Full wwPDB X-ray Structure Validation Report ⓘ

Dec 15, 2024 – 04:40 PM EST

PDB ID	:	1ETU
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:

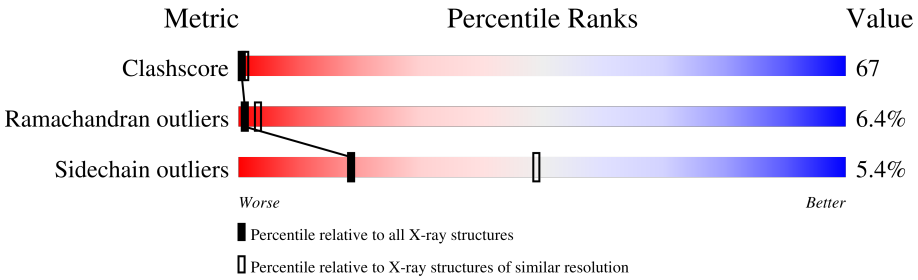
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

1 Overall quality at a glance (i)

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	180529	2564 (2.90-2.90)
Ramachandran outliers	177936	2514 (2.90-2.90)
Sidechain outliers	177891	2516 (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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	393	15% 20% 10% · 55%

2 Entry composition

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.

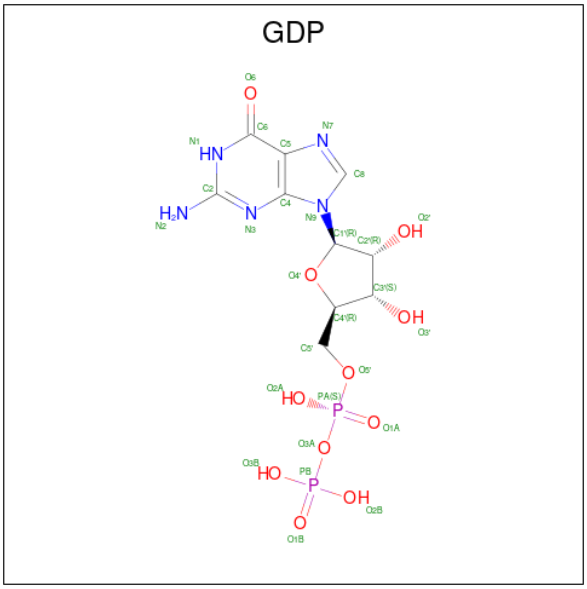
- Molecule 1 is a protein called ELONGATION FACTOR TU.

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 (three-letter code: MG) (formula: Mg).

