



Full wwPDB X-ray Structure Validation Report ⓘ

May 24, 2020 – 09:24 am BST

PDB ID : 2BM1
Title : Ribosomal elongation factor G (EF-G) Fusidic acid resistant mutant G16V
Authors : Hansson, S.; Singh, R.; Gudkov, A.T.; Liljas, A.; Logan, D.T.
Deposited on : 2005-03-09
Resolution : 2.60 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

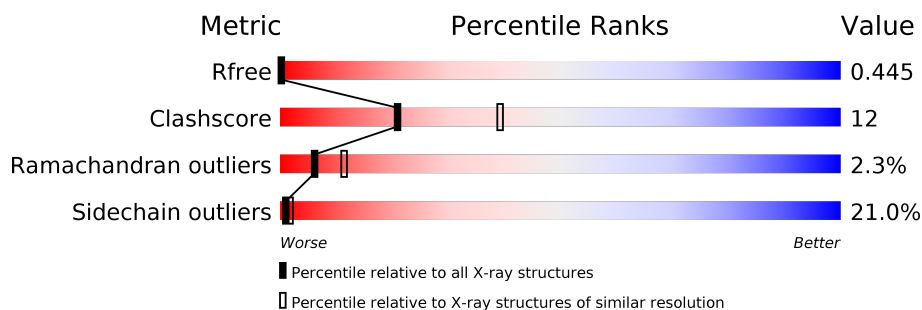
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


The reported resolution of this entry is 2.60 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}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (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 on 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	691	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 5258 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.

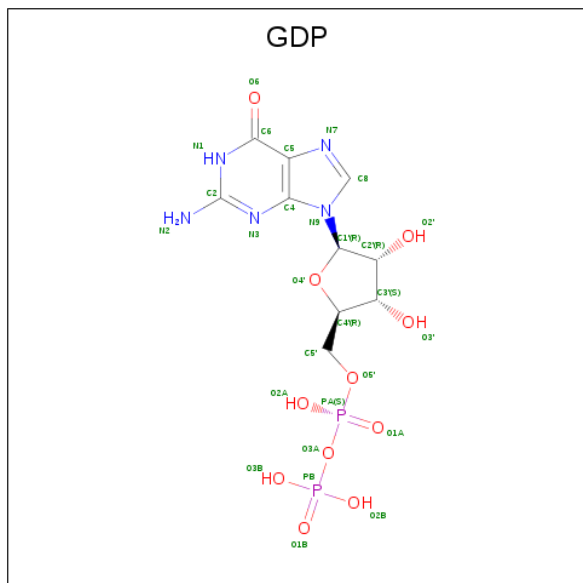
- Molecule 1 is a protein called ELONGATION FACTOR G.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	660	5167	3286	882	981	18	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	16	VAL	GLY	engineered mutation	UNP P13551

