



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:34 AM UTC

PDB ID : 2BM0 / pdb_00002bm0
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 ⓘ 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

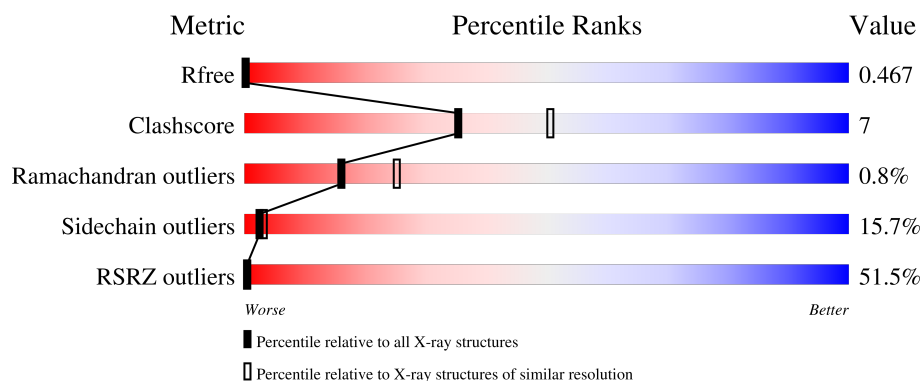
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (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 $\leq 5\%$. 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	50% 71% 21% • •

2 Entry composition [i](#)

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.

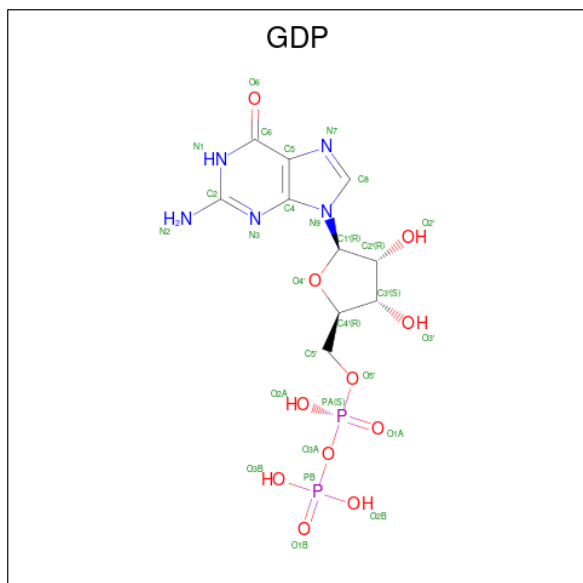
- Molecule 1 is a protein called ELONGATION FACTOR G.

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

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 (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