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

- Molecule 3 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



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

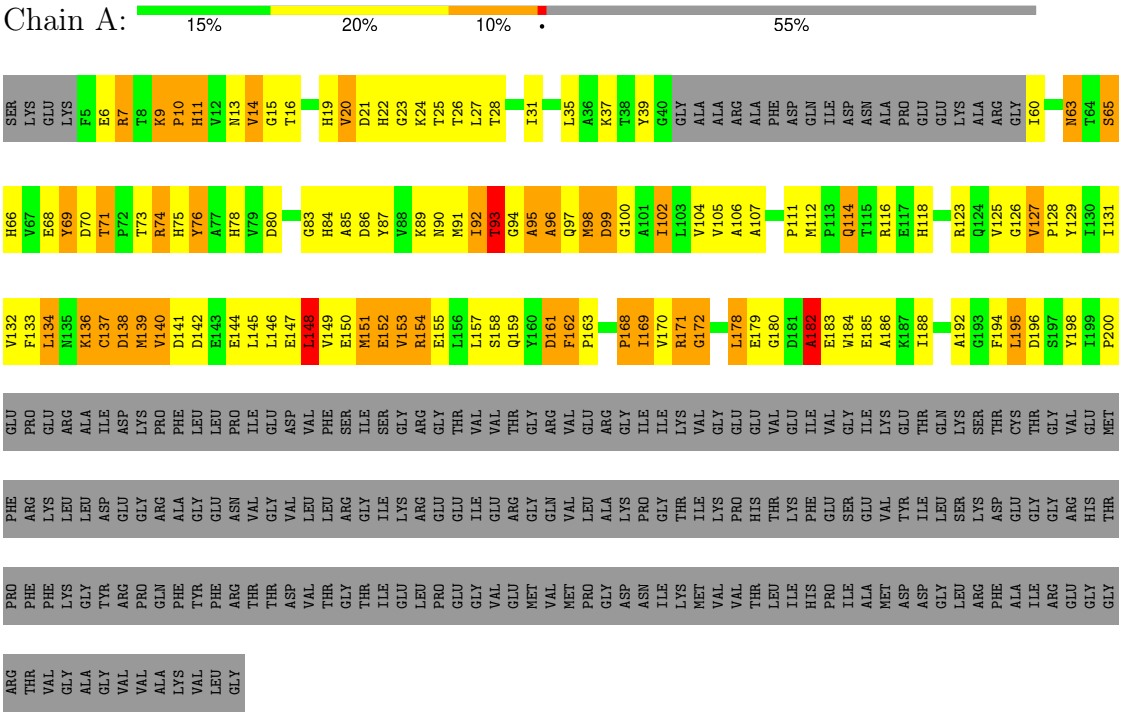
3 Residue-property plots (i)

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. 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: ELONGATION FACTOR TU

Chain A:



4 Data and refinement statistics (i)

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	1.40	7/1394 (0.5%)	2.17	82/1899 (4.3%)

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 (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	7	ARG	N-CA	7.63	1.61	1.46
1	A	9	LYS	N-CA	-6.93	1.32	1.46
1	A	60	ILE	C-N	5.69	1.47	1.34
1	A	71	THR	C-N	5.17	1.44	1.34
1	A	9	LYS	C-N	-5.15	1.24	1.34
1	A	152	GLU	C-N	-5.13	1.22	1.34
1	A	153	VAL	C-N	-5.07	1.22	1.34

