



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 05:16 PM UTC

PDB ID : 4MYT / pdb_00004myt
Title : Crystal structure of elongation factor G (EFG)
Authors : Liu, G.; Dong, J.; Gong, W.; Qin, Y.
Deposited on : 2013-09-28
Resolution : 3.50 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

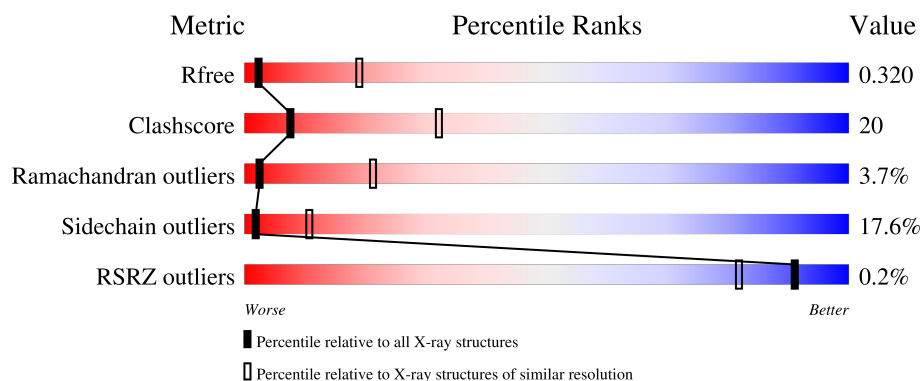
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)

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	691	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 5130 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 G.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	656	5101	3242	873	968	18	0	0	0

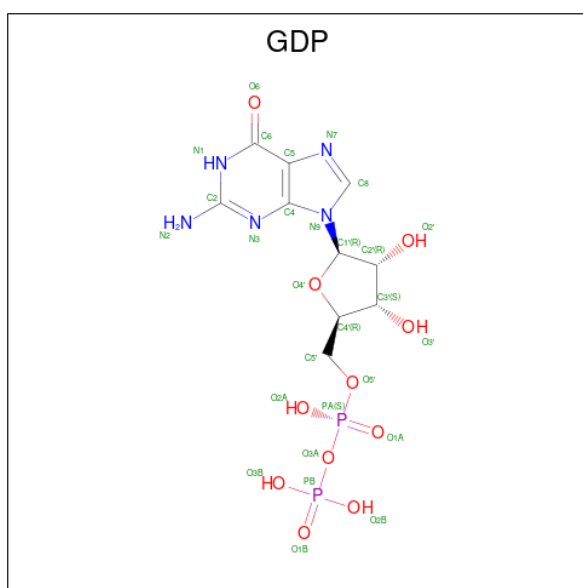
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	579	ALA	GLU	engineered mutation	UNP P13551

- 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		

- Molecule 1: Elongation factor G



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	74.88Å 101.36Å 114.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.93 – 3.50 37.93 – 3.50	Depositor EDS
% Data completeness (in resolution range)	97.6 (37.93-3.50) 97.6 (37.93-3.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.52 (at 3.48Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.207 , 0.308 0.216 , 0.320	Depositor DCC
R_{free} test set	537 reflections (4.71%)	wwPDB-VP
Wilson B-factor (Å ²)	72.4	Xtriage
Anisotropy	0.600	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 46.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.37$, $\langle L^2 \rangle = 0.19$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	5130	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.62% 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: 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	0.58	0/5196	1.05	19/7043 (0.3%)

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	173	THR	N-CA-C	-6.13	104.58	114.09
1	A	304	ASP	CA-C-N	5.84	125.70	119.28
1	A	304	ASP	C-N-CA	5.84	125.70	119.28
1	A	443	HIS	CA-C-N	5.83	127.13	119.84
1	A	443	HIS	C-N-CA	5.83	127.13	119.84
1	A	474	ALA	N-CA-C	5.83	115.53	107.73
1	A	534	ILE	CA-C-N	5.76	125.69	119.76
1	A	534	ILE	C-N-CA	5.76	125.69	119.76
1	A	140	ASP	N-CA-C	-5.74	106.41	113.41
1	A	301	ILE	N-CA-C	5.60	115.39	106.88
1	A	132	ARG	N-CA-C	5.42	116.52	108.60
1	A	551	GLN	N-CA-C	-5.33	105.08	113.02
1	A	328	ILE	N-CA-C	5.33	115.95	108.17
1	A	645	ALA	N-CA-C	5.21	116.20	108.86
1	A	563	ILE	CB-CA-C	-5.19	104.08	111.40
1	A	315	LYS	N-CA-C	5.11	117.12	108.02
1	A	563	ILE	N-CA-C	5.02	114.88	107.75
1	A	404	VAL	CA-C-N	5.02	125.30	119.93
1	A	404	VAL	C-N-CA	5.02	125.30	119.93

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5101	0	5147	208	2
2	A	1	0	0	0	0
3	A	28	0	12	4	0
All	All	5130	0	5159	208	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 20.