- Molecule 2 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	Mg	0	0
			1	1		

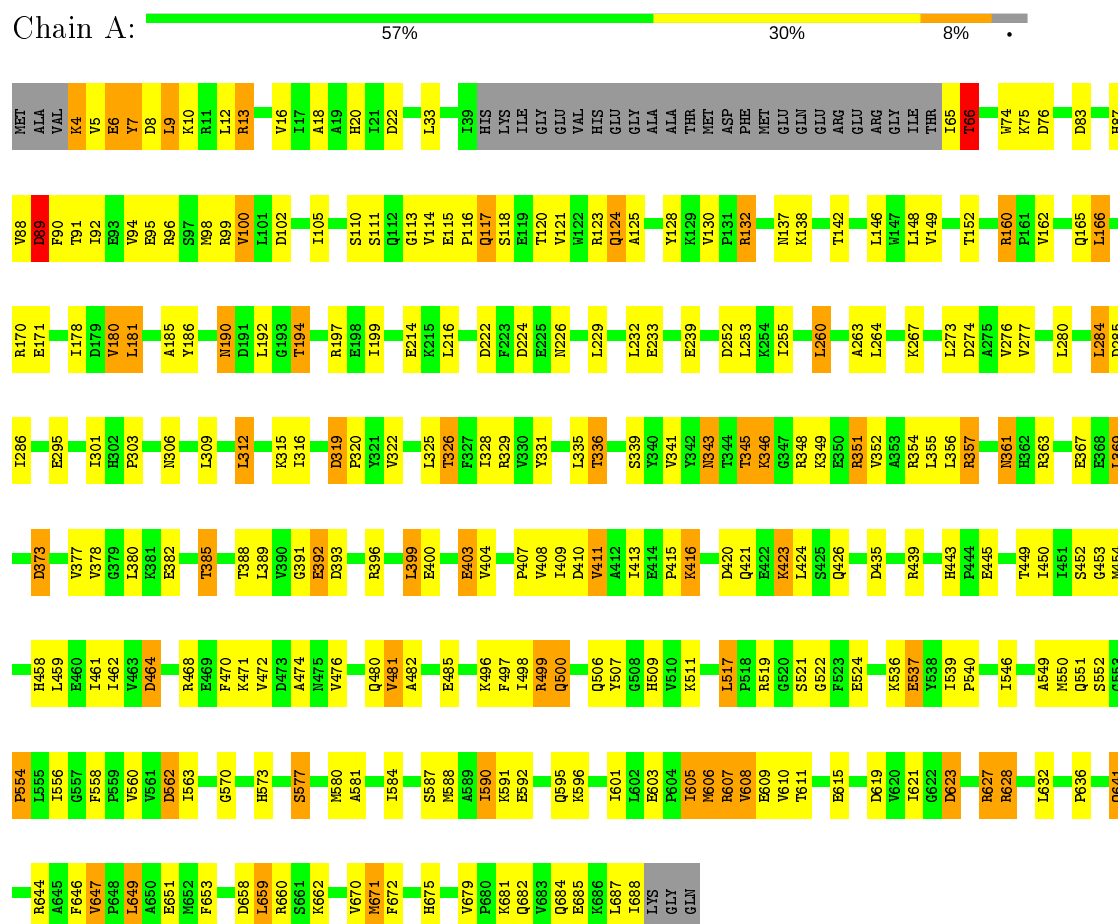
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	62	Total	O	0	0
			62	62		

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

• 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	76.30 Å 89.70 Å 114.90 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.00 – 2.60 22.52 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.2 (28.00-2.60) 98.7 (22.52-2.60)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.06 (at 2.60 Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.220 , 0.297 0.444 , 0.445	Depositor DCC
R_{free} test set	1248 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	52.9	Xtriage
Anisotropy	0.044	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 43.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.70	EDS
Total number of atoms	5258	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.88% 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	0.72	0/5264	0.93	23/7131 (0.3%)

There are no bond length outliers.

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	562	ASP	CB-CG-OD2	8.08	125.58	118.30
1	A	393	ASP	CB-CG-OD2	7.33	124.90	118.30
1	A	224	ASP	CB-CG-OD2	7.17	124.75	118.30
1	A	252	ASP	CB-CG-OD2	6.87	124.48	118.30
1	A	83	ASP	CB-CG-OD2	6.77	124.39	118.30
1	A	76	ASP	CB-CG-OD2	6.76	124.38	118.30
1	A	410	ASP	CB-CG-OD2	6.66	124.29	118.30
1	A	285	ASP	CB-CG-OD2	6.63	124.27	118.30
1	A	222	ASP	CB-CG-OD2	6.38	124.05	118.30
1	A	89	ASP	CB-CG-OD2	6.33	124.00	118.30
1	A	8	ASP	CB-CG-OD2	6.17	123.85	118.30
1	A	619	ASP	CB-CG-OD2	5.91	123.62	118.30
1	A	435	ASP	CB-CG-OD2	5.83	123.54	118.30
1	A	464	ASP	CB-CG-OD2	5.52	123.27	118.30
1	A	396	ARG	NE-CZ-NH1	5.49	123.04	120.30
1	A	102	ASP	CB-CG-OD2	5.44	123.20	118.30
1	A	13	ARG	NE-CZ-NH2	-5.43	117.58	120.30
1	A	13	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	A	274	ASP	CB-CG-OD1	5.30	123.07	118.30
1	A	319	ASP	CB-CG-OD2	5.16	122.94	118.30
1	A	658	ASP	CB-CG-OD2	5.13	122.92	118.30
1	A	623	ASP	CB-CG-OD2	5.12	122.91	118.30
1	A	357	ARG	NE-CZ-NH2	5.05	122.83	120.30

