122.57
1	A	138	ASP	N-CA-C	-10.29	97.69	113.02
1	A	169	ILE	O-C-N	10.22	134.03	123.20
1	A	152	GLU	O-C-N	-10.00	111.52	122.12
1	A	92	ILE	O-C-N	-9.79	112.31	121.91
1	A	161	ASP	O-C-N	9.71	135.51	122.59
1	A	178	LEU	CB-CA-C	-9.71	95.63	110.88
1	A	179	GLU	CB-CA-C	9.67	126.84	110.79
1	A	13	ASN	CA-C-N	9.63	135.90	123.10
1	A	13	ASN	C-N-CA	9.63	135.90	123.10
1	A	13	ASN	O-C-N	9.51	134.50	123.27
1	A	68	GLU	O-C-N	9.37	134.27	123.31
1	A	153	VAL	N-CA-C	9.27	120.09	110.36
1	A	37	LYS	CB-CA-C	-8.82	97.37	110.96
1	A	169	ILE	CA-C-N	8.65	134.37	123.12
1	A	169	ILE	C-N-CA	8.65	134.37	123.12
1	A	60	ILE	CA-C-N	8.54	136.56	122.73
1	A	60	ILE	C-N-CA	8.54	136.56	122.73
1	A	154	ARG	CB-CA-C	8.52	124.25	110.88
1	A	182	ALA	CA-C-N	8.47	131.45	120.44
1	A	182	ALA	C-N-CA	8.47	131.45	120.44
1	A	168	PRO	O-C-N	8.46	132.74	123.01
1	A	144	GLU	O-C-N	-8.43	113.38	122.07
1	A	99	ASP	O-C-N	8.39	131.72	122.15
1	A	9	LYS	N-CA-C	-8.13	91.85	109.81
1	A	92	ILE	CA-C-N	-8.02	106.22	121.54
1	A	92	ILE	C-N-CA	-8.02	106.22	121.54
1	A	137	CYS	CA-CB-SG	-7.93	96.17	114.40
1	A	112	MET	O-C-N	-7.91	112.22	121.32
1	A	11	HIS	O-C-N	7.87	132.41	123.05
1	A	81	CYS	CB-CA-C	7.70	119.81	109.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	66	HIS	O-C-N	7.61	132.54	123.33
1	A	172	GLY	O-C-N	7.56	132.53	122.70
1	A	195	LEU	CB-CA-C	-7.54	99.04	110.88
1	A	171	ARG	CB-CA-C	-7.47	98.62	110.79
1	A	134	LEU	O-C-N	7.38	131.97	123.27
1	A	68	GLU	CA-C-N	7.34	134.40	122.29
1	A	68	GLU	C-N-CA	7.34	134.40	122.29
1	A	188	ILE	N-CA-C	-7.33	102.26	110.62
1	A	121	LEU	N-CA-C	-7.25	103.38	111.28
1	A	141	ASP	CA-CB-CG	7.15	119.75	112.60
1	A	134	LEU	CA-C-N	7.11	133.02	123.00
1	A	134	LEU	C-N-CA	7.11	133.02	123.00
1	A	148	LEU	O-C-N	-7.08	114.77	122.07
1	A	17	ILE	CB-CA-C	-6.92	102.00	110.99
1	A	170	VAL	N-CA-CB	6.83	120.06	111.46
1	A	137	CYS	CB-CA-C	6.82	127.32	111.77
1	A	114	GLN	CB-CA-C	6.79	121.53	110.88
1	A	95	ALA	O-C-N	6.78	130.71	123.11
1	A	25	THR	N-CA-C	-6.75	103.85	111.07
1	A	11	HIS	CA-C-N	6.75	132.07	123.10
1	A	11	HIS	C-N-CA	6.75	132.07	123.10
1	A	93	THR	CB-CA-C	-6.74	97.01	110.42
1	A	140	VAL	CA-C-N	6.67	132.12	122.85
1	A	140	VAL	C-N-CA	6.67	132.12	122.85
1	A	7	ARG	CB-CA-C	-6.66	100.43	110.88
1	A	131	ILE	CB-CA-C	6.60	120.14	110.77
1	A	70	ASP	O-C-N	-6.50	115.43	123.36
1	A	131	ILE	N-CA-CB	-6.45	103.25	111.64
1	A	22	HIS	CA-CB-CG	-6.40	107.40	113.80
1	A	147	GLU	O-C-N	6.38	128.64	122.07
1	A	152	GLU	CA-CB-CG	-6.30	101.49	114.10
1	A	8	THR	N-CA-C	-6.28	104.44	111.28
1	A	9	LYS	CB-CA-C	6.26	122.51	110.17