All (208) 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:547:GLU:HA	1:A:550:MET:HE2	1.55	0.88
1:A:324:ARG:NH2	1:A:383:THR:O	2.14	0.79
1:A:152:THR:HB	1:A:156:ARG:HD3	1.66	0.76
1:A:268:GLY:HA2	1:A:271:LEU:HD12	1.68	0.76
1:A:418:LYS:HA	1:A:421:GLN:HB2	1.67	0.76
1:A:24:GLY:O	1:A:28:THR:OG1	2.03	0.76
1:A:439:ARG:HB2	1:A:452:SER:HB2	1.71	0.73
1:A:20:HIS:CD2	1:A:117:GLN:HB3	2.25	0.71
1:A:634:MET:HB3	1:A:643:ILE:HG12	1.71	0.71
1:A:491:VAL:HG11	1:A:596:LYS:HB3	1.71	0.71
1:A:13:ARG:HH21	1:A:282:SER:HB3	1.54	0.70
1:A:444:PRO:HG3	1:A:551:GLN:HB3	1.73	0.70
1:A:600:VAL:HA	1:A:684:GLN:HE22	1.57	0.68
1:A:348:ARG:HD3	1:A:382:GLU:HB2	1.76	0.68
1:A:74:TRP:HE1	1:A:75:LYS:HE2	1.59	0.67
1:A:319:ASP:OD2	1:A:363:ARG:NH2	2.23	0.66
1:A:514:VAL:HG22	1:A:565:VAL:HG13	1.77	0.66
1:A:151:ARG:O	1:A:155:GLU:HB2	1.96	0.65
1:A:496:LYS:HG2	1:A:509:HIS:CD2	2.32	0.64
1:A:160:ARG:NH2	1:A:222:ASP:OD2	2.31	0.62
1:A:250:THR:HG23	1:A:257:PRO:HD2	1.82	0.62
1:A:316:ILE:HG12	1:A:385:THR:HG23	1.82	0.62
1:A:462:ILE:HA	1:A:465:ARG:HB3	1.83	0.61
1:A:82:ILE:HD13	1:A:101:LEU:HB3	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:THR:O	1:A:32:ILE:N	2.30	0.61
1:A:19:ALA:HB1	1:A:23:ALA:HB3	1.83	0.61
1:A:74:TRP:NE1	1:A:75:LYS:HE2	2.17	0.60
1:A:264:LEU:HB2	3:A:702:GDP:C6	2.36	0.60
1:A:555:LEU:HD21	1:A:599:PRO:HB2	1.82	0.60
1:A:115:GLU:HB2	1:A:118:SER:HB2	1.84	0.60
1:A:101:LEU:HD13	1:A:103:GLY:O	2.03	0.59
1:A:264:LEU:HD23	3:A:702:GDP:C5	2.38	0.59
1:A:259:PHE:HZ	1:A:279:TYR:HE2	1.51	0.59
1:A:169:GLY:HA3	1:A:174:PHE:HA	1.85	0.58
1:A:617:MET:SD	1:A:641:GLN:HG2	2.44	0.58
1:A:549:ALA:HB1	1:A:591:LYS:HG2	1.85	0.58
1:A:247:ARG:NH2	1:A:281:PRO:HA	2.19	0.57
1:A:335:LEU:HG	1:A:355:LEU:HD11	1.87	0.57
1:A:466:LEU:HA	1:A:470:PHE:HB2	1.87	0.57
1:A:90:PHE:O	1:A:92:ILE:N	2.38	0.56
1:A:523:PHE:HD1	1:A:524:GLU:H	1.54	0.56
1:A:356:LEU:HB2	1:A:376:ALA:HB3	1.88	0.56
1:A:153:MET:HA	1:A:157:LEU:HD12	1.87	0.56
1:A:171:GLU:HB3	1:A:172:ASP:OD1	2.06	0.55
1:A:606:MET:HE2	1:A:671:MET:HB3	1.88	0.55
1:A:238:THR:OG1	1:A:241:GLU:HB2	2.07	0.55
1:A:259:PHE:HZ	1:A:279:TYR:CE2	2.25	0.55
1:A:635:GLU:OE2	1:A:644:ARG:NH1	2.40	0.55
1:A:117:GLN:O	1:A:121:VAL:HG13	2.07	0.55
1:A:248:LYS:NZ	1:A:252:ASP:OD2	2.40	0.54
1:A:343:ASN:HD22	1:A:346:LYS:H	1.53	0.54
1:A:519:ARG:HD2	1:A:602:LEU:HD13	1.90	0.54
