



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 04:17 AM UTC

PDB ID : 3X1D / pdb_00003x1d
Title : Crystal Structure of Atlantin from *Drosophila melanogaster*
Authors : Liu, X.
Deposited on : 2014-11-14
Resolution : 2.87 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

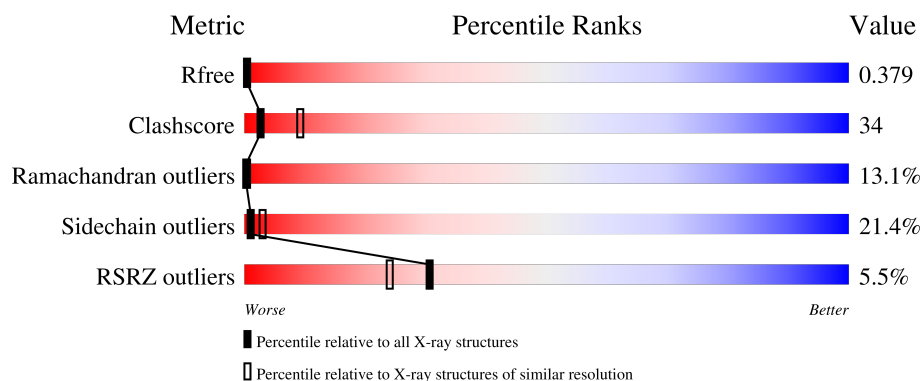
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.87 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	3557 (2.90-2.86)
Clashscore	190562	3801 (2.90-2.86)
Ramachandran outliers	187476	3699 (2.90-2.86)
Sidechain outliers	187428	3702 (2.90-2.86)
RSRZ outliers	180081	3558 (2.90-2.86)

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	541	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 3017 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 Atlastin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	381	Total	C	N	O	S	0	0	0
			2982	1905	512	551	14			

- 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
4	A	6	Total	O	0	0
			6	6		

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	71.62Å 63.91Å 107.76Å 90.00° 101.60° 90.00°	Depositor
Resolution (Å)	27.79 – 2.87 27.79 – 2.87	Depositor EDS
% Data completeness (in resolution range)	92.0 (27.79-2.87) 91.9 (27.79-2.87)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.31 (at 2.86Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.273 , 0.379 0.274 , 0.379	Depositor DCC
R_{free} test set	494 reflections (4.46%)	wwPDB-VP
Wilson B-factor (Å ²)	64.9	Xtriage
Anisotropy	0.651	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.22 , 42.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	3017	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.34% 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 [i](#)

5.1 Standard geometry [i](#)

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	0.62	0/3043	1.10	18/4114 (0.4%)

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	49	LYS	N-CA-C	-8.69	101.99	112.59
1	A	284	ASN	N-CA-C	-7.06	104.54	113.72
1	A	139	PHE	N-CA-C	-6.88	105.44	114.31
1	A	32	GLU	N-CA-C	-6.81	101.32	111.81
1	A	362	LEU	N-CA-C	-6.59	104.13	111.71
1	A	168	PHE	N-CA-C	-6.54	107.16	114.62
1	A	262	GLN	N-CA-C	-5.85	104.49	111.69
1	A	207	GLY	N-CA-C	-5.72	105.86	112.73
1	A	144	MET	N-CA-C	-5.70	105.20	111.82
1	A	257	PHE	N-CA-C	5.67	118.46	110.23
1	A	229	ARG	N-CA-C	-5.58	105.73	112.54
1	A	219	ASP	N-CA-C	-5.54	106.03	112.89
1	A	359	THR	N-CA-C	5.44	120.78	114.04
1	A	107	HIS	CA-C-N	5.24	131.12	121.70
1	A	107	HIS	C-N-CA	5.24	131.12	121.70
1	A	265	THR	CA-C-N	5.19	124.99	119.28
1	A	265	THR	C-N-CA	5.19	124.99	119.28
1	A	157	ILE	CB-CA-C	-5.03	106.47	111.80

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	2982	0	2898	200	0
2	A	28	0	12	5	0
3	A	1	0	0	0	0
4	A	6	0	0	2	0
All	All	3017	0	2910	200	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 34.