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

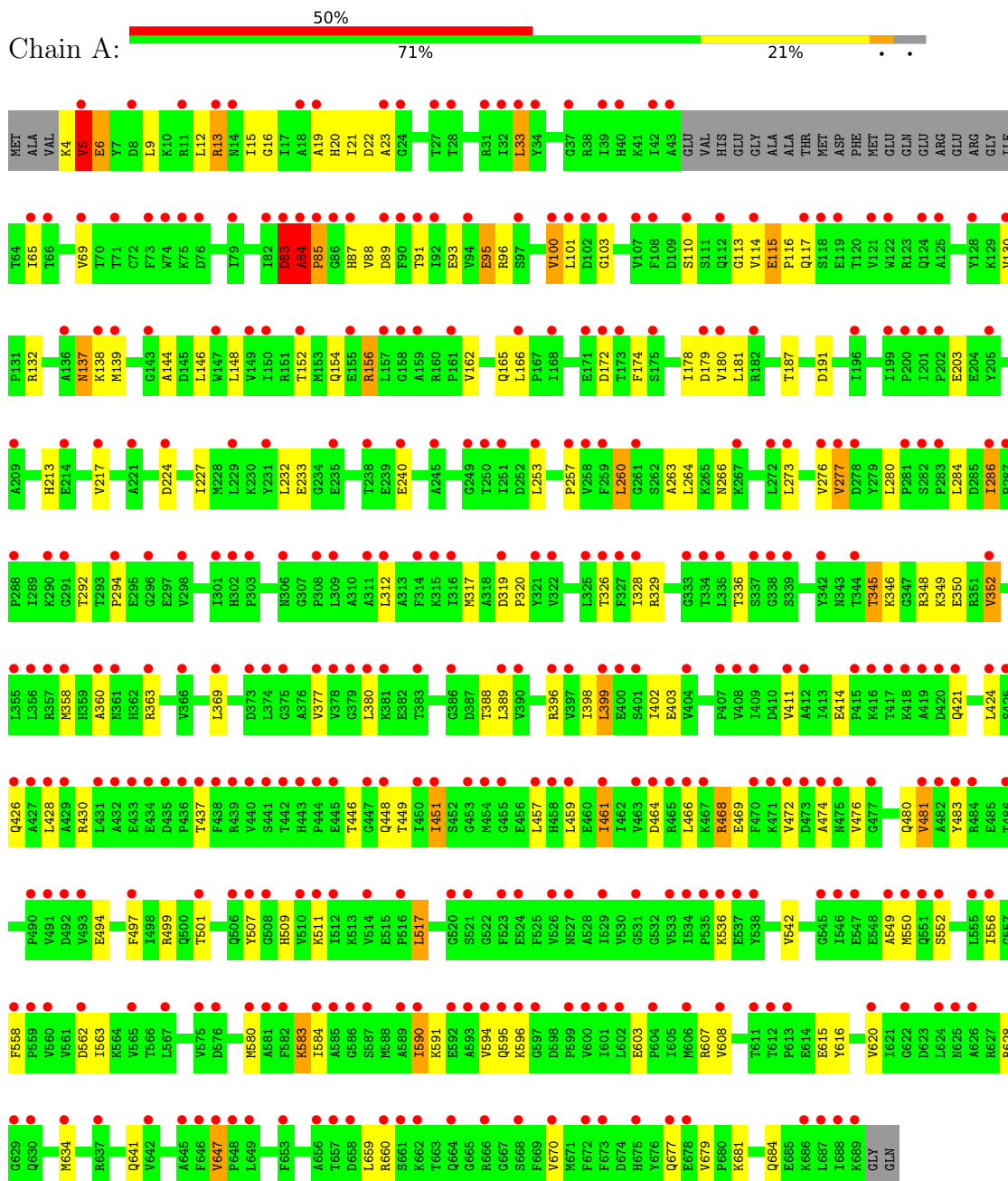
- Molecule 4 is water.

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

3 Residue-property plots

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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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	78.20Å 88.50Å 116.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 2.40 25.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.6 (25.00-2.40) 81.1 (25.00-2.50)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ 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 , 26.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	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.*

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	0.78	5/5288 (0.1%)	1.00	9/7165 (0.1%)

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 (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	85	PRO	C-N	21.41	1.63	1.33
1	A	277	VAL	CA-CB	5.72	1.61	1.54
1	A	172	ASP	C-O	5.47	1.30	1.24
1	A	174	PHE	C-O	5.15	1.30	1.24
1	A	352	VAL	CA-CB	5.13	1.59	1.53

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	84	ALA	CA-C-N	-20.07	99.69	119.76
1	A	84	ALA	C-N-CA	-20.07	99.69	119.76
1	A	84	ALA	O-C-N	18.25	142.31	121.32
1	A	83	ASP	CA-C-N	6.71	138.16	121.80
1	A	83	ASP	C-N-CA	6.71	138.16	121.80
1	A	137	ASN	N-CA-C	5.48	120.12	113.38
1	A	84	ALA	C-N-CD	5.39	147.11	125.00
1	A	277	VAL	N-CA-CB	5.07	117.06	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	83	ASP	O-C-N	5.07	129.01	122.68