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	5167	0	5230	127	9
2	A	28	0	12	1	0
3	A	1	0	0	0	1
4	A	62	0	0	10	0
All	All	5258	0	5242	127	9

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 12.

All (127) 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:190:ASN:HD22	1:A:192:LEU:H	1.23	0.82
1:A:190:ASN:ND2	1:A:192:LEU:H	1.76	0.81
1:A:636:PRO:HB3	1:A:641:GLN:HE21	1.45	0.81
1:A:361:ASN:HD22	1:A:361:ASN:H	1.27	0.81
1:A:632:LEU:HD21	1:A:646:PHE:CE2	2.18	0.79
1:A:165:GLN:NE2	1:A:260:LEU:H	1.82	0.77
1:A:132:ARG:CZ	4:A:2011:HOH:O	2.35	0.73
1:A:137:ASN:HD21	1:A:263:ALA:H	1.37	0.73
1:A:4:LYS:HA	1:A:5:VAL:C	2.15	0.67
1:A:580:MET:HG2	4:A:2055:HOH:O	1.95	0.66
1:A:90:PHE:O	1:A:670:VAL:HG12	1.95	0.65
1:A:165:GLN:HE21	1:A:260:LEU:H	1.44	0.64
1:A:18:ALA:HB1	1:A:121:VAL:HG21	1.79	0.62
1:A:415:PRO:HA	1:A:474:ALA:HB1	1.81	0.62
1:A:9:LEU:HD13	1:A:284:LEU:HD13	1.83	0.60
1:A:605:ILE:HG22	1:A:605:ILE:O	2.02	0.60
1:A:343:ASN:HD22	1:A:343:ASN:C	2.05	0.60
1:A:636:PRO:HB3	1:A:641:GLN:NE2	2.16	0.59
1:A:295:GLU:OE2	4:A:2034:HOH:O	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:PRO:O	1:A:117:GLN:HB2	2.04	0.58
1:A:316:ILE:CD1	1:A:326:THR:HB	2.35	0.57
1:A:610:VAL:HG13	1:A:659:LEU:HD11	1.85	0.57
1:A:546:ILE:HG23	1:A:590:ILE:HG13	1.87	0.57
1:A:550:MET:SD	1:A:563:ILE:HD11	2.45	0.57
1:A:113:GLY:HA2	1:A:149:VAL:HG22	1.87	0.56
1:A:391:GLY:O	1:A:392:GLU:CB	2.53	0.56
1:A:517:LEU:HD21	1:A:524:GLU:HG3	1.85	0.56
1:A:409:ILE:HD11	1:A:649:LEU:HD11	1.87	0.56
1:A:316:ILE:HG12	1:A:385:THR:HG22	1.87	0.55
1:A:89:ASP:O	1:A:124:GLN:NE2	2.40	0.55
1:A:326:THR:HG22	4:A:2039:HOH:O	2.05	0.55
1:A:485:GLU:O	1:A:560:VAL:HA	2.07	0.55
1:A:125:ALA:O	1:A:128:TYR:O	2.25	0.55
1:A:388:THR:HG23	1:A:399:LEU:HD22	1.87	0.54
1:A:415:PRO:HB2	1:A:420:ASP:HB3	1.90	0.54
1:A:160:ARG:HG2	1:A:255:ILE:HG22	1.90	0.54
1:A:536:LYS:O	1:A:537:GLU:CB	2.56	0.54
1:A:9:LEU:HD13	1:A:284:LEU:CD1	2.39	0.53