All (200) 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:208:ASP:HB3	1:A:212:LYS:HE3	1.57	0.87
1:A:40:VAL:H	1:A:118:ILE:HB	1.42	0.85
1:A:299:ASP:N	1:A:299:ASP:OD1	2.10	0.83
1:A:265:THR:HG22	1:A:267:GLU:H	1.46	0.81
1:A:319:PRO:O	1:A:321:SER:N	2.11	0.81
1:A:40:VAL:HG12	1:A:146:SER:HA	1.64	0.80
1:A:390:GLU:OE2	1:A:393:ARG:NH1	2.15	0.79
1:A:263:ASP:N	1:A:263:ASP:OD1	2.15	0.78
1:A:319:PRO:HD2	1:A:320:LYS:HG3	1.67	0.77
1:A:393:ARG:HH12	1:A:394:LYS:HG3	1.49	0.77
1:A:51:LYS:HG3	1:A:152:ASN:HD22	1.50	0.76
1:A:25:SER:HA	1:A:301:ILE:HD13	1.70	0.74
1:A:249:LEU:O	1:A:253:THR:OG1	2.05	0.74
1:A:96:THR:HA	1:A:124:GLY:HA3	1.68	0.74
1:A:51:LYS:N	2:A:601:GDP:O1B	2.17	0.73
1:A:191:VAL:HB	1:A:243:LEU:HD12	1.69	0.73
1:A:384:GLY:O	4:A:705:HOH:O	2.08	0.71
1:A:226:GLN:HA	1:A:228:LEU:HD23	1.70	0.70
1:A:99:LEU:HD12	1:A:121:ASP:HB3	1.74	0.68
1:A:22:ASP:O	1:A:26:GLU:N	2.29	0.66
1:A:67:VAL:O	1:A:69:HIS:ND1	2.29	0.66
1:A:346:MET:HE1	1:A:403:VAL:HG11	1.78	0.65
1:A:359:THR:H	1:A:360:ALA:HA	1.61	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:THR:OG1	1:A:17:PHE:N	2.18	0.64
1:A:30:ARG:O	1:A:32:GLU:N	2.32	0.63
1:A:29:MET:HE2	1:A:301:ILE:HD12	1.79	0.63
1:A:140:ALA:HA	1:A:168:PHE:HZ	1.64	0.62
1:A:300:LEU:HD22	1:A:304:PHE:HE2	1.64	0.62
1:A:346:MET:O	1:A:348:GLU:N	2.33	0.61
1:A:32:GLU:C	1:A:34:LYS:H	2.08	0.61
1:A:39:CYS:SG	1:A:286:VAL:N	2.73	0.61
1:A:112:GLY:HA3	1:A:113:ASP:O	2.01	0.61
1:A:215:LEU:HD22	1:A:229:ARG:HG2	1.81	0.61
1:A:377:PHE:O	1:A:379:ALA:N	2.33	0.61
1:A:251:VAL:O	2:A:601:GDP:O2'	2.18	0.60
1:A:321:SER:HA	1:A:323:LEU:H	1.66	0.60
1:A:62:MET:C	1:A:64:SER:H	2.08	0.60
1:A:192:ARG:HD2	1:A:244:MET:HG3	1.83	0.60
1:A:345:LEU:HD12	1:A:369:VAL:HG22	1.83	0.59
1:A:30:ARG:C	1:A:32:GLU:H	2.10	0.59
1:A:217:VAL:HG13	1:A:218:SER:H	1.67	0.59
1:A:113:ASP:HA	1:A:114:LYS:HB2	1.85	0.59
1:A:186:ARG:HA	1:A:238:GLU:O	2.03	0.58
1:A:227:SER:O	1:A:230:ARG:HG3	2.03	0.58
1:A:5:ALA:HB3	1:A:101:TRP:CZ3	2.39	0.57
1:A:62:MET:O	1:A:64:SER:N	2.37	0.57
1:A:327:ALA:HA	1:A:330:ASN:HB3	1.87	0.57
1:A:366:HIS:HD2	1:A:367:LEU:HD23	1.70	0.57
1:A:355:PRO:HB2	1:A:356:TYR:CD2	2.40	0.57
1:A:185:GLN:NE2	1:A:289:GLU:H	2.03	0.56
1:A:371:ASP:O	1:A:375:PHE:N	2.24	0.56
1:A:266:PRO:HG2	1:A:267:GLU:OE1	2.06	0.56
1:A:98:ILE:HD13	1:A:142:SER:HB2	1.88	0.55
1:A:105:PHE:HB2	1:A:117:ILE:HB	1.88	0.55
1:A:346:MET:C	1:A:348:GLU:H	2.15	0.55
1:A:49:LYS:HG3	1:A:154:SER:HB2	1.89	0.55
1:A:38:VAL:HG13	1:A:287:TYR:HA	1.89	0.55
1:A:43:VAL:HG23	1:A:150:ILE:HB	1.89	0.55
1:A:36:ARG:H	1:A:296:ARG:HD2	1.72	0.55
1:A:226:GLN:C	1:A:228:LEU:H	2.15	0.55
1:A:251:VAL:HG22	2:A:601:GDP:O2'	2.07	0.55
1:A:49:LYS:CG	1:A:154:SER:HB2	2.37	0.54
1:A:250:ASN:OD1	1:A:250:ASN:N	2.40	0.54
1:A:152:ASN:OD1	1:A:192:ARG:NH1	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:HIS:HB3	1:A:223:PRO:HD3	1.89	0.54
1:A:396:LEU:O	1:A:400:LEU:N	2.35	0.54