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	5230	77	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	5242	77	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 (77) 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
1:A:84:ALA:H	1:A:85:PRO:HD2	1.28	0.96
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	0.81
1:A:398:ILE:HG21	1:A:402:ILE:HD11	1.74	0.68
1:A:83:ASP:CG	1:A:84:ALA:N	2.56	0.63
1:A:83:ASP:CG	1:A:84:ALA:H	2.07	0.62
1:A:428:LEU:HD21	1:A:451:ILE:HD11	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:110:SER:OG	1:A:139:MET:HE3	2.02	0.58
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:517:LEU:HD22	1:A:563:ILE:C	2.32	0.54
1:A:13:ARG:HG2	1:A:276:VAL:HG12	1.90	0.53
1:A:358:MET:HE1	1:A:363:ARG:CZ	2.38	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:139:MET:HE2	1:A:139:MET:HA	1.92	0.51
1:A:88:VAL:O	1:A:89:ASP:HB2	2.12	0.50
1:A:87:HIS:HB3	1:A:88:VAL:C	2.37	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:139:MET:HE2	1:A:144:ALA:HB1	1.93	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:507:TYR:C	1:A:507:TYR:CD1	2.93	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:A:179:ASP:OD1	1:A:179:ASP:C	2.62	0.40

There are no symmetry-related clashes.

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	662/691 (96%)	627 (95%)	30 (4%)	5 (1%)	16	25

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%)	468 (84%)	87 (16%)	2 3

All (87) 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	13	ARG
1	A	21	ILE
1	A	22	ASP
1	A	33	LEU
1	A	65	ILE
1	A	69	VAL
1	A	93	GLU
1	A	95	GLU
1	A	100	VAL
1	A	115	GLU
1	A	130	VAL
1	A	132	ARG
1	A	146	LEU
1	A	154	GLN
1	A	156	ARG
1	A	166	LEU

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Mol	Chain	Res	Type
1	A	180	VAL
1	A	181	LEU
1	A	187	THR
1	A	232	LEU
1	A	233	GLU
1	A	240	GLU
1	A	253	LEU
1	A	260	LEU
1	A	264	LEU
1	A	273	LEU
1	A	277	VAL
1	A	280	LEU
1	A	284	LEU
1	A	286	ILE
1	A	292	THR
1	A	312	LEU
1	A	317	MET
1	A	326	THR
1	A	328	ILE
1	A	336	THR
1	A	345	THR
1	A	346	LYS
1	A	348	ARG
1	A	349	LYS
1	A	350	GLU
1	A	352	VAL
1	A	369	LEU
1	A	377	VAL
1	A	389	LEU
1	A	399	LEU
1	A	403	GLU
1	A	414	GLU
1	A	421	GLN
1	A	426	GLN
1	A	430	ARG
1	A	437	THR
1	A	446	THR
1	A	448	GLN
1	A	449	THR
1	A	451	ILE
1	A	457	LEU
1	A	461	ILE

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Mol	Chain	Res	Type
1	A	466	LEU
1	A	468	ARG
1	A	469	GLU
1	A	480	GLN
1	A	481	VAL
1	A	499	ARG
1	A	501	THR
1	A	517	LEU
1	A	536	LYS
1	A	542	VAL
1	A	552	SER
1	A	580	MET
1	A	583	LYS
1	A	590	ILE
1	A	596	LYS
1	A	607	ARG
1	A	615	GLU
1	A	628	ARG
1	A	634	MET
1	A	647	VAL
1	A	659	LEU
1	A	660	ARG
1	A	677	GLN
1	A	681	LYS
1	A	684	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
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	458	HIS
1	A	506	GLN
1	A	543	GLN
1	A	625	ASN
1	A	664	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GDP	A	1690	3	29,30,30	0.88	1 (3%)	45,47,47	1.61	12 (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	-	3/16/32/32	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	PA-O3A	2.07	1.61	1.59

