Full wwPDB X-ray Structure Validation Report (i)

Dec 8, 2023 – 12:11 am GMT

PDB ID	:	2BM0
Title	:	Ribosomal elongation factor G (EF-G) Fusidic acid resistant mutant T84A
Authors	:	Hansson, S.; Singh, R.; Gudkov, A.T.; Liljas, A.; Logan, D.T.
Deposited on	:	2005-03-09
Resolution	:	2.40 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 (i) 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 (i)) were used in the production of this report:

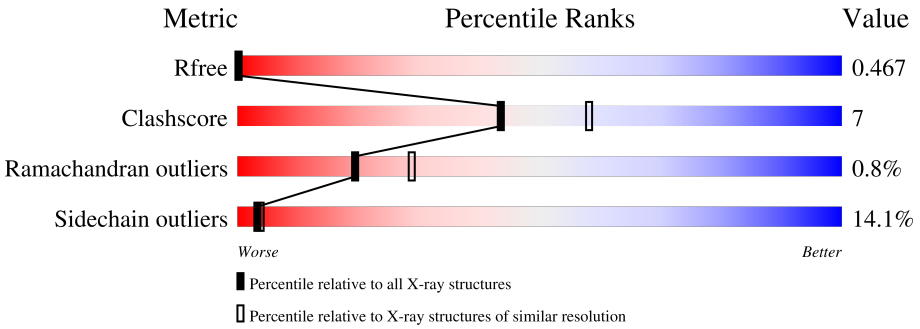
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)

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%

Mol	Chain	Length	Quality of chain
1	A	691	71% 23%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5363 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.

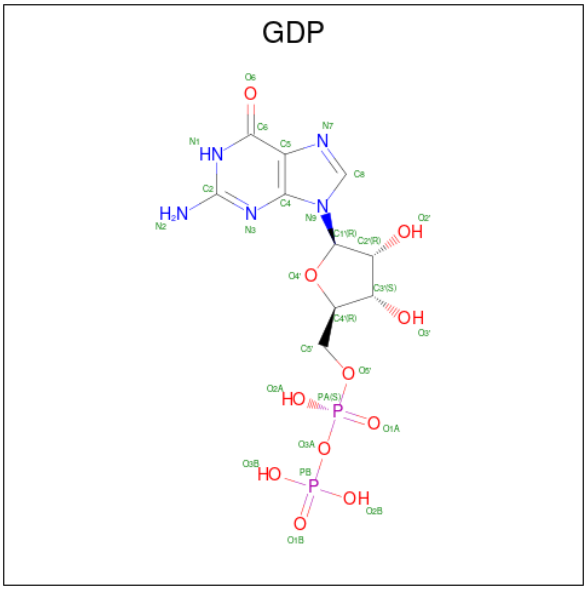
- Molecule 1 is a protein called ELONGATION FACTOR G.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	666	Total	C	N	O	S	0	0	0
			5190	3299	889	984	18			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	43	ALA	GLY	conflict	UNP P13551
A	84	ALA	THR	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
2	A	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 4 is water.