1:A:398:ASP:N	1:A:398:ASP:OD1	2.40	0.54
1:A:38:VAL:HG21	1:A:287:TYR:HD1	1.72	0.53
1:A:184:PHE:HB3	1:A:236:PHE:CE2	2.42	0.53
1:A:51:LYS:HG3	1:A:152:ASN:ND2	2.21	0.52
1:A:213:ARG:O	1:A:217:VAL:HG12	2.10	0.52
1:A:390:GLU:HG2	1:A:393:ARG:HD3	1.92	0.52
1:A:169:THR:O	1:A:173:ARG:HB2	2.11	0.51
1:A:207:GLY:HA3	1:A:241:CYS:O	2.11	0.51
1:A:362:LEU:O	1:A:366:HIS:N	2.40	0.50
1:A:192:ARG:HA	1:A:244:MET:HB2	1.93	0.50
1:A:13:GLU:O	1:A:16:THR:N	2.45	0.50
1:A:55:LEU:HA	1:A:58:PHE:CD2	2.47	0.50
1:A:320:LYS:C	1:A:322:MET:HB2	2.36	0.50
1:A:55:LEU:O	1:A:58:PHE:HB2	2.12	0.50
1:A:166:GLN:O	1:A:168:PHE:N	2.42	0.50
1:A:215:LEU:CD2	1:A:229:ARG:HG2	2.41	0.50
1:A:313:GLY:C	1:A:315:GLU:H	2.21	0.49
1:A:359:THR:N	1:A:360:ALA:HA	2.23	0.49
1:A:60:ARG:O	1:A:61:TYR:HB2	2.10	0.49
1:A:35:ASP:O	1:A:115:ILE:HA	2.11	0.49
1:A:213:ARG:O	1:A:216:GLU:N	2.37	0.49
1:A:277:PRO:O	1:A:280:LEU:N	2.46	0.49
1:A:290:ILE:O	1:A:292:GLY:N	2.38	0.49
1:A:36:ARG:N	1:A:36:ARG:HD3	2.26	0.49
1:A:39:CYS:O	1:A:118:ILE:N	2.30	0.49
1:A:213:ARG:O	1:A:215:LEU:N	2.46	0.49
1:A:359:THR:OG1	1:A:361:HIS:N	2.42	0.49
1:A:59:LEU:O	1:A:61:TYR:N	2.36	0.48
1:A:188:GLN:HE21	1:A:242:PHE:HB2	1.78	0.48
1:A:309:ASN:O	1:A:314:ASN:HB2	2.12	0.48
1:A:171:TYR:CD1	1:A:322:MET:HB3	2.49	0.48
1:A:172:GLY:O	1:A:176:LEU:N	2.42	0.48
1:A:28:LEU:HB2	1:A:301:ILE:HD11	1.96	0.48
1:A:203:GLY:HA2	1:A:242:PHE:CZ	2.48	0.48
1:A:11:ALA:HB3	1:A:97:GLY:HA2	1.96	0.48
1:A:138:VAL:HG13	1:A:141:LEU:HD12	1.96	0.48
1:A:141:LEU:O	1:A:143:THR:N	2.38	0.48
1:A:5:ALA:HB3	1:A:101:TRP:CH2	2.48	0.48
1:A:109:TYR:HD1	1:A:110:PRO:HA	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181:LYS:HB2	1:A:291:SER:O	2.14	0.47
1:A:108:ASP:N	1:A:114:LYS:H	2.13	0.47
1:A:32:GLU:C	1:A:34:LYS:N	2.71	0.47
1:A:38:VAL:HG22	1:A:288:LYS:H	1.78	0.47
1:A:139:PHE:O	1:A:143:THR:OG1	2.27	0.47
1:A:185:GLN:HA	1:A:237:THR:OG1	2.14	0.47
1:A:321:SER:HA	1:A:323:LEU:N	2.29	0.47
1:A:41:VAL:HG22	1:A:148:VAL:HB	1.95	0.47
1:A:213:ARG:C	1:A:215:LEU:H	2.23	0.47
1:A:339:LYS:NZ	1:A:399:ASP:HB3	2.29	0.47
1:A:182:LYS:HB3	1:A:234:SER:O	2.15	0.47
1:A:375:PHE:CE2	1:A:376:GLN:HG3	2.50	0.47
1:A:309:ASN:C	1:A:311:TYR:H	2.22	0.47
1:A:59:LEU:C	1:A:61:TYR:H	2.19	0.46
1:A:39:CYS:O	1:A:117:ILE:HA	2.15	0.46
1:A:271:SER:O	1:A:275:LEU:N	2.46	0.46
1:A:242:PHE:CE1	1:A:244:MET:HE3	2.51	0.46
1:A:261:LEU:O	1:A:269:LYS:NZ	2.27	0.46
1:A:22:ASP:N	1:A:22:ASP:OD1	2.47	0.46
1:A:170:GLU:OE2	1:A:173:ARG:NH1	2.38	0.46
1:A:330:ASN:OD1	1:A:383:MET:N	2.49	0.46
1:A:67:VAL:O	1:A:69:HIS:N	2.49	0.45
1:A:216:GLU:HB3	1:A:217:VAL:H	1.48	0.45
1:A:218:SER:O	1:A:218:SER:OG	2.33	0.45
1:A:154:SER:O	1:A:156:ASN:N	2.49	0.45
1:A:247:PRO:HG2	1:A:248:GLY:H	1.81	0.45
1:A:326:THR:O	1:A:330:ASN:N	2.49	0.45
1:A:275:LEU:O	1:A:278:MET:HB3	2.18	0.45
1:A:287:TYR:CG	1:A:294:ARG:HD3	2.51	0.45
1:A:247:PRO:O	1:A:265:THR:OG1	2.28	0.44