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1690	GDP	C2-N3-C4	3.94	119.08	112.30
2	A	1690	GDP	C5-C4-N3	-3.30	123.14	128.39
2	A	1690	GDP	N2-C2-N1	2.74	122.55	116.76
2	A	1690	GDP	N9-C8-N7	-2.60	108.58	113.40
2	A	1690	GDP	O6-C6-C5	-2.56	119.78	126.53
2	A	1690	GDP	O2B-PB-O3A	2.41	112.71	104.64
2	A	1690	GDP	O4'-C1'-N9	2.30	113.57	108.36
2	A	1690	GDP	C2-N1-C6	-2.29	120.95	125.11
2	A	1690	GDP	O2A-PA-O3A	2.23	113.31	107.27
2	A	1690	GDP	O4'-C4'-C3'	2.17	109.46	105.15
2	A	1690	GDP	C8-N7-C5	2.10	107.99	104.26
2	A	1690	GDP	C5-C6-N1	2.04	118.44	113.25

There are no chirality outliers.

All (3) torsion outliers are listed below:

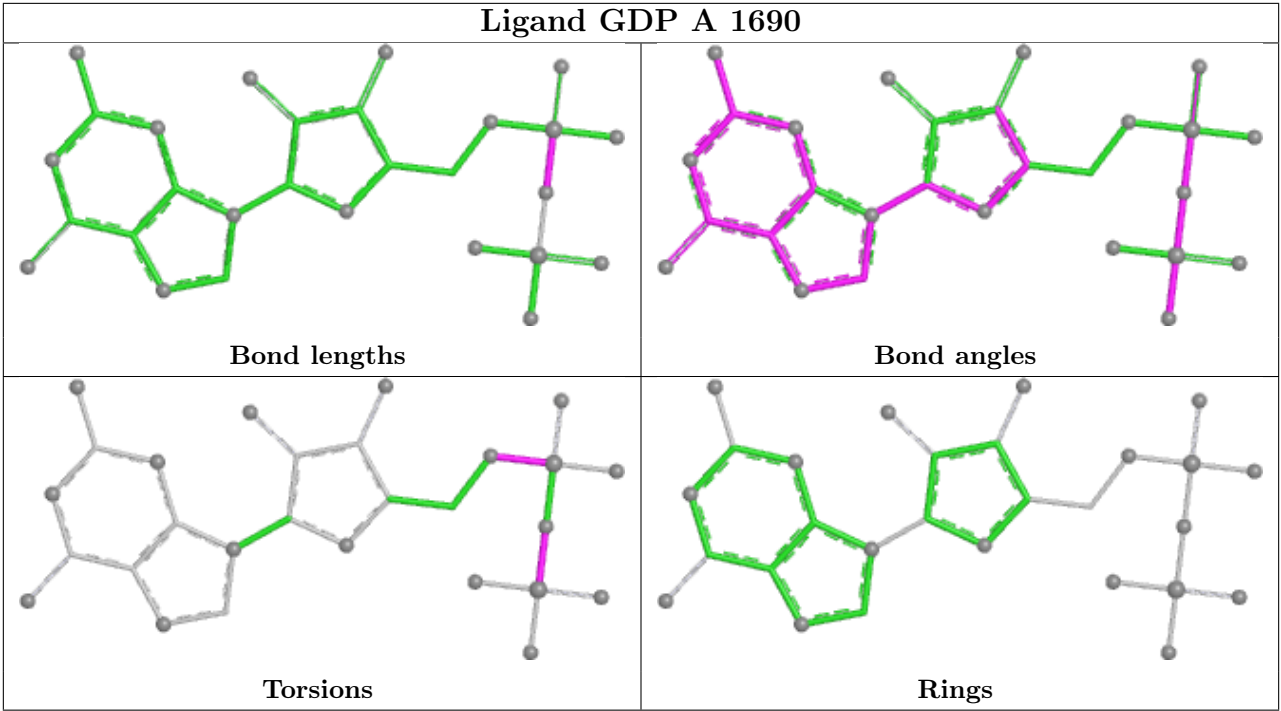
Mol	Chain	Res	Type	Atoms
2	A	1690	GDP	PA-O3A-PB-O2B
2	A	1690	GDP	PA-O3A-PB-O3B
2	A	1690	GDP	C5'-O5'-PA-O1A