All (82) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	60	ILE	CB-CA-C	14.55	140.71	111.60
1	A	60	ILE	O-C-N	11.65	141.34	122.70
1	A	60	ILE	CA-C-N	-9.91	95.40	117.20
1	A	137	CYS	CA-CB-SG	-9.91	96.17	114.00
1	A	152	GLU	CB-CA-C	9.72	129.84	110.40
1	A	63	ASN	O-C-N	9.08	137.23	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	182	ALA	O-C-N	8.85	136.86	122.70
1	A	106	ALA	O-C-N	8.81	136.79	122.70
1	A	76	TYR	CB-CG-CD1	-8.74	115.75	121.00
1	A	137	CYS	O-C-N	8.61	136.48	122.70
1	A	137	CYS	CB-CA-C	8.46	127.32	110.40
1	A	69	TYR	CB-CG-CD2	-8.34	115.99	121.00
1	A	179	GLU	CB-CA-C	8.22	126.84	110.40
1	A	140	VAL	O-C-N	8.14	135.72	122.70
1	A	161	ASP	O-C-N	8.01	135.51	122.70
1	A	116	ARG	NE-CZ-NH2	7.91	124.25	120.30
1	A	178	LEU	CB-CA-C	-7.67	95.63	110.20
1	A	74	ARG	NE-CZ-NH2	7.47	124.03	120.30
1	A	6	GLU	O-C-N	-7.44	110.80	122.70
1	A	180	GLY	O-C-N	7.43	134.59	122.70
1	A	13	ASN	O-C-N	7.37	134.50	122.70
1	A	68	GLU	O-C-N	7.23	134.27	122.70
1	A	154	ARG	NE-CZ-NH2	7.21	123.90	120.30
1	A	9	LYS	N-CA-C	-7.09	91.85	111.00
1	A	169	ILE	O-C-N	7.08	134.03	122.70
1	A	152	GLU	O-C-N	-6.99	111.52	122.70
1	A	154	ARG	CB-CA-C	6.93	124.25	110.40
1	A	71	THR	O-C-N	-6.83	108.13	121.10
1	A	63	ASN	CA-C-N	-6.81	102.21	117.20
1	A	182	ALA	CA-C-N	-6.72	102.41	117.20
1	A	106	ALA	CA-C-N	-6.70	102.46	117.20
1	A	137	CYS	CA-C-N	-6.67	102.52	117.20
1	A	7	ARG	NE-CZ-NH2	6.60	123.60	120.30
1	A	178	LEU	O-C-N	6.56	133.20	122.70
1	A	37	LYS	CB-CA-C	-6.51	97.37	110.40
1	A	92	ILE	O-C-N	-6.49	112.31	122.70
1	A	91	MET	CG-SD-CE	6.46	110.54	100.20
1	A	112	MET	CG-SD-CE	6.39	110.43	100.20
1	A	171	ARG	NE-CZ-NH2	6.31	123.45	120.30
1	A	168	PRO	O-C-N	6.28	132.74	122.70
1	A	92	ILE	C-N-CA	-6.19	106.22	121.70
1	A	98	MET	CG-SD-CE	6.17	110.07	100.20
1	A	66	HIS	O-C-N	6.15	132.54	122.70
1	A	172	GLY	O-C-N	6.14	132.53	122.70
1	A	180	GLY	CA-C-N	-6.12	103.73	117.20
1	A	140	VAL	CA-C-N	-6.11	103.75	117.20
1	A	11	HIS	O-C-N	6.07	132.41	122.70
1	A	9	LYS	CB-CA-C	6.05	122.51	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	139	MET	CG-SD-CE	6.04	109.87	100.20
1	A	60	ILE	C-N-CA	5.94	136.56	121.70
1	A	161	ASP	C-N-CA	5.93	136.53	121.70
1	A	171	ARG	CB-CA-C	-5.89	98.62	110.40
1	A	195	LEU	CB-CA-C	-5.87	99.04	110.20
1	A	69	TYR	CD1-CG-CD2	5.82	124.31	117.90
1	A	144	GLU	O-C-N	-5.82	113.38	122.70
1	A	10	PRO	CA-N-CD	5.82	119.84	111.70
1	A	111	PRO	CA-N-CD	5.81	119.84	111.70
1	A	134	LEU	O-C-N	5.80	131.97	122.70
1	A	162	PHE	CB-CG-CD2	-5.79	116.75	120.80
1	A	13	ASN	CA-C-N	-5.78	104.48	117.20
1	A	68	GLU	CA-C-N	-5.75	104.54	117.20
1	A	151	MET	CG-SD-CE	5.72	109.35	100.20
1	A	13	ASN	C-N-CA	5.68	135.90	121.70
1	A	114	GLN	CB-CA-C	5.57	121.53	110.40
1	A	7	ARG	C-N-CA	5.52	135.50	121.70
1	A	161	ASP	CA-C-N	-5.52	105.06	117.20
1	A	39	TYR	N-CA-C	5.50	125.84	111.00
1	A	71	THR	CA-C-N	5.48	132.45	117.10
1	A	141	ASP	N-CA-CB	-5.43	100.83	110.60
1	A	152	GLU	CA-CB-CG	-5.41	101.49	113.40
1	A	93	THR	CB-CA-C	-5.40	97.01	111.60
1	A	123	ARG	NE-CZ-NH2	5.32	122.96	120.30
1	A	6	GLU	CA-C-N	5.22	128.68	117.20
1	A	178	LEU	CA-C-N	-5.21	105.73	117.20
1	A	148	LEU	CB-CA-C	5.20	120.07	110.20
1	A	76	TYR	CB-CA-C	-5.08	100.23	110.40
1	A	68	GLU	C-N-CA	5.08	134.40	121.70
1	A	169	ILE	C-N-CA	5.07	134.37	121.70
1	A	14	VAL	C-N-CA	5.04	132.88	122.30
1	A	179	GLU	C-N-CA	-5.03	111.74	122.30
1	A	99	ASP	O-C-N	5.01	131.72	123.20
1	A	95	ALA	O-C-N	5.00	130.71	122.70