1:A:175:ALA:HA	1:A:178:ASP:HB3	1.99	0.44
1:A:166:GLN:C	1:A:168:PHE:H	2.25	0.44
1:A:185:GLN:N	1:A:185:GLN:OE1	2.50	0.44
1:A:14:GLU:HA	1:A:15:HIS:HA	1.50	0.44
1:A:55:LEU:HD13	1:A:58:PHE:HD2	1.82	0.44
1:A:323:LEU:O	1:A:323:LEU:HD23	2.18	0.44
1:A:406:ASN:HB3	1:A:407:TYR:CD2	2.52	0.44
1:A:46:ALA:O	1:A:49:LYS:HB2	2.18	0.44
1:A:202:TYR:CD2	1:A:245:PRO:HG3	2.52	0.44
1:A:59:LEU:C	1:A:61:TYR:N	2.76	0.44
1:A:108:ASP:O	1:A:109:TYR:HB2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:378:ALA:HA	1:A:382:LYS:NZ	2.33	0.44
1:A:380:LYS:HA	1:A:381:ARG:HA	1.74	0.44
1:A:140:ALA:HA	1:A:168:PHE:CZ	2.49	0.44
1:A:207:GLY:O	1:A:241:CYS:HB3	2.18	0.43
1:A:310:ILE:C	1:A:311:TYR:HD2	2.26	0.43
1:A:290:ILE:HG12	1:A:303:TYR:CE1	2.53	0.43
1:A:38:VAL:HG13	1:A:286:VAL:O	2.18	0.43
1:A:260:ARG:HH11	1:A:260:ARG:HG3	1.83	0.43
1:A:310:ILE:HD13	1:A:322:MET:H	1.84	0.43
1:A:30:ARG:C	1:A:32:GLU:N	2.77	0.43
1:A:70:ASP:HB3	1:A:71:ALA:H	1.72	0.43
1:A:151:TYR:HB2	1:A:187:LEU:HD11	2.01	0.43
1:A:172:GLY:O	1:A:176:LEU:HG	2.19	0.43
1:A:39:CYS:HA	1:A:40:VAL:C	2.44	0.43
1:A:51:LYS:HB2	2:A:601:GDP:O2B	2.19	0.43
1:A:51:LYS:HB2	1:A:51:LYS:HE2	1.57	0.43
1:A:355:PRO:HB2	1:A:356:TYR:H	1.56	0.42
1:A:24:LEU:HG	1:A:28:LEU:HD12	2.01	0.42
1:A:246:HIS:ND1	1:A:247:PRO:HD2	2.34	0.42
1:A:231:HIS:O	1:A:234:SER:OG	2.26	0.42
1:A:309:ASN:O	1:A:311:TYR:N	2.51	0.42
1:A:59:LEU:HD13	1:A:101:TRP:CZ3	2.55	0.42
1:A:106:LEU:HG	1:A:107:HIS:H	1.85	0.42
1:A:282:PRO:HA	1:A:284:ASN:H	1.84	0.42
1:A:209:LYS:O	1:A:213:ARG:HG3	2.19	0.42
1:A:185:GLN:HE21	1:A:289:GLU:H	1.67	0.42
1:A:193:ASP:OD2	2:A:601:GDP:N2	2.35	0.42
1:A:313:GLY:N	1:A:318:GLU:OE2	2.50	0.42
1:A:346:MET:C	1:A:348:GLU:N	2.78	0.42
1:A:389:THR:HG23	1:A:390:GLU:H	1.83	0.42
1:A:36:ARG:HG3	1:A:294:ARG:HD2	2.02	0.41
1:A:68:HIS:C	1:A:70:ASP:H	2.28	0.41
1:A:242:PHE:HE1	1:A:244:MET:HE3	1.85	0.41
1:A:261:LEU:HA	1:A:261:LEU:HD22	1.80	0.41
1:A:357:LEU:HD13	1:A:357:LEU:HA	1.67	0.41
1:A:361:HIS:HB2	1:A:364:THR:OG1	2.20	0.41
1:A:296:ARG:N	1:A:299:ASP:OD2	2.52	0.41
1:A:37:PHE:N	1:A:295:VAL:O	2.40	0.41
1:A:330:ASN:OD1	1:A:383:MET:HG3	2.20	0.41
1:A:314:ASN:HB3	1:A:315:GLU:OE2	2.20	0.41
1:A:381:ARG:HH11	1:A:381:ARG:HB2	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:343:GLY:HA2	1:A:347:GLU:OE1	2.21	0.41
1:A:49:LYS:HD3	1:A:49:LYS:HA	1.63	0.41
1:A:55:LEU:HD13	1:A:58:PHE:HB2	2.02	0.41
1:A:296:ARG:HB2	1:A:299:ASP:OD1	2.21	0.41
1:A:373:ALA:O	1:A:377:PHE:HB2	2.21	0.41
1:A:182:LYS:HE3	1:A:234:SER:O	2.21	0.41
1:A:277:PRO:O	1:A:278:MET:C	2.64	0.41
1:A:340:GLU:OE1	4:A:706:HOH:O	2.21	0.40
1:A:338:ALA:HB3	1:A:377:PHE:HD1	1.86	0.40
1:A:20:ASN:OD1	1:A:20:ASN:N	2.54	0.40
1:A:254:ASN:HA	1:A:255:PRO:HD3	1.76	0.40
1:A:25:SER:HA	1:A:301:ILE:CD1	2.47	0.40
1:A:224:GLU:OE1	1:A:224:GLU:N	2.49	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	375/541 (69%)	254 (68%)	72 (19%)	49 (13%)	0 0