1:A:100:VAL:HG22	1:A:329:ARG:HB2	1.90	0.53
1:A:316:ILE:HD13	1:A:326:THR:HB	1.91	0.52
1:A:181:LEU:HD22	1:A:216:LEU:HD21	1.92	0.52
1:A:549:ALA:HB1	1:A:591:LYS:HD3	1.92	0.52
1:A:94:VAL:HG12	1:A:94:VAL:O	2.10	0.51
1:A:116:PRO:O	1:A:117:GLN:CB	2.59	0.51
1:A:409:ILE:CG1	1:A:649:LEU:HD11	2.42	0.50
1:A:351:ARG:HB2	1:A:351:ARG:CZ	2.41	0.50
1:A:603:GLU:CD	1:A:679:VAL:HG12	2.32	0.50
1:A:632:LEU:HD11	1:A:646:PHE:CE1	2.47	0.49
1:A:96:ARG:HG3	1:A:400:GLU:OE2	2.12	0.49
1:A:7:TYR:OH	1:A:9:LEU:HG	2.12	0.49
1:A:605:ILE:HG21	1:A:675:HIS:CE1	2.48	0.48
1:A:100:VAL:HG22	1:A:329:ARG:CB	2.43	0.48
1:A:148:LEU:O	1:A:152:THR:HG22	2.13	0.48
1:A:351:ARG:HB2	1:A:351:ARG:NH2	2.29	0.48
1:A:549:ALA:HB3	1:A:590:ILE:CG2	2.43	0.48
1:A:361:ASN:HD22	1:A:361:ASN:N	2.02	0.48
1:A:539:ILE:N	1:A:540:PRO:CD	2.76	0.48
1:A:536:LYS:O	1:A:537:GLU:CD	2.52	0.47
1:A:509:HIS:HD1	1:A:570:GLY:HA2	1.78	0.47
1:A:536:LYS:O	1:A:537:GLU:OE1	2.33	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:481:VAL:HG23	1:A:482:ALA:N	2.29	0.47
1:A:301:ILE:HD13	1:A:399:LEU:HD11	1.97	0.46
1:A:165:GLN:HA	1:A:178:ILE:O	2.14	0.46
1:A:190:ASN:C	1:A:190:ASN:HD22	2.18	0.46
1:A:319:ASP:OD1	1:A:363:ARG:NH2	2.44	0.46
1:A:506:GLN:HE21	1:A:581:ALA:HB2	1.80	0.46
1:A:65:ILE:O	1:A:66:THR:C	2.54	0.46
1:A:454:MET:CG	1:A:458:HIS:CD2	2.99	0.46
1:A:20:HIS:ND1	1:A:116:PRO:O	2.49	0.46
1:A:166:LEU:HD22	1:A:180:VAL:HG11	1.98	0.46
1:A:355:LEU:HD22	1:A:369:LEU:CD2	2.46	0.46
1:A:114:VAL:H	1:A:152:THR:HG21	1.81	0.45
1:A:325:LEU:HD21	1:A:356:LEU:HD12	1.98	0.45
1:A:415:PRO:O	1:A:416:LYS:HB2	2.16	0.45
1:A:458:HIS:ND1	1:A:462:ILE:HD11	2.32	0.45
1:A:345:THR:C	1:A:346:LYS:O	2.52	0.45
1:A:5:VAL:O	1:A:6:GLU:C	2.55	0.45
1:A:354:ARG:HB2	1:A:378:VAL:HB	1.98	0.45
1:A:411:VAL:O	1:A:450:ILE:HA	2.17	0.45
1:A:573:HIS:O	1:A:577:SER:HB2	2.17	0.45
1:A:536:LYS:O	1:A:537:GLU:CG	2.65	0.45
1:A:584:ILE:O	1:A:588:MET:HG3	2.17	0.44
1:A:166:LEU:HD22	1:A:180:VAL:CG1	2.47	0.44