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 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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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 ⓘ

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	666/691 (96%)	2.20	343 (51%) 0 0	17, 28, 58, 72	0

All (343) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	472	VAL	15.5
1	A	110	SER	7.2
1	A	86	GLY	6.7
1	A	491	VAL	6.1
1	A	429	ALA	6.1
1	A	389	LEU	5.7
1	A	586	GLY	5.7
1	A	24	GLY	5.6
1	A	326	THR	5.5
1	A	590	ILE	5.3
1	A	421	GLN	5.2
1	A	83	ASP	5.0
1	A	645	ALA	4.9
1	A	158	GLY	4.9
1	A	114	VAL	4.9
1	A	42	ILE	4.8
1	A	420	ASP	4.8
1	A	366	VAL	4.8
1	A	545	GLY	4.6
1	A	453	GLY	4.5
1	A	400	GLU	4.5
1	A	538	TYR	4.4
1	A	565	VAL	4.4
1	A	482	ALA	4.3
1	A	102	ASP	4.2
1	A	444	PRO	4.2
1	A	375	GLY	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	214	GLU	4.2
1	A	585	ALA	4.2
1	A	28	THR	4.1
1	A	471	LYS	4.1
1	A	514	VAL	4.1
1	A	534	ILE	4.1
1	A	581	ALA	4.1
1	A	584	ILE	4.1
1	A	536	LYS	4.1
1	A	450	ILE	4.0
1	A	97	SER	4.0
1	A	84	ALA	4.0
1	A	334	THR	4.0
1	A	481	VAL	4.0
1	A	130	VAL	3.9
1	A	408	VAL	3.9
1	A	470	PHE	3.9
1	A	373	ASP	3.9
1	A	13	ARG	3.9
1	A	459	LEU	3.9
1	A	425	SER	3.9
1	A	171	GLU	3.8
1	A	23	ALA	3.8
1	A	316	ILE	3.8
1	A	319	ASP	3.8
1	A	325	LEU	3.8
1	A	555	LEU	3.8
1	A	281	PRO	3.8
1	A	436	PRO	3.8
1	A	576	ASP	3.8
1	A	173	THR	3.8
1	A	401	SER	3.8
1	A	594	VAL	3.8
1	A	356	LEU	3.8
1	A	447	GLY	3.7
1	A	418	LYS	3.7
1	A	397	VAL	3.7
1	A	582	PHE	3.7
1	A	122	TRP	3.7
1	A	646	PHE	3.7
1	A	547	GLU	3.7
1	A	267	LYS	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	473	ASP	3.7
1	A	575	VAL	3.6
1	A	662	LYS	3.6
1	A	294	PRO	3.6
1	A	396	ARG	3.6
1	A	74	TRP	3.6
1	A	136	ALA	3.6
1	A	464	ASP	3.6
1	A	589	ALA	3.6
1	A	624	LEU	3.6
1	A	497	PHE	3.6
1	A	79	ILE	3.6
1	A	128	TYR	3.6
1	A	647	VAL	3.6
1	A	240	GLU	3.5
1	A	445	GLU	3.5
1	A	411	VAL	3.5
1	A	486	THR	3.5
1	A	435	ASP	3.5
1	A	670	VAL	3.5
1	A	613	PRO	3.5
1	A	521	SER	3.5
1	A	510	VAL	3.4
1	A	157	LEU	3.4
1	A	253	LEU	3.4
1	A	511	LYS	3.4
1	A	549	ALA	3.4
1	A	417	THR	3.4
1	A	622	GLY	3.4
1	A	205	TYR	3.4
1	A	672	PHE	3.4