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 (i)

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	1337	130	1
2	A	1	0	0	0	0
3	A	28	0	12	6	0
All	All	1395	0	1349	130	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 (130) 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:105:VAL:O	1:A:134:LEU:HD12	1.47	1.15
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: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:136:LYS:C	1:A:137:CYS:SG	2.46	0.93
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: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: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:136:LYS:O	1:A:137:CYS:SG	2.45	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:15:GLY:C	1:A:98:MET:CE	2.57	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:C	1:A:98:MET:HE3	2.12	0.69
1:A:28:THR:HG23	1:A:78:HIS:CD2	2.27	0.69
1:A:139:MET:HE2	3:A:395:GDP:HN22	1.56	0.69
1:A:93:THR:HG1	1:A:94:GLY:H	1.36	0.69
1:A:129:TYR:HD2	1:A:198:TYR:CE1	2.09	0.69
1:A:84:HIS:ND1	1:A:118:HIS:NE2	2.37	0.68
1:A:15:GLY:O	1:A:98:MET:HE2	1.95	0.67
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:136:LYS:C	1:A:137:CYS:HG	1.90	0.65
1:A:9:LYS:O	1:A:11:HIS:CD2	2.49	0.65
1:A:139:MET:HE2	3:A:395:GDP:N2	2.10	0.64
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:139:MET:HE3	3:A:395:GDP:N2	2.13	0.63
1:A:15:GLY:CA	1:A:98:MET:CE	2.76	0.63
1:A:19:HIS:CB	1:A:22:HIS:CE1	2.66	0.62
1:A:15:GLY:C	1:A:98:MET:HE2	2.20	0.61
1:A:87:TYR:CD2	1:A:118:HIS:HE1	2.18	0.61
1:A:15:GLY:O	1:A:98:MET:CE	2.48	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:CA	1:A:98:MET:HE2	2.30	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:15:GLY:HA3	1:A:98:MET:HE2	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:138:ASP:C	1:A:139:MET:CG	2.73	0.55
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:94:GLY:O	1:A:95:ALA:C	2.44	0.54
1:A:14:VAL:CG1	1:A:102:ILE:HG13	2.38	0.53
1:A:198:TYR:O	1:A:200:PRO:HD3	2.07	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:145:LEU:O	1:A:149:VAL:N	2.39	0.52
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: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:158:SER:O	1:A:159:GLN:C	2.51	0.48
1:A:70:ASP:OD1	1:A:75:HIS:HB2	2.14	0.48
1:A:24:LYS:HG2	3:A:395:GDP:O2B	2.15	0.47
1:A:146:LEU:O	1:A:147:GLU:C	2.51	0.47
1:A:92:ILE:O	1:A:93:THR:O	2.33	0.47
1:A:153:VAL:O	1:A:154:ARG:C	2.49	0.47
1:A:183:GLU:O	1:A:186:ALA:HB3	2.15	0.47
1:A:70:ASP:CG	1:A:75:HIS:HD1	2.14	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:134:LEU:O	1:A:171:ARG:HA	2.17	0.45
1:A:92:ILE:O	1:A:93:THR:C	2.53	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:16:THR:HG21	1:A:24:LYS:HB2	2.00	0.43
1:A:9:LYS:O	1:A:10:PRO:C	2.55	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:138:ASP:C	1:A:139:MET:HG3	2.38	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
1:A:86:ASP:C	1:A:90:ASN:OD1	2.57	0.41
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 (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	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%)	140 (95%)	8 (5%)	18 49