1:A:361:ASN:H	1:A:361:ASN:ND2	2.06	0.44
1:A:409:ILE:O	1:A:452:SER:HA	2.18	0.44
1:A:609:GLU:HB3	1:A:670:VAL:CG2	2.47	0.44
1:A:497:PHE:CZ	1:A:499:ARG:HD2	2.53	0.44
1:A:607:ARG:C	4:A:2057:HOH:O	2.56	0.44
1:A:185:ALA:HB3	1:A:199:ILE:HG13	2.00	0.44
1:A:114:VAL:HG23	1:A:152:THR:HG23	2.01	0.43
1:A:336:THR:HG22	1:A:339:SER:HB3	1.99	0.43
1:A:312:LEU:O	1:A:328:ILE:HA	2.18	0.43
1:A:407:PRO:HA	1:A:453:GLY:O	2.19	0.43
1:A:186:TYR:HA	1:A:197:ARG:O	2.18	0.43
1:A:413:ILE:HG23	1:A:413:ILE:O	2.19	0.43
1:A:601:ILE:HG13	1:A:684:GLN:HE21	1.84	0.43
1:A:105:ILE:HD11	1:A:276:VAL:CG2	2.49	0.42
1:A:309:LEU:HD21	1:A:335:LEU:CD1	2.49	0.42
1:A:415:PRO:HG2	1:A:421:GLN:HG2	2.01	0.42
1:A:409:ILE:CG2	1:A:459:LEU:HD13	2.49	0.42
1:A:115:GLU:O	1:A:118:SER:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:408:VAL:HG21	1:A:606:MET:HE2	2.01	0.42
1:A:409:ILE:HG21	1:A:459:LEU:HD13	2.00	0.42
1:A:423:LYS:HA	1:A:426:GLN:HB2	2.02	0.42
1:A:498:ILE:HA	1:A:506:GLN:O	2.18	0.42
1:A:522:GLY:O	1:A:562:ASP:HA	2.19	0.42
1:A:554:PRO:HB3	1:A:595:GLN:HG2	2.01	0.42
1:A:413:ILE:HD13	1:A:424:LEU:HD21	2.01	0.42
1:A:132:ARG:NH1	4:A:2011:HOH:O	2.49	0.41
1:A:644:ARG:HB3	4:A:2058:HOH:O	2.20	0.41
1:A:671:MET:CG	4:A:2057:HOH:O	2.68	0.41
1:A:409:ILE:CD1	1:A:649:LEU:HD11	2.50	0.41
1:A:138:LYS:HG2	2:A:1689:GDP:C6	2.55	0.41
1:A:357:ARG:NH1	1:A:373:ASP:OD2	2.54	0.41
1:A:608:VAL:CG2	1:A:647:VAL:CG1	2.99	0.41
1:A:627:ARG:HB2	1:A:651:GLU:O	2.21	0.41
1:A:123:ARG:HG3	1:A:611:THR:HG21	2.02	0.41
1:A:74:TRP:CD1	1:A:75:LYS:HG2	2.56	0.41
1:A:498:ILE:HG12	1:A:507:TYR:CD2	2.55	0.41
1:A:335:LEU:HD11	1:A:341:VAL:HG11	2.02	0.41
1:A:499:ARG:NE	4:A:2049:HOH:O	2.54	0.41
1:A:506:GLN:NE2	1:A:581:ALA:HB2	2.36	0.41
1:A:94:VAL:O	1:A:94:VAL:CG1	2.69	0.41
1:A:303:PRO:HA	1:A:331:TYR:O	2.21	0.40
1:A:413:ILE:HD11	1:A:424:LEU:HD11	2.03	0.40
1:A:470:PHE:HB3	1:A:472:VAL:HG23	2.01	0.40
1:A:601:ILE:HG12	4:A:2048:HOH:O	2.22	0.40