1:A:574:GLU:HG2	1:A:575:VAL:N	2.22	0.54
1:A:20:HIS:HB2	1:A:118:SER:HB2	1.90	0.54
1:A:103:GLY:HA3	1:A:280:LEU:HG	1.89	0.54
1:A:470:PHE:HB3	1:A:472:VAL:HG23	1.89	0.54
1:A:310:ALA:HA	1:A:389:LEU:O	2.08	0.53
1:A:142:THR:HA	1:A:171:GLU:HG3	1.90	0.53
1:A:188:TYR:HB2	1:A:267:LYS:HE3	1.89	0.53
1:A:247:ARG:NH1	1:A:278:ASP:O	2.35	0.53
1:A:562:ASP:OD2	1:A:562:ASP:N	2.42	0.53
1:A:355:LEU:CD2	1:A:377:VAL:HG12	2.39	0.52
1:A:427:ALA:HB1	1:A:470:PHE:CD1	2.44	0.52
1:A:600:VAL:HA	1:A:684:GLN:NE2	2.25	0.52
1:A:213:HIS:O	1:A:217:VAL:HG23	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:TYR:CG	1:A:267:LYS:HG2	2.45	0.52
1:A:681:LYS:H	1:A:681:LYS:HD2	1.74	0.51
1:A:496:LYS:HG2	1:A:509:HIS:HD2	1.76	0.51
1:A:247:ARG:HG3	1:A:279:TYR:HA	1.93	0.51
1:A:19:ALA:HB2	1:A:107:VAL:HB	1.92	0.51
1:A:356:LEU:HA	1:A:364:GLU:O	2.11	0.51
1:A:20:HIS:CD2	1:A:115:GLU:HB3	2.46	0.50
1:A:88:VAL:HG21	1:A:121:VAL:HG12	1.93	0.50
1:A:388:THR:HG21	1:A:399:LEU:HD13	1.94	0.50
1:A:569:ASP:CG	1:A:570:GLY:H	2.18	0.50
1:A:573:HIS:CB	1:A:576:ASP:HB2	2.41	0.50
1:A:573:HIS:O	1:A:575:VAL:N	2.37	0.50
1:A:96:ARG:O	1:A:99:ARG:N	2.43	0.50
1:A:343:ASN:HA	1:A:389:LEU:HD12	1.94	0.50
1:A:549:ALA:HB3	1:A:590:ILE:HG22	1.94	0.50
1:A:135:PHE:CD1	1:A:272:LEU:HD22	2.48	0.49
1:A:142:THR:HA	1:A:171:GLU:CG	2.42	0.49
1:A:9:LEU:HD13	1:A:284:LEU:HD11	1.93	0.49
1:A:243:VAL:HG13	1:A:279:TYR:CE1	2.47	0.49
1:A:256:THR:O	1:A:258:VAL:HG23	2.12	0.49
1:A:330:VAL:HG12	1:A:371:ALA:HA	1.93	0.49
1:A:176:GLY:O	1:A:177:ILE:HG13	2.11	0.49
1:A:344:THR:HG22	1:A:390:VAL:HG22	1.95	0.49
1:A:186:TYR:CE2	1:A:271:LEU:HD21	2.48	0.49
1:A:247:ARG:NH2	1:A:280:LEU:O	2.43	0.49
1:A:165:GLN:HA	1:A:178:ILE:O	2.13	0.49
1:A:116:PRO:O	1:A:119:GLU:HB3	2.13	0.48
1:A:251:ILE:C	1:A:253:LEU:H	2.21	0.48
1:A:582:PHE:HA	1:A:585:ALA:HB3	1.95	0.48
1:A:314:PHE:CD1	1:A:315:LYS:HB2	2.48	0.48
1:A:680:PRO:HD2	1:A:683:VAL:HG21	1.95	0.48
1:A:95:GLU:O	1:A:98:MET:HB2	2.13	0.48
1:A:484:ARG:HH11	1:A:559:PRO:HG2	1.78	0.48
1:A:406:GLU:O	1:A:408:VAL:HG22	2.12	0.48
1:A:85:PRO:HB3	1:A:90:PHE:HD2	1.77	0.48
1:A:112:GLN:HG3	1:A:115:GLU:CD	2.37	0.48
1:A:230:LYS:NZ	1:A:237:PRO:HA	2.28	0.48
1:A:319:ASP:HB2	1:A:325:LEU:CD1	2.44	0.48
1:A:206:LEU:O	1:A:210:ARG:HG3	2.14	0.48
1:A:625:ASN:ND2	1:A:629:GLY:O	2.46	0.48