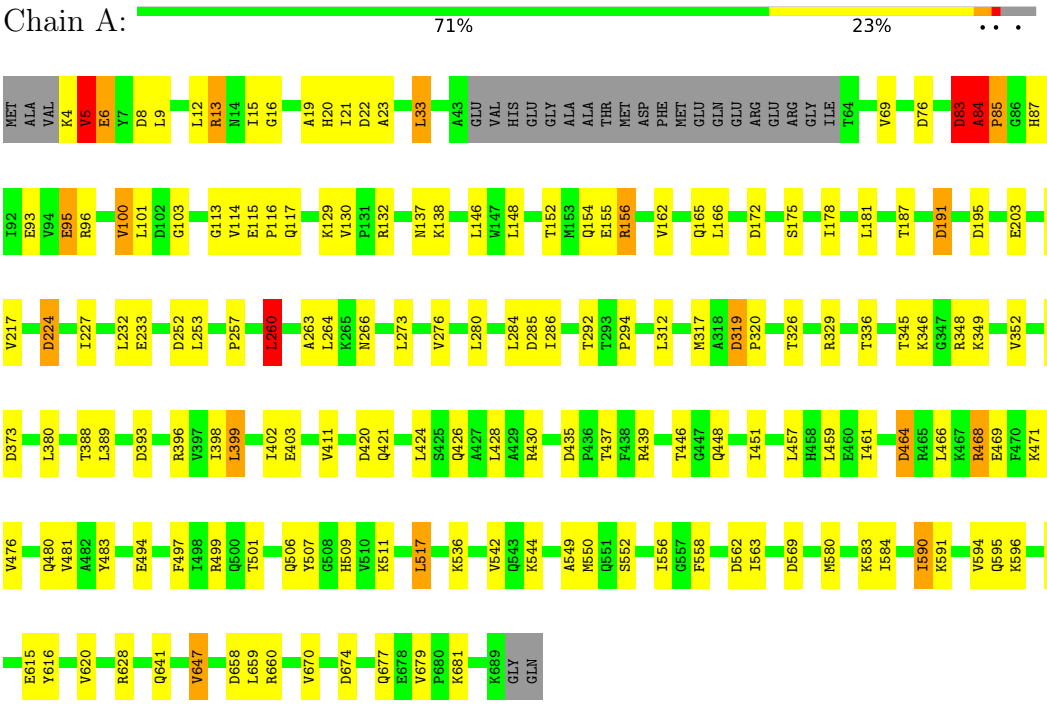
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	144	Total O 144 144	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	78.20Å 88.50Å 116.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 2.40 14.75 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.6 (25.00-2.40) 81.6 (14.75-2.50)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	8.80 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.210 , 0.274 0.460 , 0.467	Depositor DCC
R_{free} test set	1192 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å^2)	46.2	Xtriage
Anisotropy	0.668	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 36.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.69	EDS
Total number of atoms	5363	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.99% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: MG, GDP

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	1/5288 (0.0%)	0.85	24/7165 (0.3%)

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 (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	85	PRO	C-N	16.82	1.63	1.33

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	84	ALA	O-C-N	11.16	142.31	121.10
1	A	84	ALA	C-N-CD	8.91	147.11	128.40
1	A	191	ASP	CB-CG-OD2	6.86	124.47	118.30
1	A	13	ARG	NE-CZ-NH2	-6.75	116.93	120.30
1	A	83	ASP	C-N-CA	6.58	138.16	121.70
1	A	84	ALA	CA-C-N	-6.49	98.93	117.10
1	A	658	ASP	CB-CG-OD2	6.42	124.08	118.30
1	A	195	ASP	CB-CG-OD2	6.31	123.98	118.30
1	A	285	ASP	CB-CG-OD2	6.13	123.82	118.30
1	A	224	ASP	CB-CG-OD2	6.01	123.71	118.30
1	A	435	ASP	CB-CG-OD2	5.92	123.63	118.30
1	A	569	ASP	CB-CG-OD2	5.86	123.57	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	420	ASP	CB-CG-OD2	5.78	123.50	118.30
1	A	319	ASP	CB-CG-OD2	5.77	123.49	118.30
1	A	172	ASP	CB-CG-OD2	5.75	123.48	118.30
1	A	252	ASP	CB-CG-OD2	5.74	123.46	118.30
1	A	674	ASP	CB-CG-OD2	5.72	123.45	118.30
1	A	393	ASP	CB-CG-OD2	5.63	123.37	118.30
1	A	8	ASP	CB-CG-OD2	5.56	123.30	118.30
1	A	84	ALA	C-N-CA	-5.31	99.69	122.00
1	A	76	ASP	CB-CG-OD2	5.25	123.03	118.30
1	A	13	ARG	NE-CZ-NH1	5.17	122.89	120.30
1	A	464	ASP	CB-CG-OD2	5.16	122.94	118.30
1	A	260	LEU	CA-CB-CG	5.02	126.85	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	83	ASP	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	5190	0	5229	70	0
2	A	28	0	12	1	0
3	A	1	0	0	0	0
4	A	144	0	0	4	0
All	All	5363	0	5241	70	0

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 7.