1	A	437	THR	3.4
1	A	455	GLY	3.4
1	A	592	GLU	3.4
1	A	438	PHE	3.4
1	A	416	LYS	3.4
1	A	467	LYS	3.4
1	A	567	LEU	3.3
1	A	426	GLN	3.3
1	A	506	GLN	3.3
1	A	172	ASP	3.3
1	A	484	ARG	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	688	ILE	3.3
1	A	399	LEU	3.3
1	A	424	LEU	3.3
1	A	649	LEU	3.3
1	A	94	VAL	3.3
1	A	558	PHE	3.2
1	A	620	VAL	3.2
1	A	235	GLU	3.2
1	A	386	GLY	3.2
1	A	245	ALA	3.2
1	A	412	ALA	3.2
1	A	492	ASP	3.2
1	A	69	VAL	3.2
1	A	71	THR	3.2
1	A	201	ILE	3.2
1	A	224	ASP	3.1
1	A	559	PRO	3.1
1	A	152	THR	3.1
1	A	434	GLU	3.1
1	A	196	ILE	3.1
1	A	90	PHE	3.1
1	A	612	THR	3.1
1	A	272	LEU	3.1
1	A	427	ALA	3.0
1	A	552	SER	3.0
1	A	66	THR	3.0
1	A	231	TYR	3.0
1	A	458	HIS	3.0
1	A	562	ASP	3.0
1	A	199	ILE	3.0
1	A	551	GLN	3.0
1	A	608	VAL	3.0
1	A	442	THR	3.0
1	A	687	LEU	3.0
1	A	32	ILE	3.0
1	A	404	VAL	3.0
1	A	221	ALA	3.0
1	A	73	PHE	3.0
1	A	249	GLY	3.0
1	A	322	VAL	2.9
1	A	390	VAL	2.9
1	A	501	THR	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	419	ALA	2.9
1	A	483	TYR	2.9
1	A	92	ILE	2.9
1	A	529	ILE	2.9
1	A	377	VAL	2.9
1	A	477	GLY	2.9
1	A	43	ALA	2.9
1	A	161	PRO	2.9
1	A	474	ALA	2.9
1	A	648	PRO	2.9
1	A	259	PHE	2.9
1	A	118	SER	2.9
1	A	100	VAL	2.9
1	A	85	PRO	2.9
1	A	657	THR	2.9
1	A	355	LEU	2.9
1	A	597	GLY	2.9
1	A	306	ASN	2.8
1	A	138	LYS	2.8
1	A	290	LYS	2.8
1	A	360	ALA	2.8
1	A	457	LEU	2.8
1	A	537	GLU	2.8
1	A	660	ARG	2.8
1	A	287	PRO	2.8
1	A	352	VAL	2.8
1	A	600	VAL	2.8
1	A	369	LEU	2.8
1	A	656	ALA	2.8
1	A	119	GLU	2.8
1	A	124	GLN	2.8
1	A	11	ARG	2.8
1	A	321	TYR	2.8
1	A	556	ILE	2.8
1	A	202	PRO	2.8
1	A	526	VAL	2.8
1	A	432	ALA	2.8
1	A	302	HIS	2.8
1	A	296	GLY	2.7
1	A	301	ILE	2.7
1	A	166	LEU	2.7
1	A	87	HIS	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	675	HIS	2.7
1	A	276	VAL	2.7
1	A	378	VAL	2.7
1	A	587	SER	2.7
1	A	661	SER	2.7
1	A	448	GLN	2.7
1	A	108	PHE	2.7
1	A	461	ILE	2.7
1	A	180	VAL	2.7
1	A	277	VAL	2.7
1	A	311	ALA	2.7
1	A	653	PHE	2.7
1	A	673	PHE	2.7
1	A	112	GLN	2.7
1	A	328	ILE	2.6
1	A	121	VAL	2.6
1	A	560	VAL	2.6
1	A	18	ALA	2.6
1	A	428	LEU	2.6
1	A	117	GLN	2.6
1	A	303	PRO	2.6
1	A	82	ILE	2.6
1	A	546	ILE	2.6
1	A	40	HIS	2.6
1	A	76	ASP	2.6
1	A	103	GLY	2.6