1:A:432:ALA:HA	1:A:438:PHE:CZ	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:520:GLY:N	1:A:562:ASP:OD1	2.38	0.47
1:A:523:PHE:CD1	1:A:524:GLU:N	2.82	0.47
1:A:272:LEU:O	1:A:275:ALA:HB3	2.14	0.47
1:A:312:LEU:HD11	1:A:386:GLY:HA2	1.95	0.47
1:A:154:GLN:HA	1:A:159:ALA:H	1.79	0.47
1:A:145:ASP:OD1	1:A:148:LEU:N	2.45	0.47
1:A:529:ILE:HG22	1:A:531:GLY:N	2.30	0.47
1:A:280:LEU:HD12	1:A:281:PRO:HD2	1.97	0.47
1:A:535:PRO:HB2	1:A:537:GLU:HG3	1.96	0.47
1:A:35:TYR:OH	1:A:266:ASN:HB3	2.15	0.47
1:A:280:LEU:HD12	1:A:280:LEU:HA	1.56	0.47
1:A:326:THR:O	1:A:377:VAL:HG22	2.15	0.46
1:A:415:PRO:CG	1:A:418:LYS:HE2	2.45	0.46
1:A:580:MET:HE2	1:A:580:MET:HB3	1.67	0.46
1:A:115:GLU:O	1:A:119:GLU:N	2.45	0.46
1:A:142:THR:HG22	1:A:171:GLU:HG2	1.98	0.46
1:A:541:ALA:O	1:A:583:LYS:HA	2.15	0.46
1:A:416:LYS:HD3	1:A:416:LYS:HA	1.73	0.46
1:A:660:ARG:HG2	1:A:665:GLY:HA2	1.98	0.46
1:A:127:LYS:HE3	1:A:637:ARG:HH12	1.80	0.46
1:A:190:ASN:OD1	1:A:192:LEU:HB2	2.16	0.46
1:A:427:ALA:HB1	1:A:470:PHE:HD1	1.80	0.46
1:A:153:MET:HG2	1:A:157:LEU:HD12	1.98	0.46
1:A:454:MET:HE2	1:A:458:HIS:HB2	1.98	0.46
1:A:604:PRO:HG2	1:A:649:LEU:HD23	1.98	0.46
1:A:504:ARG:HH22	1:A:578:SER:CB	2.29	0.45
1:A:523:PHE:HD1	1:A:524:GLU:N	2.14	0.45
1:A:355:LEU:HD13	1:A:369:LEU:HB2	1.98	0.45
1:A:346:LYS:NZ	1:A:384:ILE:HG12	2.32	0.45
1:A:507:TYR:O	1:A:577:SER:HA	2.17	0.45
1:A:513:LYS:HG3	1:A:568:TYR:CD1	2.51	0.45
1:A:660:ARG:O	1:A:665:GLY:N	2.49	0.45
1:A:299:VAL:HG12	1:A:300:GLU:H	1.81	0.45
1:A:74:TRP:CD1	1:A:75:LYS:HG3	2.52	0.45
1:A:139:MET:HG3	1:A:260:LEU:HD23	2.00	0.44
1:A:216:LEU:O	1:A:219:VAL:N	2.46	0.44
1:A:674:ASP:OD1	1:A:675:HIS:ND1	2.31	0.44
1:A:118:SER:O	1:A:121:VAL:HG22	2.17	0.44
1:A:402:ILE:HD12	1:A:402:ILE:HA	1.89	0.44
1:A:590:ILE:HA	1:A:590:ILE:HD12	1.71	0.44
1:A:165:GLN:OE1	1:A:259:PHE:HB3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:453:GLY:HA3	1:A:459:LEU:HD21	2.00	0.44
1:A:494:GLU:OE2	1:A:511:LYS:HE3	2.16	0.44
1:A:85:PRO:HG2	1:A:94:VAL:HG22	2.00	0.44
1:A:127:LYS:O	1:A:129:LYS:HD2	2.18	0.44
1:A:111:SER:HA	1:A:143:GLY:O	2.17	0.44
1:A:20:HIS:HB2	1:A:118:SER:CB	2.48	0.44
1:A:119:GLU:CD	1:A:666:ARG:HG2	2.43	0.44
1:A:327:PHE:HZ	1:A:358:MET:HE2	1.83	0.43
1:A:146:LEU:HD22	1:A:150:ILE:HD11	2.00	0.43
1:A:344:THR:OG1	1:A:388:THR:HB	2.18	0.43