1	A	143	GLU	N-CA-C	-6.19	104.53	111.28
1	A	73	THR	O-C-N	6.05	129.53	122.09
1	A	161	ASP	CA-C-N	6.04	136.53	121.80
1	A	161	ASP	C-N-CA	6.04	136.53	121.80
1	A	76	TYR	O-C-N	6.03	130.63	123.27
1	A	159	GLN	O-C-N	5.95	128.20	122.07
1	A	160	TYR	CB-CA-C	5.88	120.19	110.90
1	A	85	ALA	N-CA-C	-5.86	104.80	111.07
1	A	148	LEU	CB-CA-C	5.85	120.07	110.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	14	VAL	CA-C-N	5.85	132.88	121.41
1	A	14	VAL	C-N-CA	5.85	132.88	121.41
1	A	188	ILE	CB-CA-C	5.84	119.69	112.04
1	A	194	PHE	N-CA-C	-5.82	104.94	111.28
1	A	141	ASP	N-CA-CB	-5.80	100.83	110.39
1	A	120	LEU	O-C-N	5.79	128.04	122.07
1	A	154	ARG	N-CA-C	-5.75	104.92	111.07
1	A	132	VAL	O-C-N	5.74	129.40	123.03
1	A	80	ASP	CA-CB-CG	5.72	118.32	112.60
1	A	77	ALA	N-CA-C	-5.72	99.09	108.76
1	A	66	HIS	CA-C-N	5.71	130.93	122.71
1	A	66	HIS	C-N-CA	5.71	130.93	122.71
1	A	83	GLY	O-C-N	5.67	128.76	123.54
1	A	104	VAL	O-C-N	5.62	129.16	123.20
1	A	116	ARG	NE-CZ-NH2	5.61	124.25	119.20
1	A	8	THR	CB-CA-C	-5.61	101.47	110.79
1	A	179	GLU	N-CA-C	-5.61	105.17	111.28
1	A	10	PRO	CA-N-CD	5.60	119.84	112.00
1	A	111	PRO	CA-N-CD	5.60	119.84	112.00
1	A	113	PRO	O-C-N	5.57	128.46	122.17
1	A	10	PRO	O-C-N	5.55	130.13	122.64
1	A	106	ALA	CA-C-N	5.54	132.12	121.54
1	A	106	ALA	C-N-CA	5.54	132.12	121.54
1	A	126	GLY	N-CA-C	-5.53	107.38	115.63
1	A	97	GLN	N-CA-C	-5.51	99.07	110.80
1	A	83	GLY	CA-C-N	5.50	127.59	120.44
1	A	83	GLY	C-N-CA	5.50	127.59	120.44
1	A	39	TYR	O-C-N	5.49	128.02	122.09
1	A	124	GLN	CB-CA-C	5.46	119.85	110.79
1	A	74	ARG	NE-CZ-NH2	5.37	124.03	119.20
1	A	173	SER	O-C-N	5.33	129.68	122.59
1	A	93	THR	O-C-N	5.28	129.61	122.59
1	A	149	VAL	O-C-N	5.25	127.06	121.91
1	A	154	ARG	NE-CZ-NH2	5.23	123.90	119.20
1	A	170	VAL	O-C-N	5.18	129.16	123.10
1	A	10	PRO	CB-CA-C	5.16	120.08	111.56
1	A	147	GLU	N-CA-C	-5.16	105.54	111.07
1	A	125	VAL	CB-CA-C	5.16	119.10	112.14
1	A	159	GLN	CB-CA-C	-5.12	102.84	110.88
1	A	37	LYS	N-CA-C	5.10	116.53	110.97
1	A	149	VAL	N-CA-CB	5.10	116.52	110.55
1	A	70	ASP	CB-CA-C	-5.09	100.74	109.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	65	SER	O-C-N	5.08	129.26	123.31
1	A	7	ARG	O-C-N	5.08	127.31	122.07
1	A	38	THR	CA-C-N	5.06	127.32	120.44
1	A	38	THR	C-N-CA	5.06	127.32	120.44
1	A	162	PHE	N-CA-C	5.06	120.99	109.81
1	A	160	TYR	CA-CB-CG	-5.04	104.82	113.90
1	A	171	ARG	N-CA-C	5.04	116.91	107.99
1	A	37	LYS	CA-C-N	-5.03	114.01	120.65
1	A	37	LYS	C-N-CA	-5.03	114.01	120.65
1	A	12	VAL	N-CA-C	5.02	115.09	107.75