All (49) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	61	TYR
1	A	63	TYR
1	A	68	HIS
1	A	217	VAL
1	A	221	GLN
1	A	319	PRO
1	A	320	LYS
1	A	347	GLU

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Mol	Chain	Res	Type
1	A	378	ALA
1	A	34	LYS
1	A	38	VAL
1	A	96	THR
1	A	142	SER
1	A	143	THR
1	A	167	LEU
1	A	178	ASP
1	A	214	ARG
1	A	222	HIS
1	A	223	PRO
1	A	259	GLY
1	A	308	MET
1	A	310	ILE
1	A	316	LEU
1	A	361	HIS
1	A	17	PHE
1	A	31	ASP
1	A	33	VAL
1	A	60	ARG
1	A	67	VAL
1	A	71	ALA
1	A	155	GLN
1	A	184	PHE
1	A	255	PRO
1	A	278	MET
1	A	322	MET
1	A	345	LEU
1	A	69	HIS
1	A	110	PRO
1	A	355	PRO
1	A	36	ARG
1	A	37	PHE
1	A	109	TYR
1	A	113	ASP
1	A	125	ALA
1	A	292	GLY
1	A	53	PHE
1	A	247	PRO
1	A	281	ALA
1	A	27	VAL

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	309/456 (68%)	243 (79%)	66 (21%)	1 3