1:A:430:ARG:HD2	1:A:430:ARG:H	1.83	0.43
1:A:430:ARG:HD2	1:A:430:ARG:N	2.34	0.43
1:A:170:ARG:N	1:A:173:THR:OG1	2.51	0.43
1:A:74:TRP:O	1:A:75:LYS:C	2.61	0.43
1:A:122:TRP:NE1	1:A:126:GLU:HG3	2.33	0.43
1:A:592:GLU:OE1	1:A:596:LYS:HE2	2.19	0.43
1:A:408:VAL:HA	1:A:482:ALA:CB	2.49	0.42
1:A:416:LYS:HG2	1:A:473:ASP:O	2.19	0.42
1:A:76:ASP:OD2	1:A:76:ASP:N	2.51	0.42
1:A:335:LEU:O	1:A:369:LEU:N	2.50	0.42
1:A:423:LYS:O	1:A:427:ALA:HB2	2.19	0.42
1:A:443:HIS:HA	1:A:444:PRO:HD2	1.70	0.42
1:A:292:THR:O	1:A:292:THR:OG1	2.33	0.42
1:A:425:SER:HA	1:A:428:LEU:HG	2.01	0.42
1:A:539:ILE:O	1:A:543:GLN:HG3	2.19	0.42
1:A:7:TYR:OH	1:A:371:ALA:O	2.38	0.42
1:A:95:GLU:HA	1:A:128:TYR:CZ	2.55	0.42
1:A:139:MET:HE2	1:A:260:LEU:HD23	2.02	0.42
1:A:306:ASN:N	1:A:306:ASN:OD1	2.52	0.42
1:A:627:ARG:O	1:A:648:PRO:HD2	2.20	0.42
1:A:190:ASN:ND2	1:A:195:ASP:HB2	2.35	0.41
1:A:256:THR:O	1:A:257:PRO:C	2.63	0.41
1:A:316:ILE:HG12	1:A:385:THR:CG2	2.49	0.41
1:A:542:VAL:O	1:A:546:ILE:HD13	2.20	0.41
1:A:152:THR:CB	1:A:156:ARG:HD3	2.45	0.41
1:A:313:ALA:O	1:A:386:GLY:N	2.23	0.41
1:A:681:LYS:O	1:A:685:GLU:HG3	2.21	0.41
1:A:335:LEU:HD12	1:A:335:LEU:HA	1.88	0.41
1:A:464:ASP:OD1	1:A:468:ARG:HD2	2.20	0.41
1:A:27:THR:OG1	3:A:702:GDP:O2A	2.38	0.41
1:A:493:VAL:HG23	1:A:593:ALA:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:646:PHE:HD1	1:A:646:PHE:HA	1.77	0.41
1:A:100:VAL:HG13	1:A:329:ARG:HB2	2.03	0.41
1:A:171:GLU:C	1:A:173:THR:H	2.29	0.41
1:A:488:THR:O	1:A:516:PRO:HG3	2.21	0.41
1:A:531:GLY:C	1:A:533:VAL:H	2.29	0.41
1:A:660:ARG:CG	1:A:665:GLY:HA2	2.51	0.41
1:A:293:THR:OG1	1:A:295:GLU:HG2	2.21	0.41
1:A:32:ILE:HD12	1:A:269:VAL:HG13	2.01	0.40
1:A:36:THR:HG22	1:A:73:PHE:O	2.21	0.40
1:A:164:MET:HE3	1:A:164:MET:HB3	1.55	0.40
1:A:431:LEU:HD11	1:A:465:ARG:NE	2.36	0.40
1:A:484:ARG:HD3	1:A:561:VAL:HG11	2.02	0.40
1:A:9:LEU:HD22	1:A:284:LEU:HD13	2.02	0.40
1:A:150:ILE:H	1:A:150:ILE:HG12	1.64	0.40
1:A:569:ASP:CG	1:A:570:GLY:N	2.79	0.40
1:A:34:TYR:C	1:A:34:TYR:CD2	2.99	0.40
1:A:31:ARG:HD3	1:A:266:ASN:OD1	2.22	0.40
1:A:152:THR:O	1:A:156:ARG:HB2	2.22	0.40
1:A:264:LEU:HD23	3:A:702:GDP:C4	2.56	0.40
1:A:275:ALA:O	1:A:278:ASP:HB2	2.22	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:212:TYR:OH	1:A:574:GLU:OE1[2_555]	2.02	0.18
1:A:151:ARG:NH1	1:A:537:GLU:OE1[2_555]	2.12	0.08