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ARG
1	A	65	SER
1	A	99	ASP
1	A	138	ASP
1	A	148	LEU
1	A	161	ASP
1	A	162	PHE
1	A	178	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	HIS
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 (i)

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	25,30,30	1.88	5 (20%)	30,47,47	1.46	4 (13%)

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	-	2/12/32/32	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-C6	-4.49	1.38	1.47
3	A	395	GDP	C4-N3	-4.19	1.27	1.37
3	A	395	GDP	O4'-C1'	3.53	1.45	1.40
3	A	395	GDP	C8-N7	2.97	1.39	1.34
3	A	395	GDP	C6-N1	-2.76	1.33	1.37

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	395	GDP	C2'-C3'-C4'	3.02	108.44	102.61
3	A	395	GDP	C8-N7-C5	2.86	107.42	102.55
3	A	395	GDP	O4'-C1'-N9	2.17	111.63	108.75
3	A	395	GDP	O3B-PB-O3A	2.12	111.73	104.64

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

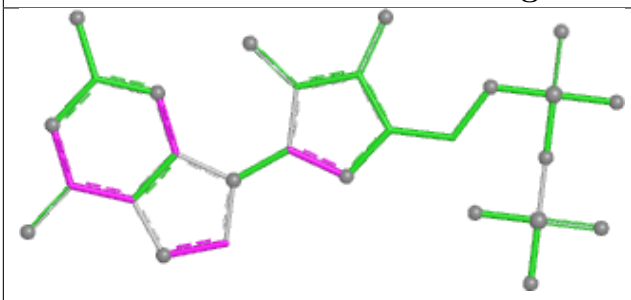
There are no ring outliers.

1 monomer is involved in 6 short contacts:

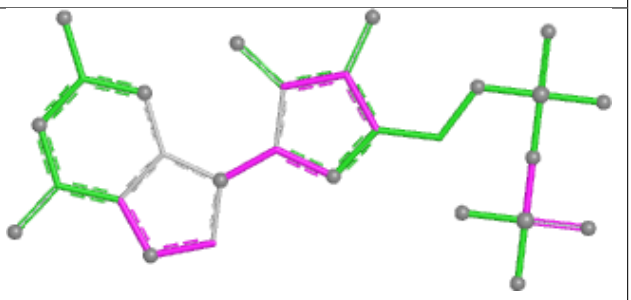
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	395	GDP	6	0

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 then 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.

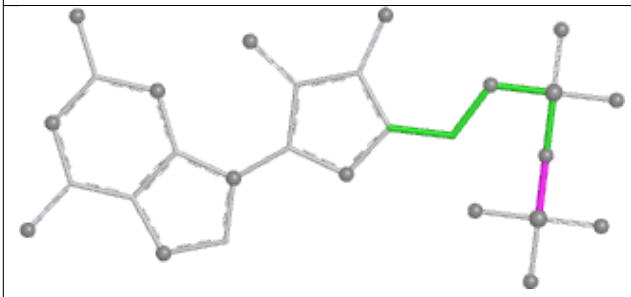
Ligand GDP A 395



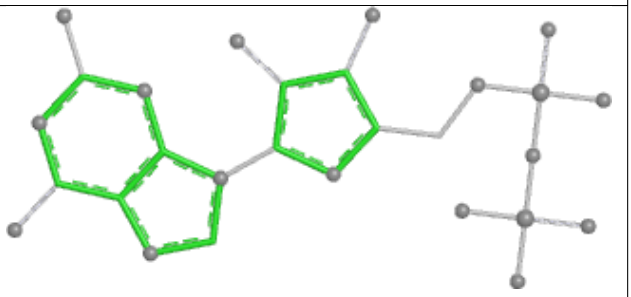
Bond lengths



Bond angles



Torsions



Rings

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.