All (9) 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:295:GLU:OE2	3:A:1690:MG:MG[3_555]	1.18	1.02
1:A:226:ASN:ND2	1:A:685:GLU:OE1[1_655]	1.49	0.71
1:A:367:GLU:OE1	1:A:500:GLN:OE1[1_655]	1.59	0.61
1:A:194:THR:O	1:A:521:SER:O[3_545]	2.05	0.15
1:A:367:GLU:CB	1:A:500:GLN:CB[1_655]	2.06	0.14
1:A:306:ASN:ND2	1:A:496:LYS:CE[1_655]	2.15	0.05
1:A:194:THR:CA	1:A:521:SER:O[3_545]	2.16	0.04
1:A:194:THR:OG1	1:A:521:SER:O[3_545]	2.17	0.03
1:A:367:GLU:CD	1:A:500:GLN:OE1[1_655]	2.18	0.02

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	656/691 (95%)	578 (88%)	63 (10%)	15 (2%)	6	11

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	66	THR
1	A	416	LYS
1	A	537	GLU
1	A	91	THR
1	A	117	GLN
1	A	392	GLU
1	A	403	GLU
1	A	171	GLU
1	A	628	ARG
1	A	346	LYS
1	A	380	LEU
1	A	87	HIS
1	A	320	PRO
1	A	554	PRO
1	A	556	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	558/583 (96%)	441 (79%)	117 (21%)	1	2

All (117) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LYS
1	A	6	GLU
1	A	7	TYR
1	A	9	LEU
1	A	10	LYS
1	A	12	LEU
1	A	13	ARG
1	A	16	VAL
1	A	22	ASP
1	A	33	LEU
1	A	66	THR
1	A	88	VAL
1	A	89	ASP
1	A	92	ILE
1	A	95	GLU
1	A	98	MET
1	A	99	ARG
1	A	100	VAL
1	A	110	SER
1	A	111	SER
1	A	120	THR
1	A	124	GLN
1	A	130	VAL
1	A	132	ARG
1	A	142	THR
1	A	146	LEU
1	A	160	ARG
1	A	162	VAL
1	A	166	LEU
1	A	170	ARG
1	A	180	VAL
1	A	181	LEU
1	A	190	ASN
1	A	194	THR
1	A	214	GLU
1	A	229	LEU
1	A	232	LEU
1	A	233	GLU
1	A	239	GLU
1	A	253	LEU
1	A	260	LEU
1	A	264	LEU

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Mol	Chain	Res	Type
1	A	267	LYS
1	A	273	LEU
1	A	277	VAL
1	A	280	LEU
1	A	284	LEU
1	A	286	ILE
1	A	312	LEU
1	A	315	LYS
1	A	322	VAL
1	A	326	THR
1	A	336	THR
1	A	343	ASN
1	A	345	THR
1	A	348	ARG
1	A	349	LYS
1	A	351	ARG
1	A	352	VAL
1	A	361	ASN
1	A	369	LEU
1	A	373	ASP
1	A	377	VAL
1	A	382	GLU
1	A	385	THR
1	A	389	LEU
1	A	399	LEU
1	A	403	GLU
1	A	404	VAL
1	A	411	VAL
1	A	423	LYS
1	A	439	ARG
1	A	443	HIS
1	A	445	GLU
1	A	449	THR
1	A	461	ILE
1	A	464	ASP
1	A	468	ARG
1	A	471	LYS
1	A	476	VAL
1	A	480	GLN
1	A	481	VAL
1	A	499	ARG
1	A	500	GLN

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Mol	Chain	Res	Type
1	A	511	LYS
1	A	517	LEU
1	A	519	ARG
1	A	551	GLN
1	A	552	SER
1	A	558	PHE
1	A	577	SER
1	A	587	SER
1	A	590	ILE
1	A	592	GLU
1	A	596	LYS
1	A	605	ILE
1	A	606	MET
1	A	607	ARG
1	A	608	VAL
1	A	615	GLU
1	A	621	ILE
1	A	623	ASP
1	A	627	ARG
1	A	628	ARG
1	A	641	GLN
1	A	647	VAL
1	A	649	LEU
1	A	653	PHE
1	A	659	LEU
1	A	660	ARG
1	A	662	LYS
1	A	671	MET
1	A	672	PHE
1	A	681	LYS
1	A	682	GLN
1	A	687	LEU
1	A	688	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	77	HIS
1	A	124	GLN
1	A	137	ASN
1	A	154	GLN
1	A	165	GLN