All (70) 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:137:ASN:O	1:A:137:ASN:ND2	1.92	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:562:ASP:OD1	4:A:2122:HOH:O	1.85	0.93
1:A:84:ALA:N	1:A:85:PRO:CD	2.32	0.92
1:A:84:ALA:N	1:A:85:PRO:HD2	1.91	0.84
1:A:148:LEU:O	1:A:152:THR:HG22	1.81	0.81
1:A:137:ASN:O	1:A:137:ASN:CG	2.22	0.76
1:A:398:ILE:HG21	1:A:402:ILE:HD11	1.74	0.68
1:A:428:LEU:HD21	1:A:451:ILE:HD11	1.81	0.61
1:A:616:TYR:O	1:A:620:VAL:HG23	2.01	0.61
1:A:497:PHE:CD1	1:A:584:ILE:HG21	2.36	0.60
1:A:137:ASN:HD21	1:A:263:ALA:H	1.49	0.60
1:A:4:LYS:O	1:A:5:VAL:HG23	2.01	0.59
1:A:83:ASP:CG	1:A:84:ALA:N	2.56	0.59
1:A:641:GLN:NE2	4:A:2135:HOH:O	2.38	0.57
1:A:608:VAL:HG21	1:A:647:VAL:HG13	1.87	0.55
1:A:137:ASN:ND2	1:A:263:ALA:H	2.05	0.54
1:A:13:ARG:HG2	1:A:276:VAL:HG12	1.90	0.53
1:A:83:ASP:OD2	1:A:85:PRO:HD2	2.08	0.53
1:A:87:HIS:CE1	1:A:461:ILE:HG21	2.45	0.52
1:A:138:LYS:HG2	2:A:1690:GDP:C6	2.45	0.52
1:A:87:HIS:HB3	1:A:88:VAL:O	2.09	0.52
1:A:203:GLU:HA	4:A:2050:HOH:O	2.10	0.51
1:A:88:VAL:O	1:A:89:ASP:HB2	2.12	0.50
1:A:424:LEU:HD12	1:A:472:VAL:HG11	1.93	0.49
1:A:91:THR:HG21	1:A:670:VAL:HG12	1.94	0.49
1:A:517:LEU:HD22	1:A:563:ILE:C	2.32	0.49
1:A:165:GLN:NE2	1:A:260:LEU:H	2.11	0.49
1:A:474:ALA:O	1:A:476:VAL:HG23	2.12	0.49
1:A:556:ILE:HD12	1:A:558:PHE:CD2	2.48	0.49
1:A:583:LYS:HD2	4:A:2120:HOH:O	2.13	0.49
1:A:591:LYS:O	1:A:595:GLN:HG3	2.13	0.48
1:A:87:HIS:HB3	1:A:88:VAL:HB	1.95	0.48
1:A:88:VAL:O	1:A:88:VAL:HG12	2.13	0.48
1:A:224:ASP:HB3	1:A:227:ILE:HD12	1.96	0.48
1:A:590:ILE:O	1:A:594:VAL:HG23	2.14	0.47
1:A:608:VAL:HG21	1:A:647:VAL:CG1	2.44	0.47
1:A:213:HIS:O	1:A:217:VAL:HG23	2.15	0.47
1:A:19:ALA:HB1	1:A:23:ALA:HB3	1.96	0.46
1:A:165:GLN:HA	1:A:178:ILE:O	2.15	0.46
1:A:116:PRO:HA	1:A:156:ARG:HH22	1.80	0.46
1:A:91:THR:CG2	1:A:670:VAL:HG12	2.47	0.45
1:A:162:VAL:HG13	1:A:257:PRO:HA	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:HIS:HB3	1:A:88:VAL:C	2.37	0.45
1:A:481:VAL:HG22	1:A:483:TYR:CE2	2.52	0.45
1:A:294:PRO:HD3	1:A:396:ARG:O	2.18	0.44
1:A:603:GLU:HG2	1:A:679:VAL:HG12	1.99	0.44
1:A:165:GLN:HE22	1:A:260:LEU:H	1.64	0.44
1:A:20:HIS:NE2	1:A:117:GLN:HB2	2.33	0.43
1:A:424:LEU:CD1	1:A:472:VAL:HG11	2.47	0.43
1:A:550:MET:SD	1:A:563:ILE:HD11	2.58	0.43
1:A:494:GLU:HG2	1:A:511:LYS:HG2	2.00	0.43
1:A:100:VAL:O	1:A:329:ARG:NH1	2.52	0.43
1:A:388:THR:HG23	1:A:399:LEU:HD22	2.00	0.43
1:A:16:GLY:HA3	1:A:101:LEU:HD22	2.00	0.42
1:A:13:ARG:HG2	1:A:276:VAL:CG1	2.49	0.42
1:A:114:VAL:O	1:A:115:GLU:HG2	2.19	0.42
1:A:191:ASP:O	1:A:266:ASN:ND2	2.44	0.42
1:A:286:ILE:H	1:A:286:ILE:HG13	1.74	0.42
1:A:494:GLU:OE1	1:A:509:HIS:NE2	2.53	0.42
1:A:411:VAL:HG23	1:A:459:LEU:HD23	2.01	0.42
1:A:507:TYR:C	1:A:507:TYR:CD1	2.93	0.42
1:A:33:LEU:HG	1:A:360:ALA:HB2	2.01	0.42
1:A:345:THR:HG23	1:A:402:ILE:HD12	2.00	0.42
1:A:464:ASP:O	1:A:468:ARG:HB2	2.19	0.42
1:A:95:GLU:HG3	1:A:96:ARG:N	2.32	0.41
1:A:549:ALA:HB1	1:A:591:LYS:HD3	2.02	0.41
1:A:15:ILE:HA	1:A:103:GLY:O	2.20	0.41
1:A:87:HIS:HB3	1:A:88:VAL:CB	2.51	0.41
1:A:87:HIS:HB3	1:A:88:VAL:CA	2.51	0.41
1:A:319:ASP:HA	1:A:320:PRO:HD3	1.93	0.40