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	652/691 (94%)	534 (82%)	94 (14%)	24 (4%)	2	21

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	68	ALA
1	A	91	THR
1	A	320	PRO
1	A	401	SER
1	A	444	PRO
1	A	75	LYS
1	A	97	SER
1	A	445	GLU
1	A	596	LYS
1	A	215	LYS
1	A	392	GLU
1	A	496	LYS
1	A	574	GLU
1	A	128	TYR
1	A	497	PHE
1	A	687	LEU
1	A	85	PRO
1	A	214	GLU
1	A	242	LEU
1	A	303	PRO
1	A	255	ILE
1	A	482	ALA
1	A	495	GLY
1	A	402	ILE

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	546/581 (94%)	450 (82%)	96 (18%)	2	11

All (96) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LEU
1	A	13	ARG
1	A	26	THR
1	A	32	ILE
1	A	33	LEU
1	A	36	THR
1	A	69	VAL
1	A	76	ASP
1	A	79	ILE
1	A	106	VAL
1	A	112	GLN
1	A	114	VAL
1	A	118	SER
1	A	130	VAL
1	A	146	LEU
1	A	148	LEU
1	A	150	ILE
1	A	155	GLU
1	A	162	VAL
1	A	164	MET
1	A	171	GLU
1	A	172	ASP
1	A	177	ILE
1	A	180	VAL
1	A	181	LEU
1	A	194	THR
1	A	196	ILE
1	A	199	ILE
1	A	201	ILE
1	A	203	GLU
1	A	232	LEU
1	A	241	GLU
1	A	253	LEU
1	A	260	LEU
1	A	264	LEU
1	A	270	GLN
1	A	274	ASP
1	A	277	VAL
1	A	280	LEU
1	A	284	LEU
1	A	289	ILE
1	A	292	THR
1	A	299	VAL

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Mol	Chain	Res	Type
1	A	306	ASN
1	A	309	LEU
1	A	312	LEU
1	A	326	THR
1	A	336	THR
1	A	349	LYS
1	A	352	VAL
1	A	367	GLU
1	A	374	LEU
1	A	389	LEU
1	A	408	VAL
1	A	411	VAL
1	A	417	THR
1	A	418	LYS
1	A	431	LEU
1	A	434	GLU
1	A	449	THR
1	A	454	MET
1	A	457	LEU
1	A	467	LYS
1	A	473	ASP
1	A	481	VAL
1	A	484	ARG
1	A	486	THR
1	A	491	VAL
1	A	493	VAL
1	A	526	VAL
1	A	546	ILE
1	A	556	ILE
1	A	562	ASP
1	A	565	VAL
1	A	572	TYR
1	A	574	GLU
1	A	575	VAL
1	A	577	SER
1	A	588	MET
1	A	590	ILE
1	A	596	LYS
1	A	600	VAL
1	A	609	GLU
1	A	615	GLU
1	A	619	ASP