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Mol	Chain	Res	Type
1	A	190	ASN
1	A	208	GLN
1	A	343	ASN
1	A	361	ASN
1	A	448	GLN
1	A	480	GLN
1	A	506	GLN
1	A	551	GLN
1	A	630	GLN
1	A	641	GLN
1	A	675	HIS
1	A	677	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 carbohydrates 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	$\# Z > 2$
2	GDP	A	1689	3	24,30,30	1.33	3 (12%)	31,47,47	1.87	7 (22%)

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	GDP	A	1689	3	-	2/12/32/32	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1689	GDP	C6-N1	3.52	1.39	1.33
2	A	1689	GDP	O4'-C1'	-2.87	1.37	1.41
2	A	1689	GDP	C2-N1	2.00	1.39	1.35

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1689	GDP	N3-C2-N1	-5.40	120.02	127.22
2	A	1689	GDP	C5-C6-N1	-4.18	117.71	123.43
2	A	1689	GDP	C6-N1-C2	3.57	121.60	115.93
2	A	1689	GDP	C2-N3-C4	3.26	119.08	115.36
2	A	1689	GDP	O3B-PB-O2B	2.75	118.15	107.64
2	A	1689	GDP	PA-O3A-PB	-2.62	123.83	132.83
2	A	1689	GDP	C1'-N9-C4	-2.40	122.42	126.64

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1689	GDP	PA-O3A-PB-O2B
2	A	1689	GDP	PA-O3A-PB-O3B

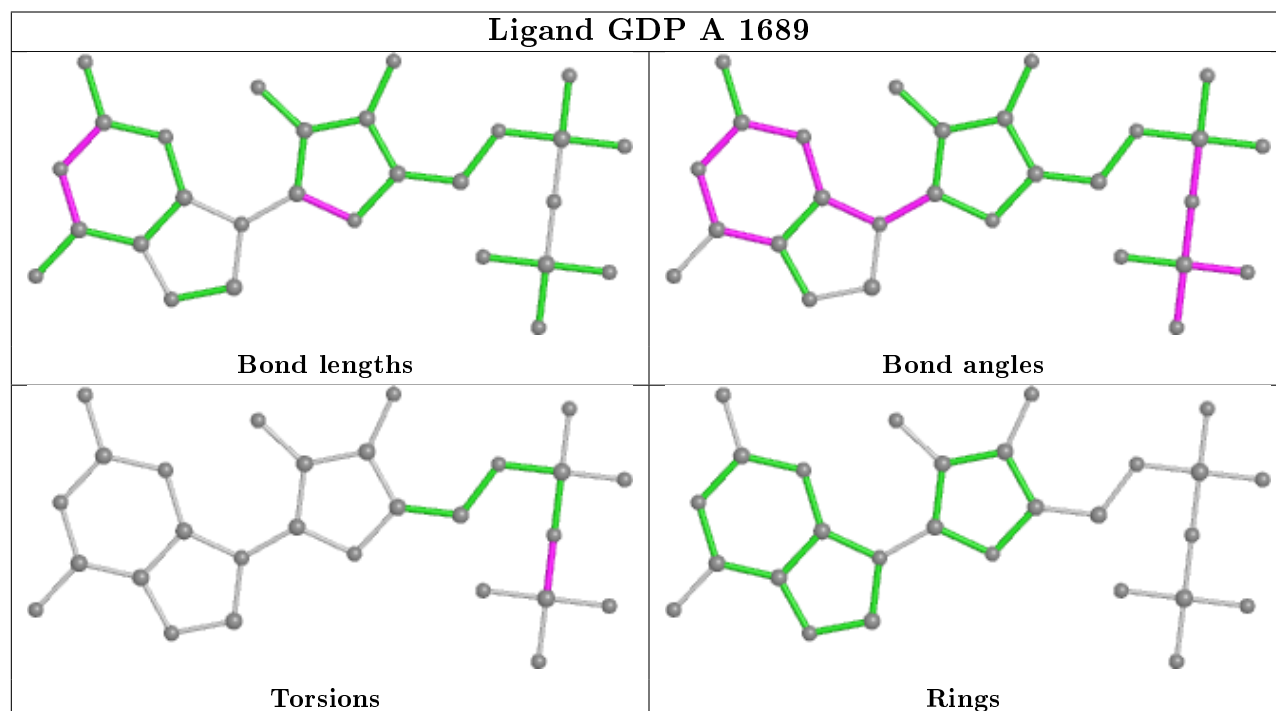
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1689	GDP	1	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 ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