There are no symmetry-related clashes.

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	662/691 (96%)	627 (95%)	30 (4%)	5 (1%)	19 29

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	84	ALA
1	A	5	VAL
1	A	6	GLU
1	A	113	GLY
1	A	380	LEU

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	555/581 (96%)	477 (86%)	78 (14%)	3 4

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	VAL
1	A	6	GLU
1	A	9	LEU
1	A	12	LEU
1	A	21	ILE
1	A	22	ASP
1	A	33	LEU
1	A	69	VAL
1	A	90	PHE
1	A	93	GLU
1	A	95	GLU
1	A	100	VAL
1	A	129	LYS
1	A	130	VAL
1	A	132	ARG
1	A	146	LEU

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Mol	Chain	Res	Type
1	A	154	GLN
1	A	155	GLU
1	A	156	ARG
1	A	166	LEU
1	A	175	SER
1	A	181	LEU
1	A	187	THR
1	A	206	LEU
1	A	232	LEU
1	A	233	GLU
1	A	253	LEU
1	A	260	LEU
1	A	264	LEU
1	A	273	LEU
1	A	280	LEU
1	A	284	LEU
1	A	292	THR
1	A	312	LEU
1	A	317	MET
1	A	326	THR
1	A	336	THR
1	A	346	LYS
1	A	348	ARG
1	A	349	LYS
1	A	352	VAL
1	A	369	LEU
1	A	373	ASP
1	A	389	LEU
1	A	399	LEU
1	A	403	GLU
1	A	421	GLN
1	A	426	GLN
1	A	430	ARG
1	A	437	THR
1	A	439	ARG
1	A	446	THR
1	A	448	GLN
1	A	457	LEU
1	A	466	LEU
1	A	468	ARG
1	A	469	GLU
1	A	471	LYS

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Mol	Chain	Res	Type
1	A	480	GLN
1	A	499	ARG
1	A	501	THR
1	A	506	GLN
1	A	517	LEU
1	A	536	LYS
1	A	542	VAL
1	A	544	LYS
1	A	552	SER
1	A	580	MET
1	A	590	ILE
1	A	596	LYS
1	A	607	ARG
1	A	615	GLU
1	A	628	ARG
1	A	647	VAL
1	A	659	LEU
1	A	660	ARG
1	A	677	GLN
1	A	681	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	HIS
1	A	117	GLN
1	A	137	ASN
1	A	165	GLN
1	A	208	GLN
1	A	226	ASN
1	A	270	GLN
1	A	421	GLN
1	A	506	GLN
1	A	543	GLN
1	A	641	GLN
1	A	684	GLN