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	102	ILE	Peptide

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	1366	0	1338	129	1
2	A	1	0	0	0	0
3	A	28	0	12	5	0
All	All	1395	0	1350	129	1

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 67.

All (129) 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:A:19:HIS:HB3	1:A:22:HIS:CE1	1.72	1.22
1:A:15:GLY:C	1:A:98:MET:HE3	1.67	1.19
1:A:105:VAL:O	1:A:134:LEU:HD12	1.47	1.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139:MET:HE2	3:A:395:GDP:N2	1.71	1.06
1:A:15:GLY:CA	1:A:98:MET:HE3	1.87	1.05
1:A:19:HIS:O	1:A:20:VAL:HB	1.61	1.00
1:A:93:THR:OG1	1:A:94:GLY:N	1.81	0.99
1:A:136:LYS:C	1:A:137:CYS:SG	2.46	0.98
1:A:19:HIS:CD2	1:A:20:VAL:HG12	1.99	0.98
1:A:71:THR:HG21	1:A:196:ASP:OD1	1.66	0.96
1:A:19:HIS:HB3	1:A:22:HIS:HE1	1.17	0.95
1:A:20:VAL:HG13	1:A:20:VAL:O	1.66	0.95
1:A:15:GLY:HA3	1:A:98:MET:HE3	1.48	0.92
1:A:27:LEU:O	1:A:31:ILE:HG13	1.71	0.90
1:A:137:CYS:O	1:A:184:TRP:CZ2	2.26	0.87
1:A:139:MET:HE2	3:A:395:GDP:HN22	1.37	0.86
1:A:126:GLY:O	1:A:128:PRO:HD3	1.75	0.85
1:A:86:ASP:O	1:A:90:ASN:OD1	1.94	0.84
1:A:147:GLU:O	1:A:151:MET:N	2.10	0.84
1:A:182:ALA:O	1:A:185:GLU:HB2	1.77	0.83
1:A:23:GLY:O	1:A:27:LEU:N	2.11	0.81
1:A:133:PHE:HA	1:A:170:VAL:O	1.80	0.81
1:A:129:TYR:HD2	1:A:198:TYR:HE1	1.29	0.79
1:A:35:LEU:CD2	1:A:69:TYR:CD1	2.66	0.79
1:A:70:ASP:OD1	1:A:75:HIS:ND1	2.16	0.78
1:A:136:LYS:C	1:A:137:CYS:HG	1.86	0.78
1:A:20:VAL:O	1:A:20:VAL:CG1	2.30	0.78
1:A:168:PRO:HB3	1:A:194:PHE:CD1	2.20	0.76
1:A:129:TYR:CD2	1:A:198:TYR:CE1	2.74	0.75
1:A:15:GLY:C	1:A:98:MET:CE	2.57	0.75
1:A:23:GLY:HA2	3:A:395:GDP:O1A	1.87	0.75
1:A:15:GLY:HA3	1:A:98:MET:CE	2.16	0.75
1:A:19:HIS:CB	1:A:22:HIS:HE1	1.96	0.74
1:A:35:LEU:CD2	1:A:69:TYR:HD1	2.00	0.74
1:A:139:MET:CE	3:A:395:GDP:N2	2.52	0.72
1:A:129:TYR:CD2	1:A:198:TYR:HE1	2.07	0.72
1:A:19:HIS:O	1:A:114:GLN:NE2	2.24	0.71
1:A:83:GLY:O	1:A:86:ASP:HB2	1.91	0.71