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	VAL
1	A	9	ILE
1	A	15	HIS
1	A	16	THR
1	A	17	PHE
1	A	21	GLU
1	A	22	ASP
1	A	27	VAL
1	A	36	ARG
1	A	40	VAL
1	A	49	LYS
1	A	55	LEU
1	A	64	SER
1	A	67	VAL
1	A	68	HIS
1	A	101	TRP
1	A	104	ILE
1	A	107	HIS
1	A	146	SER
1	A	162	LEU
1	A	163	GLN
1	A	179	THR
1	A	196	PHE
1	A	205	LEU
1	A	216	GLU
1	A	224	GLU
1	A	225	LEU
1	A	228	LEU
1	A	233	SER
1	A	237	THR

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Mol	Chain	Res	Type
1	A	238	GLU
1	A	239	VAL
1	A	243	LEU
1	A	244	MET
1	A	249	LEU
1	A	250	ASN
1	A	251	VAL
1	A	260	ARG
1	A	261	LEU
1	A	263	ASP
1	A	271	SER
1	A	285	LEU
1	A	288	LYS
1	A	294	ARG
1	A	295	VAL
1	A	299	ASP
1	A	306	SER
1	A	312	LYS
1	A	314	ASN
1	A	316	LEU
1	A	320	LYS
1	A	323	LEU
1	A	345	LEU
1	A	357	LEU
1	A	361	HIS
1	A	366	HIS
1	A	375	PHE
1	A	380	LYS
1	A	381	ARG
1	A	382	LYS
1	A	387	GLU
1	A	389	THR
1	A	390	GLU
1	A	391	LYS
1	A	398	ASP
1	A	402	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	149	GLN
1	A	158	GLN

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Mol	Chain	Res	Type
1	A	231	HIS
1	A	302	GLN
1	A	331	HIS

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	601	3	29,30,30	1.22	4 (13%)	45,47,47	1.85	8 (17%)

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	601	3	-	3/16/32/32	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	GDP	C5-C4	2.74	1.46	1.38
2	A	601	GDP	C5-N7	-2.45	1.34	1.39
2	A	601	GDP	C6-N1	-2.29	1.34	1.38
2	A	601	GDP	C4-N9	-2.20	1.32	1.38