5.3.3 RNA

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 monosaccharides 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	1690	3	24,30,30	1.12	1 (4%)	30,47,47	1.56	8 (26%)

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	1690	3	-	2/12/32/32	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1690	GDP	C5-C6	-3.81	1.39	1.47

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1690	GDP	PA-O3A-PB	-3.69	120.17	132.83
2	A	1690	GDP	N2-C2-N1	2.74	122.55	116.71
2	A	1690	GDP	C8-N7-C5	2.63	107.99	102.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1690	GDP	C5-C6-N1	2.54	118.44	113.95
2	A	1690	GDP	O2B-PB-O3A	2.41	112.71	104.64
2	A	1690	GDP	O6-C6-C5	-2.35	119.78	124.37
2	A	1690	GDP	C2-N1-C6	-2.25	120.95	125.10
2	A	1690	GDP	O4'-C4'-C3'	2.20	109.46	105.11

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1690	GDP	PA-O3A-PB-O2B
2	A	1690	GDP	PA-O3A-PB-O3B

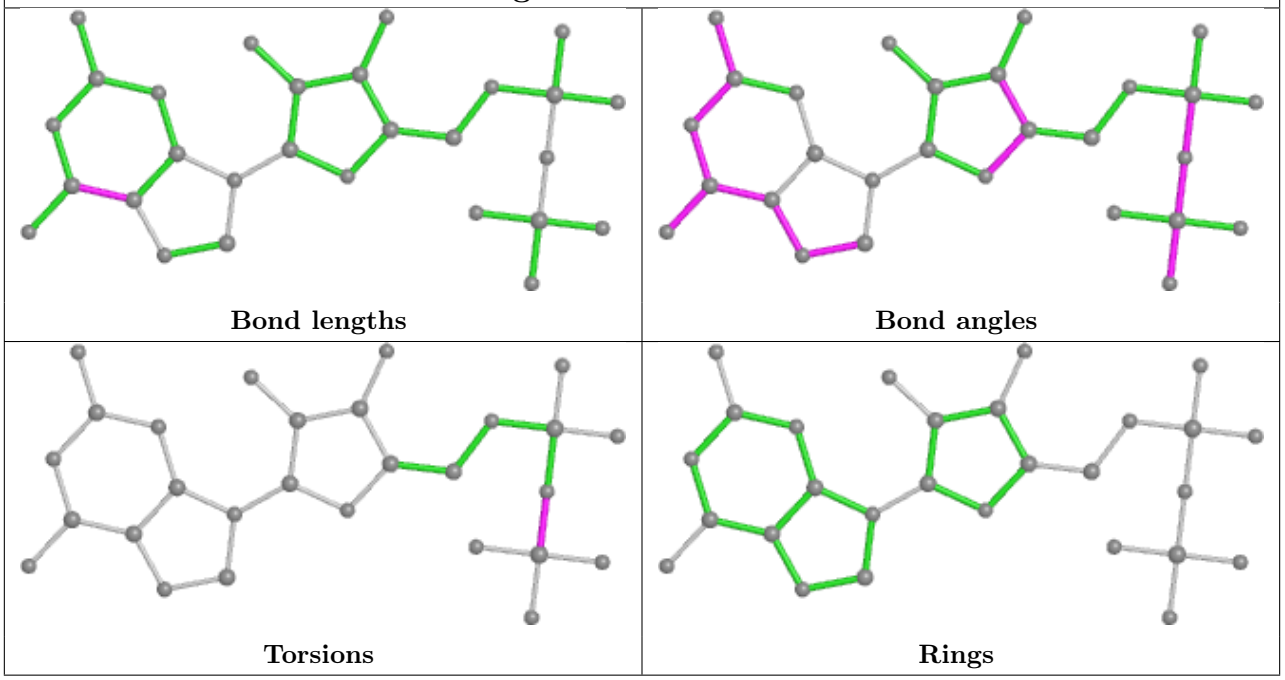
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1690	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 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 1690



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	85:PRO	C	86:GLY	N	1.63

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.