1:A:153:VAL:O	1:A:157:LEU:HG	1.90	0.70
1:A:105:VAL:O	1:A:134:LEU:CD1	2.34	0.70
1:A:15:GLY:O	1:A:98:MET:HE3	1.92	0.70
1:A:28:THR:HG23	1:A:78:HIS:CD2	2.27	0.69
1:A:136:LYS:O	1:A:137:CYS:SG	2.45	0.69
1:A:129:TYR:HD2	1:A:198:TYR:CE1	2.09	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:HIS:ND1	1:A:118:HIS:NE2	2.37	0.68
1:A:24:LYS:HD2	1:A:87:TYR:OH	1.95	0.66
1:A:140:VAL:CG1	1:A:146:LEU:HD21	2.25	0.65
1:A:9:LYS:O	1:A:11:HIS:CD2	2.49	0.65
1:A:134:LEU:N	1:A:170:VAL:O	2.27	0.64
1:A:85:ALA:O	1:A:89:LYS:HG2	1.96	0.64
1:A:84:HIS:CE1	1:A:118:HIS:HE2	2.16	0.63
1:A:125:VAL:HG12	1:A:127:VAL:HG23	1.80	0.63
1:A:19:HIS:CB	1:A:22:HIS:CE1	2.66	0.62
1:A:93:THR:HG1	1:A:94:GLY:H	1.42	0.62
1:A:87:TYR:CD2	1:A:118:HIS:HE1	2.18	0.61
1:A:140:VAL:HG12	1:A:146:LEU:HD21	1.82	0.61
1:A:73:THR:HG22	1:A:74:ARG:HG3	1.83	0.60
1:A:15:GLY:O	1:A:98:MET:CE	2.48	0.60
1:A:138:ASP:C	1:A:139:MET:CG	2.73	0.60
1:A:19:HIS:ND1	1:A:114:GLN:HG3	2.15	0.60
1:A:35:LEU:HD22	1:A:69:TYR:CD1	2.37	0.60
1:A:19:HIS:O	1:A:20:VAL:CB	2.45	0.60
1:A:19:HIS:ND1	1:A:114:GLN:HB2	2.16	0.59
1:A:145:LEU:O	1:A:148:LEU:HB2	2.02	0.59
1:A:14:VAL:HA	1:A:100:GLY:O	2.01	0.59
1:A:94:GLY:O	1:A:95:ALA:C	2.44	0.59
1:A:194:PHE:O	1:A:198:TYR:N	2.27	0.58
1:A:15:GLY:HA3	1:A:98:MET:HG3	1.86	0.57
1:A:125:VAL:CG1	1:A:127:VAL:HG23	2.34	0.57
1:A:132:VAL:O	1:A:169:ILE:HA	2.04	0.57
1:A:25:THR:HA	1:A:80:ASP:OD2	2.06	0.56
1:A:114:GLN:O	1:A:118:HIS:CD2	2.59	0.55
1:A:168:PRO:HB3	1:A:194:PHE:CE1	2.42	0.55
1:A:16:THR:CG2	1:A:24:LYS:HB2	2.37	0.54
1:A:105:VAL:HG11	1:A:153:VAL:CG2	2.36	0.54
1:A:84:HIS:CE1	1:A:118:HIS:NE2	2.76	0.54
1:A:14:VAL:CG1	1:A:102:ILE:HG13	2.38	0.53
1:A:93:THR:HG1	1:A:94:GLY:N	2.02	0.53
1:A:198:TYR:O	1:A:200:PRO:HD3	2.07	0.53
1:A:158:SER:O	1:A:159:GLN:C	2.51	0.53
1:A:15:GLY:HA3	1:A:98:MET:SD	2.48	0.53
1:A:23:GLY:O	1:A:26:THR:HB	2.10	0.52
1:A:146:LEU:O	1:A:147:GLU:C	2.51	0.52
1:A:145:LEU:O	1:A:149:VAL:N	2.39	0.52