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	GDP	C5-C4-N3	-5.72	119.29	128.39
2	A	601	GDP	C2-N3-C4	4.93	120.79	112.30
2	A	601	GDP	C6-C5-N7	4.05	137.66	130.29
2	A	601	GDP	N9-C4-N3	3.98	133.90	125.95
2	A	601	GDP	C4-C5-N7	-3.44	105.22	110.67
2	A	601	GDP	C8-N7-C5	2.61	108.91	104.26
2	A	601	GDP	N9-C8-N7	-2.10	109.51	113.40
2	A	601	GDP	O3'-C3'-C2'	-2.09	105.13	111.82

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	GDP	C5'-O5'-PA-O3A
2	A	601	GDP	C5'-O5'-PA-O2A
2	A	601	GDP	C5'-O5'-PA-O1A

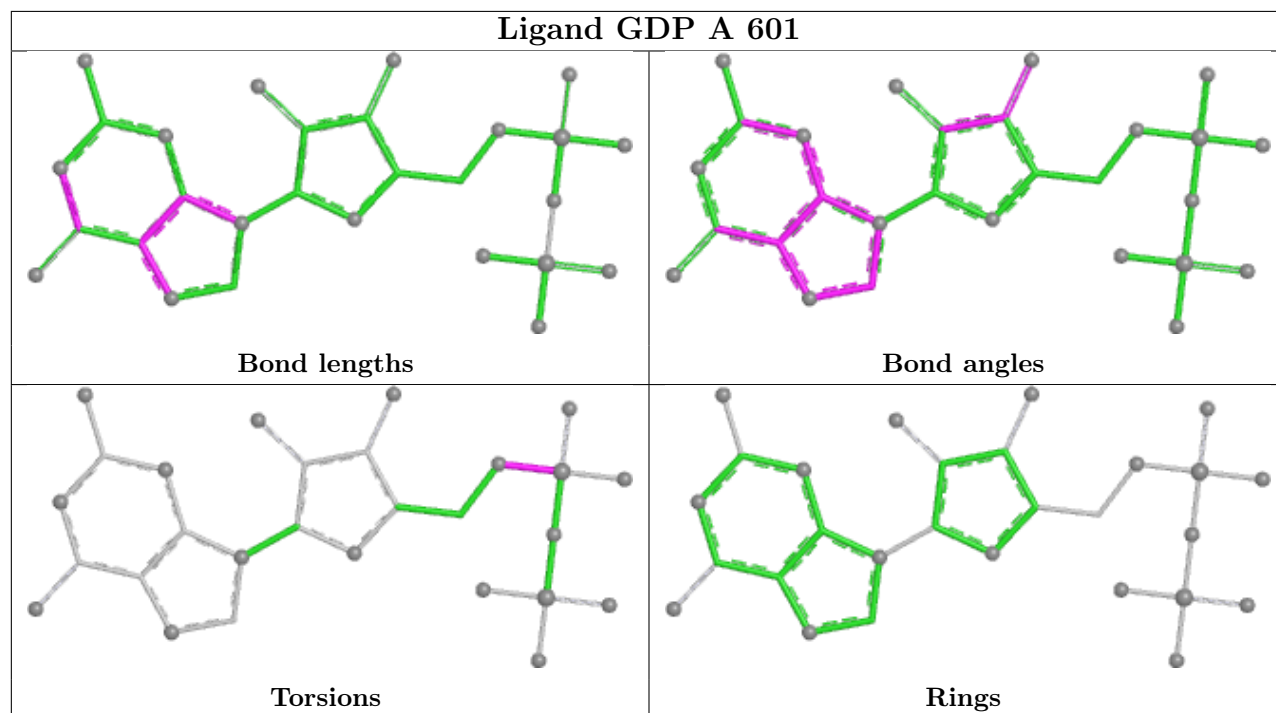
There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	GDP	5	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	381/541 (70%)	0.57	21 (5%) 30 24	18, 41, 70, 91	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	116	ALA	3.9
1	A	357	LEU	3.6
1	A	99	LEU	3.3
1	A	249	LEU	3.2
1	A	40	VAL	2.9
1	A	338	ALA	2.9
1	A	308	MET	2.8
1	A	38	VAL	2.8
1	A	48	ARG	2.7
1	A	356	TYR	2.7
1	A	165	LEU	2.5
1	A	344	GLN	2.5
1	A	361	HIS	2.5
1	A	10	ASN	2.5
1	A	104	ILE	2.4
1	A	95	THR	2.4
1	A	232	ILE	2.3
1	A	136	ALA	2.3
1	A	166	GLN	2.2
1	A	360	ALA	2.1
1	A	135	CYS	2.1