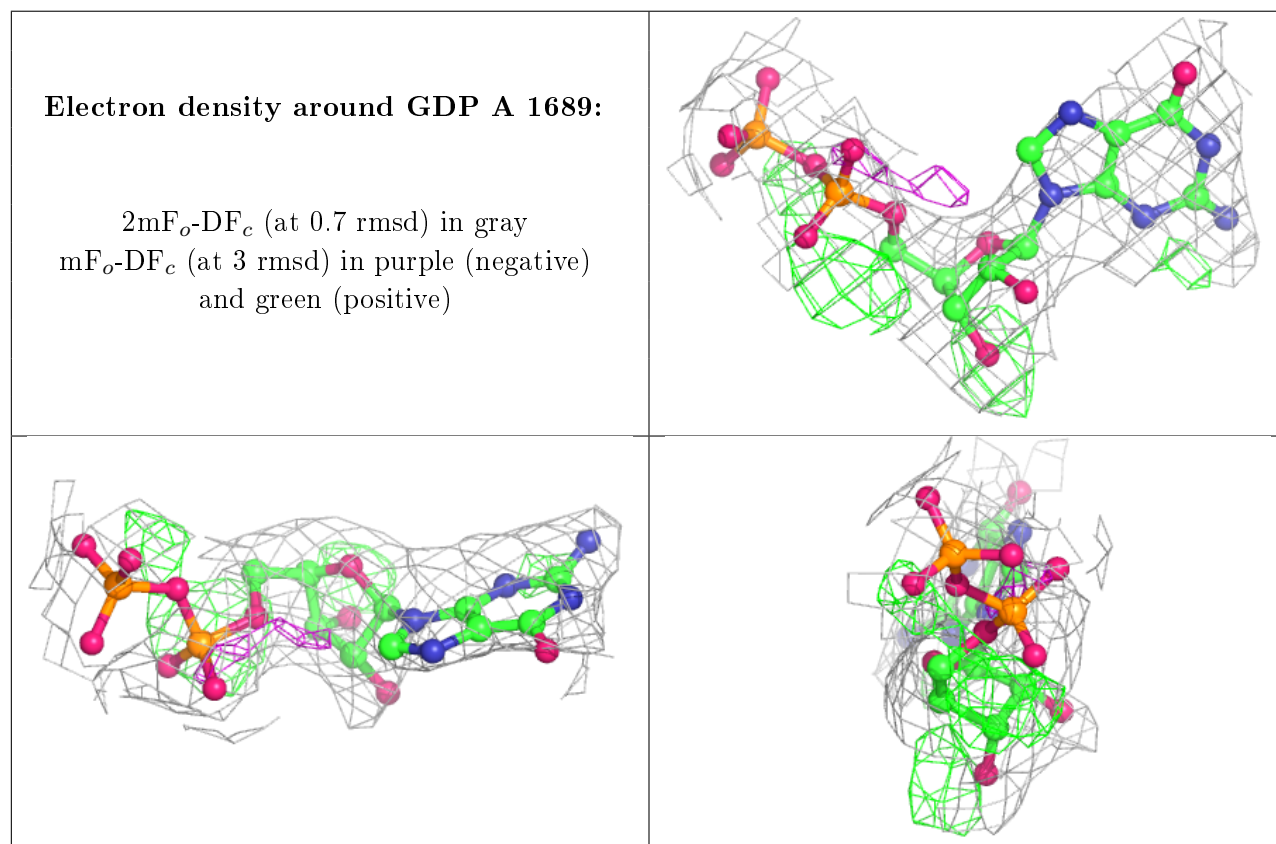
6.3 Carbohydrates ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.