1:A:153:VAL:O	1:A:154:ARG:C	2.49	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:ASP:CG	1:A:75:HIS:HD1	2.14	0.51
1:A:126:GLY:O	1:A:128:PRO:CD	2.55	0.51
1:A:95:ALA:O	1:A:96:ALA:HB3	2.08	0.51
1:A:19:HIS:ND1	1:A:114:GLN:CG	2.73	0.51
1:A:27:LEU:O	1:A:31:ILE:CG1	2.53	0.51
1:A:15:GLY:HA3	1:A:98:MET:CG	2.41	0.50
1:A:92:ILE:O	1:A:93:THR:C	2.53	0.49
1:A:35:LEU:HD21	1:A:69:TYR:CD1	2.46	0.48
1:A:150:GLU:O	1:A:154:ARG:HG3	2.14	0.48
1:A:14:VAL:HG13	1:A:102:ILE:HG13	1.95	0.48
1:A:70:ASP:OD1	1:A:75:HIS:HB2	2.14	0.48
1:A:9:LYS:O	1:A:10:PRO:C	2.55	0.47
1:A:24:LYS:HG2	3:A:395:GDP:O2B	2.15	0.47
1:A:92:ILE:O	1:A:93:THR:O	2.33	0.47
1:A:183:GLU:O	1:A:186:ALA:HB3	2.15	0.47
1:A:138:ASP:C	1:A:139:MET:HG3	2.38	0.47
1:A:16:THR:HG22	1:A:24:LYS:HB2	1.95	0.47
1:A:19:HIS:CE1	1:A:114:GLN:HG3	2.50	0.47
1:A:137:CYS:HB2	1:A:172:GLY:O	2.15	0.47
1:A:192:ALA:O	1:A:195:LEU:HB2	2.14	0.46
1:A:86:ASP:C	1:A:90:ASN:OD1	2.57	0.45
1:A:134:LEU:O	1:A:171:ARG:HA	2.17	0.45
1:A:22:HIS:HB3	1:A:104:VAL:HG12	1.99	0.45
1:A:19:HIS:NE2	1:A:20:VAL:HG12	2.30	0.44
1:A:168:PRO:CB	1:A:194:PHE:CD1	2.96	0.44
1:A:140:VAL:CG1	1:A:146:LEU:CD2	2.95	0.44
1:A:74:ARG:HD2	1:A:196:ASP:HA	2.00	0.43
1:A:146:LEU:O	1:A:150:GLU:HB2	2.18	0.43
1:A:187:LYS:O	1:A:188:ILE:C	2.60	0.43
1:A:16:THR:HG21	1:A:24:LYS:HB2	2.00	0.43
1:A:105:VAL:HG11	1:A:153:VAL:HG22	2.01	0.43
1:A:152:GLU:HG2	1:A:155:GLU:OE1	2.19	0.42
1:A:168:PRO:HD3	1:A:198:TYR:CE2	2.54	0.42
1:A:19:HIS:HA	1:A:114:GLN:HB2	2.01	0.42
1:A:145:LEU:O	1:A:148:LEU:N	2.53	0.42
1:A:19:HIS:ND1	1:A:114:GLN:CB	2.81	0.42
1:A:31:ILE:HA	1:A:188:ILE:HG21	2.01	0.42
1:A:70:ASP:OD1	1:A:75:HIS:CG	2.73	0.41
1:A:14:VAL:HG21	1:A:76:TYR:CE2	2.55	0.41
1:A:31:ILE:HA	1:A:188:ILE:CG2	2.50	0.41
1:A:168:PRO:CD	1:A:198:TYR:CD2	3.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:ASP:OD1	1:A:75:HIS:CB	2.70	0.40
1:A:102:ILE:HA	1:A:131:ILE:O	2.20	0.40
1:A:35:LEU:HD22	1:A:69:TYR:HB2	2.04	0.40