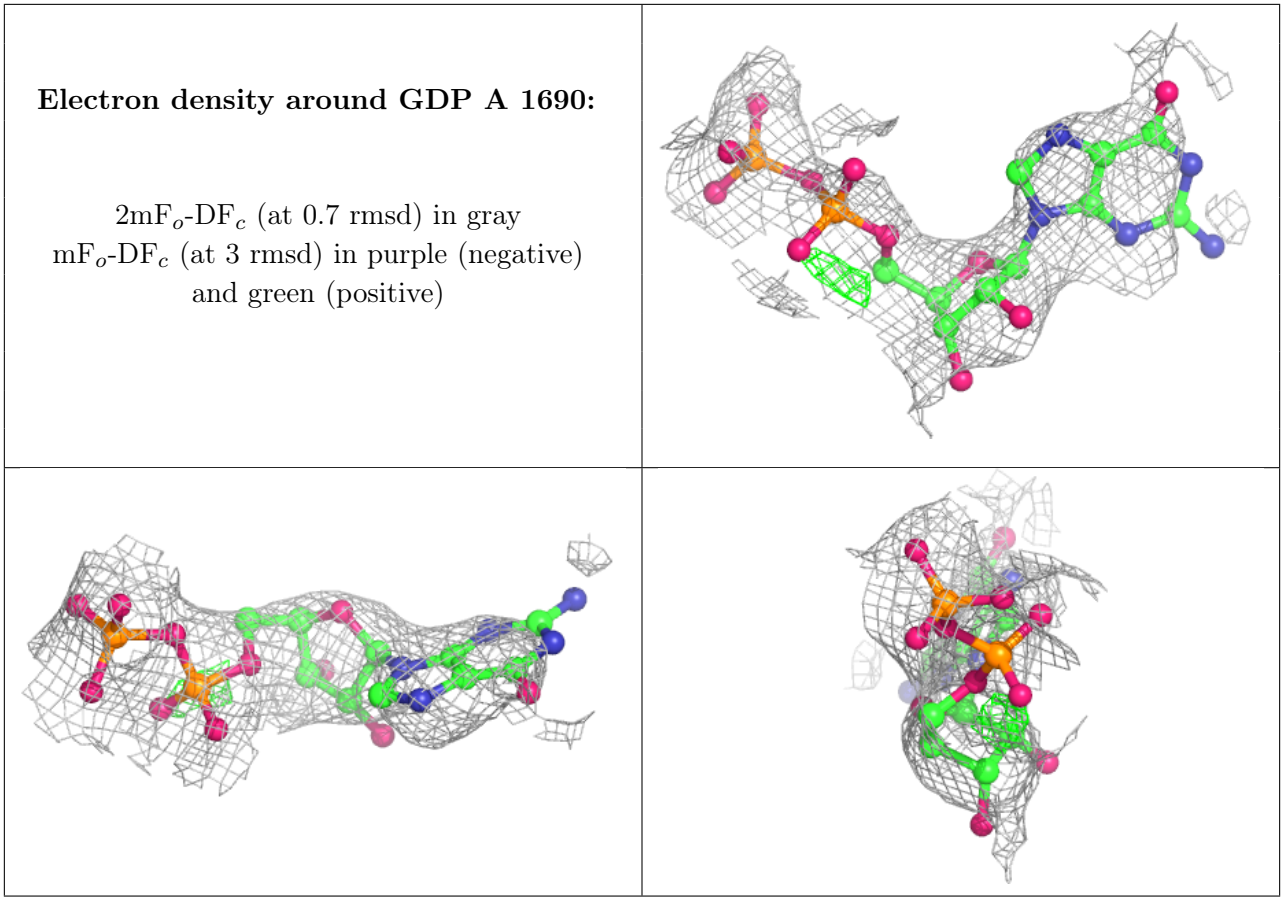
6.4 Ligands

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.

Electron density around GDP A 1690:

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



6.5 Other polymers (i)

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