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Mol	Chain	Res	Type
1	A	634	MET
1	A	635	GLU
1	A	646	PHE
1	A	659	LEU
1	A	664	GLN
1	A	670	VAL
1	A	678	GLU
1	A	681	LYS
1	A	682	GLN
1	A	687	LEU
1	A	688	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	343	ASN
1	A	359	HIS
1	A	682	GLN
1	A	684	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	702	2	29,30,30	1.17	2 (6%)	45,47,47	2.02	9 (20%)

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	702	2	-	6/16/32/32	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	702	GDP	C5-C4	3.07	1.47	1.38
3	A	702	GDP	C6-N1	-2.79	1.33	1.38

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	702	GDP	C5-C4-N3	-7.47	116.50	128.39
3	A	702	GDP	N9-C4-N3	5.72	137.40	125.95
3	A	702	GDP	C2-N3-C4	5.42	121.64	112.30
3	A	702	GDP	C4-C5-N7	-2.88	106.10	110.67
3	A	702	GDP	C6-C5-N7	2.82	135.41	130.29
3	A	702	GDP	C8-N7-C5	2.39	108.52	104.26
3	A	702	GDP	C2-N1-C6	-2.32	120.90	125.11
3	A	702	GDP	C5-C6-N1	2.06	118.51	113.25
3	A	702	GDP	O6-C6-C5	-2.02	121.20	126.53

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	702	GDP	C5'-O5'-PA-O3A
3	A	702	GDP	C5'-O5'-PA-O1A
3	A	702	GDP	C5'-O5'-PA-O2A

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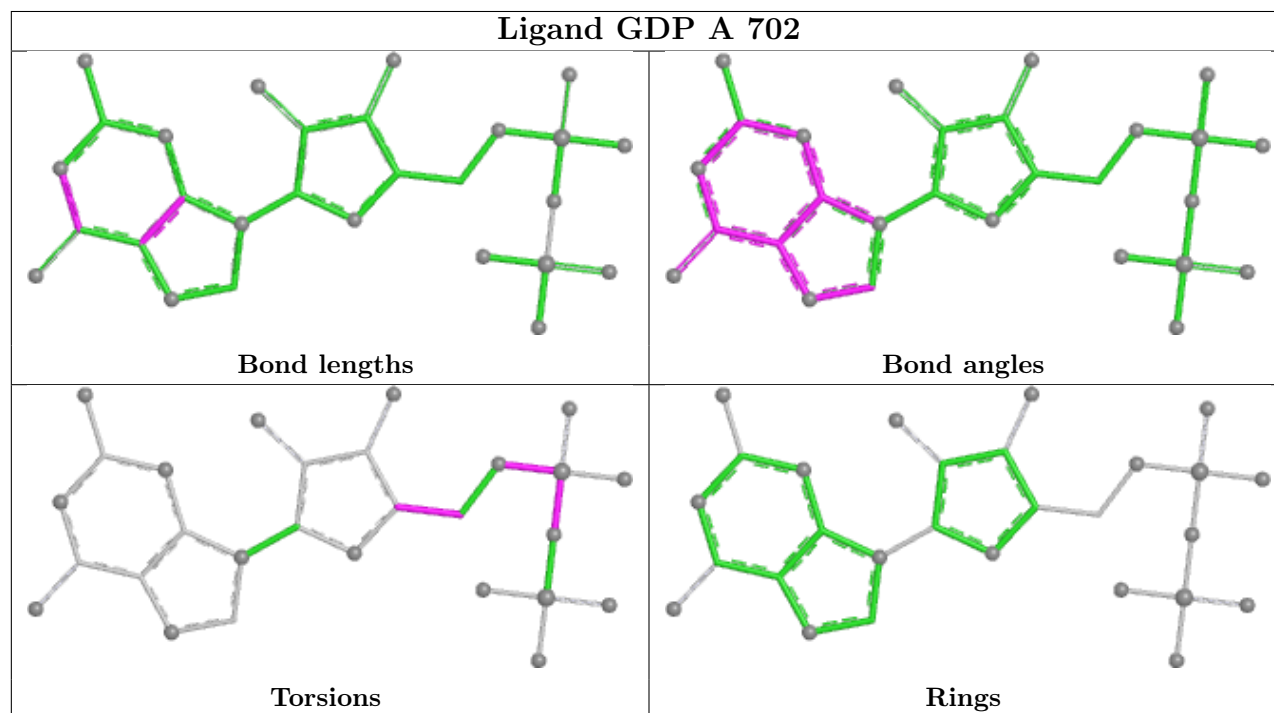
Mol	Chain	Res	Type	Atoms
3	A	702	GDP	O4'-C4'-C5'-O5'
3	A	702	GDP	C3'-C4'-C5'-O5'
3	A	702	GDP	PB-O3A-PA-O2A