All (1) 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:A:63:ASN:ND2	1:A:65:SER:OG[3_755]	1.38	0.82

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	173/393 (44%)	148 (86%)	14 (8%)	11 (6%)	1 3

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	20	VAL
1	A	136	LYS
1	A	142	ASP
1	A	182	ALA
1	A	21	ASP
1	A	93	THR
1	A	97	GLN
1	A	107	ALA
1	A	163	PRO
1	A	96	ALA
1	A	127	VAL

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	148/325 (46%)	138 (93%)	10 (7%)	14	42

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ARG
1	A	60	ILE
1	A	65	SER
1	A	79	VAL
1	A	131	ILE
1	A	138	ASP
1	A	148	LEU
1	A	161	ASP
1	A	175	LEU
1	A	178	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	114	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	GDP	A	395	2	29,30,30	1.89	5 (17%)	45,47,47	1.69	7 (15%)

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
3	GDP	A	395	2	-	2/16/32/32	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	395	GDP	C5-N7	-6.54	1.26	1.39
3	A	395	GDP	C4-N3	-3.09	1.27	1.34
3	A	395	GDP	C8-N9	-2.98	1.30	1.37
3	A	395	GDP	C6-N1	-2.82	1.33	1.38
3	A	395	GDP	C8-N7	2.49	1.39	1.32

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	395	GDP	C5-C4-N3	-5.45	119.71	128.39
3	A	395	GDP	C2-N3-C4	4.34	119.77	112.30
3	A	395	GDP	C2'-C3'-C4'	3.02	108.44	102.61
3	A	395	GDP	C6-C5-C4	2.89	123.18	118.83
3	A	395	GDP	N9-C4-N3	2.35	130.66	125.95
3	A	395	GDP	O3B-PB-O3A	2.12	111.73	104.64
3	A	395	GDP	C5-C4-N9	2.06	109.35	105.66

There are no chirality outliers.

All (2) torsion outliers are listed below:

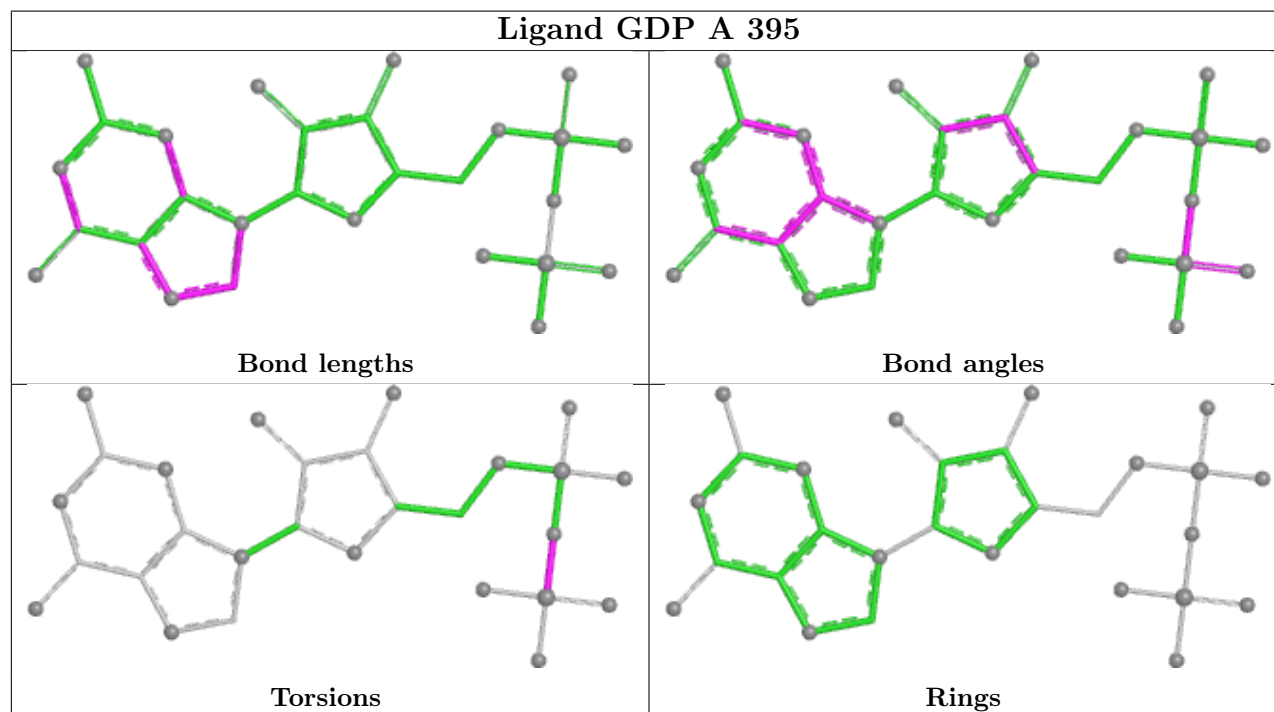
Mol	Chain	Res	Type	Atoms
3	A	395	GDP	PA-O3A-PB-O1B
3	A	395	GDP	PA-O3A-PB-O2B

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	395	GDP	5	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [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.