1	A	357	ARG	2.5
1	A	257	PRO	2.5
1	A	335	LEU	2.5
1	A	463	VAL	2.5
1	A	677	GLN	2.5
1	A	443	HIS	2.5
1	A	611	THR	2.5
1	A	291	GLY	2.5
1	A	338	GLY	2.5
1	A	535	PRO	2.5
1	A	431	LEU	2.5
1	A	595	GLN	2.5
1	A	630	GLN	2.5
1	A	512	ILE	2.5
1	A	664	GLN	2.5
1	A	125	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	666	ARG	2.5
1	A	250	THR	2.5
1	A	282	SER	2.5
1	A	358	MET	2.5
1	A	606	MET	2.5
1	A	451	ILE	2.5
1	A	75	LYS	2.5
1	A	686	LYS	2.5
1	A	490	PRO	2.4
1	A	101	LEU	2.4
1	A	314	PHE	2.4
1	A	363	ARG	2.4
1	A	516	PRO	2.4
1	A	5	VAL	2.4
1	A	258	VAL	2.4
1	A	283	PRO	2.4
1	A	415	PRO	2.4
1	A	520	GLY	2.4
1	A	39	ILE	2.4
1	A	309	LEU	2.4
1	A	637	ARG	2.4
1	A	34	TYR	2.4
1	A	625	ASN	2.4
1	A	383	THR	2.4
1	A	642	VAL	2.4
1	A	433	GLU	2.4
1	A	407	PRO	2.3
1	A	31	ARG	2.3
1	A	466	LEU	2.3
1	A	440	VAL	2.3
1	A	337	SER	2.3
1	A	339	SER	2.3
1	A	33	LEU	2.3
1	A	286	ILE	2.3
1	A	601	ILE	2.3
1	A	658	ASP	2.3
1	A	37	GLY	2.3
1	A	147	TRP	2.3
1	A	139	MET	2.3
1	A	315	LYS	2.3
1	A	596	LYS	2.3
1	A	217	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	599	PRO	2.3
1	A	143	GLY	2.3
1	A	668	SER	2.3
1	A	238	THR	2.2
1	A	175	SER	2.2
1	A	251	ILE	2.2
1	A	580	MET	2.2
1	A	602	LEU	2.2
1	A	179	ASP	2.2
1	A	342	TYR	2.2
1	A	91	THR	2.2
1	A	381	LYS	2.2
1	A	380	LEU	2.2
1	A	634	MET	2.2
1	A	168	ILE	2.2
1	A	409	ILE	2.2
1	A	441	SER	2.2
1	A	475	ASN	2.2
1	A	550	MET	2.2
1	A	150	ILE	2.2
1	A	678	GLU	2.2
1	A	298	VAL	2.2
1	A	229	LEU	2.2
1	A	524	GLU	2.2
1	A	604	PRO	2.2
1	A	523	PHE	2.2
1	A	493	VAL	2.1
1	A	27	THR	2.1
1	A	273	LEU	2.1
1	A	344	THR	2.1
1	A	155	GLU	2.1
1	A	439	ARG	2.1
1	A	465	ARG	2.1
1	A	89	ASP	2.1
1	A	288	PRO	2.1
1	A	107	VAL	2.1
1	A	533	VAL	2.1
1	A	19	ALA	2.1
1	A	626	ALA	2.1
1	A	182	ARG	2.1
1	A	507	TYR	2.1
1	A	327	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	454	MET	2.1
1	A	209	ALA	2.1
1	A	361	ASN	2.1
1	A	312	LEU	2.1
1	A	508	GLY	2.1
1	A	629	GLY	2.1
1	A	278	ASP	2.1
1	A	308	PRO	2.1
1	A	159	ALA	2.1
1	A	593	ALA	2.1
1	A	374	LEU	2.1
1	A	527	ASN	2.1
1	A	261	GLY	2.1
1	A	65	ILE	2.1
1	A	149	VAL	2.0
1	A	14	ASN	2.0
1	A	689	LYS	2.0
1	A	333	GLY	2.0
1	A	379	GLY	2.0
1	A	531	GLY	2.0
1	A	8	ASP	2.0
1	A	200	PRO	2.0