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	702	GDP	4	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 [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	656/691 (94%)	-0.58	1 (0%) 91 82	28, 52, 95, 123	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	124	GLN	2.3

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](#)

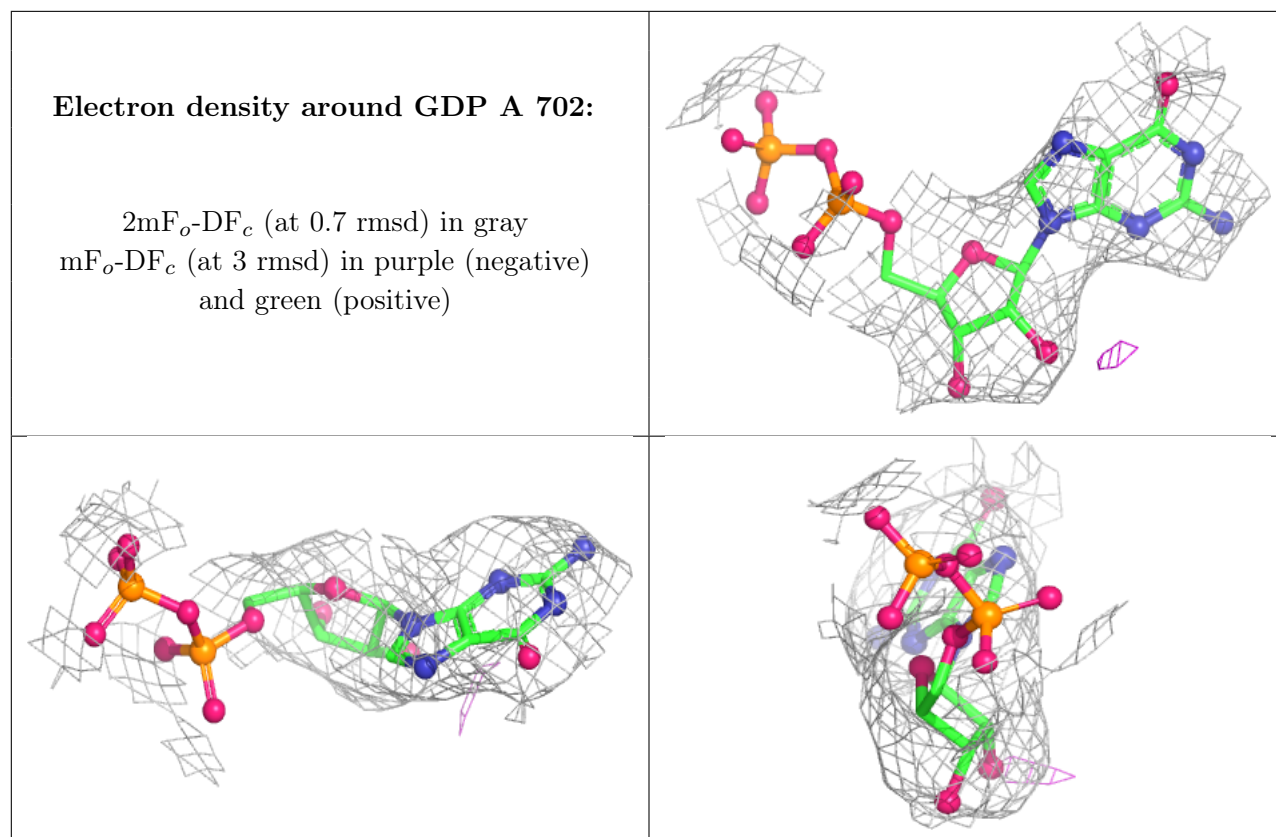
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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	MG	A	701	1/1	0.91	0.06	67,67,67,67	0
3	GDP	A	702	28/28	0.96	0.07	29,46,56,62	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.



6.5 Other polymers [i](#)

There are no such residues in this entry.