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](#)

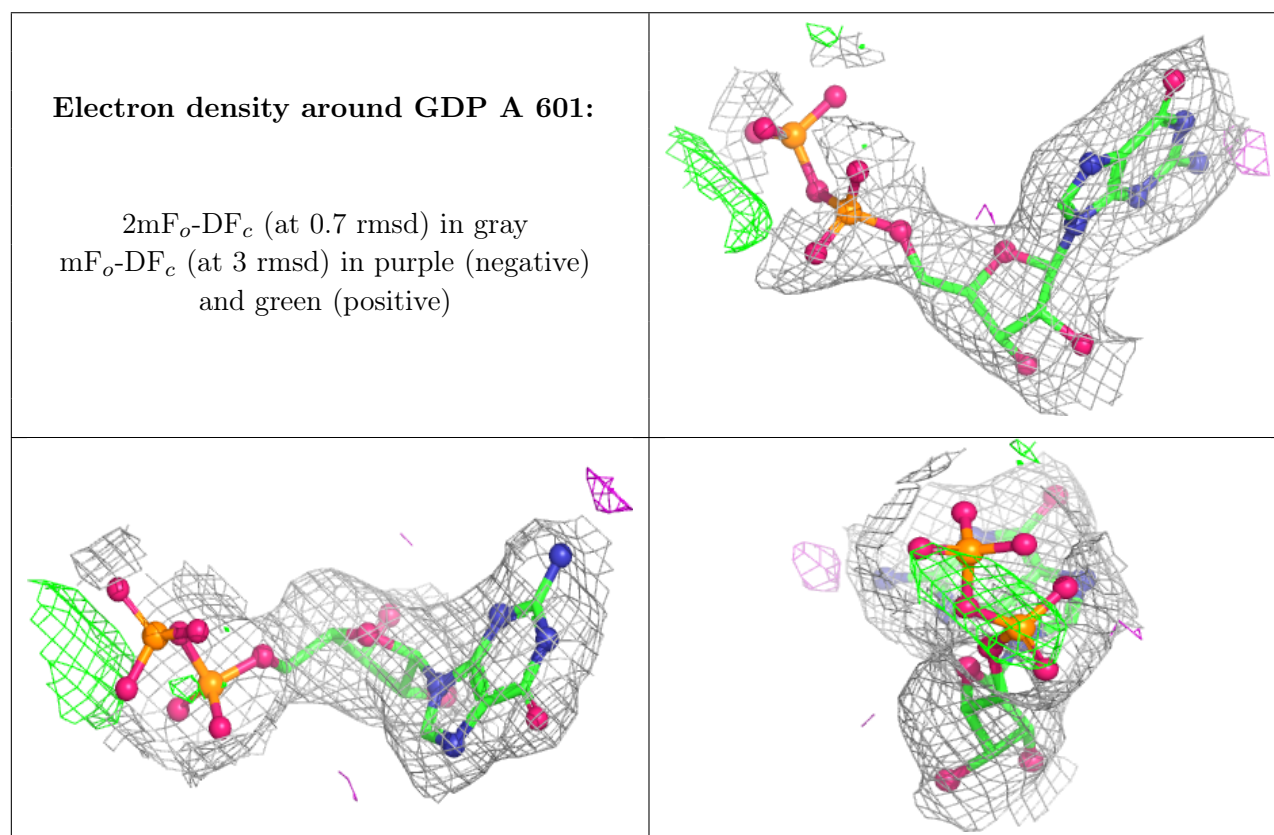
There are no oligosaccharides in this entry.

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
3	MG	A	602	1/1	0.81	0.16	26,26,26,26	0
2	GDP	A	601	28/28	0.90	0.10	18,28,36,41	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.