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.

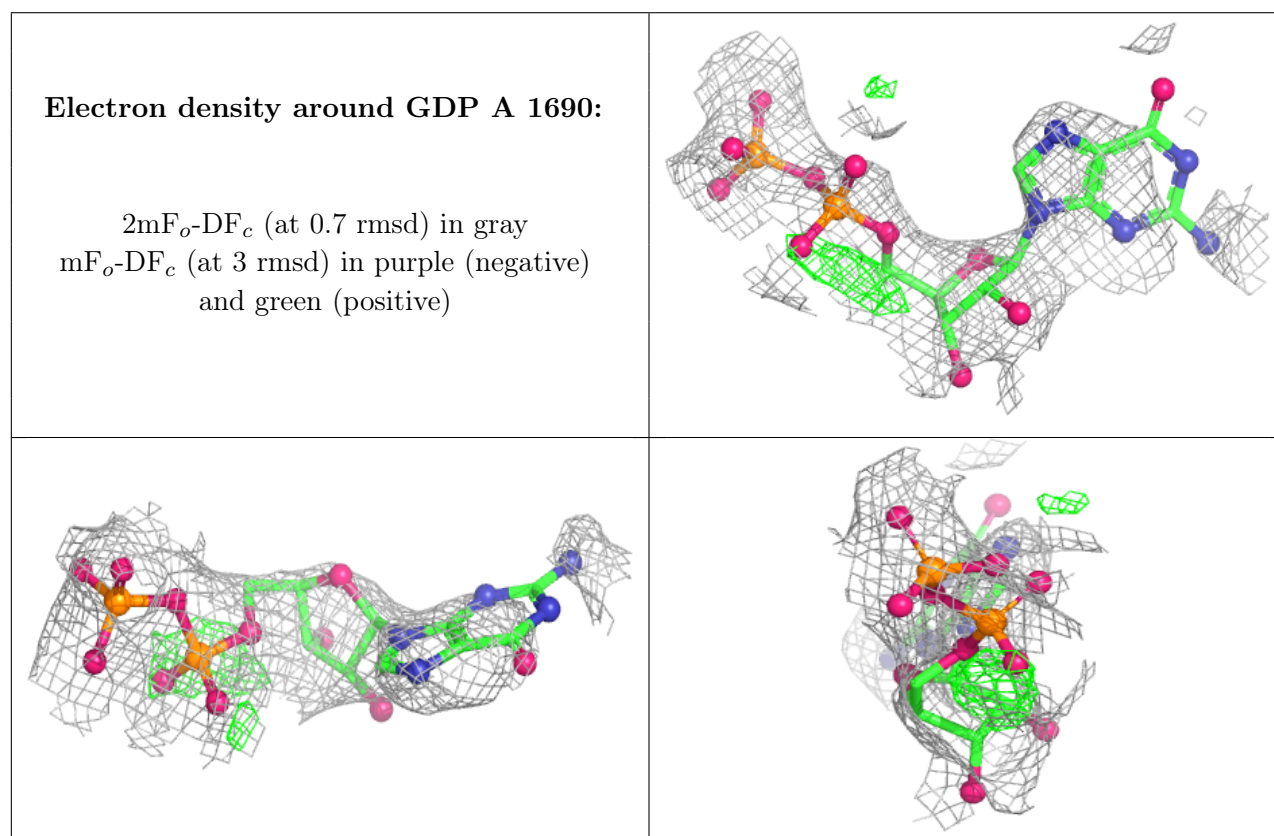
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	MG	A	1691	1/1	0.45	0.34	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	GDP	A	1690	28/28	0.67	0.21	58,62,65,66	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.